



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2025 – 04:20 pm BST

PDB ID : 9HJS / pdb_00009hjs
Title : Crystal structure of human geranylgeranyl diphosphate synthase mutant R235C
Authors : Yehia, R.; Giladi, M.; Haitin, Y.
Deposited on : 2024-12-01
Resolution : 2.51 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

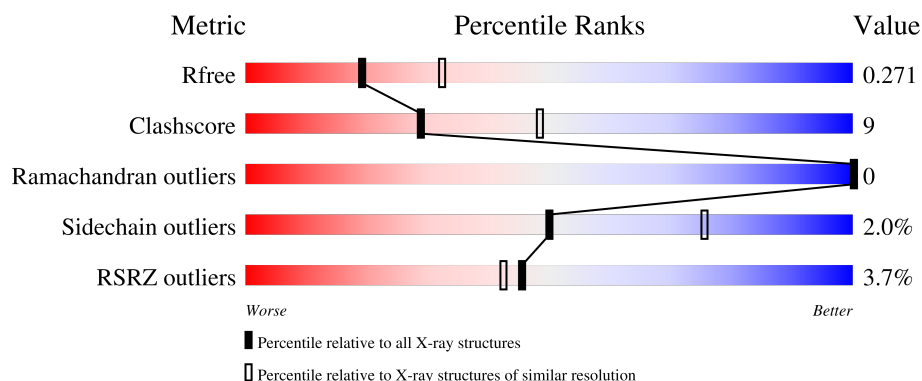
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	307	<div> <div>7%</div> <div>79% 16% .</div> </div>
1	B	307	<div> <div>6%</div> <div>76% 17% . 7%</div> </div>
1	C	307	<div> <div>%</div> <div>80% 15% 5%</div> </div>
1	D	307	<div> <div>%</div> <div>78% 17% 5%</div> </div>
1	E	307	<div> <div>2%</div> <div>76% 18% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	307	<div><div></div><div>3%</div><div>74%</div><div>21%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13669 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 Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2166	1386	365	408	7			
1	B	287	Total	C	N	O	S	0	0	0
			2152	1397	347	401	7			
1	C	293	Total	C	N	O	S	0	0	0
			2289	1476	378	427	8			
1	D	293	Total	C	N	O	S	0	0	0
			2329	1503	385	433	8			
1	E	291	Total	C	N	O	S	0	0	0
			2232	1448	366	410	8			
1	F	294	Total	C	N	O	S	0	0	0
			2234	1446	366	415	7			

There are 54 discrepancies between the modelled and reference sequences:

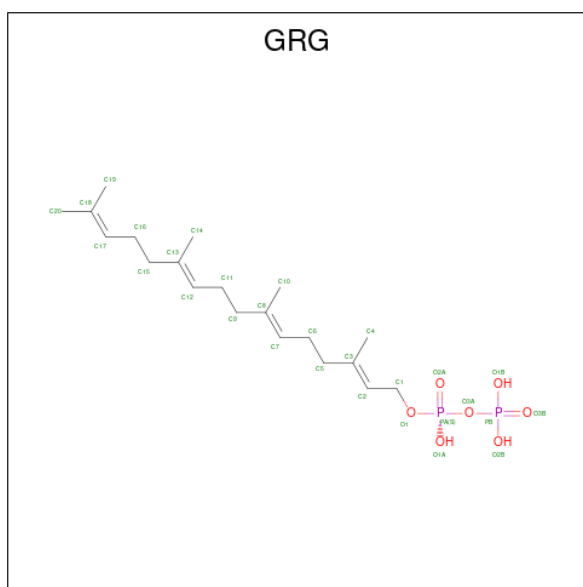
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O95749
A	-5	SER	-	expression tag	UNP O95749
A	-4	GLY	-	expression tag	UNP O95749
A	-3	SER	-	expression tag	UNP O95749
A	-2	GLY	-	expression tag	UNP O95749
A	-1	SER	-	expression tag	UNP O95749
A	0	GLY	-	expression tag	UNP O95749
A	109	GLN	PRO	variant	UNP O95749
A	235	CYS	ARG	engineered mutation	UNP O95749
B	-6	GLY	-	expression tag	UNP O95749
B	-5	SER	-	expression tag	UNP O95749
B	-4	GLY	-	expression tag	UNP O95749
B	-3	SER	-	expression tag	UNP O95749
B	-2	GLY	-	expression tag	UNP O95749
B	-1	SER	-	expression tag	UNP O95749
B	0	GLY	-	expression tag	UNP O95749
B	109	GLN	PRO	variant	UNP O95749

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Chain	Residue	Modelled	Actual	Comment	Reference
B	235	CYS	ARG	engineered mutation	UNP O95749
C	-6	GLY	-	expression tag	UNP O95749
C	-5	SER	-	expression tag	UNP O95749
C	-4	GLY	-	expression tag	UNP O95749
C	-3	SER	-	expression tag	UNP O95749
C	-2	GLY	-	expression tag	UNP O95749
C	-1	SER	-	expression tag	UNP O95749
C	0	GLY	-	expression tag	UNP O95749
C	109	GLN	PRO	variant	UNP O95749
C	235	CYS	ARG	engineered mutation	UNP O95749
D	-6	GLY	-	expression tag	UNP O95749
D	-5	SER	-	expression tag	UNP O95749
D	-4	GLY	-	expression tag	UNP O95749
D	-3	SER	-	expression tag	UNP O95749
D	-2	GLY	-	expression tag	UNP O95749
D	-1	SER	-	expression tag	UNP O95749
D	0	GLY	-	expression tag	UNP O95749
D	109	GLN	PRO	variant	UNP O95749
D	235	CYS	ARG	engineered mutation	UNP O95749
E	-6	GLY	-	expression tag	UNP O95749
E	-5	SER	-	expression tag	UNP O95749
E	-4	GLY	-	expression tag	UNP O95749
E	-3	SER	-	expression tag	UNP O95749
E	-2	GLY	-	expression tag	UNP O95749
E	-1	SER	-	expression tag	UNP O95749
E	0	GLY	-	expression tag	UNP O95749
E	109	GLN	PRO	variant	UNP O95749
E	235	CYS	ARG	engineered mutation	UNP O95749
F	-6	GLY	-	expression tag	UNP O95749
F	-5	SER	-	expression tag	UNP O95749
F	-4	GLY	-	expression tag	UNP O95749
F	-3	SER	-	expression tag	UNP O95749
F	-2	GLY	-	expression tag	UNP O95749
F	-1	SER	-	expression tag	UNP O95749
F	0	GLY	-	expression tag	UNP O95749
F	109	GLN	PRO	variant	UNP O95749
F	235	CYS	ARG	engineered mutation	UNP O95749

- Molecule 2 is GERANYLGERANYL DIPHOSPHATE (CCD ID: GRG) (formula: $C_{20}H_{36}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 29	C 20	O 7	P 2	0	0
2	B	1	Total 29	C 20	O 7	P 2	0	0
2	C	1	Total 29	C 20	O 7	P 2	0	0
2	D	1	Total 29	C 20	O 7	P 2	0	0
2	E	1	Total 29	C 20	O 7	P 2	0	0
2	F	1	Total 29	C 20	O 7	P 2	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Mg	0	0
			2	2		

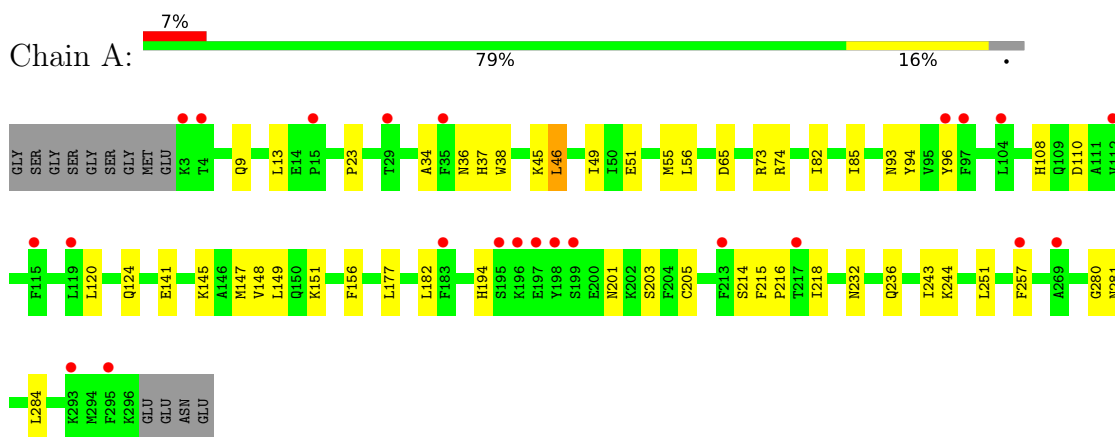
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	11	Total	O	0	0
			11	11		
4	C	17	Total	O	0	0
			17	17		
4	D	27	Total	O	0	0
			27	27		
4	E	6	Total	O	0	0
			6	6		
4	F	11	Total	O	0	0
			11	11		

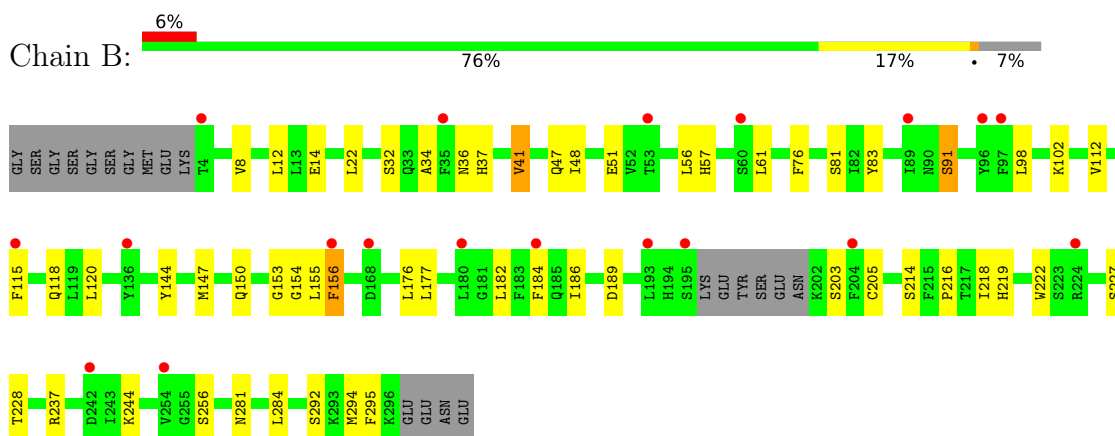
3 Residue-property plots [i](#)

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.

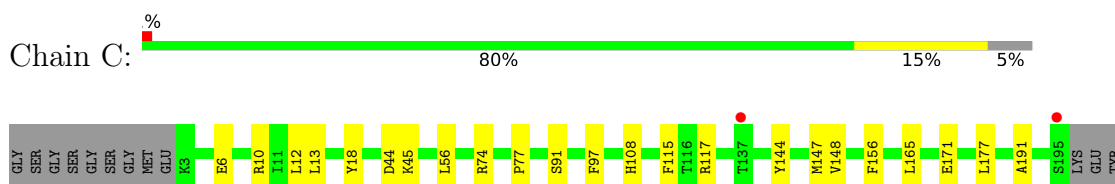
- Molecule 1: Geranylgeranyl pyrophosphate synthase



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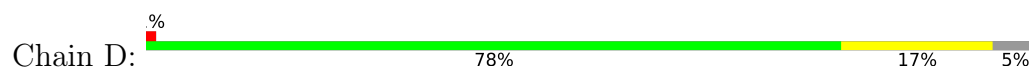


- Molecule 1: Geranylgeranyl pyrophosphate synthase

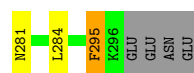
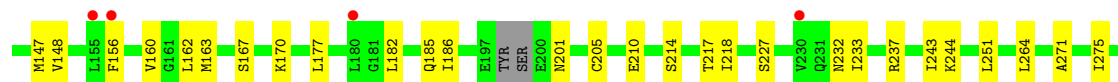
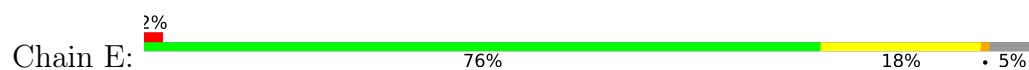




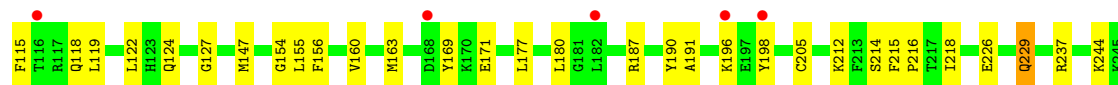
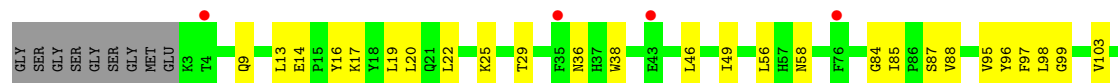
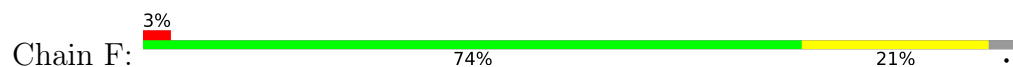
- Molecule 1: Geranylgeranyl pyrophosphate synthase



- Molecule 1: Geranylgeranyl pyrophosphate synthase



- Molecule 1: Geranylgeranyl pyrophosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.62Å 69.08Å 154.99Å 90.00° 97.39° 90.00°	Depositor
Resolution (Å)	45.19 – 2.51 45.19 – 2.51	Depositor EDS
% Data completeness (in resolution range)	77.0 (45.19-2.51) 72.7 (45.19-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.227 , 0.271 0.227 , 0.271	Depositor DCC
R_{free} test set	54877 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.6	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	0.93	EDS
Total number of atoms	13669	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: GRG, 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	0.41	1/2216 (0.0%)	0.47	0/3033
1	B	0.34	1/2201 (0.0%)	0.47	0/3010
1	C	0.23	0/2338	0.39	0/3178
1	D	0.26	0/2380	0.41	0/3229
1	E	0.24	0/2281	0.42	0/3108
1	F	0.29	2/2284 (0.1%)	0.44	0/3115
All	All	0.30	4/13700 (0.0%)	0.43	0/18673

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	ILE	CA-CB	13.58	1.61	1.54
1	F	85	ILE	CA-CB	-6.05	1.51	1.54
1	B	294	MET	SD-CE	5.41	1.93	1.79
1	F	119	LEU	CG-CD1	-5.12	1.35	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2166	0	1899	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2152	0	1969	34	0
1	C	2289	0	2170	30	0
1	D	2329	0	2266	37	0
1	E	2232	0	2083	43	0
1	F	2234	0	2065	42	0
2	A	29	0	33	8	0
2	B	29	0	33	4	0
2	C	29	0	33	2	0
2	D	29	0	33	4	0
2	E	29	0	33	3	0
2	F	29	0	33	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	9	0	0	0	0
4	B	11	0	0	0	0
4	C	17	0	0	0	0
4	D	27	0	0	0	0
4	E	6	0	0	1	0
4	F	11	0	0	0	0
All	All	13669	0	12650	226	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 (226) 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:D:243:ILE:HD11	1:E:81:SER:HB3	1.57	0.85
1:E:12:LEU:HD11	1:F:124:GLN:HA	1.67	0.76
1:D:117:ARG:NH1	1:D:118:GLN:OE1	2.20	0.75
1:A:65:ASP:OD1	1:A:73:ARG:NH1	2.21	0.74
1:A:23:PRO:HD2	1:A:74:ARG:HB3	1.71	0.73
1:E:271:ALA:O	1:E:275:ILE:HG13	1.91	0.71
1:A:124:GLN:HA	1:B:12:LEU:HD21	1.73	0.70
1:C:171:GLU:HB3	1:C:278:ARG:NH2	2.08	0.69
1:A:120:LEU:O	1:A:124:GLN:HG2	1.94	0.68
1:F:191:ALA:HB2	1:F:294:MET:HE1	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:LEU:HD21	1:E:115:PHE:HE2	1.59	0.67
1:D:39:LEU:HD23	1:D:169:TYR:HB3	1.79	0.64
1:B:228:THR:HG22	1:F:14:GLU:OE2	1.99	0.62
1:D:56:LEU:HD11	1:D:115:PHE:HE2	1.64	0.62
1:F:160:VAL:HG21	1:F:177:LEU:HD11	1.82	0.61
1:A:156:PHE:HB3	1:A:177:LEU:HD23	1.82	0.61
1:F:25:LYS:O	1:F:29:THR:OG1	2.18	0.61
1:F:212:LYS:NZ	2:F:401:GRG:O2A	2.33	0.60
1:E:100:LEU:HD23	1:E:115:PHE:CD1	2.35	0.60
1:B:281:ASN:HB3	1:B:284:LEU:HB3	1.83	0.60
1:A:38:TRP:CH2	1:A:281:ASN:HB2	2.36	0.60
1:B:34:ALA:O	1:B:281:ASN:ND2	2.27	0.60
1:D:160:VAL:HG23	2:D:401:GRG:H193	1.83	0.60
1:D:187:ARG:NH1	1:D:291:LEU:O	2.35	0.59
1:E:205:CYS:HB2	1:E:244:LYS:HD2	1.84	0.59
1:E:74:ARG:HA	1:E:201:ASN:HA	1.85	0.58
1:E:160:VAL:HA	1:E:163:MET:HE3	1.85	0.58
1:F:290:HIS:HA	1:F:293:LYS:HE3	1.86	0.57
1:F:169:TYR:CE1	1:F:171:GLU:HB2	2.39	0.57
1:E:12:LEU:HD22	1:F:127:GLY:HA3	1.87	0.57
1:F:268:GLU:CD	1:F:296:LYS:HZ1	2.13	0.57
1:F:56:LEU:HD11	1:F:115:PHE:HE2	1.70	0.57
1:C:12:LEU:HD21	1:D:124:GLN:HA	1.87	0.57
1:A:73:ARG:HH22	2:A:501:GRG:PB	2.27	0.56
1:B:22:LEU:HD21	1:B:76:PHE:HB2	1.86	0.56
1:A:73:ARG:NH2	2:A:501:GRG:O1B	2.37	0.56
1:F:122:LEU:HD22	1:F:155:LEU:HD21	1.85	0.56
1:B:32:SER:HA	2:B:401:GRG:H203	1.86	0.56
1:B:218:ILE:O	1:B:222:TRP:HD1	1.87	0.56
1:A:214:SER:O	1:A:218:ILE:HG13	2.06	0.56
1:F:99:GLY:O	1:F:103:VAL:HG23	2.05	0.56
1:A:74:ARG:HA	1:A:201:ASN:HA	1.87	0.55
1:E:100:LEU:O	1:E:103:VAL:HG12	2.07	0.55
1:E:56:LEU:HD21	1:E:115:PHE:CE2	2.42	0.54
1:A:205:CYS:HB2	1:A:244:LYS:HD2	1.88	0.54
1:C:97:PHE:CZ	1:D:119:LEU:HD23	2.43	0.54
1:E:160:VAL:HG21	1:E:177:LEU:HD21	1.90	0.54
1:B:216:PRO:O	1:B:256:SER:OG	2.24	0.54
1:F:205:CYS:HB2	1:F:244:LYS:HD2	1.88	0.54
1:B:48:ILE:HG23	1:B:102:LYS:HG2	1.90	0.54
1:C:214:SER:O	1:C:218:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASN:ND2	1:A:46:LEU:HD21	2.22	0.53
1:E:12:LEU:CD1	1:F:124:GLN:HA	2.36	0.53
1:F:38:TRP:CZ2	1:F:281:ASN:HB2	2.44	0.53
1:D:237:ARG:HG3	1:D:237:ARG:HH11	1.73	0.53
1:C:56:LEU:HD11	1:C:115:PHE:HE2	1.73	0.53
1:F:156:PHE:HB3	1:F:177:LEU:HD23	1.89	0.53
1:B:205:CYS:HB2	1:B:244:LYS:HD2	1.90	0.53
1:C:171:GLU:HB3	1:C:278:ARG:HH21	1.72	0.53
1:E:119:LEU:HD13	1:F:97:PHE:CZ	2.44	0.53
1:A:51:GLU:O	1:A:55:MET:HG3	2.09	0.52
1:A:148:VAL:HG21	1:A:182:LEU:HD23	1.90	0.52
1:C:211:GLY:HA3	1:C:237:ARG:HH11	1.73	0.52
1:E:237:ARG:HG3	1:E:237:ARG:HH11	1.74	0.52
1:A:145:LYS:O	1:A:149:LEU:HD13	2.09	0.52
1:E:217:THR:HA	1:E:251:LEU:HD21	1.91	0.52
1:F:237:ARG:HH11	1:F:237:ARG:HG3	1.75	0.52
1:E:11:ILE:HG22	1:E:12:LEU:HD23	1.92	0.52
1:D:284:LEU:O	1:D:288:VAL:HG23	2.10	0.52
1:E:133:ARG:HD2	1:E:210:GLU:O	2.09	0.51
1:A:194:HIS:HD2	1:A:257:PHE:CD1	2.28	0.51
1:D:141:GLU:HG2	1:D:145:LYS:HE2	1.93	0.51
2:E:401:GRG:O1B	2:E:401:GRG:HC12	2.11	0.50
1:C:205:CYS:HB2	1:C:244:LYS:HD2	1.92	0.50
1:D:142:GLU:H	1:D:142:GLU:CD	2.20	0.50
1:E:132:TRP:CE2	1:E:139:PRO:HB3	2.47	0.50
1:B:176:LEU:HD21	1:B:284:LEU:HD21	1.94	0.50
1:D:66:ILE:HD13	1:D:85:ILE:HG23	1.93	0.50
1:A:232:ASN:HB3	1:D:82:ILE:O	2.12	0.49
1:F:226:GLU:OE2	1:F:226:GLU:N	2.33	0.49
1:A:9:GLN:O	1:A:13:LEU:HD12	2.12	0.49
1:D:44:ASP:OD1	1:D:44:ASP:N	2.45	0.49
1:F:214:SER:O	1:F:218:ILE:HG13	2.12	0.49
1:A:38:TRP:CZ2	1:A:281:ASN:HB2	2.47	0.49
1:A:56:LEU:HD12	1:A:96:TYR:HD1	1.78	0.49
1:E:8:VAL:O	1:E:12:LEU:HG	2.13	0.49
1:E:264:LEU:HD13	1:E:295:PHE:CE1	2.47	0.49
1:F:118:GLN:HB3	1:F:154:GLY:O	2.13	0.49
1:B:118:GLN:HB3	1:B:154:GLY:O	2.13	0.49
1:B:156:PHE:CD1	1:B:177:LEU:HD22	2.47	0.48
1:F:187:ARG:HH11	1:F:294:MET:HG2	1.76	0.48
1:A:65:ASP:CG	1:A:73:ARG:HH11	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:SER:O	1:D:218:ILE:HG13	2.12	0.48
1:C:156:PHE:CD1	1:C:177:LEU:HD22	2.47	0.48
1:C:211:GLY:HA3	1:C:237:ARG:NH1	2.29	0.48
1:E:148:VAL:HG22	1:E:185:GLN:HG2	1.94	0.48
1:F:103:VAL:HG21	1:F:115:PHE:CD2	2.48	0.48
1:D:7:THR:C	1:D:9:GLN:H	2.20	0.48
1:E:214:SER:O	1:E:218:ILE:HG13	2.14	0.48
1:F:147:MET:HE3	1:F:147:MET:HB3	1.81	0.47
2:B:401:GRG:HC11	2:B:401:GRG:HC41	1.69	0.47
1:B:237:ARG:HG3	1:B:237:ARG:HH11	1.80	0.47
2:C:401:GRG:HC11	2:C:401:GRG:HC41	1.59	0.47
1:A:147:MET:HE3	1:A:147:MET:HB3	1.78	0.47
1:A:45:LYS:O	1:A:49:ILE:HG23	2.15	0.47
1:A:56:LEU:HD12	1:A:96:TYR:CD1	2.50	0.47
1:A:141:GLU:O	1:A:145:LYS:HG3	2.14	0.47
1:D:294:MET:HG3	1:D:295:PHE:N	2.30	0.47
1:E:167:SER:O	1:E:170:LYS:HE3	2.14	0.47
1:F:19:LEU:HA	1:F:22:LEU:HD13	1.96	0.47
2:A:501:GRG:HC7	2:A:501:GRG:H111	1.51	0.46
1:B:12:LEU:O	1:B:91:SER:HB2	2.16	0.46
1:A:215:PHE:HB3	1:A:216:PRO:HD3	1.96	0.46
1:E:38:TRP:CZ2	1:E:281:ASN:HB2	2.50	0.46
1:F:95:VAL:HA	1:F:98:LEU:HB2	1.97	0.46
1:E:34:ALA:HB1	1:E:284:LEU:HB2	1.98	0.46
1:E:128:LEU:HD12	1:E:132:TRP:CZ2	2.50	0.46
2:F:401:GRG:H112	2:F:401:GRG:H141	1.70	0.46
1:B:147:MET:HE3	1:B:147:MET:HB3	1.66	0.46
1:C:144:TYR:O	1:C:148:VAL:HG23	2.15	0.46
1:D:56:LEU:HD11	1:D:115:PHE:CE2	2.49	0.46
1:E:114:LEU:HD23	1:E:162:LEU:HG	1.97	0.46
2:A:501:GRG:H112	2:A:501:GRG:H141	1.66	0.46
1:C:284:LEU:O	1:C:288:VAL:HG23	2.15	0.46
1:D:147:MET:HE3	1:D:147:MET:HB3	1.65	0.46
1:F:187:ARG:NH1	1:F:294:MET:HG2	2.31	0.46
1:F:56:LEU:HD23	1:F:96:TYR:HD1	1.81	0.45
1:A:34:ALA:O	1:A:281:ASN:ND2	2.29	0.45
1:A:94:TYR:CE2	1:B:120:LEU:HD22	2.52	0.45
1:B:47:GLN:O	1:B:51:GLU:HG3	2.16	0.45
2:D:401:GRG:H141	2:D:401:GRG:H112	1.70	0.45
1:C:74:ARG:HA	1:C:201:ASN:HA	1.99	0.45
1:F:9:GLN:O	1:F:13:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:HD12	1:D:163:MET:HE2	1.99	0.45
1:F:17:LYS:HA	1:F:20:LEU:HD12	1.99	0.45
1:A:156:PHE:CD2	2:A:501:GRG:HC92	2.52	0.44
1:A:93:ASN:HA	1:A:96:TYR:HD2	1.83	0.44
1:A:232:ASN:O	1:A:236:GLN:HG2	2.16	0.44
1:C:56:LEU:HD11	1:C:115:PHE:CE2	2.51	0.44
1:C:97:PHE:CE2	1:D:119:LEU:HD23	2.53	0.44
1:D:244:LYS:O	1:D:248:VAL:HG23	2.18	0.44
1:C:240:ASN:ND2	1:C:243:ILE:HG13	2.33	0.44
1:A:108:HIS:CE1	1:A:110:ASP:HB2	2.53	0.44
1:B:57:HIS:O	1:B:61:LEU:HG	2.17	0.44
1:A:82:ILE:O	1:E:232:ASN:HB3	2.17	0.44
1:D:51:GLU:O	1:D:55:MET:HG3	2.17	0.44
1:E:147:MET:HB3	1:E:147:MET:HE3	1.67	0.44
1:E:295:PHE:CD1	1:E:295:PHE:N	2.84	0.44
1:C:217:THR:O	1:C:221:ILE:HG12	2.18	0.43
1:A:243:ILE:HD11	1:D:81:SER:HB2	1.99	0.43
1:C:221:ILE:HD12	1:C:231:GLN:HG3	2.00	0.43
1:F:56:LEU:HD11	1:F:115:PHE:CE2	2.52	0.43
1:F:229:GLN:OE1	1:F:246:TYR:OH	2.25	0.43
2:A:501:GRG:HC2	2:A:501:GRG:HC61	1.65	0.43
1:B:156:PHE:HZ	1:B:184:PHE:CE2	2.36	0.43
1:D:182:LEU:HD23	1:D:182:LEU:HA	1.86	0.43
1:B:14:GLU:HG2	1:B:83:TYR:CE1	2.53	0.43
1:C:147:MET:HE3	1:C:147:MET:HB3	1.74	0.43
1:E:16:TYR:HE1	1:E:58:ASN:HB2	1.84	0.43
1:A:34:ALA:HB1	1:A:284:LEU:HB2	2.00	0.43
1:C:261:ARG:HG2	1:C:295:PHE:HB2	2.00	0.43
1:D:39:LEU:HD23	1:D:39:LEU:HA	1.90	0.43
1:D:133:ARG:HG3	1:D:211:GLY:O	2.18	0.43
2:A:501:GRG:H191	2:A:501:GRG:H162	1.67	0.43
1:B:37:HIS:C	1:B:37:HIS:CD2	2.96	0.43
2:C:401:GRG:H101	2:C:401:GRG:HC61	1.64	0.43
2:D:401:GRG:HC61	2:D:401:GRG:H101	1.78	0.43
2:E:401:GRG:H201	2:E:401:GRG:H162	1.76	0.43
1:C:12:LEU:O	1:C:91:SER:OG	2.28	0.43
1:D:40:LYS:HE3	1:D:40:LYS:HB2	1.80	0.43
1:E:57:HIS:O	1:E:61:LEU:HG	2.19	0.43
1:F:84:GLY:O	1:F:88:VAL:HG23	2.19	0.43
1:C:44:ASP:OD2	1:C:45:LYS:N	2.51	0.43
1:C:274:GLN:O	1:C:278:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ILE:HG21	1:F:163:MET:HG3	2.00	0.43
1:B:36:ASN:OD1	1:B:41:VAL:HG12	2.19	0.42
1:B:214:SER:O	1:B:218:ILE:HG13	2.19	0.42
1:E:51:GLU:O	1:E:55:MET:HG3	2.20	0.42
1:E:7:THR:HA	4:E:501:HOH:O	2.17	0.42
1:E:182:LEU:O	1:E:186:ILE:HD13	2.20	0.42
1:E:264:LEU:HB3	1:E:295:PHE:CZ	2.54	0.42
1:D:228:THR:HG22	1:E:14:GLU:CD	2.44	0.42
1:D:7:THR:C	1:D:9:GLN:N	2.78	0.42
1:C:6:GLU:O	1:C:10:ARG:HG3	2.19	0.42
1:A:82:ILE:HG23	1:E:233:ILE:HG13	2.02	0.42
1:A:94:TYR:HE2	1:B:120:LEU:HD22	1.84	0.42
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.89	0.42
1:E:12:LEU:O	1:E:91:SER:OG	2.18	0.42
1:B:56:LEU:HD11	1:B:115:PHE:HE1	1.84	0.41
1:F:196:LYS:C	1:F:198:TYR:N	2.77	0.41
1:A:151:LYS:HD2	2:A:501:GRG:HC11	2.02	0.41
1:D:38:TRP:CZ2	1:D:281:ASN:HB2	2.55	0.41
1:B:98:LEU:HD23	1:B:98:LEU:HA	1.82	0.41
1:B:155:LEU:HB3	2:B:401:GRG:H142	2.01	0.41
1:B:182:LEU:O	1:B:186:ILE:HD13	2.20	0.41
1:C:117:ARG:HH11	1:C:117:ARG:HG2	1.86	0.41
1:A:9:GLN:HG2	1:A:13:LEU:HD11	2.02	0.41
1:C:18:TYR:OH	1:C:77:PRO:O	2.34	0.41
1:D:36:ASN:ND2	1:D:46:LEU:HD22	2.35	0.41
2:D:401:GRG:HC11	2:D:401:GRG:HC41	1.71	0.41
1:F:275:ILE:HD11	1:F:284:LEU:HG	2.02	0.41
1:C:191:ALA:HB2	1:C:294:MET:SD	2.60	0.41
1:B:118:GLN:NE2	1:B:153:GLY:O	2.52	0.41
1:B:292:SER:HA	1:B:295:PHE:CE1	2.55	0.41
1:D:56:LEU:HD22	1:D:119:LEU:HD21	2.01	0.41
1:F:16:TYR:HE1	1:F:58:ASN:HB2	1.85	0.41
1:F:156:PHE:CD1	1:F:177:LEU:HG	2.56	0.41
1:A:37:HIS:NE2	1:A:280:GLY:O	2.53	0.41
1:B:144:TYR:OH	1:B:189:ASP:OD2	2.33	0.41
1:C:250:TYR:O	1:C:254:VAL:HG22	2.20	0.41
2:B:401:GRG:H162	2:B:401:GRG:H191	1.66	0.41
1:C:264:LEU:HD13	1:C:295:PHE:CD2	2.56	0.41
1:E:31:LEU:C	2:E:401:GRG:H192	2.46	0.41
1:F:36:ASN:ND2	1:F:46:LEU:HD22	2.35	0.41
2:F:401:GRG:HC61	2:F:401:GRG:HC2	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:HIS:HB3	1:B:256:SER:OG	2.20	0.41
1:D:11:ILE:H	1:D:11:ILE:HD12	1.86	0.41
1:E:119:LEU:HD23	1:E:119:LEU:HA	1.92	0.41
1:F:190:TYR:HB2	1:F:260:THR:HG21	2.03	0.41
1:F:215:PHE:HB3	1:F:216:PRO:HD3	2.03	0.40
1:B:8:VAL:O	1:B:12:LEU:HD13	2.21	0.40
1:D:215:PHE:HB3	1:D:216:PRO:HD3	2.03	0.40
1:A:251:LEU:HB2	1:A:257:PHE:HE2	1.85	0.40
1:C:108:HIS:CD2	1:C:165:LEU:HB3	2.57	0.40
1:D:51:GLU:OE2	1:D:102:LYS:HE2	2.22	0.40
1:E:275:ILE:HG13	1:E:275:ILE:H	1.75	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	292/307 (95%)	285 (98%)	7 (2%)	0	100	100
1	B	283/307 (92%)	276 (98%)	7 (2%)	0	100	100
1	C	289/307 (94%)	281 (97%)	8 (3%)	0	100	100
1	D	291/307 (95%)	282 (97%)	9 (3%)	0	100	100
1	E	287/307 (94%)	280 (98%)	7 (2%)	0	100	100
1	F	292/307 (95%)	280 (96%)	12 (4%)	0	100	100
All	All	1734/1842 (94%)	1684 (97%)	50 (3%)	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	197/275 (72%)	195 (99%)	2 (1%)	73	88
1	B	207/275 (75%)	199 (96%)	8 (4%)	27	52
1	C	231/275 (84%)	229 (99%)	2 (1%)	75	90
1	D	245/275 (89%)	240 (98%)	5 (2%)	50	75
1	E	217/275 (79%)	211 (97%)	6 (3%)	38	65
1	F	215/275 (78%)	212 (99%)	3 (1%)	62	83
All	All	1312/1650 (80%)	1286 (98%)	26 (2%)	50	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	203	SER
1	B	41	VAL
1	B	81	SER
1	B	91	SER
1	B	112	VAL
1	B	150	GLN
1	B	156	PHE
1	B	203	SER
1	B	227	SER
1	C	13	LEU
1	C	229	GLN
1	D	27	VAL
1	D	103	VAL
1	D	156	PHE
1	D	203	SER
1	D	276	ASP
1	E	103	VAL
1	E	128	LEU
1	E	156	PHE
1	E	227	SER
1	E	243	ILE

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Mol	Chain	Res	Type
1	E	295	PHE
1	F	87	SER
1	F	180	LEU
1	F	229	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	164	GLN
1	A	194	HIS
1	A	290	HIS
1	B	37	HIS
1	B	58	ASN
1	B	135	ASN
1	B	194	HIS
1	B	232	ASN
1	C	80	HIS
1	C	192	ASN
1	C	290	HIS
1	D	164	GLN
1	D	274	GLN
1	E	21	GLN
1	E	69	ASN
1	E	194	HIS
1	F	37	HIS
1	F	118	GLN
1	F	194	HIS

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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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
2	GRG	D	401	3	26,28,28	1.22	1 (3%)	33,37,37	1.57	7 (21%)
2	GRG	F	401	3	26,28,28	1.24	3 (11%)	33,37,37	1.58	7 (21%)
2	GRG	E	401	3	26,28,28	1.30	3 (11%)	33,37,37	1.65	10 (30%)
2	GRG	A	501	3	26,28,28	1.16	0	33,37,37	1.70	9 (27%)
2	GRG	C	401	3	26,28,28	1.17	0	33,37,37	1.75	8 (24%)
2	GRG	B	401	3	26,28,28	1.26	1 (3%)	33,37,37	1.56	9 (27%)

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
2	GRG	D	401	3	-	9/31/31/31	-
2	GRG	F	401	3	-	9/31/31/31	-
2	GRG	E	401	3	-	8/31/31/31	-
2	GRG	A	501	3	-	6/31/31/31	-
2	GRG	C	401	3	-	4/31/31/31	-
2	GRG	B	401	3	-	9/31/31/31	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	GRG	C9-C8	2.71	1.56	1.51
2	E	401	GRG	O1-C1	-2.17	1.40	1.43
2	D	401	GRG	C9-C8	2.15	1.55	1.51
2	F	401	GRG	O1-C1	-2.13	1.40	1.43
2	E	401	GRG	C15-C13	2.12	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	GRG	C9-C8	2.11	1.55	1.51
2	B	401	GRG	C9-C8	2.10	1.55	1.51
2	F	401	GRG	C15-C13	2.06	1.55	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	GRG	C1-C2-C3	-4.32	118.56	126.04
2	E	401	GRG	C14-C13-C15	3.52	121.20	115.27
2	F	401	GRG	C1-C2-C3	-3.52	119.96	126.04
2	F	401	GRG	C6-C7-C8	-3.52	119.19	127.66
2	C	401	GRG	C6-C7-C8	-3.46	119.32	127.66
2	D	401	GRG	C1-C2-C3	-3.41	120.15	126.04
2	C	401	GRG	C11-C12-C13	-3.38	119.53	127.66
2	B	401	GRG	PA-O3A-PB	-3.37	121.27	132.83
2	D	401	GRG	C11-C12-C13	-3.33	119.63	127.66
2	E	401	GRG	C10-C8-C9	3.29	120.81	115.27
2	A	501	GRG	C10-C8-C9	3.26	120.76	115.27
2	A	501	GRG	C11-C12-C13	-3.22	119.91	127.66
2	A	501	GRG	PA-O3A-PB	-3.12	122.14	132.83
2	C	401	GRG	C10-C8-C9	3.05	120.40	115.27
2	A	501	GRG	C14-C13-C15	3.01	120.34	115.27
2	A	501	GRG	C1-C2-C3	-2.93	120.98	126.04
2	D	401	GRG	C10-C8-C9	2.93	120.20	115.27
2	F	401	GRG	C4-C3-C5	2.92	120.18	115.27
2	B	401	GRG	C4-C3-C5	2.89	120.13	115.27
2	D	401	GRG	PA-O3A-PB	-2.87	122.99	132.83
2	C	401	GRG	PA-O3A-PB	-2.84	123.07	132.83
2	B	401	GRG	C14-C13-C15	2.77	119.94	115.27
2	D	401	GRG	C6-C7-C8	-2.72	121.11	127.66
2	C	401	GRG	C4-C3-C5	2.71	119.82	115.27
2	E	401	GRG	C4-C3-C5	2.69	119.79	115.27
2	B	401	GRG	C6-C7-C8	-2.65	121.28	127.66
2	F	401	GRG	C11-C12-C13	-2.64	121.30	127.66
2	F	401	GRG	C10-C8-C9	2.62	119.68	115.27
2	E	401	GRG	PA-O3A-PB	-2.61	123.89	132.83
2	E	401	GRG	C6-C7-C8	-2.60	121.39	127.66
2	E	401	GRG	C1-C2-C3	-2.60	121.54	126.04
2	B	401	GRG	C11-C12-C13	-2.60	121.41	127.66
2	D	401	GRG	C4-C3-C5	2.57	119.59	115.27
2	B	401	GRG	C1-C2-C3	-2.56	121.61	126.04
2	E	401	GRG	C15-C13-C12	-2.50	116.06	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	GRG	C19-C18-C20	2.47	120.06	114.60
2	C	401	GRG	C14-C13-C15	2.42	119.34	115.27
2	B	401	GRG	C19-C18-C20	2.36	119.82	114.60
2	E	401	GRG	C9-C11-C12	-2.33	104.21	111.88
2	E	401	GRG	C19-C18-C20	2.27	119.62	114.60
2	B	401	GRG	C16-C17-C18	-2.25	120.05	127.75
2	E	401	GRG	C16-C17-C18	-2.19	120.26	127.75
2	C	401	GRG	C19-C18-C20	2.15	119.35	114.60
2	A	501	GRG	C16-C17-C18	-2.12	120.50	127.75
2	B	401	GRG	C10-C8-C9	2.12	118.84	115.27
2	A	501	GRG	C4-C3-C5	2.12	118.83	115.27
2	A	501	GRG	C6-C7-C8	-2.11	122.58	127.66
2	F	401	GRG	C14-C13-C15	2.04	118.71	115.27
2	F	401	GRG	PA-O3A-PB	-2.02	125.90	132.83
2	D	401	GRG	C14-C13-C15	2.01	118.64	115.27

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GRG	C1-O1-PA-O1A
2	E	401	GRG	C12-C11-C9-C8
2	A	501	GRG	C13-C15-C16-C17
2	A	501	GRG	C12-C11-C9-C8
2	E	401	GRG	C13-C15-C16-C17
2	F	401	GRG	C3-C5-C6-C7
2	F	401	GRG	C14-C13-C15-C16
2	A	501	GRG	C10-C8-C9-C11
2	D	401	GRG	C14-C13-C15-C16
2	A	501	GRG	C2-C3-C5-C6
2	F	401	GRG	C12-C13-C15-C16
2	A	501	GRG	C4-C3-C5-C6
2	D	401	GRG	C10-C8-C9-C11
2	A	501	GRG	C7-C8-C9-C11
2	D	401	GRG	C12-C13-C15-C16
2	D	401	GRG	C7-C8-C9-C11
2	F	401	GRG	C4-C3-C5-C6
2	F	401	GRG	C2-C3-C5-C6
2	B	401	GRG	C4-C3-C5-C6
2	E	401	GRG	C10-C8-C9-C11
2	E	401	GRG	C4-C3-C5-C6
2	F	401	GRG	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
2	B	401	GRG	C2-C3-C5-C6
2	E	401	GRG	C7-C8-C9-C11
2	E	401	GRG	C2-C3-C5-C6
2	F	401	GRG	PB-O3A-PA-O2A
2	B	401	GRG	PB-O3A-PA-O1
2	C	401	GRG	C2-C3-C5-C6
2	B	401	GRG	C1-O1-PA-O3A
2	D	401	GRG	C1-O1-PA-O3A
2	C	401	GRG	C4-C3-C5-C6
2	D	401	GRG	C4-C3-C5-C6
2	B	401	GRG	C1-O1-PA-O2A
2	D	401	GRG	C1-O1-PA-O2A
2	B	401	GRG	C13-C15-C16-C17
2	D	401	GRG	C2-C3-C5-C6
2	D	401	GRG	C13-C15-C16-C17
2	E	401	GRG	C14-C13-C15-C16
2	F	401	GRG	C10-C8-C9-C11
2	F	401	GRG	C7-C8-C9-C11
2	B	401	GRG	C14-C13-C15-C16
2	B	401	GRG	C12-C13-C15-C16
2	E	401	GRG	C12-C13-C15-C16
2	C	401	GRG	C9-C11-C12-C13
2	C	401	GRG	C10-C8-C9-C11

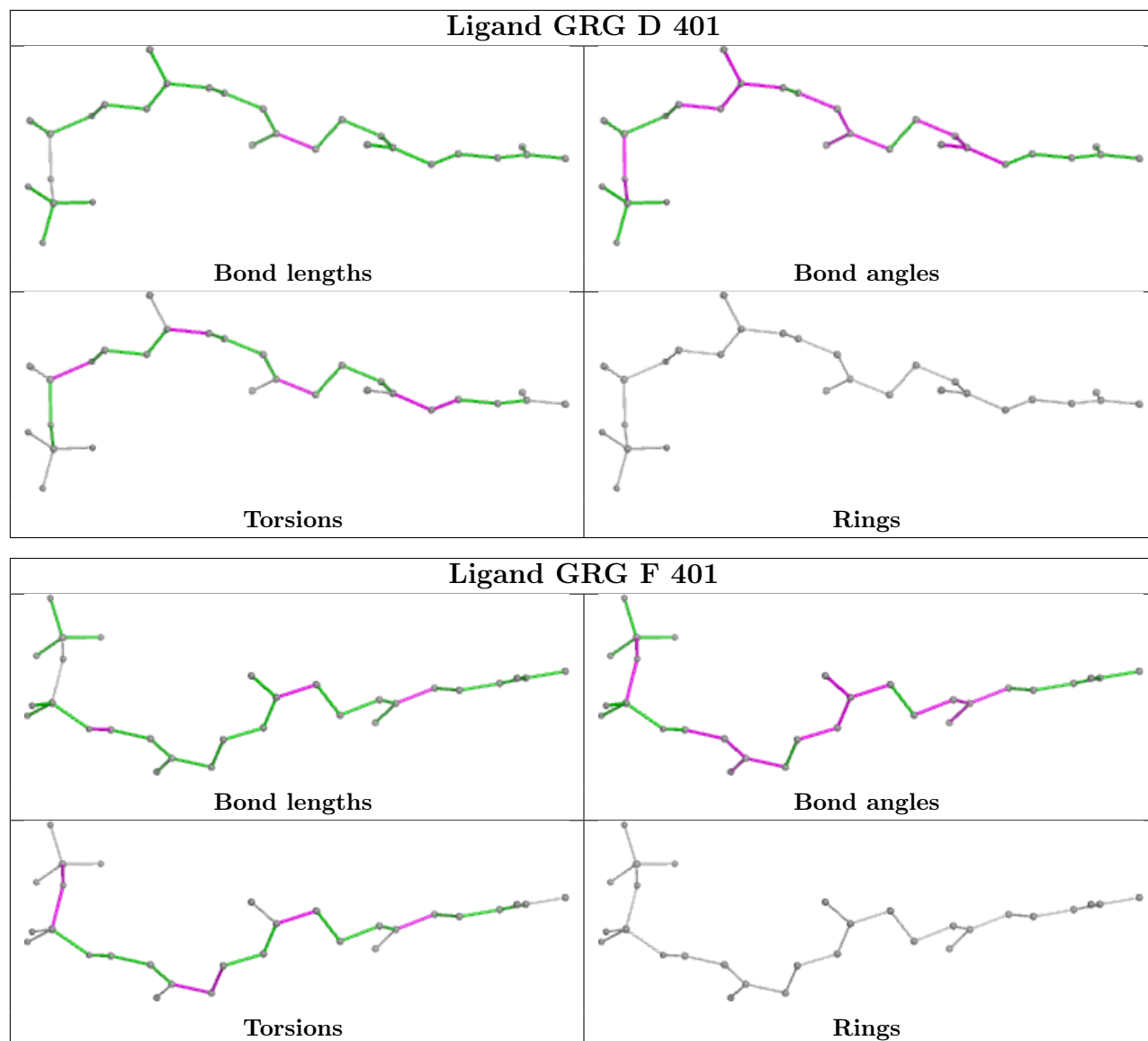
There are no ring outliers.

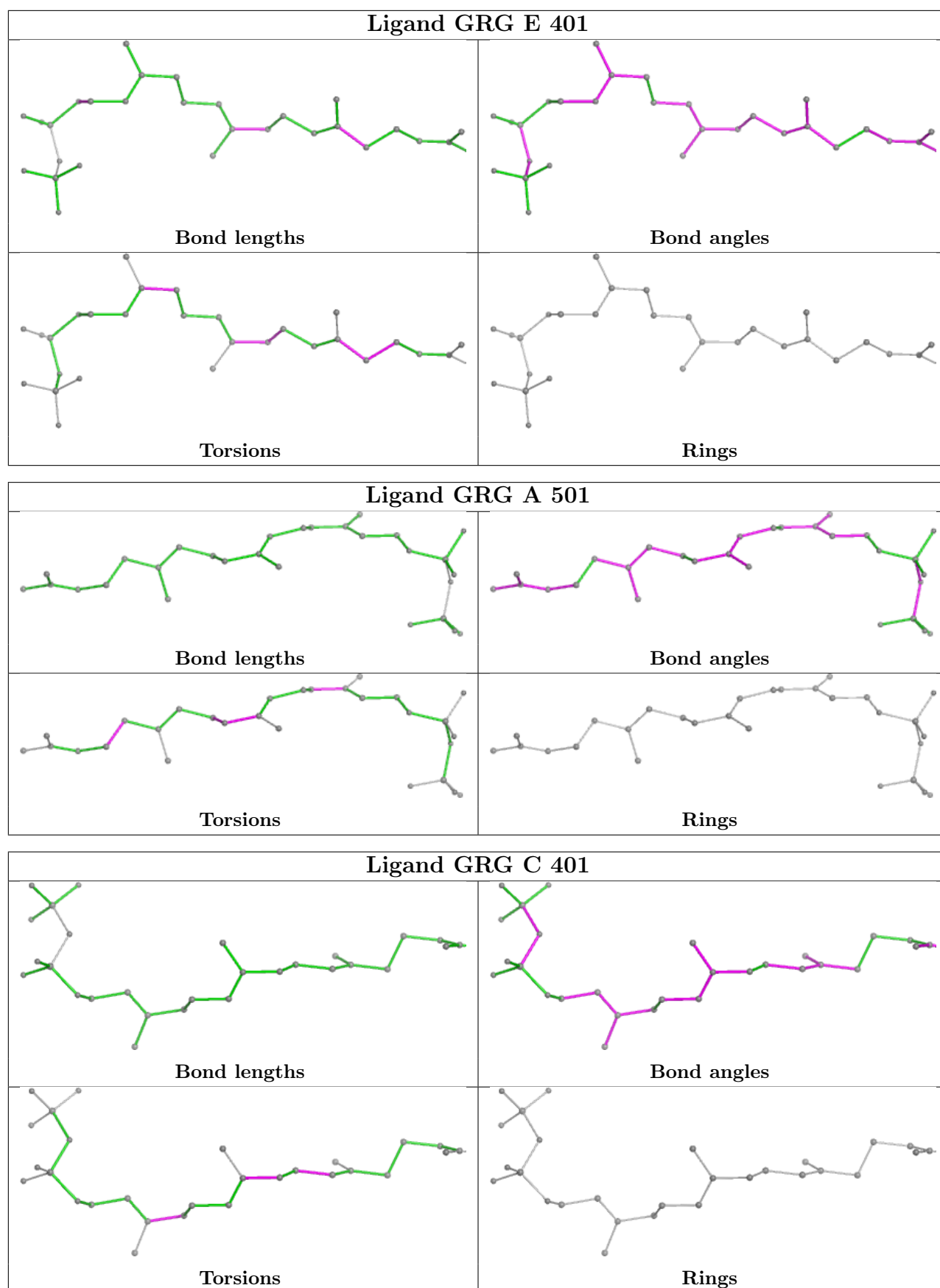
6 monomers are involved in 24 short contacts:

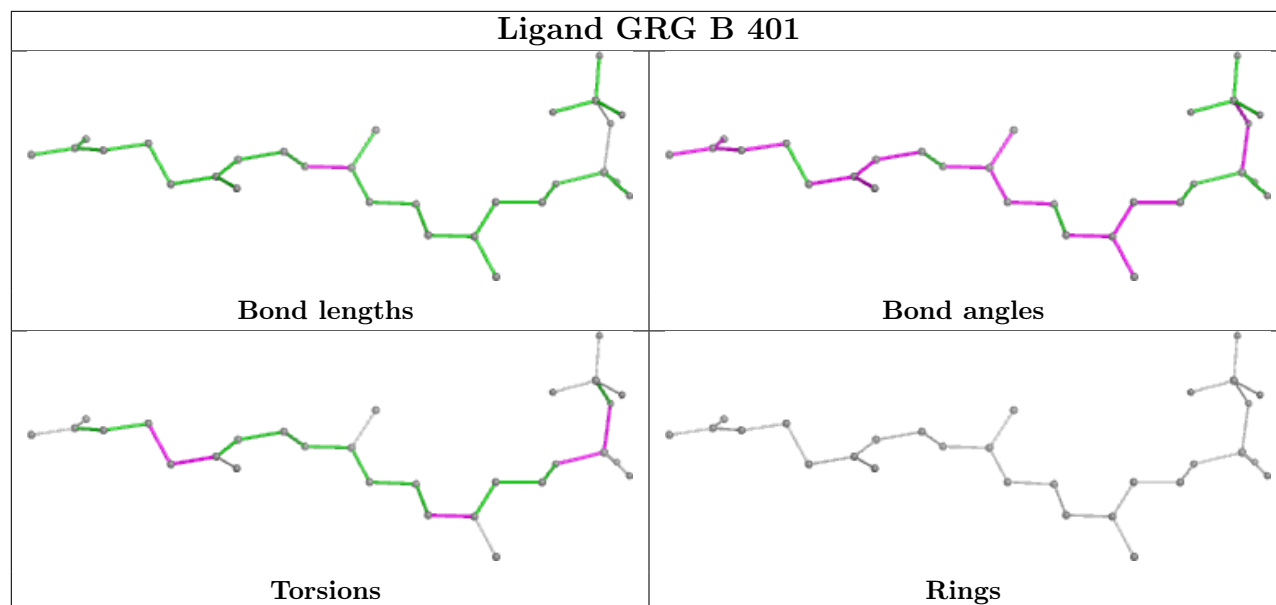
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	GRG	4	0
2	F	401	GRG	3	0
2	E	401	GRG	3	0
2	A	501	GRG	8	0
2	C	401	GRG	2	0
2	B	401	GRG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	294/307 (95%)	0.77	23 (7%)	20 19	64, 87, 116, 126	0
1	B	287/307 (93%)	0.72	19 (6%)	26 24	66, 87, 107, 116	0
1	C	293/307 (95%)	0.11	4 (1%)	73 70	42, 64, 79, 95	0
1	D	293/307 (95%)	0.06	4 (1%)	73 70	47, 56, 71, 99	0
1	E	291/307 (94%)	0.44	6 (2%)	63 60	55, 80, 98, 105	0
1	F	294/307 (95%)	0.47	9 (3%)	51 48	51, 73, 103, 123	0
All	All	1752/1842 (95%)	0.43	65 (3%)	45 42	42, 74, 105, 126	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	TYR	4.0
1	F	43	GLU	3.4
1	A	97	PHE	3.4
1	A	4	THR	3.3
1	B	136	TYR	3.3
1	B	195	SER	3.2
1	A	199	SER	3.2
1	B	35	PHE	3.2
1	E	180	LEU	3.1
1	C	137	THR	3.1
1	D	76	PHE	3.0
1	E	156	PHE	3.0
1	A	112	VAL	3.0
1	B	4	THR	2.9
1	B	193	LEU	2.9
1	F	76	PHE	2.9
1	F	198	TYR	2.8
1	F	168	ASP	2.8
1	E	5	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	35	PHE	2.8
1	D	287	LEU	2.8
1	B	97	PHE	2.7
1	B	96	TYR	2.7
1	A	35	PHE	2.7
1	B	60	SER	2.7
1	E	230	VAL	2.7
1	A	29	THR	2.7
1	A	213	PHE	2.7
1	A	115	PHE	2.6
1	D	198	TYR	2.6
1	B	204	PHE	2.6
1	B	254	VAL	2.5
1	B	53	THR	2.5
1	A	96	TYR	2.5
1	A	293	LYS	2.5
1	F	116	THR	2.5
1	F	4	THR	2.4
1	A	269	ALA	2.4
1	A	196	LYS	2.4
1	B	180	LEU	2.4
1	F	182	LEU	2.4
1	A	295	PHE	2.4
1	B	89	ILE	2.4
1	E	155	LEU	2.3
1	A	119	LEU	2.3
1	C	199	SER	2.3
1	B	242	ASP	2.3
1	B	168	ASP	2.3
1	F	196	LYS	2.2
1	A	195	SER	2.2
1	C	298	GLU	2.2
1	A	217	THR	2.2
1	A	257	PHE	2.2
1	B	224	ARG	2.2
1	E	35	PHE	2.2
1	B	156	PHE	2.2
1	A	104	LEU	2.1
1	B	115	PHE	2.1
1	A	183	PHE	2.1
1	A	15	PRO	2.1
1	C	195	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	184	PHE	2.0
1	A	197	GLU	2.0
1	A	3	LYS	2.0
1	D	200	GLU	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](#)

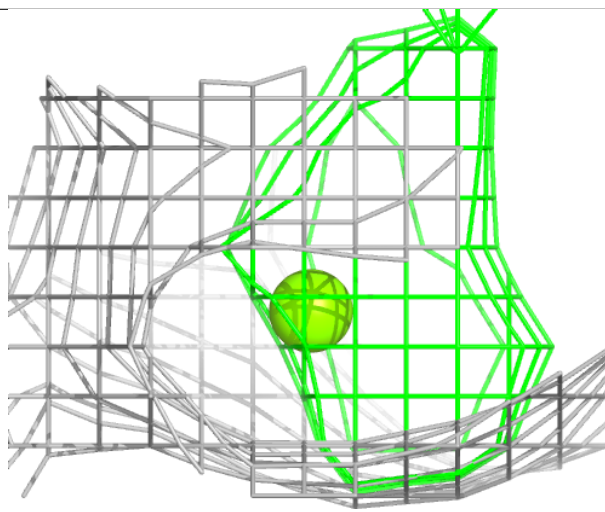
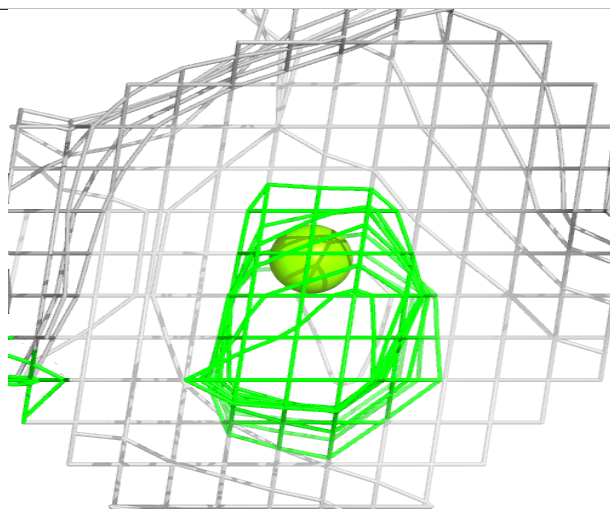
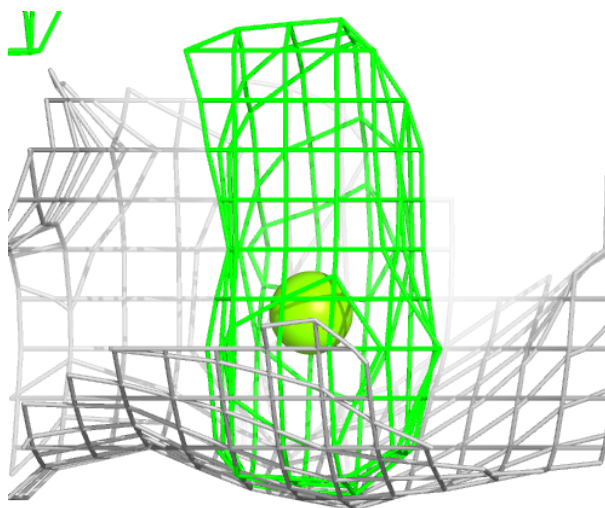
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	403	1/1	0.91	0.22	67,67,67,67	0
2	GRG	A	501	29/29	0.92	0.17	75,81,89,95	0
2	GRG	E	401	29/29	0.93	0.15	67,75,81,84	0
3	MG	B	402	1/1	0.94	0.11	71,71,71,71	0
2	GRG	B	401	29/29	0.94	0.14	73,80,92,93	0
3	MG	D	403	1/1	0.94	0.12	52,52,52,52	0
3	MG	F	403	1/1	0.94	0.12	63,63,63,63	0
2	GRG	F	401	29/29	0.95	0.12	62,68,75,76	0
3	MG	E	402	1/1	0.95	0.12	66,66,66,66	0
3	MG	A	502	1/1	0.95	0.12	71,71,71,71	0
2	GRG	C	401	29/29	0.96	0.11	54,58,62,63	0
2	GRG	D	401	29/29	0.97	0.11	46,52,57,73	0
3	MG	E	403	1/1	0.98	0.07	73,73,73,73	0
3	MG	F	402	1/1	0.98	0.09	65,65,65,65	0
3	MG	C	402	1/1	0.98	0.08	55,55,55,55	0
3	MG	C	403	1/1	0.99	0.06	56,56,56,56	0
3	MG	A	503	1/1	0.99	0.11	72,72,72,72	0
3	MG	D	402	1/1	1.00	0.04	53,53,53,53	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.

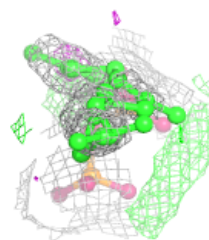
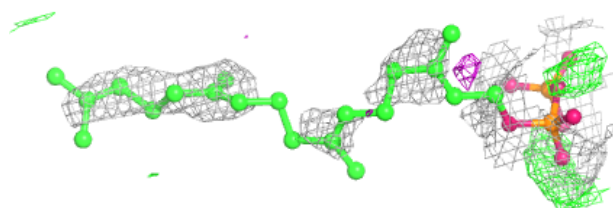
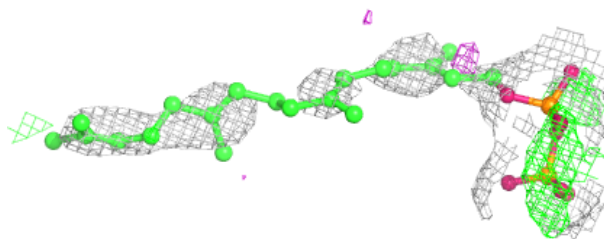
Electron density around MG B 403:

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

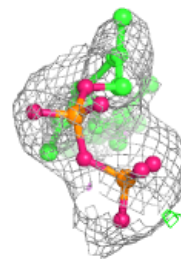
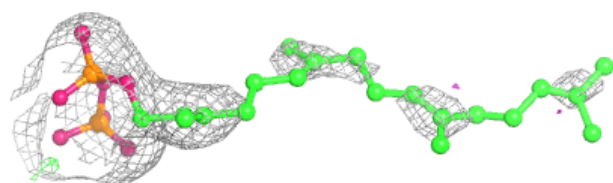
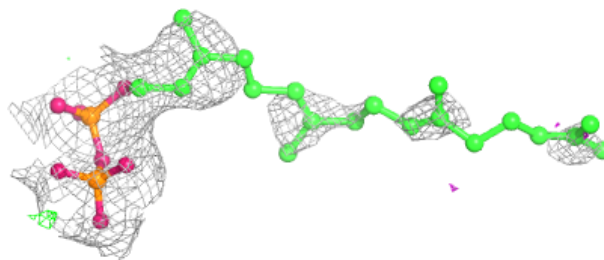


Electron density around GRG A 501:

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

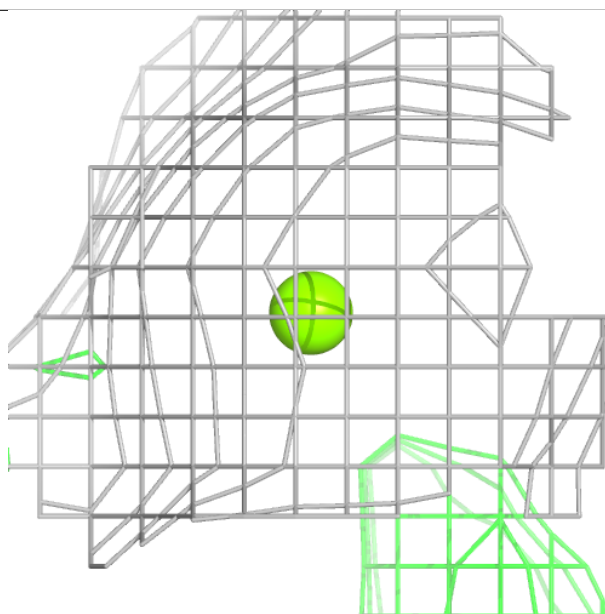
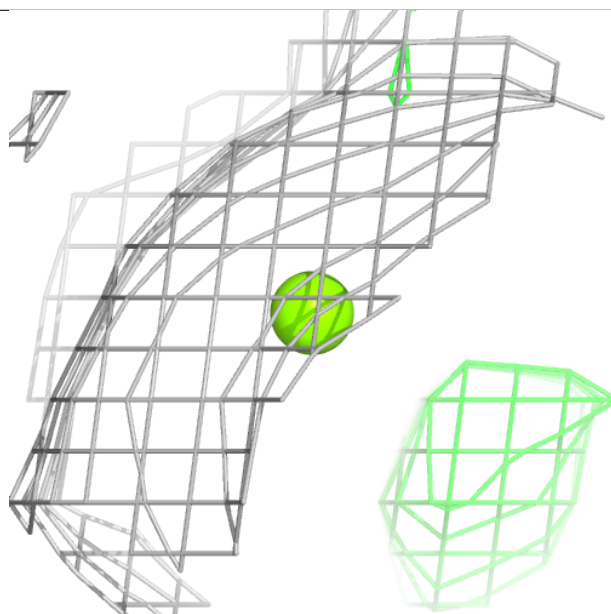
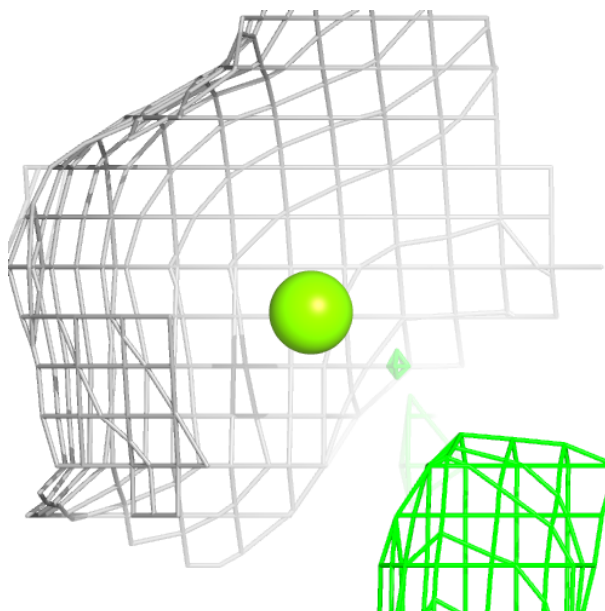
**Electron density around GRG E 401:**

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



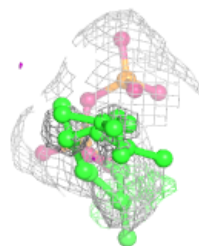
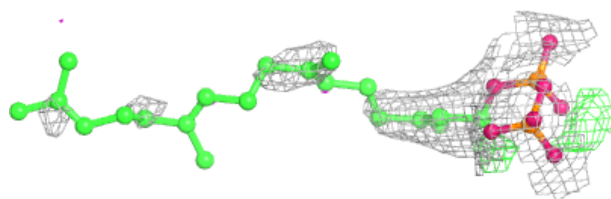
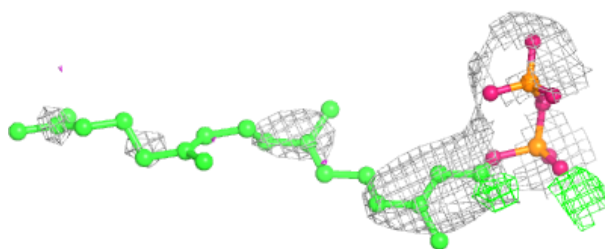
Electron density around MG B 402:

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and green (positive)



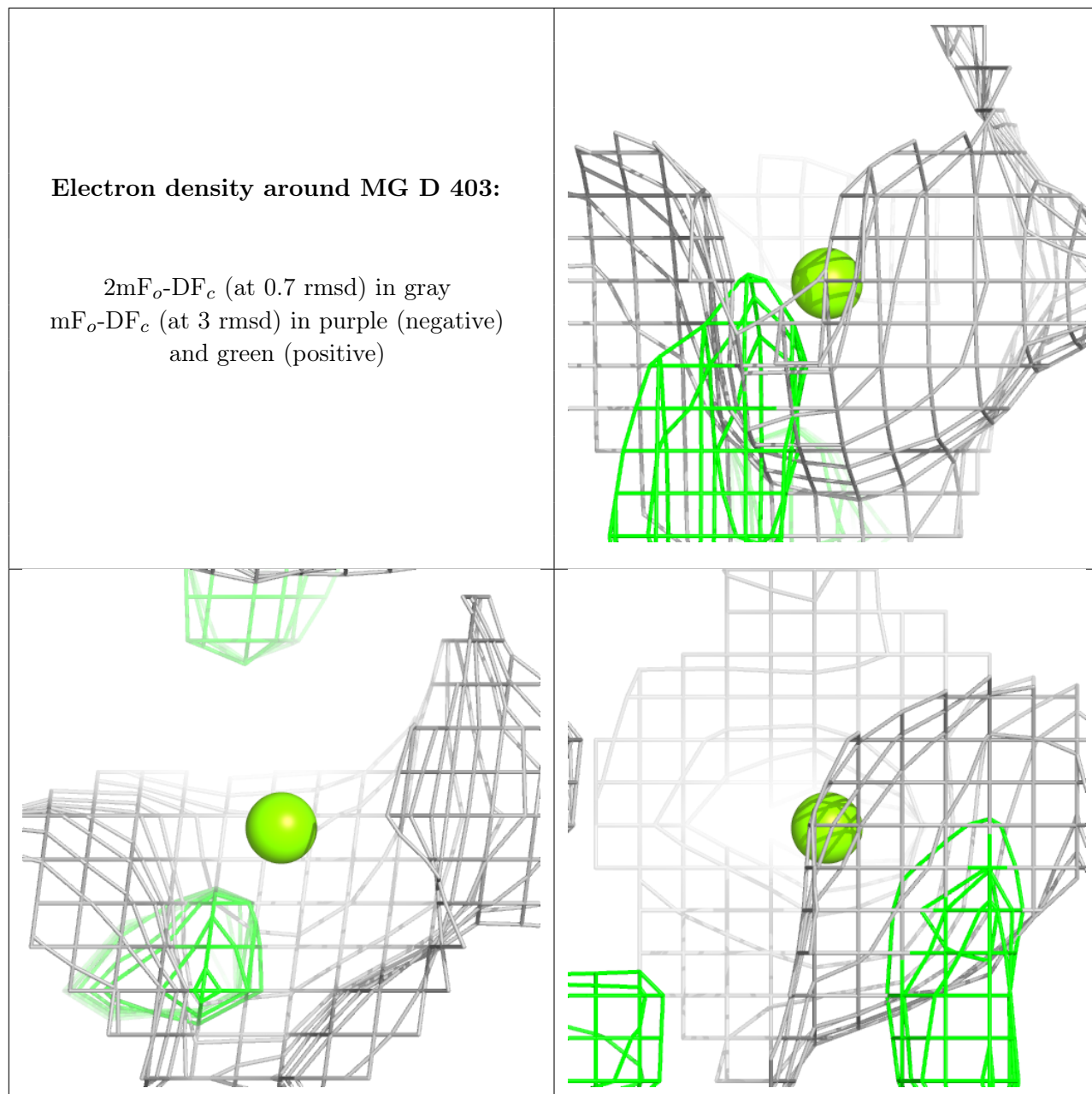
Electron density around GRG B 401:

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and green (positive)



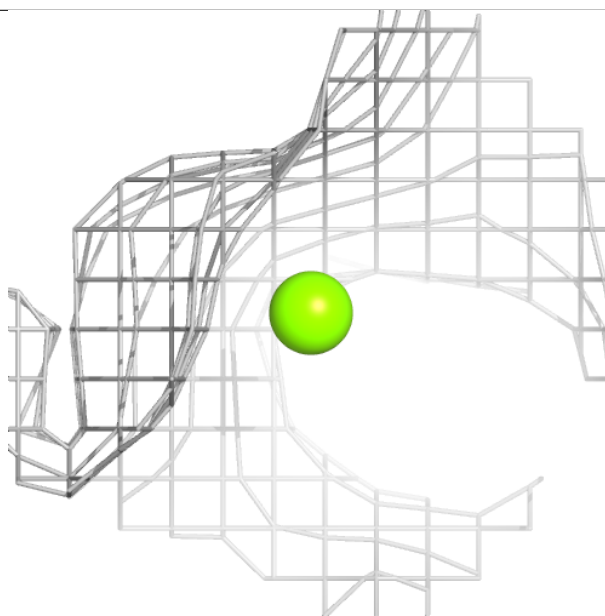
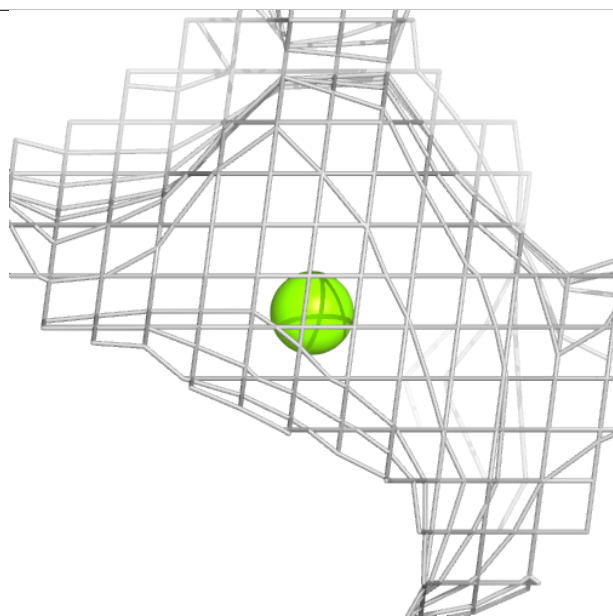
Electron density around MG D 403:

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and green (positive)



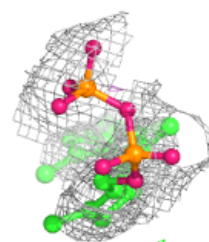
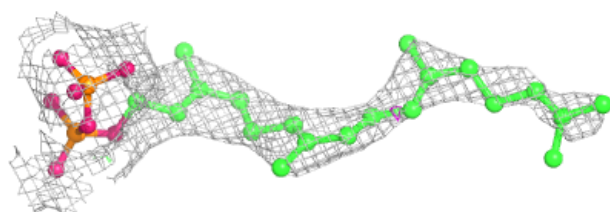
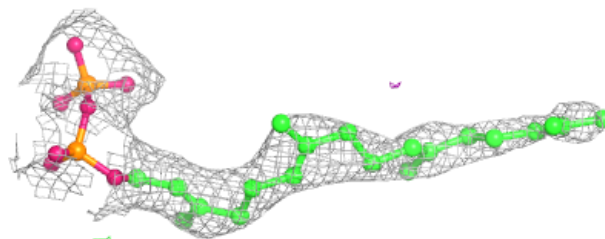
Electron density around MG F 403:

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and green (positive)



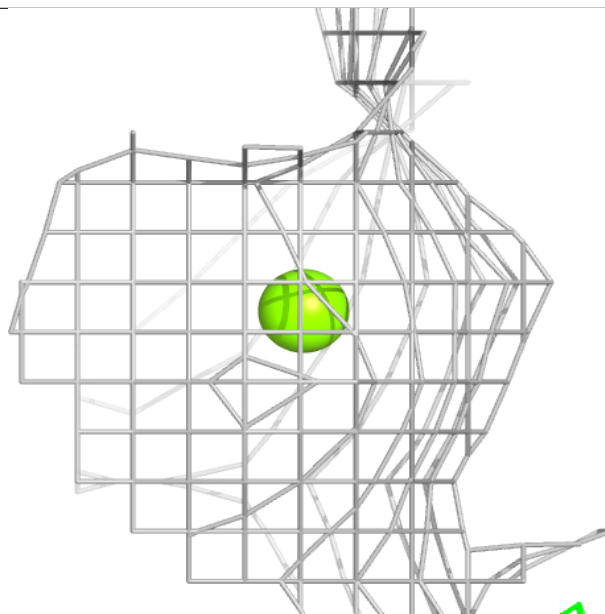
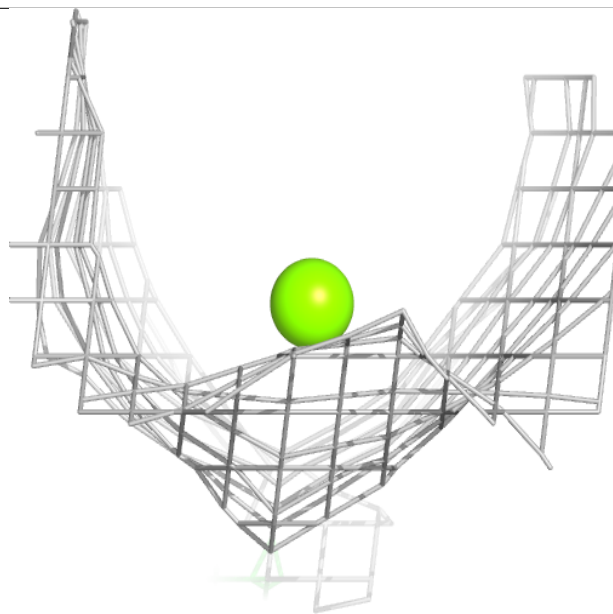
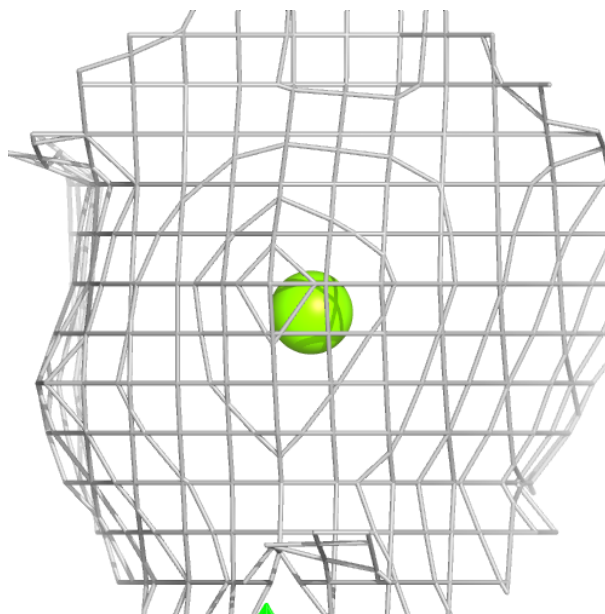
Electron density around GRG F 401:

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and green (positive)



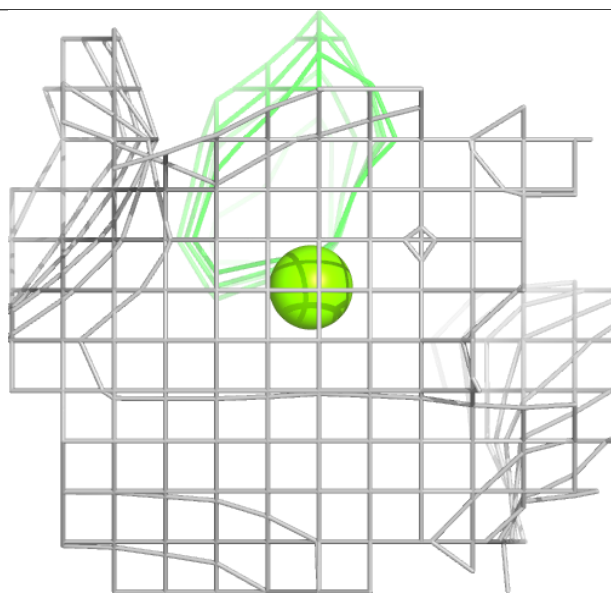
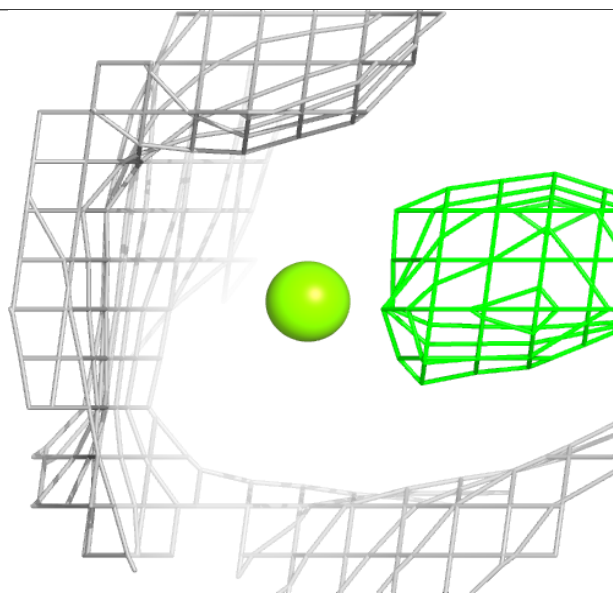
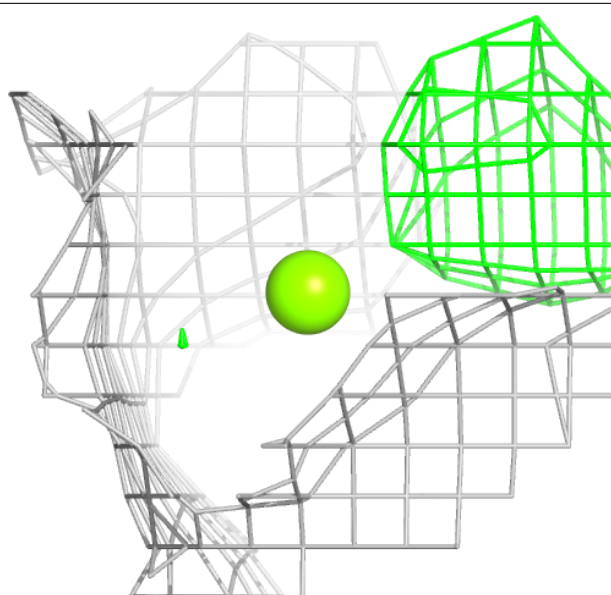
Electron density around MG E 402:

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and green (positive)



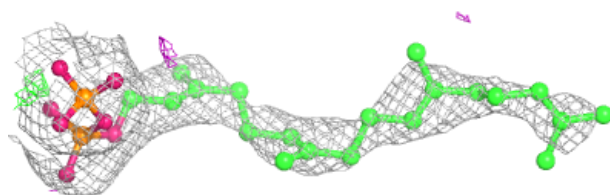
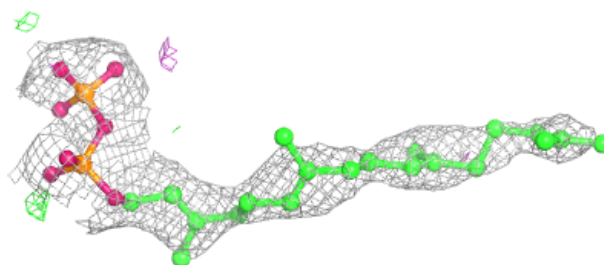
Electron density around MG A 502:

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

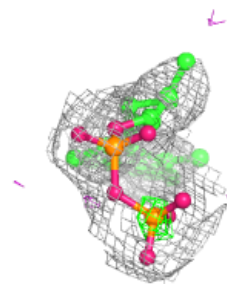
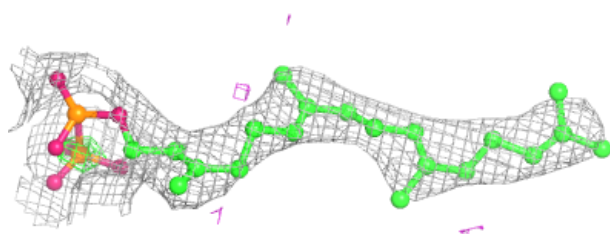
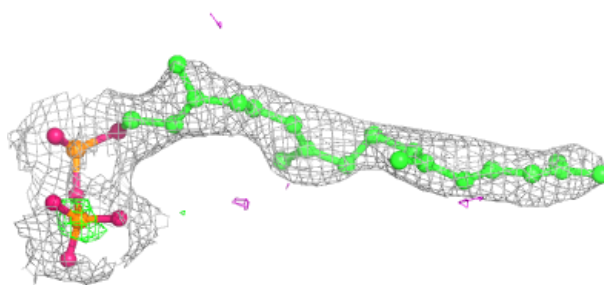


Electron density around GRG C 401:

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

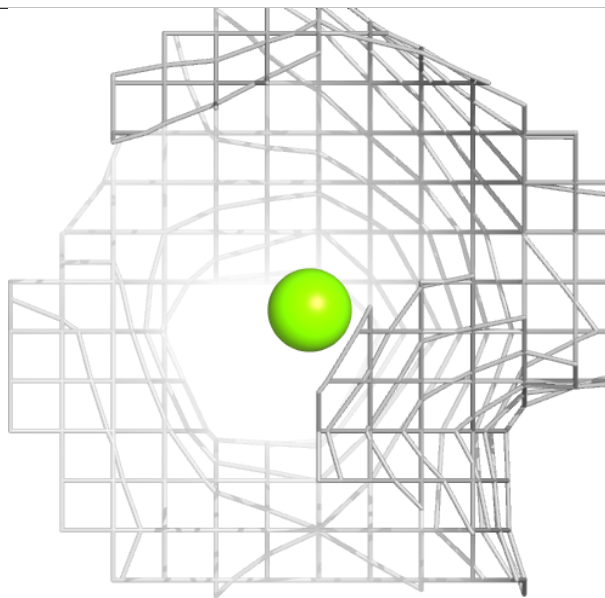
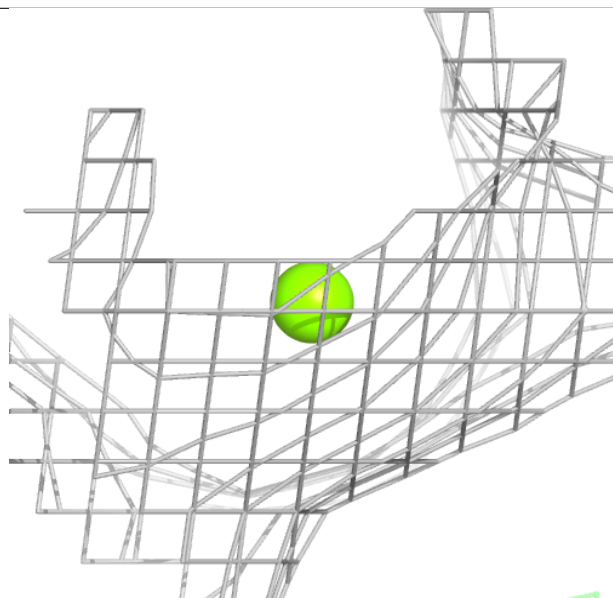
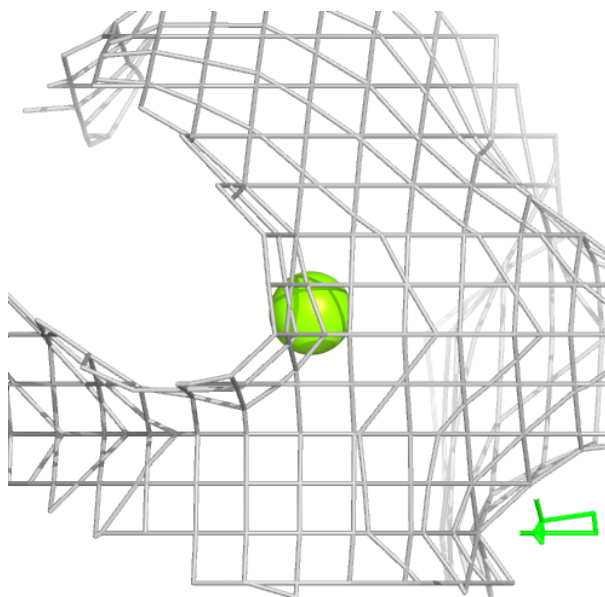
**Electron density around GRG D 401:**

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



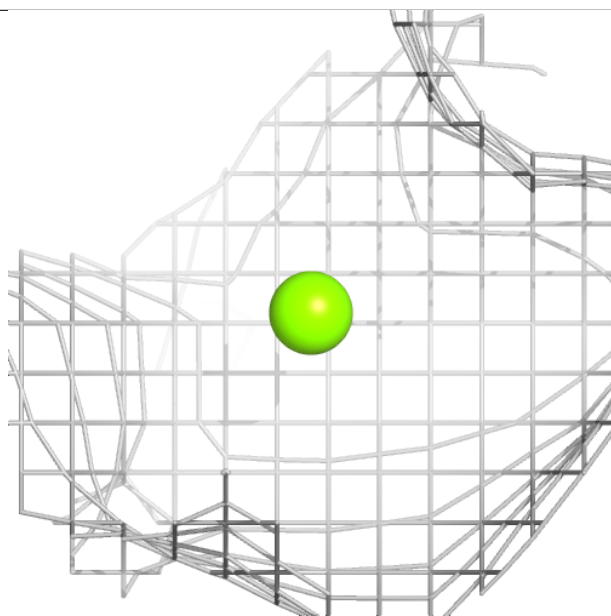
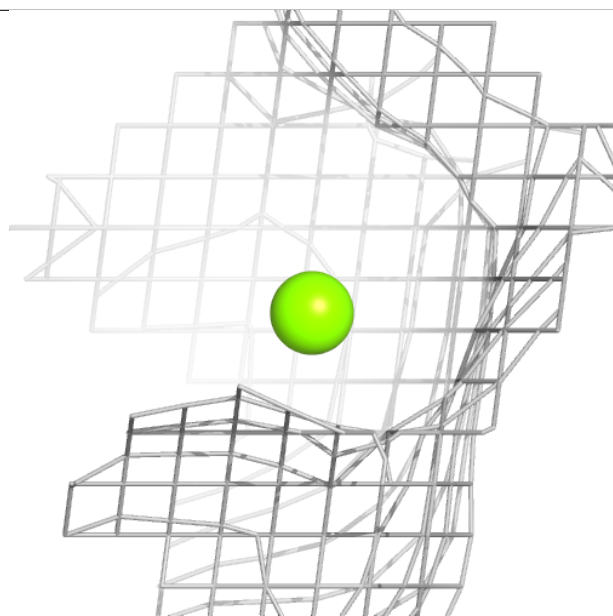
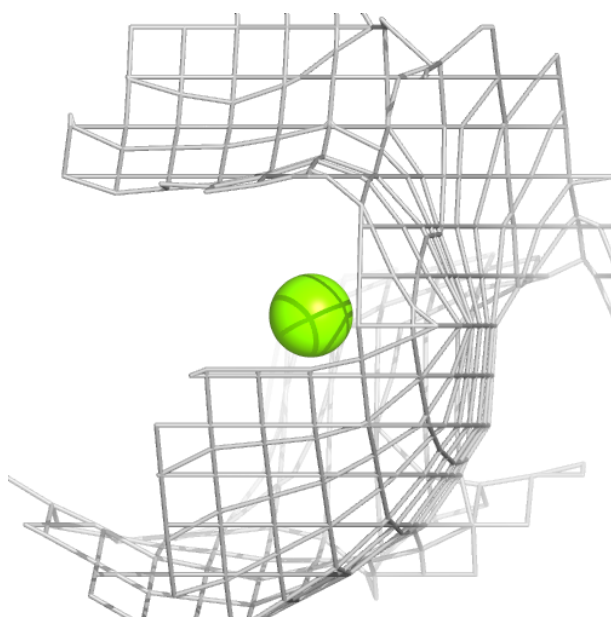
Electron density around MG E 403:

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



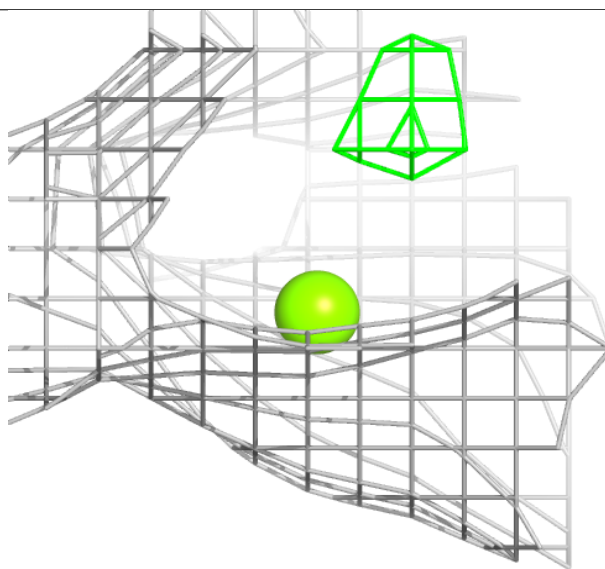
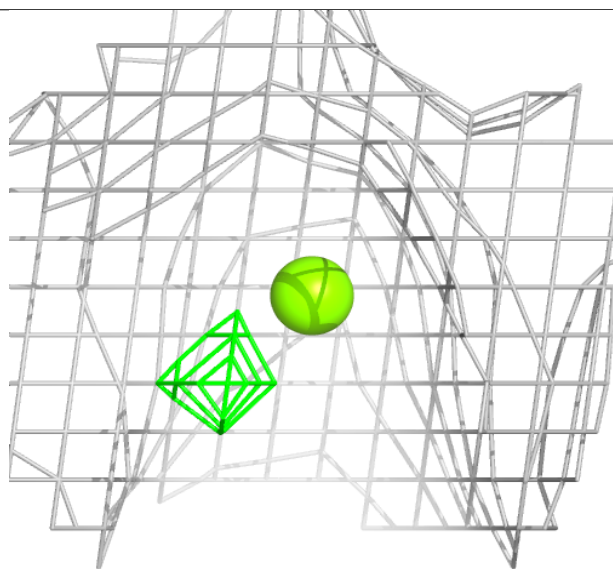
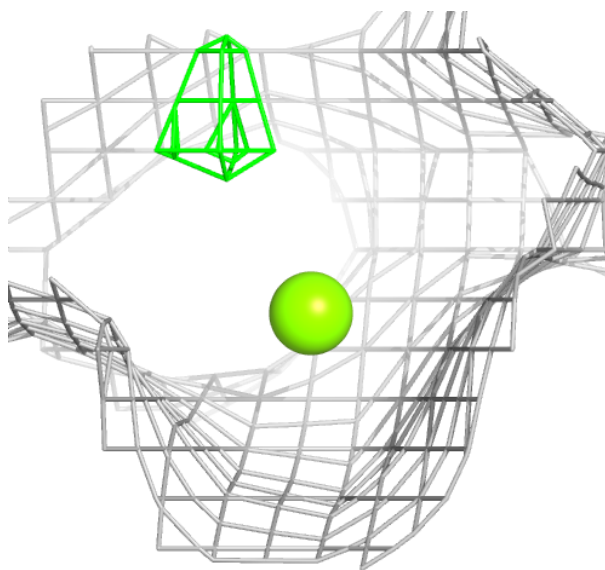
Electron density around MG F 402:

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



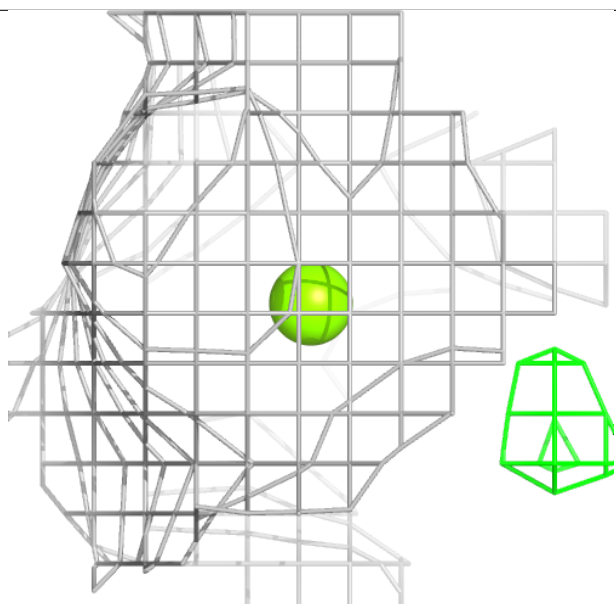
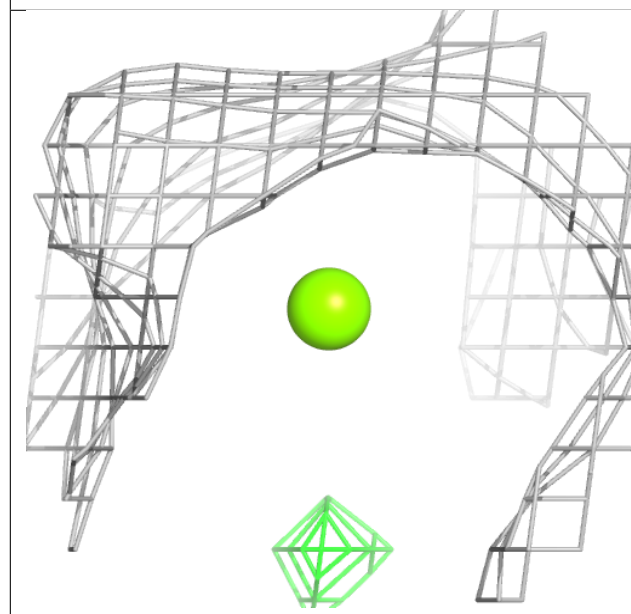
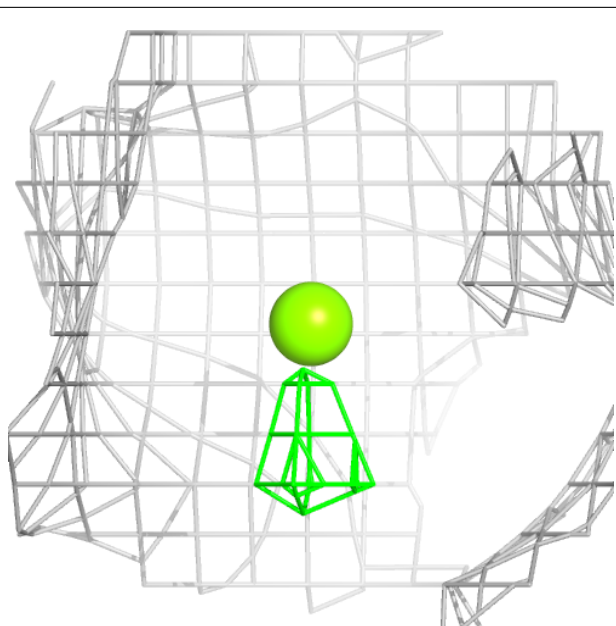
Electron density around MG C 402:

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



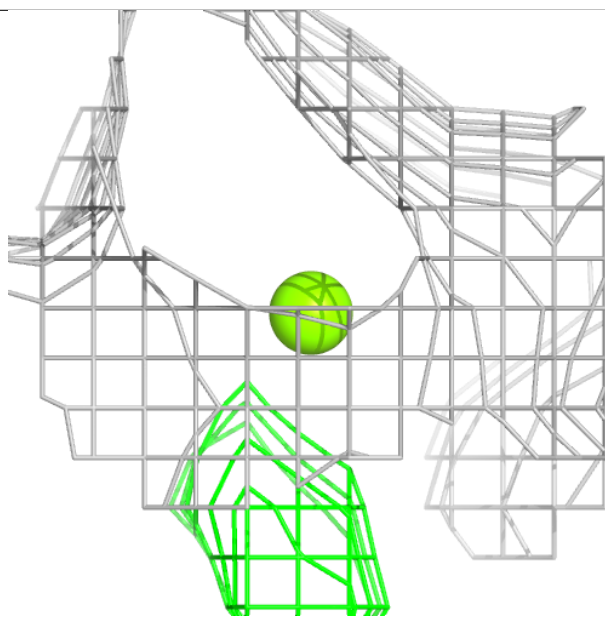
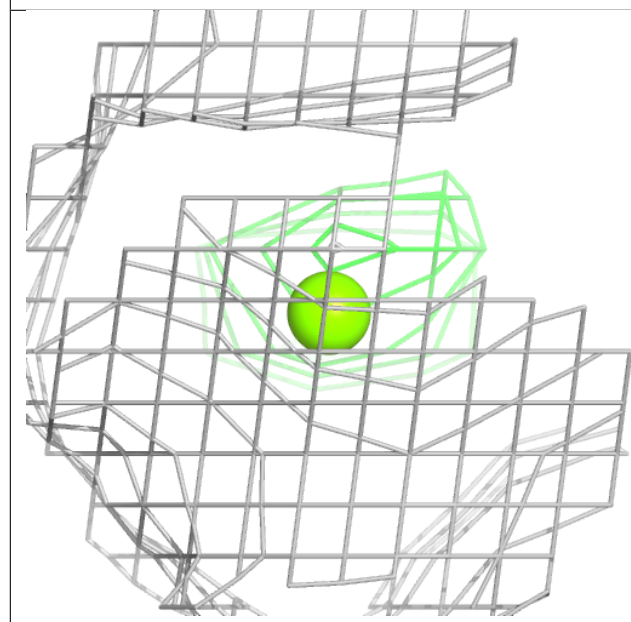
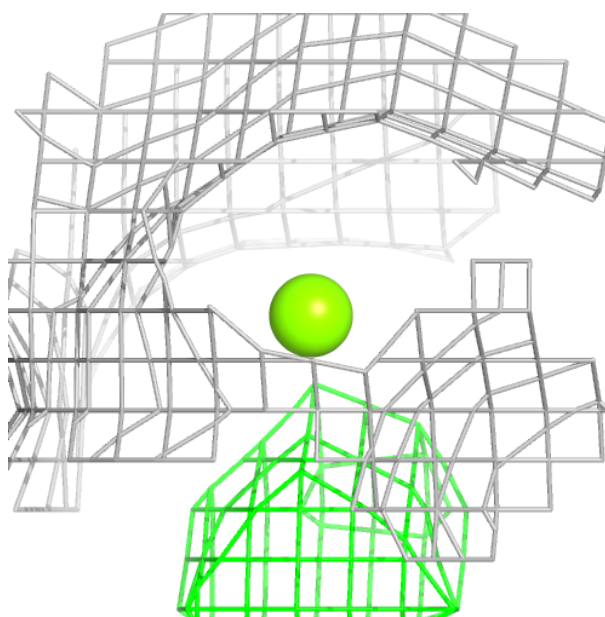
Electron density around MG C 403:

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



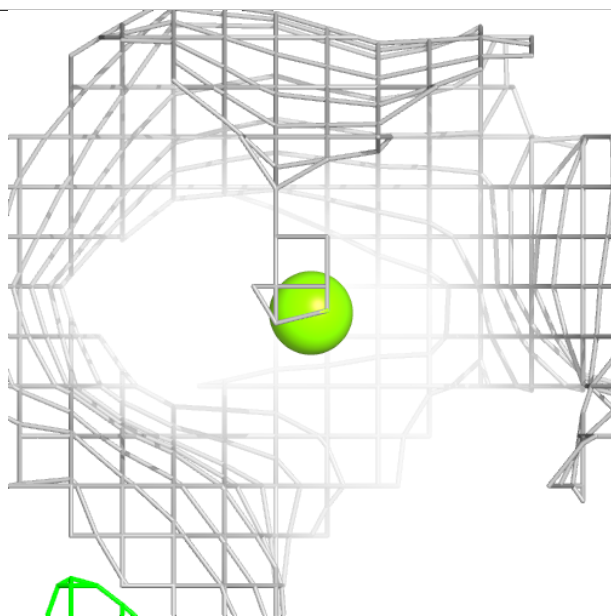
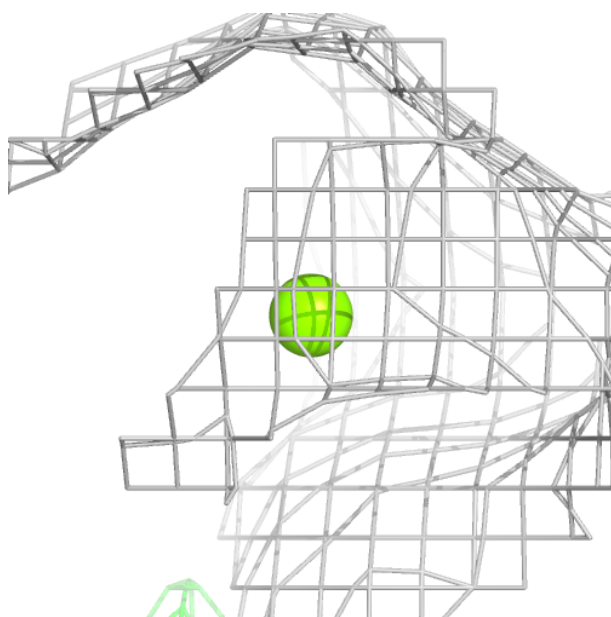
Electron density around MG A 503:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.