



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 29, 2024 – 06:09 PM JST

PDB ID : 8YP3
Title : Crystal structure of UDP-N-acetylglucosamine pyrophosphorylase from
Spodoptera frugiperda in complex with UDP-GlcNAc
Authors : Lu, Q.; Liu, T.; Zhou, Y.; Yang, Q.
Deposited on : 2024-03-15
Resolution : 2.12 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

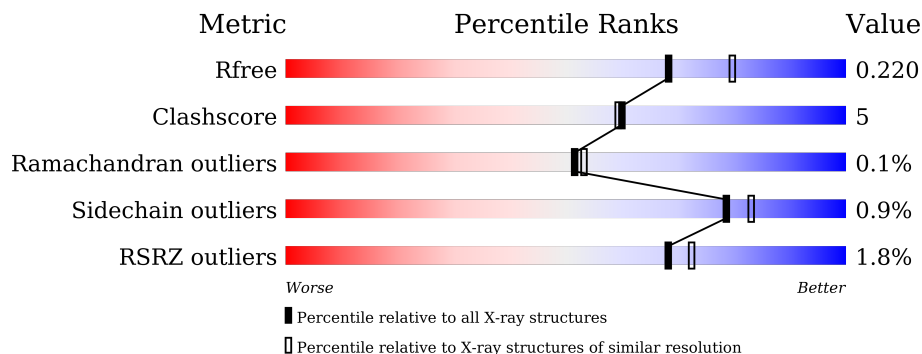
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	482	 2% 88% 9% ..
1	B	482	 3% 85% 9% 6%
1	C	482	 2% 91% 6% ..
1	D	482	 2% 87% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	502	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 15945 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 UDP-N-acetylglucosamine diphosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	471	3744	2373	642	717	12	0	0	0
1	B	454	3607	2289	616	688	14	0	0	0
1	C	467	3718	2356	643	705	14	0	0	0
1	D	466	3703	2346	636	707	14	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

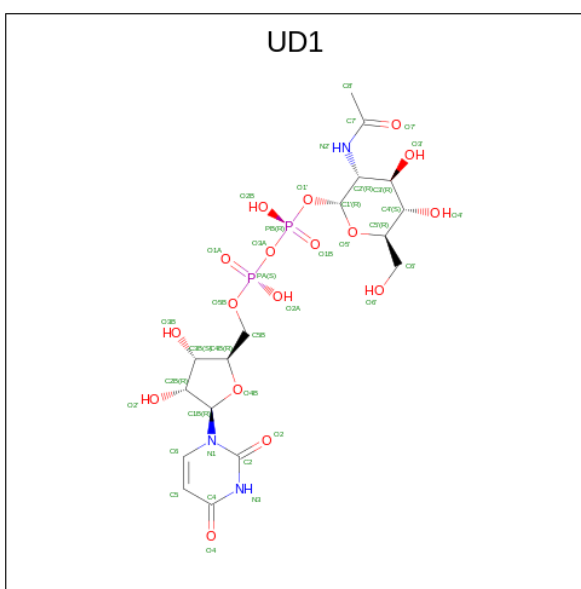
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	HIS	-	expression tag	UNP A0A2H1VI03
A	5	HIS	-	expression tag	UNP A0A2H1VI03
A	6	HIS	-	expression tag	UNP A0A2H1VI03
A	7	HIS	-	expression tag	UNP A0A2H1VI03
A	101	ARG	LYS	conflict	UNP A0A2H1VI03
A	463	THR	ALA	conflict	UNP A0A2H1VI03
A	485	ALA	-	expression tag	UNP A0A2H1VI03
B	4	HIS	-	expression tag	UNP A0A2H1VI03
B	5	HIS	-	expression tag	UNP A0A2H1VI03
B	6	HIS	-	expression tag	UNP A0A2H1VI03
B	7	HIS	-	expression tag	UNP A0A2H1VI03
B	101	ARG	LYS	conflict	UNP A0A2H1VI03
B	463	THR	ALA	conflict	UNP A0A2H1VI03
B	485	ALA	-	expression tag	UNP A0A2H1VI03
C	4	HIS	-	expression tag	UNP A0A2H1VI03
C	5	HIS	-	expression tag	UNP A0A2H1VI03
C	6	HIS	-	expression tag	UNP A0A2H1VI03
C	7	HIS	-	expression tag	UNP A0A2H1VI03
C	101	ARG	LYS	conflict	UNP A0A2H1VI03
C	463	THR	ALA	conflict	UNP A0A2H1VI03
C	485	ALA	-	expression tag	UNP A0A2H1VI03

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	HIS	-	expression tag	UNP A0A2H1VI03
D	5	HIS	-	expression tag	UNP A0A2H1VI03
D	6	HIS	-	expression tag	UNP A0A2H1VI03
D	7	HIS	-	expression tag	UNP A0A2H1VI03
D	101	ARG	LYS	conflict	UNP A0A2H1VI03
D	463	THR	ALA	conflict	UNP A0A2H1VI03
D	485	ALA	-	expression tag	UNP A0A2H1VI03

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: 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	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	247	Total	O	0	0
			247	247		

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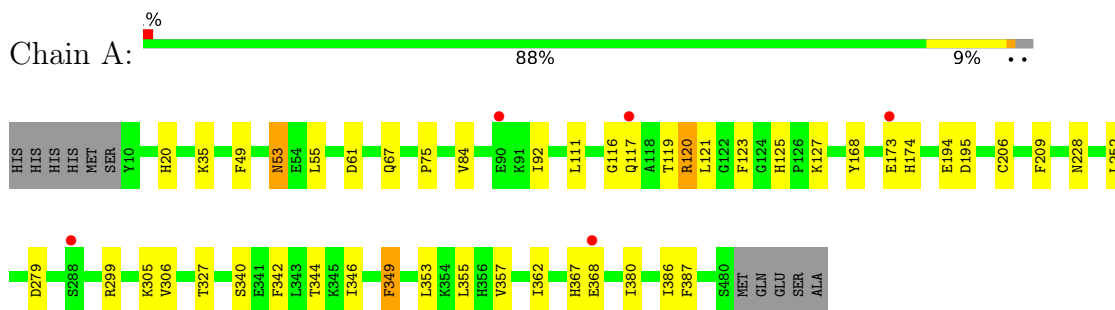
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	216	Total 216	O 216	0	0
5	C	254	Total 254	O 254	0	0
5	D	276	Total 276	O 276	0	0

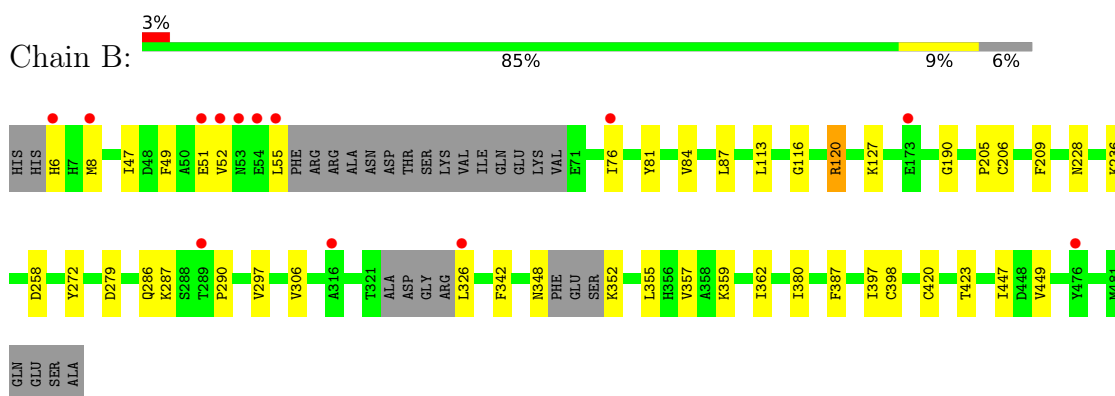
3 Residue-property plots [i](#)

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.

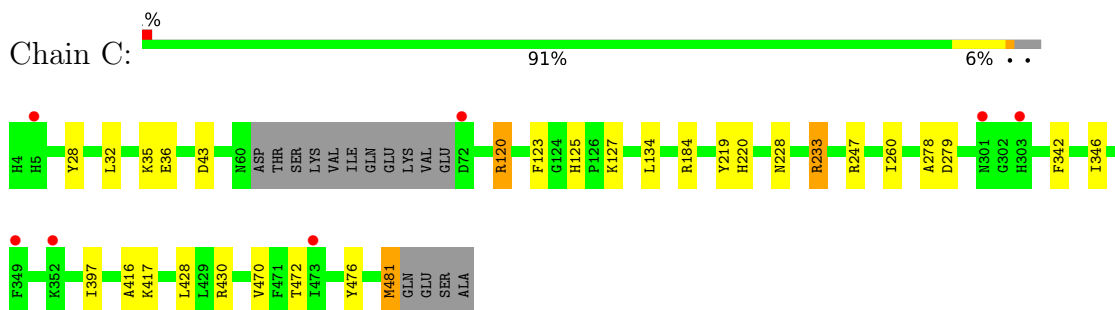
- Molecule 1: UDP-N-acetylglucosamine diphosphorylase



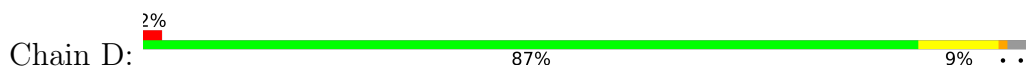
- Molecule 1: UDP-N-acetylglucosamine diphosphorylase

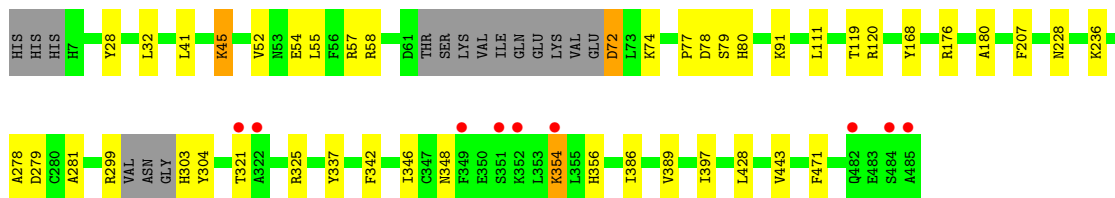


- Molecule 1: UDP-N-acetylglucosamine diphosphorylase



- Molecule 1: UDP-N-acetylglucosamine diphosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.73Å 233.53Å 98.06Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.00 – 2.12 90.41 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.00-2.12) 93.8 (90.41-2.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.192 , 0.220 0.192 , 0.220	Depositor DCC
R_{free} test set	2001 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15945	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1683e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UD1, SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3823	0.55	1/5160 (0.0%)
1	B	0.38	0/3683	0.56	1/4968 (0.0%)
1	C	0.34	0/3800	0.54	2/5127 (0.0%)
1	D	0.43	0/3781	0.54	0/5099
All	All	0.38	0/15087	0.55	4/20354 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	GLN	CA-CB-CG	-5.82	100.61	113.40
1	C	120	ARG	CA-CB-CG	5.55	125.61	113.40
1	A	252	LEU	CA-CB-CG	-5.28	103.17	115.30
1	C	233	ARG	CG-CD-NE	5.20	122.72	111.80

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	3744	0	3676	45	0
1	B	3607	0	3534	41	0
1	C	3718	0	3635	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3703	0	3621	29	0
2	A	39	0	25	2	0
2	B	39	0	25	3	0
2	C	39	0	25	1	0
2	D	39	0	25	3	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	3	0
3	D	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	247	0	0	1	0
5	B	216	0	0	3	0
5	C	254	0	0	3	0
5	D	276	0	0	2	0
All	All	15945	0	14566	135	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 5.

All (135) 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:67:GLN:CG	1:C:481:MET:HG2	1.56	1.33
1:A:67:GLN:HG2	1:C:481:MET:HG2	1.20	1.11
1:A:67:GLN:HG3	1:C:481:MET:HG2	1.47	0.93
1:A:67:GLN:CG	1:C:481:MET:CG	2.47	0.92
1:B:55:LEU:CD2	1:B:355:LEU:HB2	2.02	0.89
1:D:55:LEU:HD23	1:D:58:ARG:HH12	1.35	0.88
1:D:80:HIS:HD1	1:D:304:TYR:HH	1.22	0.88
1:A:120:ARG:HD2	1:A:120:ARG:H	1.39	0.86
1:B:55:LEU:CD1	1:B:355:LEU:HD12	2.06	0.83
1:B:55:LEU:HD21	1:B:355:LEU:HB2	1.61	0.83
1:B:76:ILE:CD1	1:B:398:CYS:CB	2.59	0.81
1:C:127:LYS:HE3	3:C:502:SO4:O2	1.82	0.80
1:A:67:GLN:HG2	1:C:481:MET:CG	2.09	0.79
1:A:67:GLN:HG3	1:C:481:MET:CG	2.10	0.78
1:C:481:MET:HE2	1:C:481:MET:H	1.47	0.78
1:B:76:ILE:CD1	1:B:398:CYS:HB3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LYS:HD2	5:B:634:HOH:O	1.86	0.76
1:B:76:ILE:HD13	1:B:398:CYS:HB3	1.66	0.75
1:C:184:ARG:NH1	5:C:601:HOH:O	2.20	0.74
1:B:55:LEU:HD13	1:B:355:LEU:HD12	1.69	0.73
1:B:55:LEU:HD22	1:B:355:LEU:HB2	1.71	0.72
1:D:278:ALA:HB2	1:D:397:ILE:HD12	1.73	0.71
1:B:55:LEU:HD11	1:B:355:LEU:HD12	1.71	0.71
1:D:176:ARG:HH12	1:D:180:ALA:HB2	1.57	0.70
1:A:20:HIS:HB3	1:A:53:ASN:ND2	2.07	0.69
1:B:76:ILE:HD11	1:B:398:CYS:HB2	1.75	0.69
1:B:76:ILE:CD1	1:B:398:CYS:HB2	2.23	0.67
1:D:54:GLU:HG2	1:D:57:ARG:HH11	1.59	0.67
1:C:247:ARG:NH1	5:C:602:HOH:O	2.20	0.66
1:B:76:ILE:HG21	1:B:81:TYR:HD2	1.59	0.65
1:D:342:PHE:CE2	1:D:346:ILE:HD11	2.31	0.65
1:B:76:ILE:HD11	1:B:398:CYS:CB	2.26	0.65
1:A:20:HIS:HB3	1:A:53:ASN:HD22	1.62	0.65
1:A:173:GLU:O	1:A:173:GLU:HG3	1.93	0.63
1:A:342:PHE:CE2	1:A:346:ILE:HD11	2.33	0.63
1:C:127:LYS:CE	3:C:502:SO4:O2	2.46	0.63
1:C:342:PHE:CE2	1:C:346:ILE:HD11	2.36	0.61
1:A:49:PHE:O	1:A:53:ASN:HB2	2.01	0.61
1:B:228:ASN:HD21	2:B:501:UD1:H8'1	1.66	0.60
1:B:297:VAL:HG22	1:B:306:VAL:HG22	1.84	0.59
1:C:481:MET:HE2	1:C:481:MET:N	2.17	0.59
1:A:116:GLY:C	3:A:502:SO4:O2	2.42	0.57
1:B:228:ASN:HD21	2:B:501:UD1:C8'	2.18	0.57
1:A:35:LYS:HZ3	1:B:352:LYS:HD3	1.70	0.56
1:B:47:ILE:HG12	1:B:205:PRO:HG3	1.87	0.56
1:A:367:HIS:C	1:A:368:GLU:HG3	2.26	0.56
1:D:91:LYS:NZ	5:D:606:HOH:O	2.39	0.56
1:A:206:CYS:HB3	1:A:362:ILE:HD13	1.88	0.56
1:D:299:ARG:HG2	1:D:303:HIS:O	2.06	0.55
1:D:354:LYS:HE2	1:D:356:HIS:CE1	2.41	0.55
1:C:43:ASP:OD2	1:C:220:HIS:ND1	2.38	0.55
1:A:119:THR:H	1:A:120:ARG:HH11	1.53	0.55
1:B:357:VAL:HG13	1:B:380:ILE:HG23	1.88	0.55
1:C:127:LYS:NZ	3:C:502:SO4:O2	2.41	0.54
1:D:279:ASP:HB2	1:D:342:PHE:HB2	1.88	0.54
1:C:123:PHE:CE2	1:C:125:HIS:HB2	2.43	0.53
1:B:127:LYS:HD3	1:B:258:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ALA:HB2	1:C:397:ILE:HD12	1.90	0.53
1:A:340:SER:O	1:A:344:THR:HG23	2.09	0.52
1:A:61:ASP:OD1	1:C:476:TYR:OH	2.26	0.52
1:C:470:VAL:HG12	1:C:472:THR:HG23	1.91	0.52
1:B:116:GLY:HA3	3:B:502:SO4:O2	2.10	0.51
1:D:228:ASN:HD21	2:D:501:UD1:C8'	2.24	0.51
1:B:447:ILE:HG22	1:B:449:VAL:HG23	1.91	0.51
1:A:209:PHE:O	1:C:472:THR:HG22	2.11	0.51
1:D:55:LEU:HD23	1:D:58:ARG:NH1	2.17	0.51
1:A:55:LEU:HB3	1:A:355:LEU:CD1	2.42	0.50
1:D:321:THR:HG22	1:D:325:ARG:O	2.10	0.50
1:A:119:THR:H	1:A:120:ARG:NH1	2.10	0.50
1:B:287:LYS:NZ	5:B:611:HOH:O	2.44	0.50
1:B:236:LYS:HE2	1:B:348:ASN:OD1	2.11	0.50
1:B:290:PRO:HG3	1:B:326:LEU:HD21	1.93	0.49
1:A:299:ARG:HG2	1:A:299:ARG:HH11	1.78	0.49
1:A:84:VAL:HG13	1:A:92:ILE:HD11	1.95	0.49
1:A:305:LYS:HG3	5:A:747:HOH:O	2.12	0.49
1:A:123:PHE:CE2	1:A:125:HIS:HB2	2.48	0.48
1:D:72:ASP:O	1:D:74:LYS:NZ	2.46	0.48
1:B:120:ARG:N	1:B:120:ARG:HD3	2.29	0.48
1:B:49:PHE:HA	1:B:52:VAL:HG12	1.96	0.48
1:B:306:VAL:HB	1:B:387:PHE:CD1	2.49	0.47
1:C:481:MET:H	1:C:481:MET:CE	2.22	0.47
1:D:41:LEU:O	1:D:45:LYS:HD3	2.14	0.47
1:B:206:CYS:HB3	1:B:362:ILE:HD13	1.96	0.47
1:C:228:ASN:HD21	2:C:501:UD1:C8'	2.28	0.47
1:D:77:PRO:HG2	1:D:80:HIS:CD2	2.51	0.46
1:C:279:ASP:HB2	1:C:342:PHE:HB2	1.98	0.46
1:A:35:LYS:NZ	1:B:352:LYS:HD3	2.31	0.46
1:D:228:ASN:HD21	2:D:501:UD1:H8'1	1.81	0.46
1:B:190:GLY:O	5:B:601:HOH:O	2.21	0.46
1:A:299:ARG:HG2	1:A:299:ARG:NH1	2.31	0.46
1:B:113:LEU:O	2:B:501:UD1:O3B	2.34	0.45
1:A:35:LYS:HD2	1:B:352:LYS:HZ3	1.82	0.45
1:C:481:MET:HE3	1:C:481:MET:HB2	1.72	0.44
1:B:76:ILE:HD13	1:B:76:ILE:HG21	1.84	0.44
1:A:357:VAL:HG13	1:A:380:ILE:HG23	2.00	0.44
1:A:386:ILE:HG22	2:A:501:UD1:H8'1	1.99	0.44
1:A:306:VAL:HB	1:A:387:PHE:CD1	2.53	0.44
1:B:420:CYS:SG	1:B:423:THR:HG23	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:TYR:HB2	5:D:688:HOH:O	2.17	0.44
1:C:127:LYS:HE3	1:C:127:LYS:HB2	1.80	0.43
1:C:416:ALA:O	1:C:417:LYS:HB2	2.18	0.43
1:B:209:PHE:HE1	1:B:359:LYS:HG2	1.83	0.43
1:D:111:LEU:HD23	1:D:168:TYR:HB2	1.99	0.43
1:D:236:LYS:NZ	1:D:348:ASN:OD1	2.41	0.43
1:C:36:GLU:HB3	1:C:219:TYR:HB3	2.00	0.43
1:D:176:ARG:NH1	1:D:180:ALA:HB2	2.31	0.43
1:A:121:LEU:HD12	1:A:127:LYS:HE2	2.00	0.43
1:B:76:ILE:HG21	1:B:81:TYR:CD2	2.46	0.43
1:A:346:ILE:HA	1:A:349:PHE:CE1	2.54	0.43
1:A:346:ILE:HA	1:A:349:PHE:CZ	2.54	0.43
1:D:78:ASP:OD1	1:D:78:ASP:N	2.52	0.42
1:D:52:VAL:HG22	1:D:207:PHE:HZ	1.84	0.42
1:A:121:LEU:HD12	1:A:127:LYS:HD3	2.02	0.42
1:D:119:THR:H	1:D:120:ARG:NH2	2.18	0.42
1:A:117:GLN:NE2	1:A:174:HIS:HB2	2.35	0.42
1:A:67:GLN:CD	1:C:481:MET:HG2	2.30	0.42
1:B:272:TYR:HE2	1:B:397:ILE:HG21	1.85	0.42
1:D:346:ILE:HG21	1:D:389:VAL:HG11	2.01	0.42
1:A:75:PRO:HG3	1:A:327:THR:HG22	2.02	0.42
1:B:279:ASP:HB2	1:B:342:PHE:HB2	2.02	0.42
1:A:194:GLU:HG2	1:A:195:ASP:N	2.36	0.41
1:A:279:ASP:HB2	1:A:342:PHE:HB2	2.01	0.41
1:D:28:TYR:O	1:D:32:LEU:HG	2.20	0.41
1:A:228:ASN:HD21	2:A:501:UD1:C8'	2.34	0.41
1:B:76:ILE:HD13	1:B:398:CYS:CB	2.34	0.41
1:C:35:LYS:HE2	1:C:35:LYS:HB2	1.97	0.41
1:D:443:VAL:HB	1:D:471:PHE:HB2	2.03	0.41
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.91	0.41
1:D:281:ALA:HB3	1:D:337:TYR:HB3	2.02	0.41
1:C:134:LEU:HD11	1:C:260:ILE:HD11	2.03	0.40
1:B:84:VAL:HA	1:B:87:LEU:HD12	2.03	0.40
1:C:28:TYR:O	1:C:32:LEU:HG	2.21	0.40
1:C:430:ARG:NH2	5:C:606:HOH:O	2.39	0.40
1:A:111:LEU:HD23	1:A:168:TYR:HB2	2.03	0.40
1:D:386:ILE:HG22	2:D:501:UD1:H8'1	2.04	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	469/482 (97%)	462 (98%)	7 (2%)	0	100	100
1	B	446/482 (92%)	437 (98%)	8 (2%)	1 (0%)	47	48
1	C	463/482 (96%)	454 (98%)	9 (2%)	0	100	100
1	D	460/482 (95%)	450 (98%)	10 (2%)	0	100	100
All	All	1838/1928 (95%)	1803 (98%)	34 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	GLU

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	406/416 (98%)	403 (99%)	3 (1%)	84	88
1	B	392/416 (94%)	389 (99%)	3 (1%)	81	86
1	C	402/416 (97%)	398 (99%)	4 (1%)	76	81
1	D	400/416 (96%)	395 (99%)	5 (1%)	69	74
All	All	1600/1664 (96%)	1585 (99%)	15 (1%)	78	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	120	ARG
1	A	349	PHE
1	B	6	HIS
1	B	8	MET
1	B	120	ARG
1	C	120	ARG
1	C	233	ARG
1	C	428	LEU
1	C	481	MET
1	D	45	LYS
1	D	72	ASP
1	D	79	SER
1	D	354	LYS
1	D	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	286	GLN
1	A	301	ASN
1	C	446	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	UD1	A	501	-	38,41,41	0.38	0	57,62,62	0.95	2 (3%)
2	UD1	D	501	-	38,41,41	0.38	0	57,62,62	0.97	2 (3%)
3	SO4	C	502	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	D	502	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	A	502	-	4,4,4	0.32	0	6,6,6	0.05	0
2	UD1	B	501	-	38,41,41	0.36	0	57,62,62	0.92	3 (5%)
2	UD1	C	501	-	38,41,41	0.38	0	57,62,62	0.99	2 (3%)
3	SO4	B	502	-	4,4,4	0.33	0	6,6,6	0.05	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
2	UD1	A	501	-	-	3/26/63/63	0/3/3/3
2	UD1	D	501	-	-	3/26/63/63	0/3/3/3
2	UD1	B	501	-	-	2/26/63/63	0/3/3/3
2	UD1	C	501	-	-	3/26/63/63	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	UD1	O5'-C1'-O1'	4.62	117.41	111.36
2	D	501	UD1	O5'-C1'-O1'	4.58	117.35	111.36
2	A	501	UD1	O5'-C1'-O1'	4.31	117.00	111.36
2	B	501	UD1	O5'-C1'-O1'	4.02	116.62	111.36
2	D	501	UD1	PB-O1'-C1'	2.38	128.93	119.74
2	B	501	UD1	C1'-C2'-N2'	-2.28	107.08	111.00
2	C	501	UD1	PB-O1'-C1'	2.27	128.53	119.74
2	A	501	UD1	PB-O1'-C1'	2.16	128.08	119.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UD1	PB-O1'-C1'	2.09	127.82	119.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

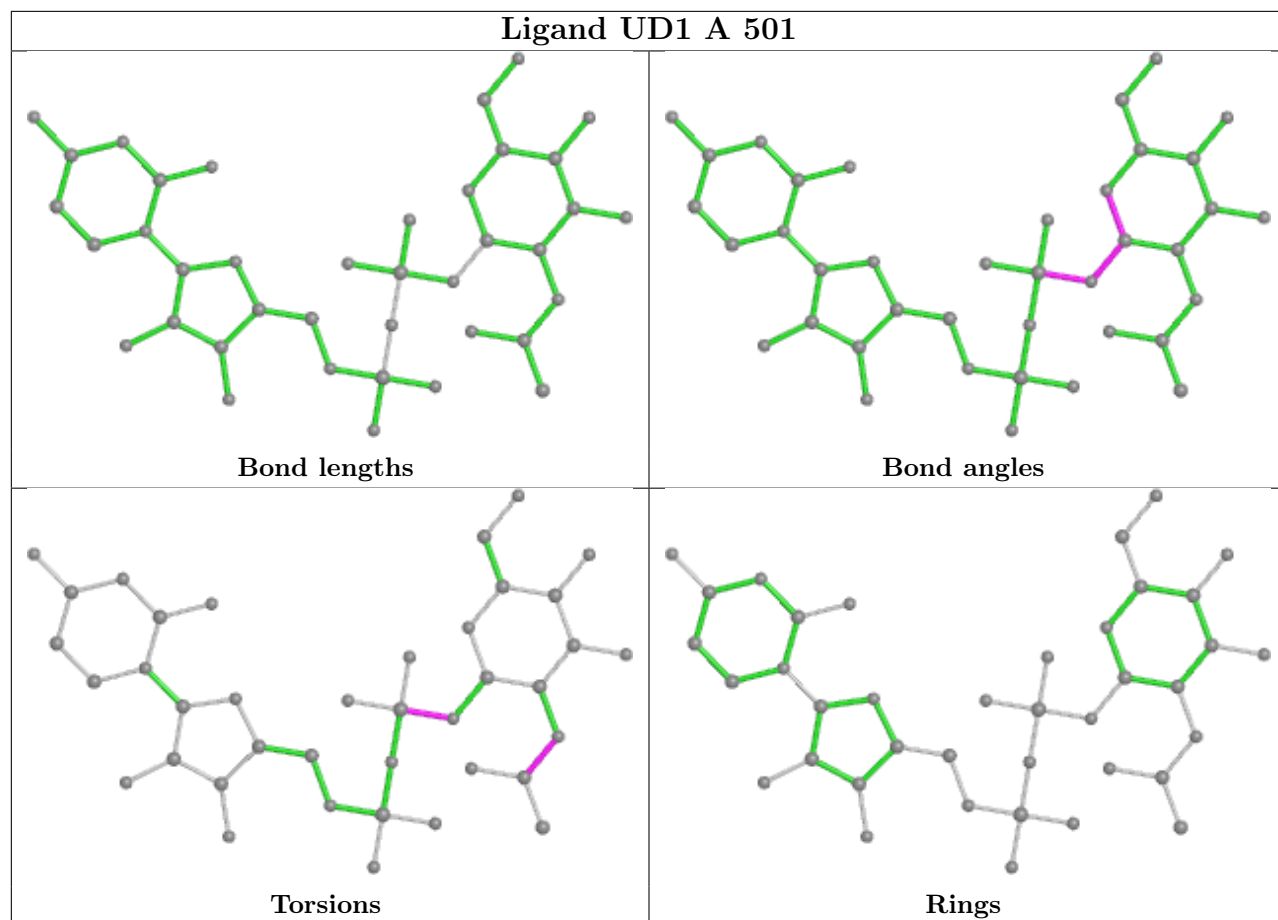
Mol	Chain	Res	Type	Atoms
2	A	501	UD1	C8'-C7'-N2'-C2'
2	A	501	UD1	O7'-C7'-N2'-C2'
2	B	501	UD1	C8'-C7'-N2'-C2'
2	B	501	UD1	O7'-C7'-N2'-C2'
2	C	501	UD1	C8'-C7'-N2'-C2'
2	C	501	UD1	O7'-C7'-N2'-C2'
2	D	501	UD1	C8'-C7'-N2'-C2'
2	D	501	UD1	O7'-C7'-N2'-C2'
2	C	501	UD1	C1'-O1'-PB-O3A
2	D	501	UD1	C1'-O1'-PB-O3A
2	A	501	UD1	C1'-O1'-PB-O3A

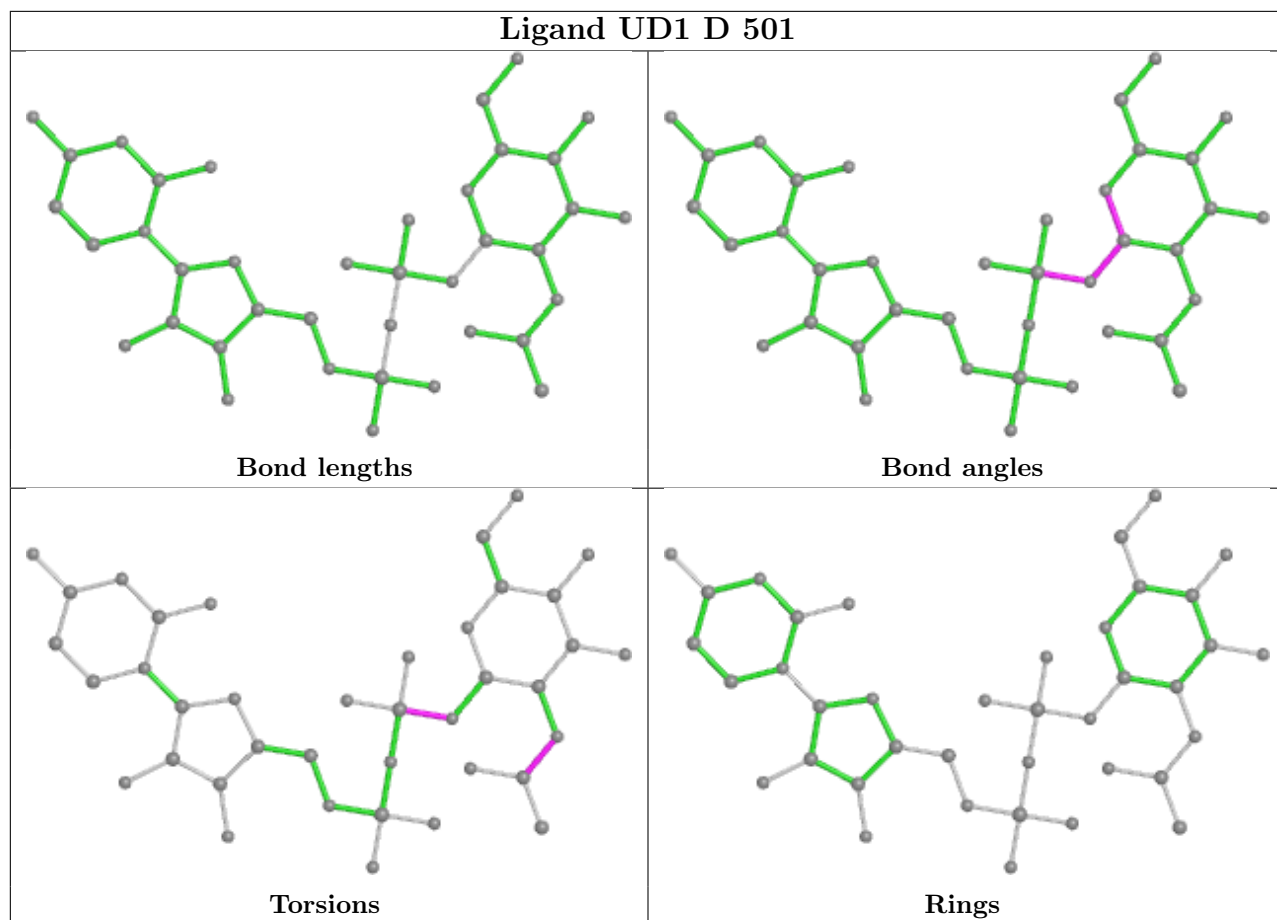
There are no ring outliers.

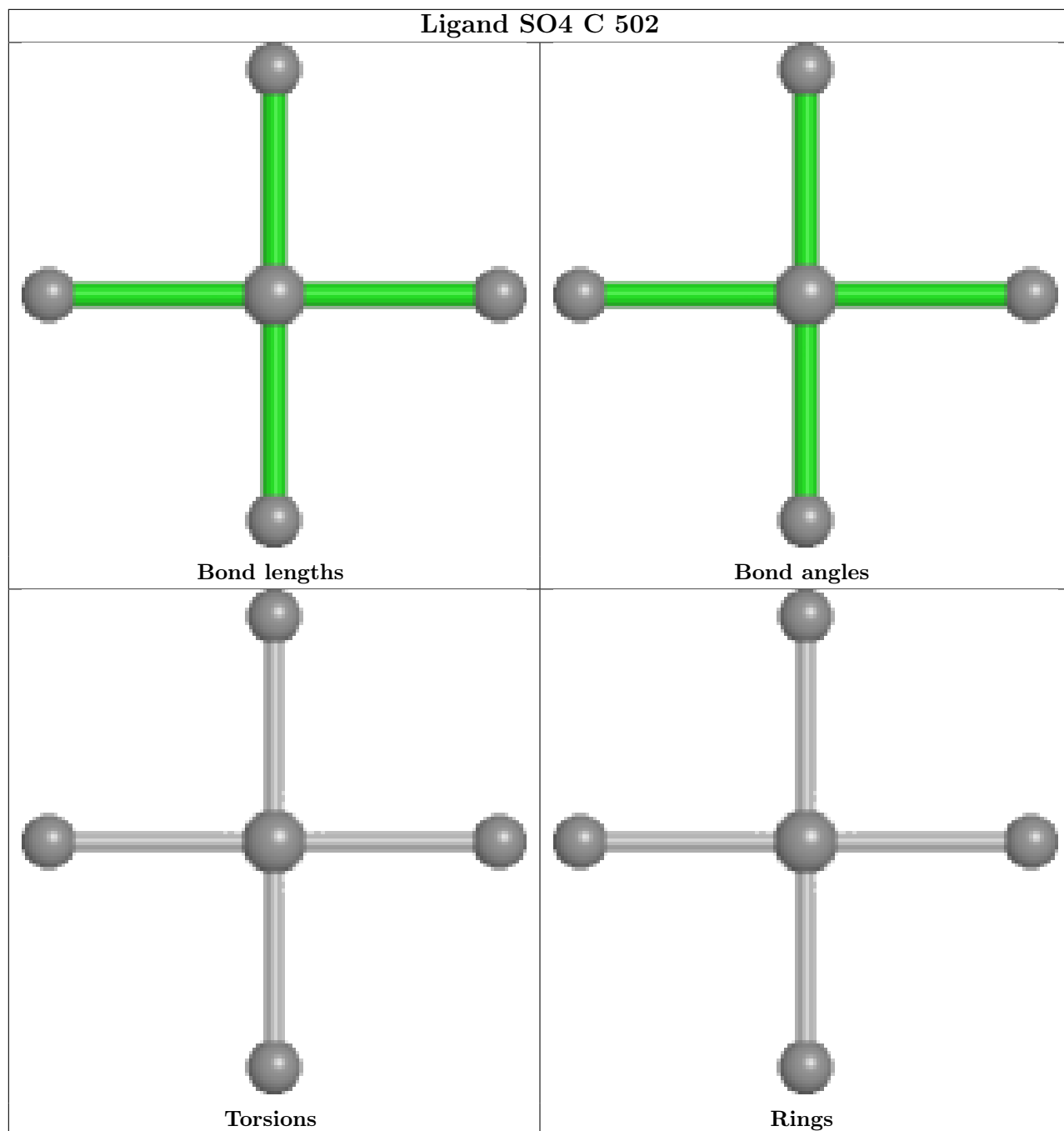
7 monomers are involved in 14 short contacts:

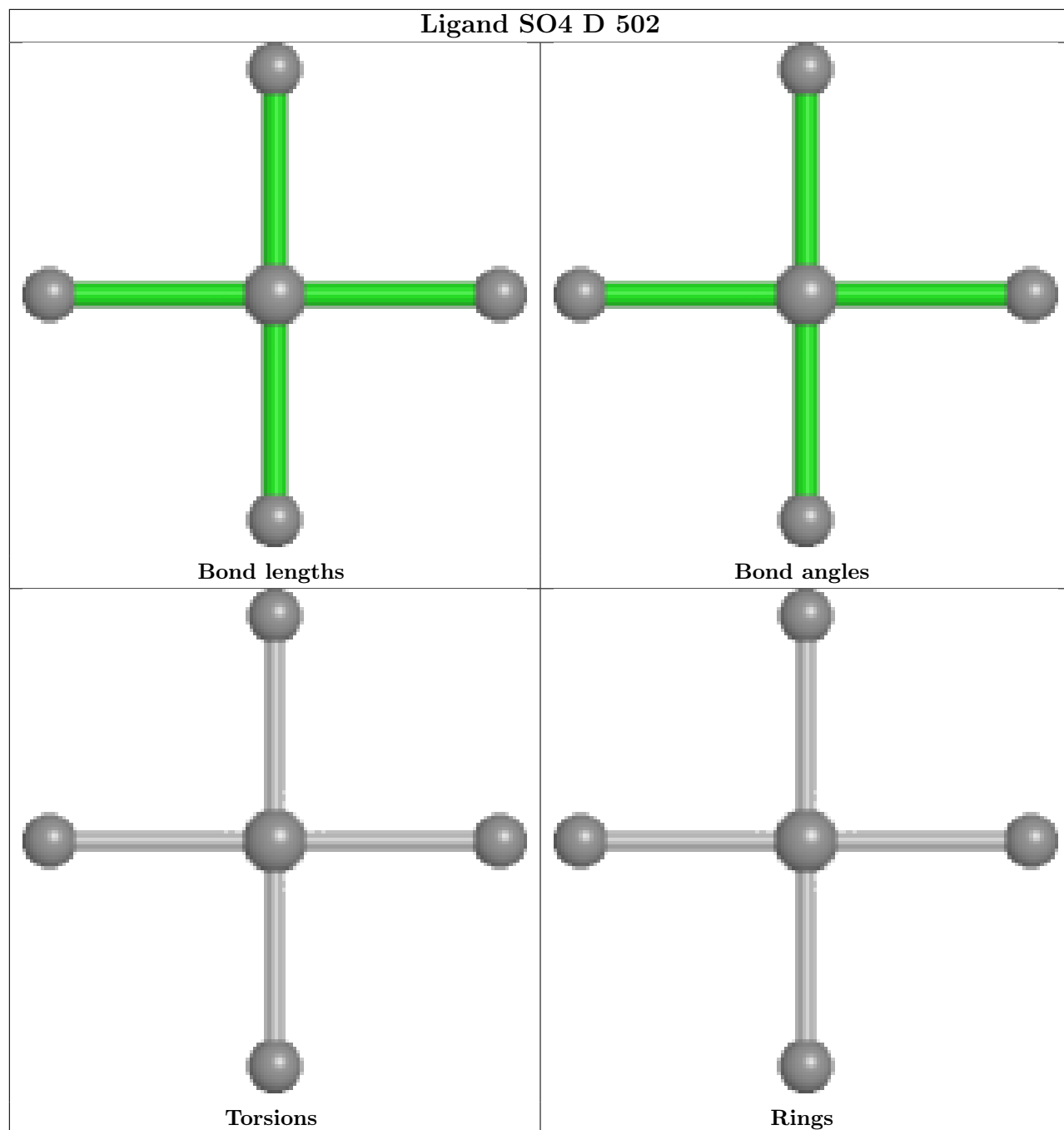
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	UD1	2	0
2	D	501	UD1	3	0
3	C	502	SO4	3	0
3	A	502	SO4	1	0
2	B	501	UD1	3	0
2	C	501	UD1	1	0
3	B	502	SO4	1	0

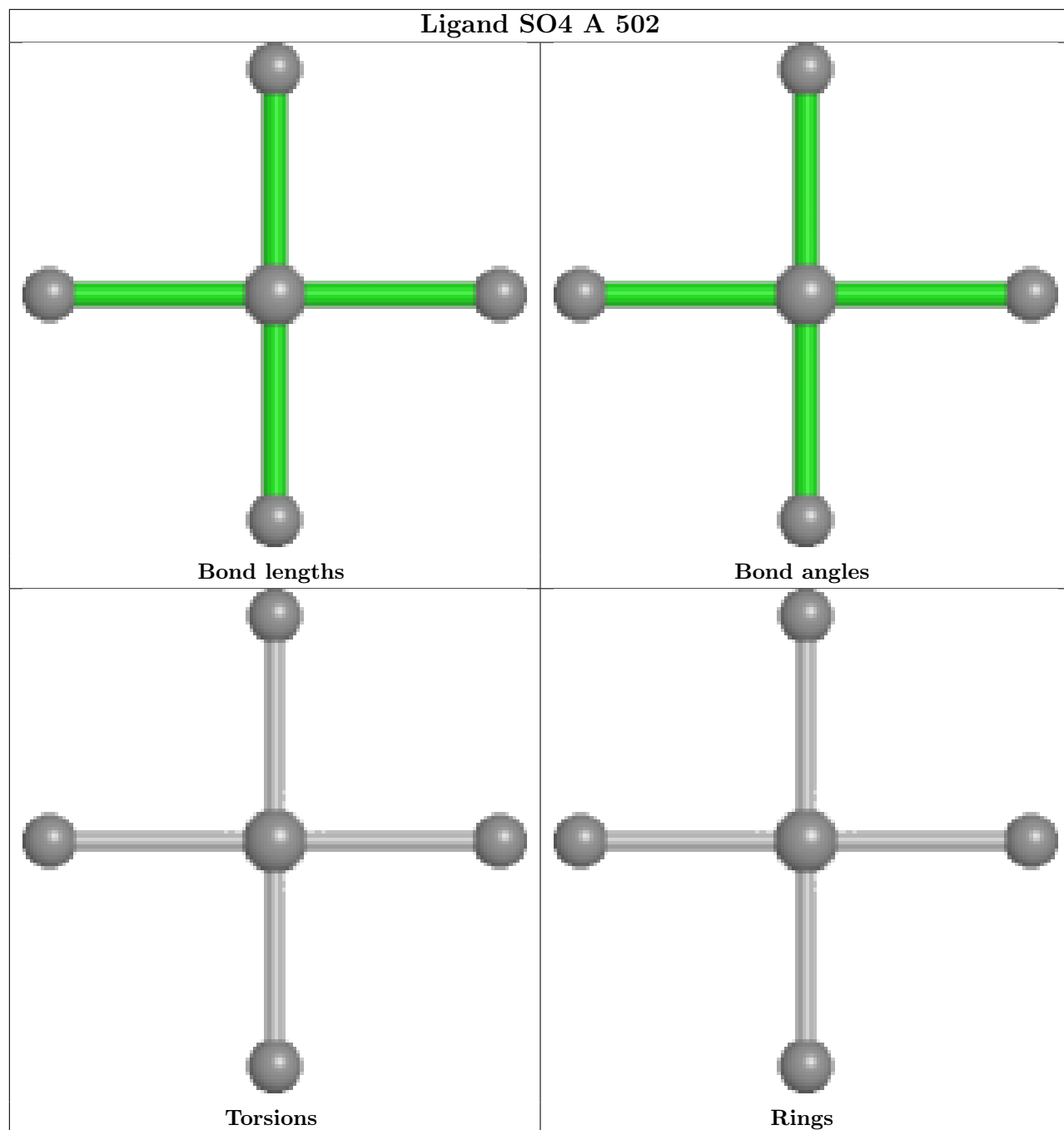
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

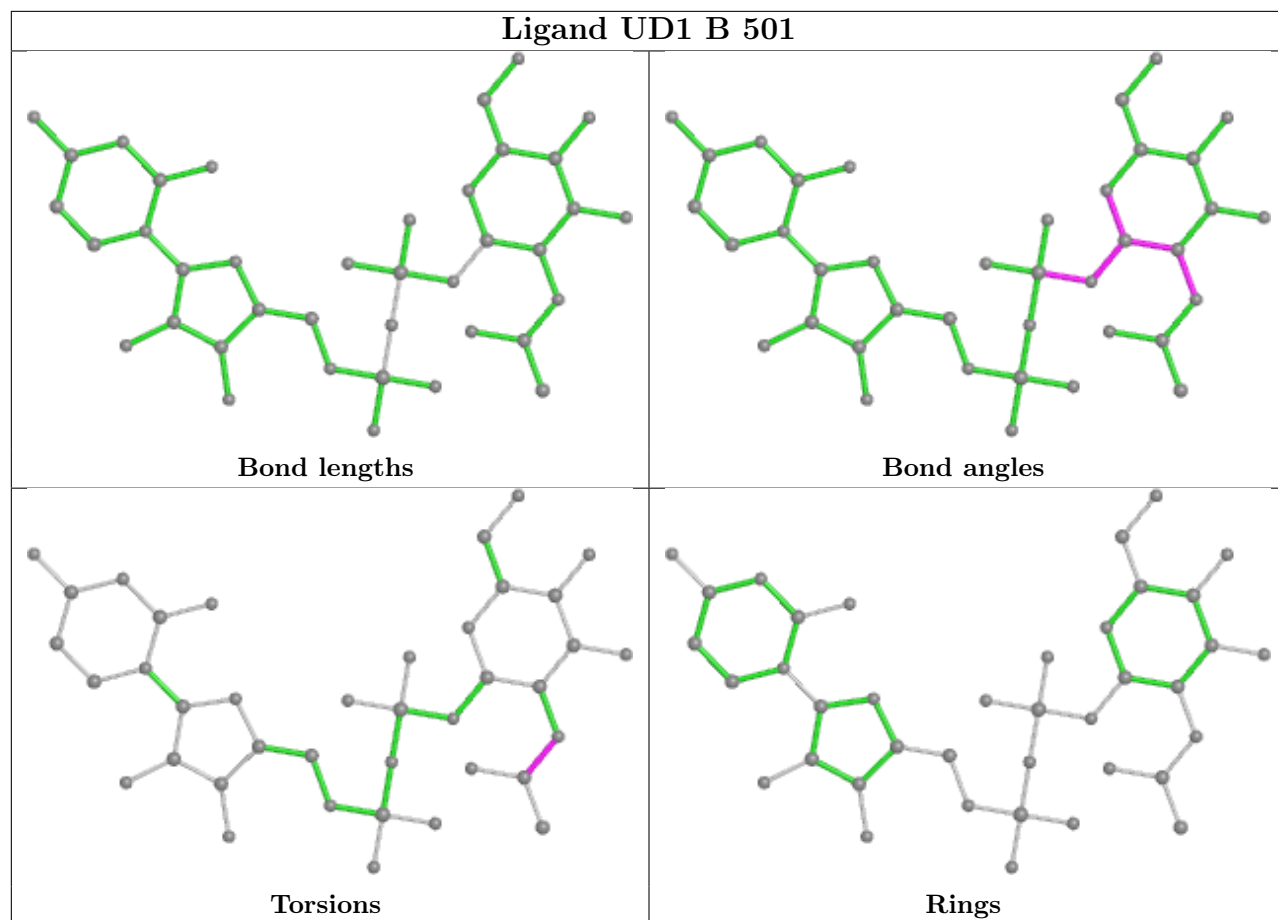


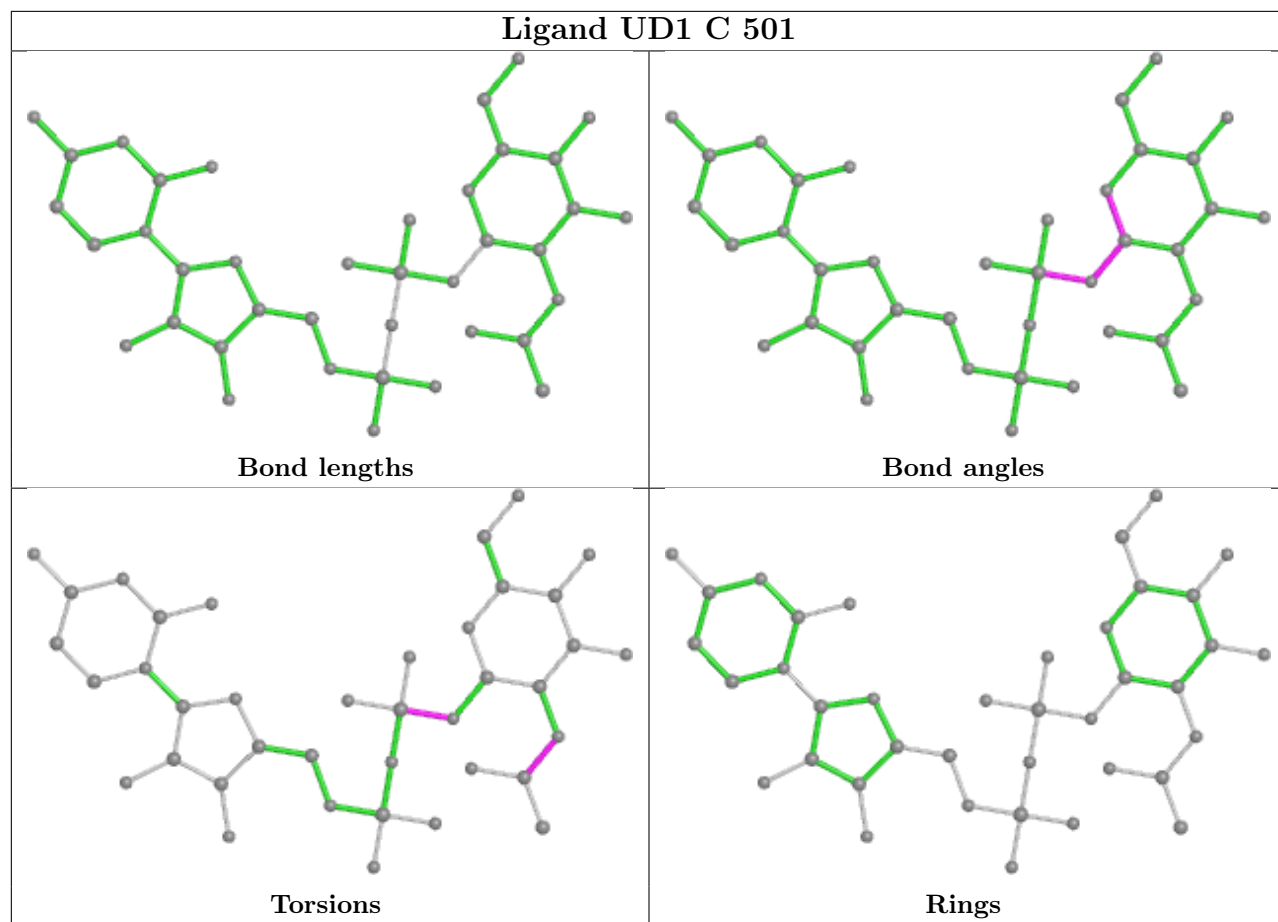


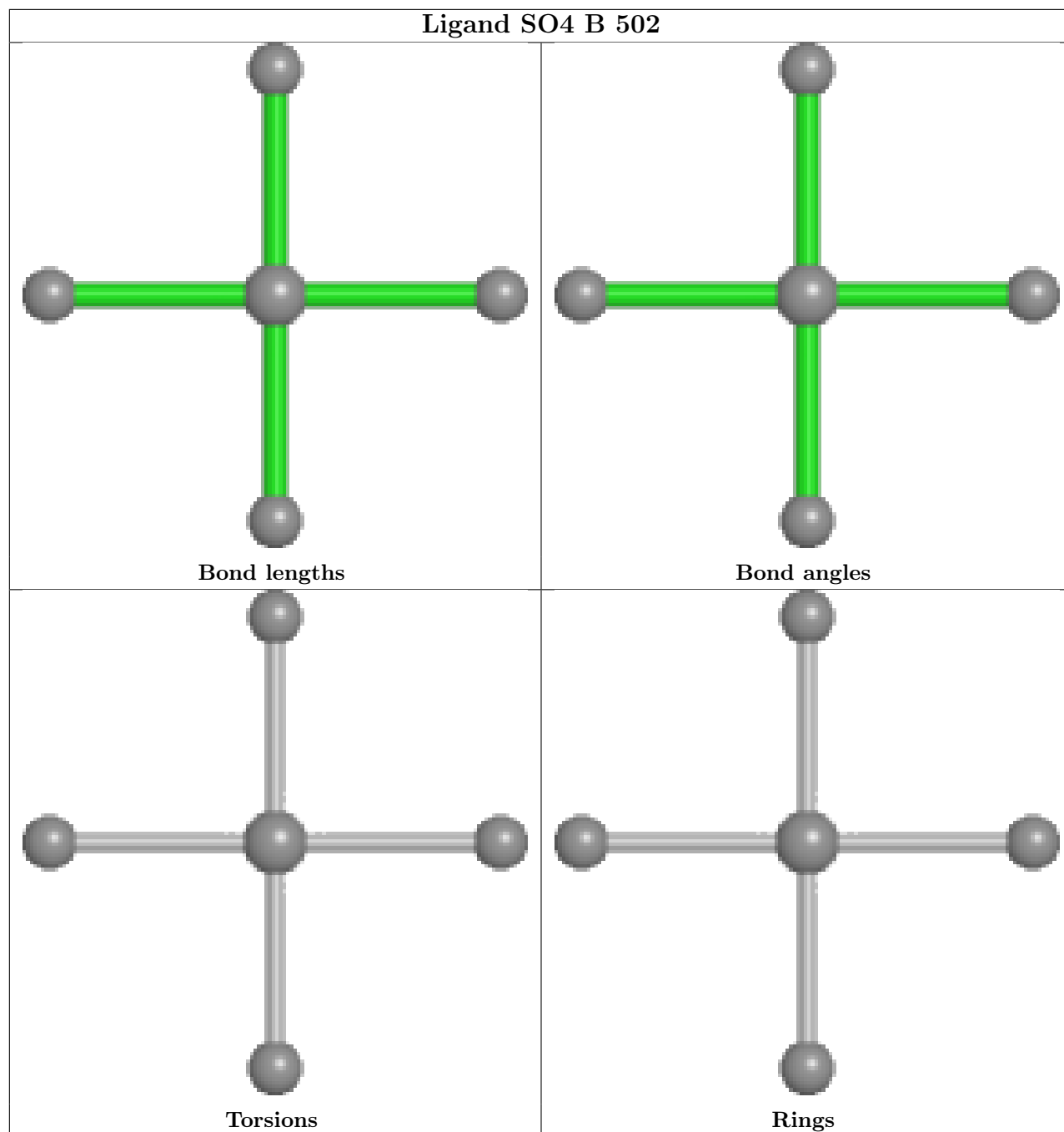












5.7 Other polymers [i](#)

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	471/482 (97%)	-0.12	5 (1%) 80 84	25, 36, 56, 71	0
1	B	454/482 (94%)	-0.07	13 (2%) 51 57	25, 38, 61, 83	0
1	C	467/482 (96%)	-0.15	7 (1%) 73 77	24, 36, 55, 73	0
1	D	466/482 (96%)	-0.15	9 (1%) 66 71	23, 35, 56, 78	0
All	All	1858/1928 (96%)	-0.12	34 (1%) 68 72	23, 36, 57, 83	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	ALA	7.2
1	D	349	PHE	7.1
1	C	5	HIS	4.0
1	B	55	LEU	4.0
1	B	173	GLU	3.8
1	B	51	GLU	3.8
1	B	6	HIS	3.7
1	B	289	THR	3.6
1	B	52	VAL	3.6
1	B	76	ILE	3.5
1	B	476	TYR	3.5
1	C	349	PHE	3.4
1	D	352	LYS	2.9
1	D	482	GLN	2.9
1	A	173	GLU	2.8
1	D	485	ALA	2.6
1	A	288	SER	2.5
1	D	354	LYS	2.5
1	D	351	SER	2.5
1	B	8	MET	2.3
1	B	326	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	301	ASN	2.3
1	B	316	ALA	2.3
1	D	484	SER	2.3
1	A	368	GLU	2.3
1	C	72	ASP	2.2
1	A	117	GLN	2.2
1	B	54	GLU	2.2
1	D	321	THR	2.2
1	A	90	GLU	2.2
1	C	352	LYS	2.2
1	B	53	ASN	2.1
1	C	303	HIS	2.1
1	C	473	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

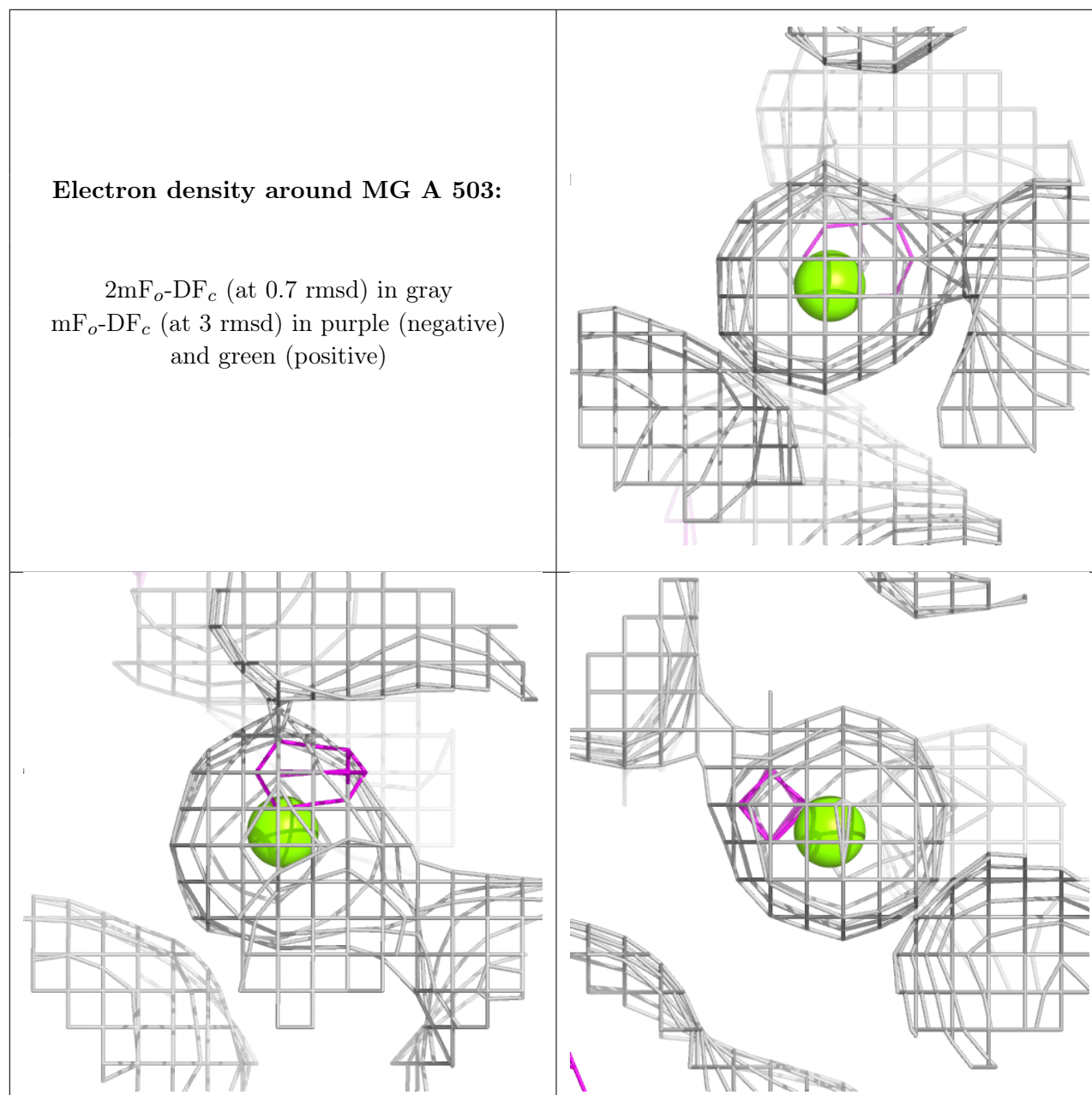
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	503	1/1	0.94	0.13	36,36,36,36	0
4	MG	C	503	1/1	0.95	0.08	36,36,36,36	0
2	UD1	D	501	39/39	0.96	0.12	18,27,31,38	0
2	UD1	A	501	39/39	0.97	0.11	25,31,38,40	0
3	SO4	B	502	5/5	0.97	0.21	45,56,57,58	0
2	UD1	B	501	39/39	0.97	0.11	28,32,37,48	0
4	MG	B	503	1/1	0.97	0.09	39,39,39,39	0
2	UD1	C	501	39/39	0.97	0.11	21,27,32,39	0
3	SO4	A	502	5/5	0.98	0.17	39,49,50,51	0
3	SO4	D	502	5/5	0.99	0.12	33,35,43,44	0

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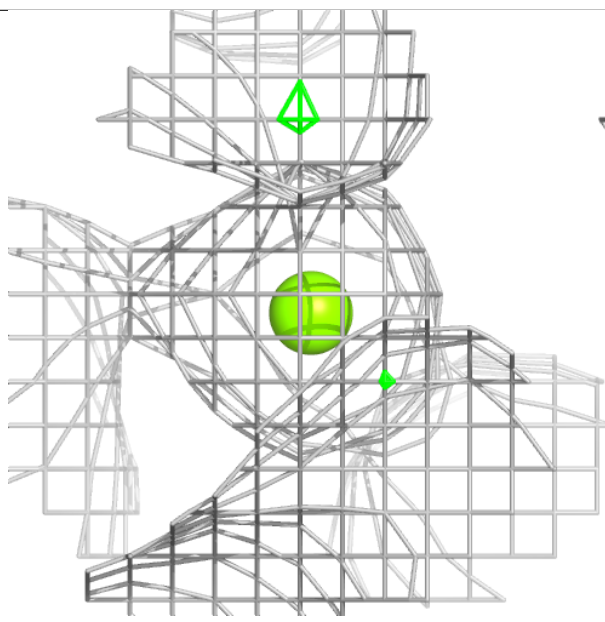
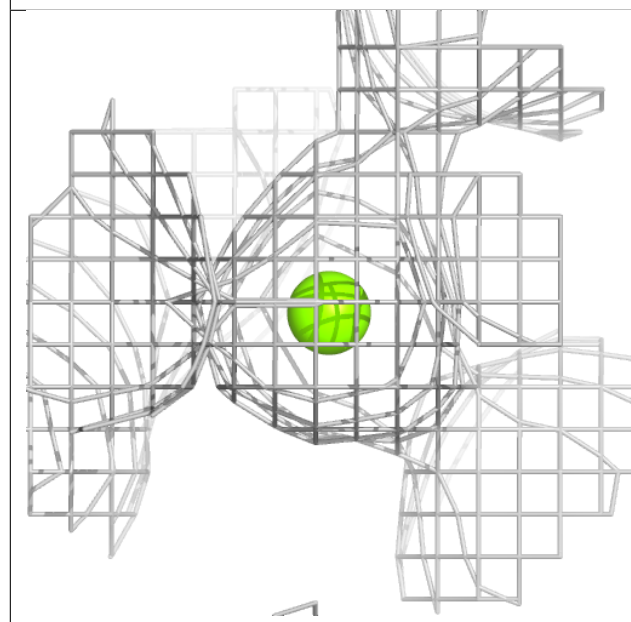
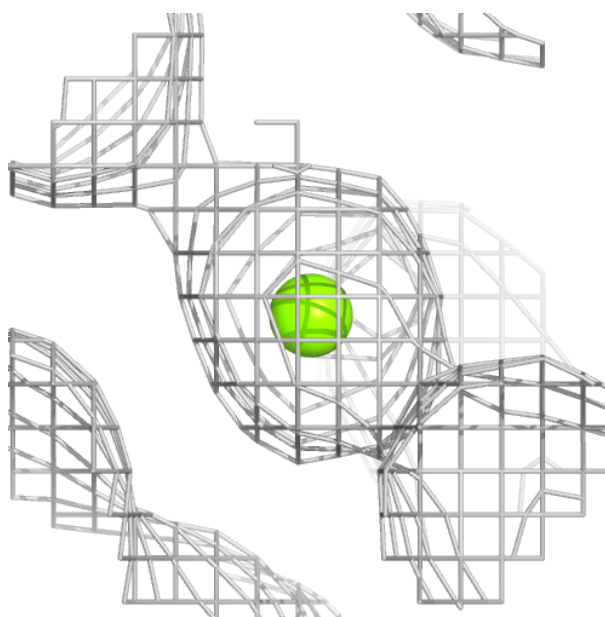
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	502	5/5	0.99	0.12	33,39,44,46	0
4	MG	D	503	1/1	0.99	0.21	37,37,37,37	0

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.



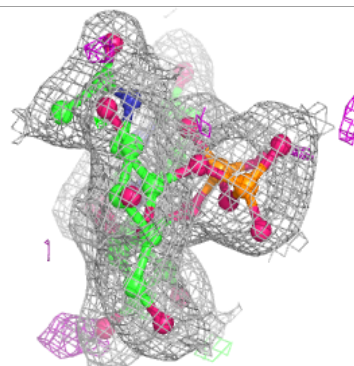
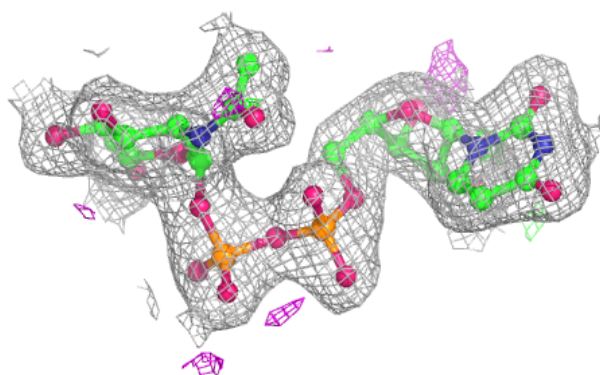
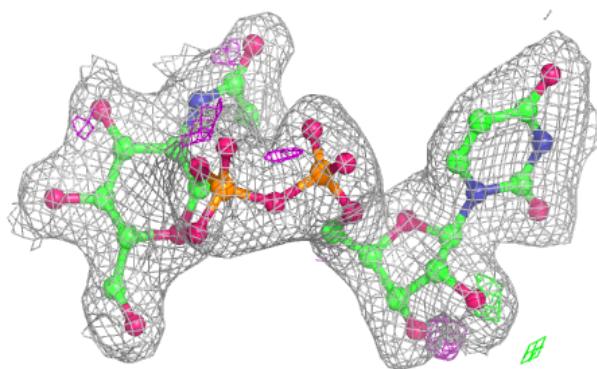
Electron density around MG C 503:

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

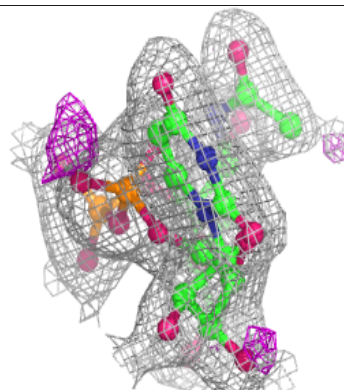
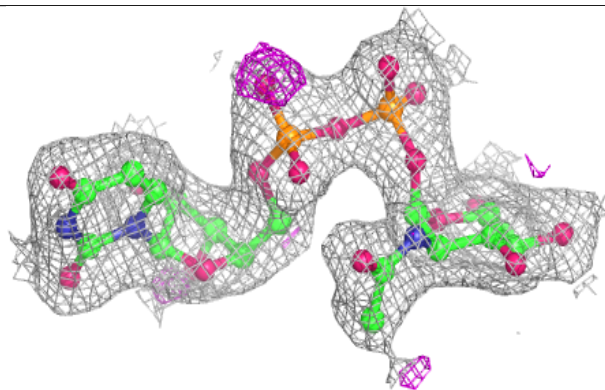
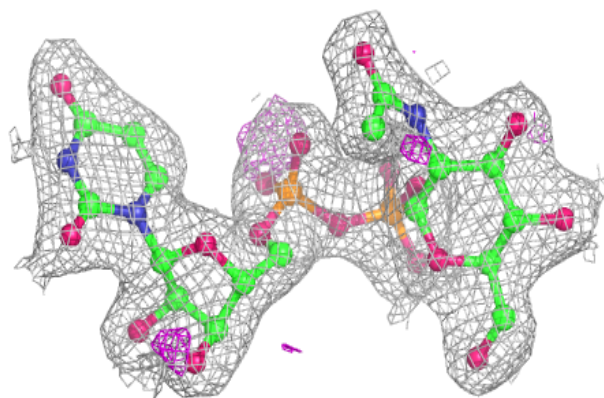


Electron density around UD1 D 501:

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

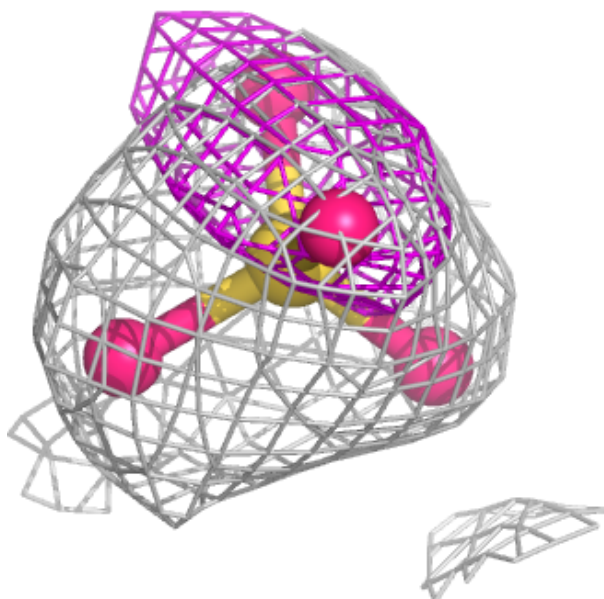
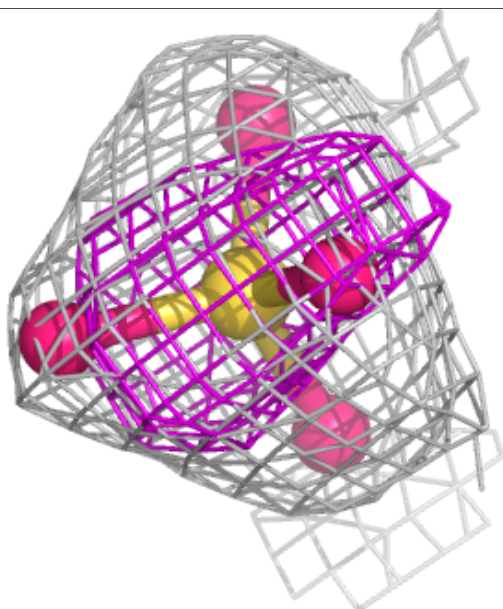
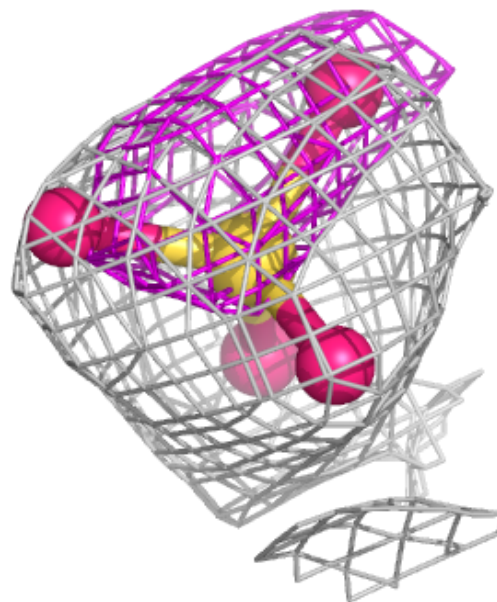
**Electron density around UD1 A 501:**

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



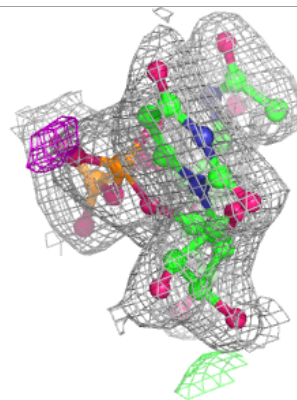
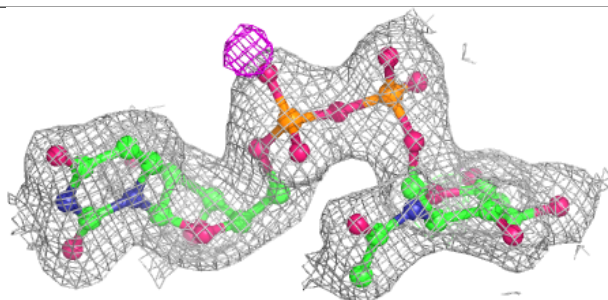
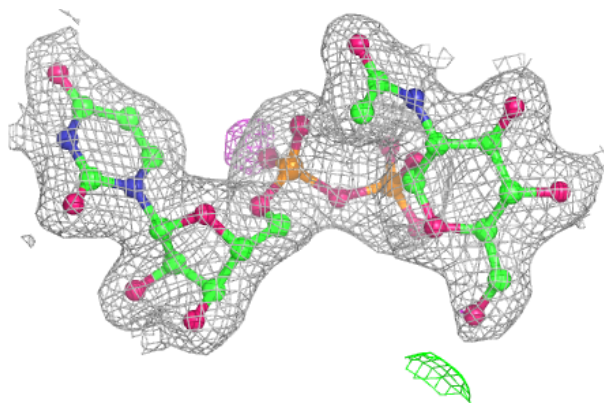
Electron density around SO4 B 502:

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



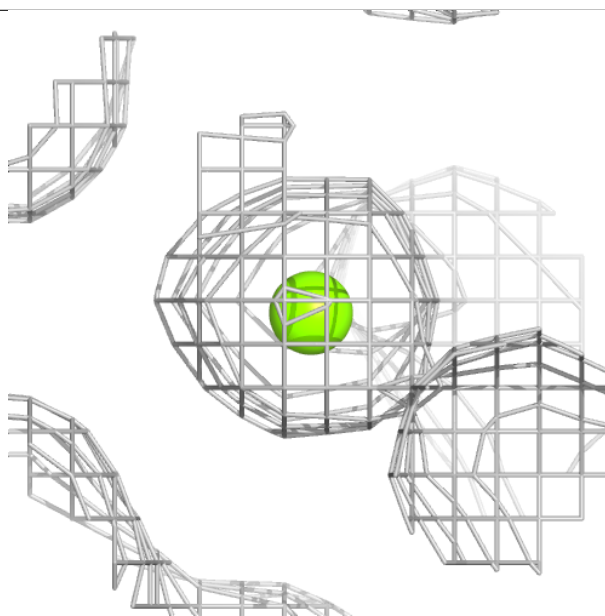
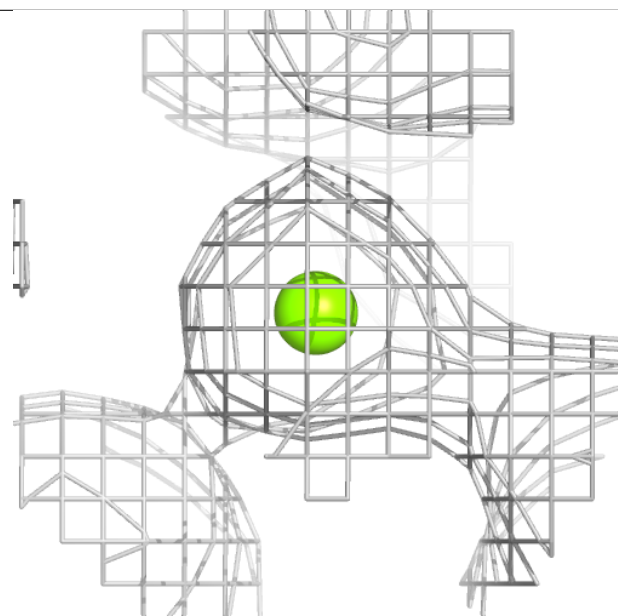
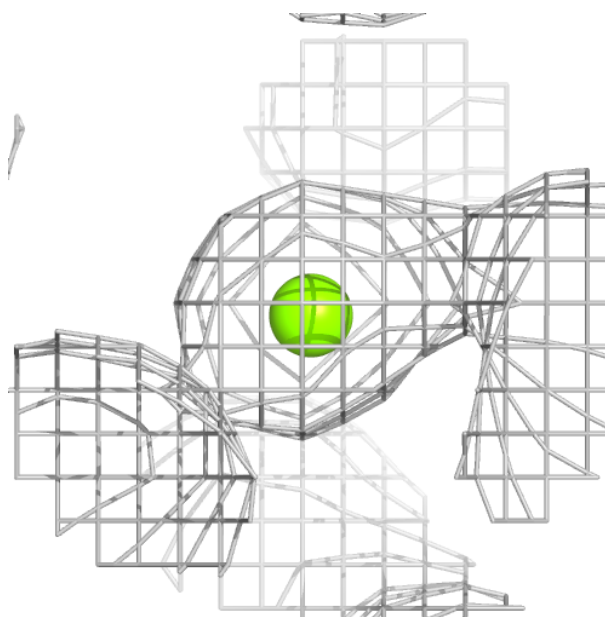
Electron density around UD1 B 501:

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



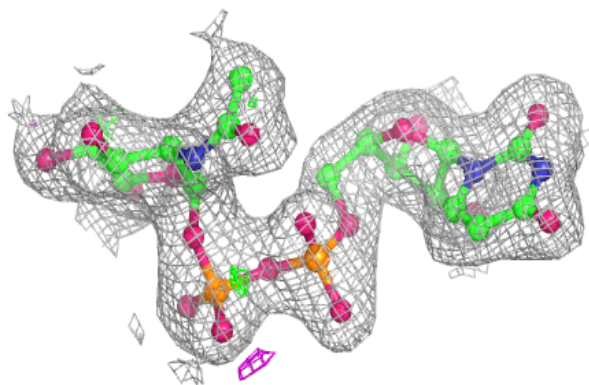
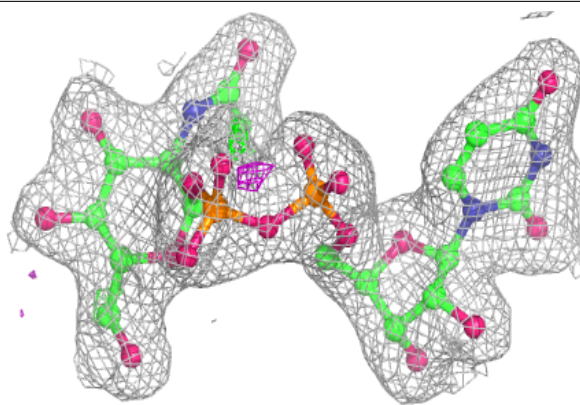
Electron density around MG B 503:

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



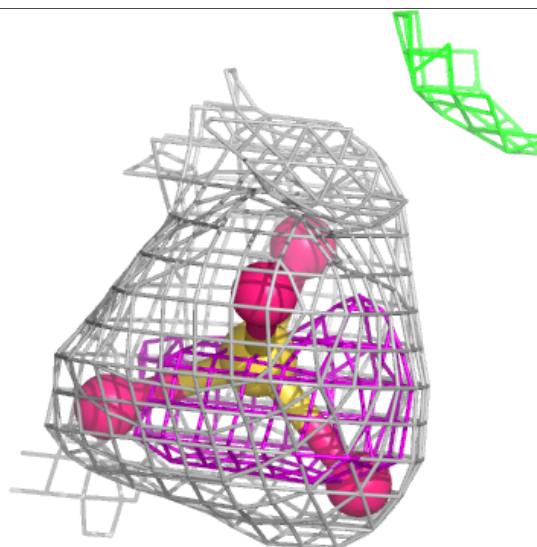
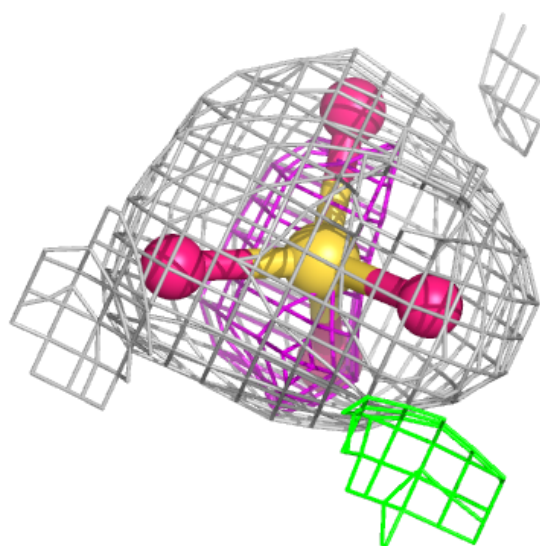
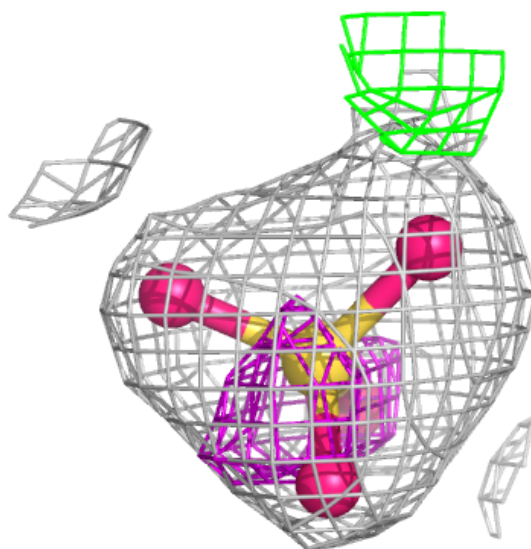
Electron density around UD1 C 501:

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



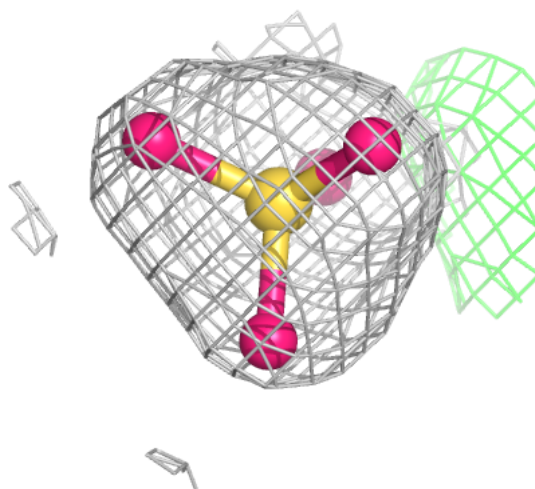
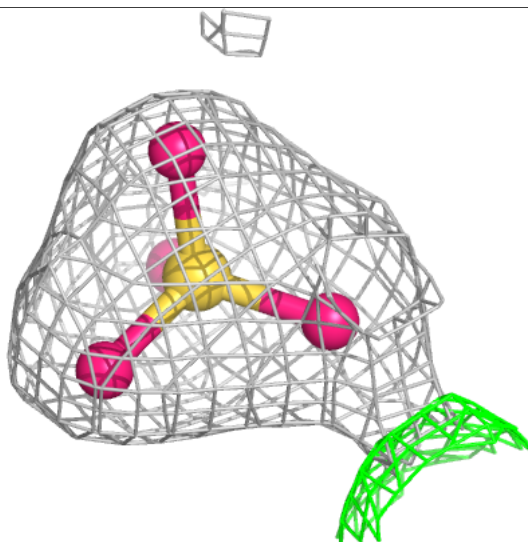
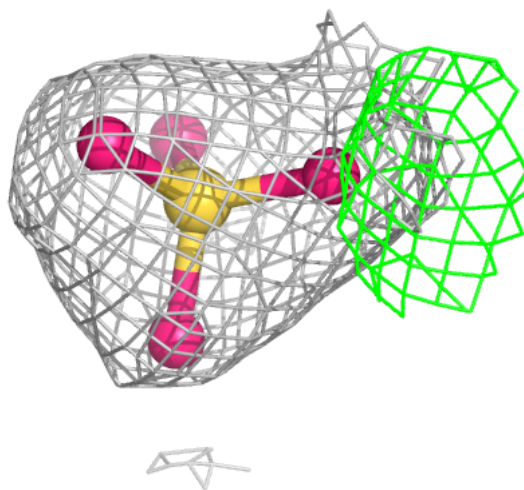
Electron density around SO4 A 502:

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



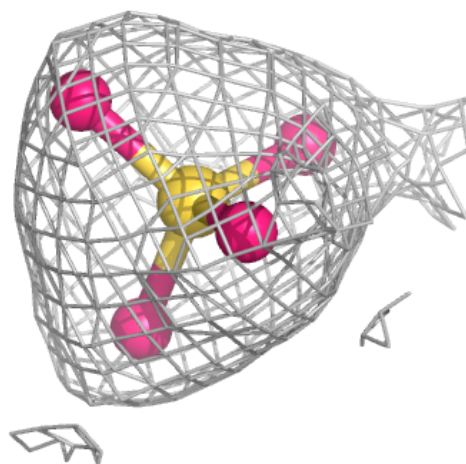
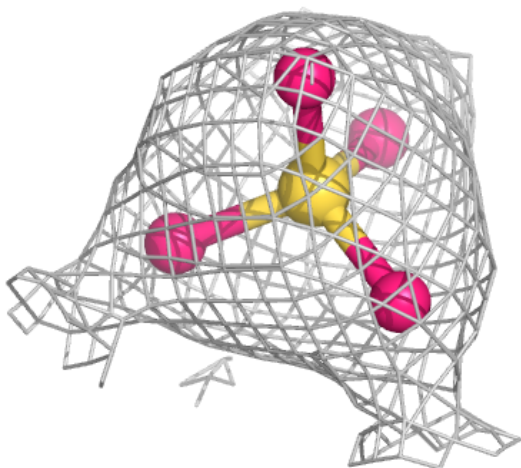
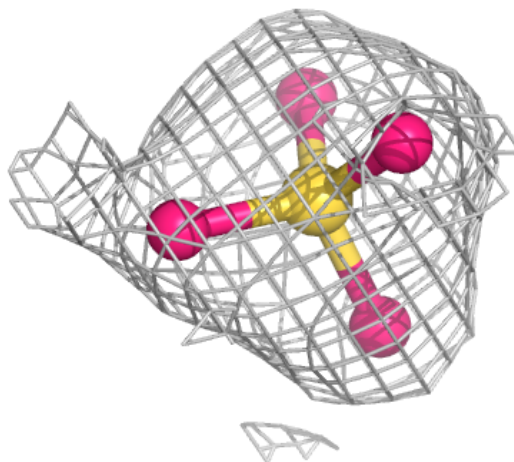
Electron density around SO4 D 502:

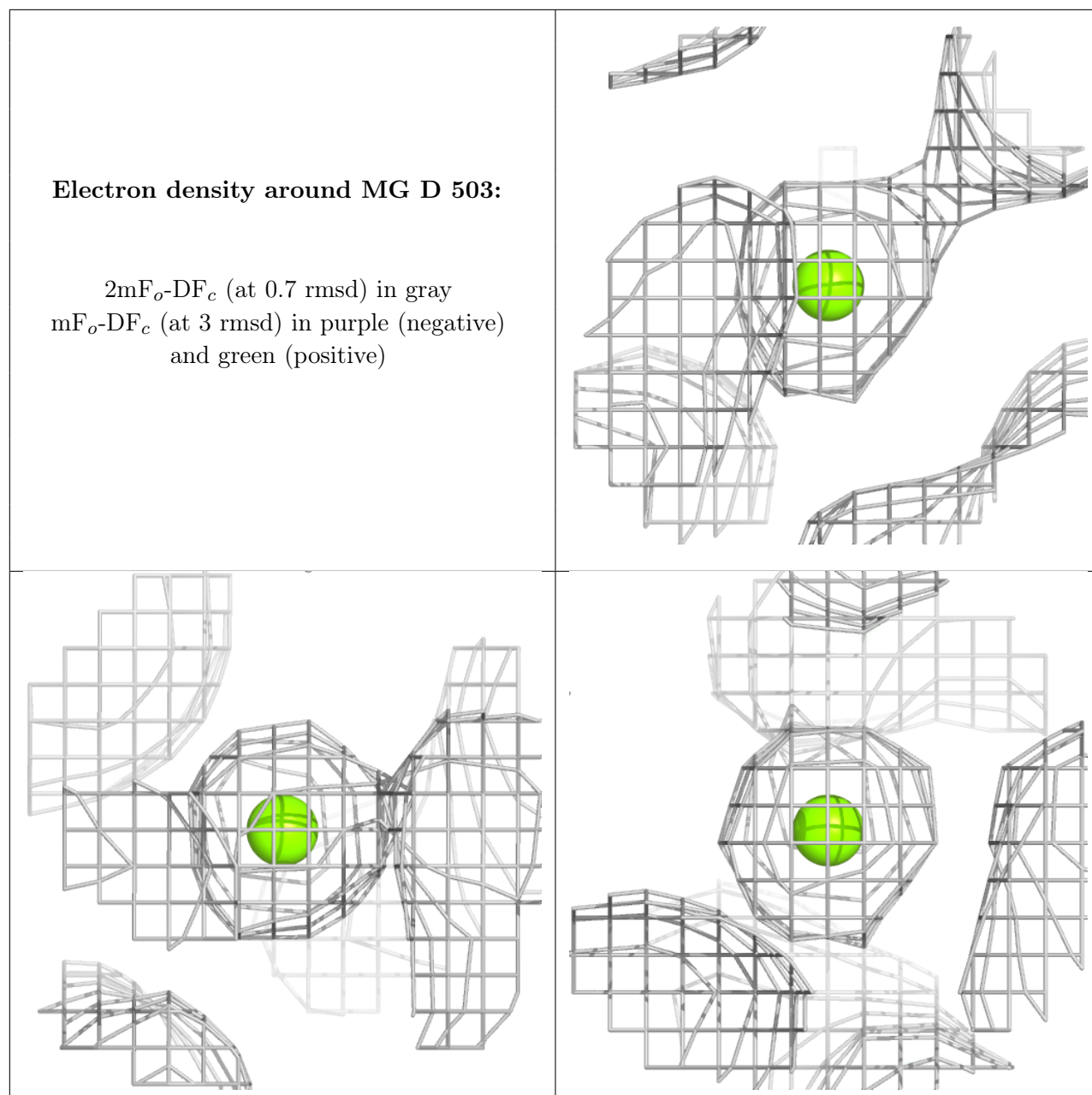
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 C 502:

$2mF_o-DF_c$ (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.