



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:02 AM EDT

PDB ID : 7QOT / pdb_00007qot
Title : Factor XI and Plasma Kallikrein apple domain structures reveals different kininogen bound complexes
Authors : Li, C.; Awital, B.; Wong, S.; Dreveny, I.; Meijers, J.; Emsley, J.
Deposited on : 2021-12-28
Resolution : 3.24 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

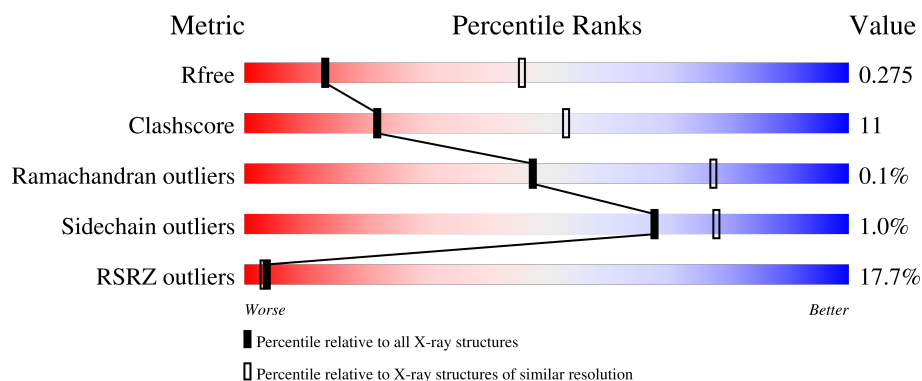
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	358	11% 79% 20% ..
1	B	358	20% 76% 23% ..
2	C	31	48% 32% 48% 19%
2	D	31	29% 39% 6% 55%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	402	X	-	-	-
3	NAG	B	401	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5910 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.

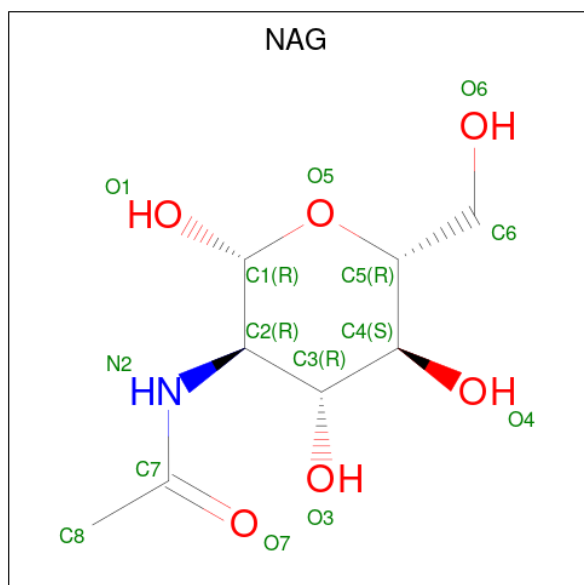
- Molecule 1 is a protein called Coagulation factor XIa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	25	0	0
			2764	1736	479	521	28			
1	B	355	Total	C	N	O	S	23	1	0
			2766	1738	479	521	28			

- Molecule 2 is a protein called Kininogen-1 light chain.

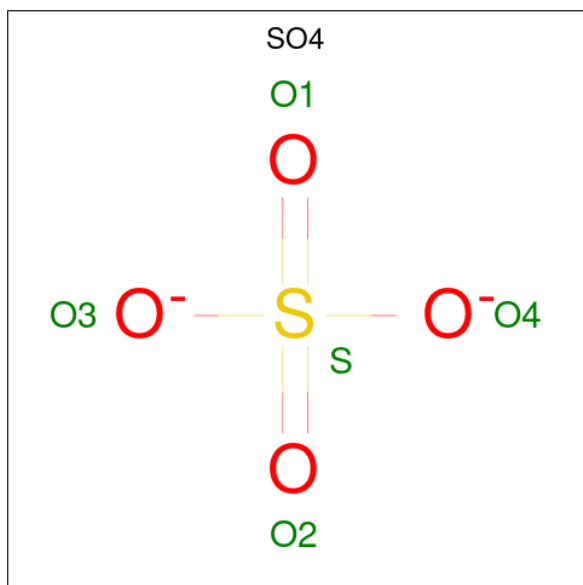
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	25	Total	C	N	O	47	0	0
			201	128	29	44			
2	D	14	Total	C	N	O	0	0	0
			107	69	16	22			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).

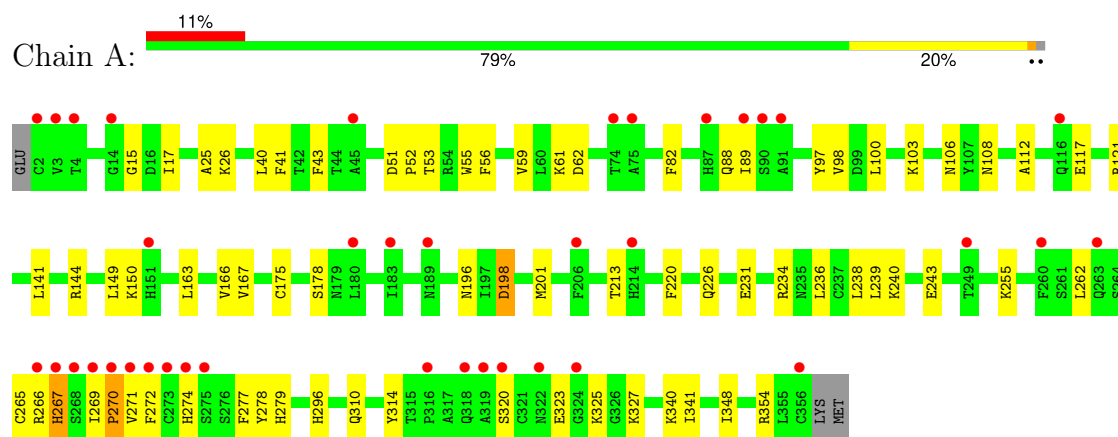


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

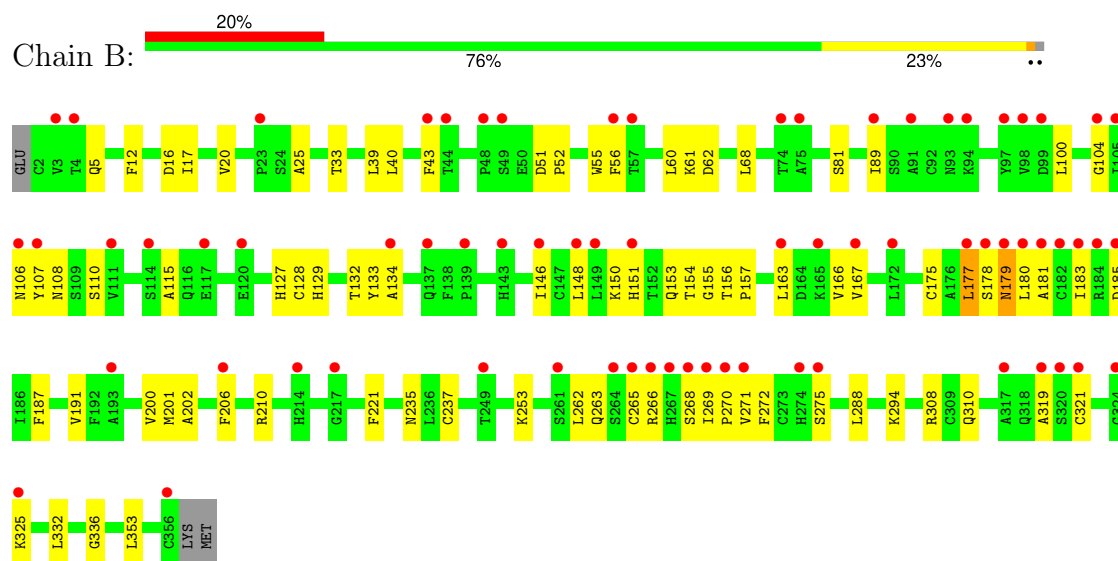
3 Residue-property plots [i](#)

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: Coagulation factor XIa heavy chain

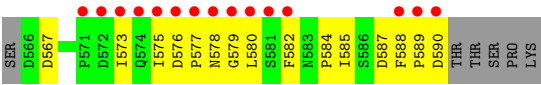


- Molecule 1: Coagulation factor XIa heavy chain

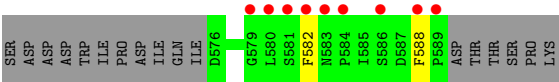
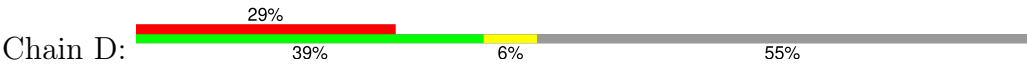


- Molecule 2: Kininogen-1 light chain





● Molecule 2: Kininogen-1 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.32Å 87.32Å 629.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.53 – 3.24 73.53 – 3.24	Depositor EDS
% Data completeness (in resolution range)	80.5 (73.53-3.24) 80.5 (73.53-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.45 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.251 , 0.284 0.251 , 0.275	Depositor DCC
R_{free} test set	1946 reflections (8.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.2	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	0.87	EDS
Total number of atoms	5910	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAG, SO4

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	0.33	1/2828 (0.0%)	0.69	3/3828 (0.1%)
1	B	0.34	0/2834	0.70	1/3836 (0.0%)
2	C	0.85	0/208	1.34	3/287 (1.0%)
2	D	0.74	0/111	1.02	0/152
All	All	0.38	1/5981 (0.0%)	0.74	7/8103 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	PRO	C-O	-5.57	1.16	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	HIS	N-CA-C	10.62	123.18	110.44
1	A	320	SER	N-CA-C	-7.84	102.33	111.03
2	C	579	GLY	N-CA-C	7.82	124.57	112.60
1	B	179	ASN	N-CA-C	-6.82	101.98	111.39
1	A	271	VAL	N-CA-C	-5.75	103.99	112.04
2	C	567	ASP	N-CA-C	-5.30	108.58	114.62
2	C	578	ASN	CA-C-O	-5.01	115.95	121.31

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	2764	0	2678	54	0
1	B	2766	0	2682	62	0
2	C	201	0	171	13	0
2	D	107	0	93	5	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
All	All	5910	0	5663	122	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 11.

All (122) 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:277:PHE:HB3	1:A:348:ILE:HD11	1.47	0.96
1:B:40:LEU:HD11	1:B:68:LEU:HD12	1.63	0.79
1:A:238:LEU:HD11	2:C:575:ILE:HG22	1.63	0.79
1:B:177:LEU:H	1:B:177:LEU:HD23	1.47	0.78
1:A:255:LYS:HA	1:A:255:LYS:HE3	1.65	0.78
1:B:269:ILE:HB	1:B:270:PRO:HD3	1.67	0.76
1:A:314:TYR:HB3	1:A:348:ILE:HG23	1.70	0.73
1:B:266:ARG:HG3	1:B:270:PRO:CG	2.22	0.70
1:B:181:ALA:O	1:B:265:CYS:HB3	1.93	0.68
1:B:107:TYR:HA	2:D:582:PHE:CE2	2.29	0.68
1:B:177:LEU:HD23	1:B:177:LEU:N	2.08	0.67
1:B:294:LYS:HD3	1:B:325:LYS:HG2	1.76	0.67
1:A:163:LEU:O	1:A:166:VAL:HG12	1.95	0.65
1:A:201:MET:HE2	1:A:340:LYS:HA	1.78	0.63
1:A:236:LEU:HD21	2:C:575:ILE:HG21	1.81	0.63
1:B:268:SER:O	1:B:272:PHE:HB2	1.99	0.63
1:A:198:ASP:HB3	1:A:239:LEU:HD12	1.81	0.62
1:B:275:SER:HB3	1:B:353:LEU:HD11	1.80	0.62
1:A:112:ALA:HB1	1:A:117:GLU:HB3	1.81	0.62
1:A:121:ARG:HG2	1:A:149:LEU:HD11	1.82	0.62
1:A:52:PRO:HA	1:A:55:TRP:CD2	2.35	0.62
1:B:51:ASP:OD1	1:B:52:PRO:HD2	2.01	0.61
1:B:52:PRO:HA	1:B:55:TRP:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:N	1:B:177:LEU:CD2	2.62	0.60
1:A:82:PHE:HD2	1:A:89:ILE:HD13	1.67	0.60
1:B:210:ARG:HB3	1:B:271:VAL:HG12	1.83	0.60
1:B:181:ALA:O	1:B:262:LEU:HD22	2.00	0.60
1:B:319:ALA:HB3	1:B:321:CYS:SG	2.41	0.60
1:A:269:ILE:HG22	1:A:272:PHE:CD2	2.37	0.60
1:A:106:ASN:OD1	1:A:150:LYS:HE3	2.02	0.59
1:B:17:ILE:HD11	1:B:62:ASP:HB2	1.84	0.59
1:A:108:ASN:HB3	1:A:149:LEU:HB2	1.84	0.59
1:A:196:ASN:O	2:C:577:PRO:HA	2.03	0.58
1:B:191:VAL:HG13	1:B:253:LYS:HB2	1.87	0.57
2:C:576:ASP:O	2:C:576:ASP:OD1	2.23	0.56
1:A:201:MET:HB3	1:A:341:ILE:HD12	1.87	0.56
1:B:40:LEU:HD12	1:B:61:LYS:HB2	1.87	0.56
1:A:243:GLU:HA	2:C:580:LEU:HD21	1.86	0.55
1:A:213:THR:HG22	1:A:267:HIS:ND1	2.23	0.54
1:A:163:LEU:HD21	2:C:588:PHE:HB2	1.90	0.54
1:A:178:SER:O	1:A:265:CYS:O	2.25	0.54
2:C:582:PHE:CE2	2:C:584:PRO:HA	2.43	0.53
1:B:183:ILE:HD11	1:B:221:PHE:HZ	1.73	0.53
1:B:129:HIS:ND1	1:B:155:GLY:HA2	2.23	0.53
1:A:226:GLN:O	1:A:234:ARG:HD3	2.08	0.53
1:B:262:LEU:O	1:B:263:GLN:HG2	2.09	0.52
1:A:269:ILE:HG22	1:A:272:PHE:HD2	1.75	0.52
1:B:39:LEU:HD11	1:B:308:ARG:HG2	1.91	0.52
2:C:573:ILE:O	2:C:573:ILE:HG23	2.09	0.52
1:B:181:ALA:O	1:B:262:LEU:CD2	2.58	0.51
1:B:266:ARG:HG3	1:B:270:PRO:HG2	1.93	0.51
1:A:52:PRO:HA	1:A:55:TRP:CE2	2.45	0.51
1:B:156:THR:OG1	1:B:157:PRO:HD2	2.10	0.51
1:B:288:LEU:HD13	1:B:332:LEU:HD23	1.93	0.50
1:A:103:LYS:NZ	1:A:106:ASN:HD21	2.09	0.50
1:A:266:ARG:O	1:A:266:ARG:HG3	2.12	0.50
1:B:16:ASP:HA	1:B:61:LYS:HG2	1.93	0.50
1:B:206:PHE:HB3	1:B:210:ARG:HH21	1.76	0.50
1:A:97:TYR:HB3	1:A:100:LEU:HD12	1.93	0.50
1:B:33:THR:HA	1:B:81:SER:HB2	1.92	0.50
1:B:202:ALA:O	1:B:235:ASN:HB3	2.12	0.50
1:B:5:GLN:HA	1:B:5:GLN:OE1	2.12	0.49
1:B:20:VAL:HB	1:B:156:THR:HG21	1.94	0.49
1:A:25:ALA:HB2	1:A:43:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HA	1:A:272:PHE:CD2	2.47	0.49
1:A:231:GLU:HA	1:A:234:ARG:HE	1.78	0.48
1:B:134:ALA:HB2	2:D:588:PHE:CE1	2.49	0.48
1:A:17:ILE:HD11	1:A:62:ASP:HB2	1.94	0.48
1:A:103:LYS:HD2	1:A:103:LYS:HA	1.56	0.48
1:B:56:PHE:CZ	1:B:100:LEU:HD11	2.49	0.48
1:B:133:TYR:HB3	1:B:167:VAL:HG23	1.96	0.48
1:A:141:LEU:HA	1:A:144:ARG:HD2	1.95	0.47
1:B:134:ALA:HB2	2:D:588:PHE:CZ	2.49	0.47
1:B:110:SER:O	1:B:146:ILE:HG23	2.15	0.47
1:B:17:ILE:N	1:B:60:LEU:O	2.41	0.47
1:B:185:ASP:O	1:B:187:PHE:CD1	2.68	0.46
1:B:107:TYR:HA	2:D:582:PHE:HE2	1.79	0.46
1:A:279:HIS:CG	1:A:348:ILE:HD13	2.51	0.46
1:A:267:HIS:O	1:A:267:HIS:CG	2.67	0.46
1:A:106:ASN:HB2	2:C:585:ILE:HB	1.98	0.46
1:B:177:LEU:O	1:B:178:SER:C	2.58	0.45
1:B:183:ILE:O	1:B:183:ILE:HG23	2.16	0.45
1:B:132:THR:O	1:B:148:LEU:HD23	2.16	0.45
1:A:56:PHE:CZ	1:A:100:LEU:HD21	2.52	0.45
1:B:177:LEU:O	1:B:177:LEU:HG	2.17	0.44
1:A:51:ASP:OD1	1:A:53:THR:HG22	2.18	0.44
1:B:177:LEU:C	1:B:179:ASN:N	2.76	0.44
1:B:115:ALA:HB2	1:B:167:VAL:HG21	2.00	0.44
1:B:200:VAL:HG13	1:B:237:CYS:HB3	1.98	0.44
2:C:576:ASP:O	2:C:576:ASP:CG	2.60	0.44
1:B:153:GLN:HG2	1:B:154:THR:HG23	1.99	0.44
1:A:269:ILE:HA	1:A:272:PHE:HD2	1.82	0.44
1:A:26:LYS:HE3	1:A:26:LYS:HB2	1.72	0.43
2:C:584:PRO:O	2:C:585:ILE:HD13	2.18	0.43
1:A:15:GLY:O	1:A:61:LYS:HA	2.19	0.43
1:A:323:GLU:HG2	1:A:325:LYS:H	1.83	0.43
1:A:327:LYS:HA	1:A:327:LYS:HD3	1.71	0.43
1:B:106:ASN:OD1	1:B:150:LYS:HG2	2.18	0.43
2:C:589:PRO:O	2:C:590:ASP:CG	2.61	0.43
1:B:25:ALA:HB2	1:B:43:PHE:CD2	2.54	0.42
1:B:166:VAL:HG21	2:D:588:PHE:CD2	2.54	0.42
1:B:108:ASN:O	1:B:148:LEU:HA	2.19	0.42
1:A:40:LEU:HB2	1:A:61:LYS:HB2	2.01	0.42
1:B:201:MET:HE3	1:B:201:MET:HB3	1.91	0.42
1:B:163:LEU:O	1:B:166:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:HG21	1:A:265:CYS:SG	2.59	0.42
1:B:12:PHE:CD2	1:B:40:LEU:HD13	2.54	0.42
1:B:310:GLN:CD	1:B:336:GLY:HA2	2.44	0.42
1:A:220:PHE:CE2	1:A:240:LYS:HB2	2.55	0.41
1:B:107:TYR:OH	1:B:128:CYS:HB2	2.19	0.41
1:A:98:VAL:HA	1:A:167:VAL:HG12	2.02	0.41
1:A:310:GLN:HG2	1:A:354:ARG:HH21	1.85	0.41
1:A:262:LEU:HB3	1:A:265:CYS:HB3	2.03	0.41
1:A:262:LEU:HD23	1:A:265:CYS:HB3	2.01	0.41
1:B:100:LEU:HD12	1:B:100:LEU:HA	1.90	0.41
1:B:132:THR:OG1	1:B:150:LYS:NZ	2.53	0.41
1:A:41:PHE:HA	1:A:59:VAL:O	2.21	0.41
1:B:104:GLY:HA3	1:B:150:LYS:HB3	2.01	0.41
1:A:103:LYS:HZ3	2:C:587:ASP:CG	2.24	0.41
1:B:127:HIS:O	1:B:151:HIS:HB3	2.21	0.41
1:A:296:HIS:HB3	1:A:348:ILE:CG2	2.52	0.40
1:A:274:HIS:NE2	1:A:278:TYR:OH	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/358 (99%)	333 (94%)	19 (5%)	1 (0%)	36	66
1	B	354/358 (99%)	331 (94%)	23 (6%)	0	100	100
2	C	23/31 (74%)	18 (78%)	5 (22%)	0	100	100
2	D	12/31 (39%)	9 (75%)	3 (25%)	0	100	100
All	All	742/778 (95%)	691 (93%)	50 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PRO

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	317/320 (99%)	314 (99%)	3 (1%)	70	79
1	B	318/320 (99%)	314 (99%)	4 (1%)	61	75
2	C	24/30 (80%)	24 (100%)	0	100	100
2	D	13/30 (43%)	13 (100%)	0	100	100
All	All	672/700 (96%)	665 (99%)	7 (1%)	68	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	175	CYS
1	A	198	ASP
1	B	89	ILE
1	B	175	CYS
1	B	177	LEU
1	B	180	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	215	HIS
1	A	233	GLN
1	A	235	ASN
1	A	343	HIS
1	B	84	GLN
1	B	235	ASN
1	B	318	GLN
1	B	343	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 ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	405	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	A	404	-	4,4,4	0.22	0	6,6,6	0.09	0
4	SO4	B	403	-	4,4,4	0.40	0	6,6,6	0.07	0
3	NAG	A	402	1	14,14,15	0.35	0	17,19,21	0.67	0
4	SO4	B	404	-	4,4,4	0.23	0	6,6,6	0.07	0
3	NAG	A	401	1	14,14,15	0.30	0	17,19,21	0.87	1 (5%)
3	NAG	B	401	1	14,14,15	0.41	0	17,19,21	0.66	0
4	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	402	1	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	401	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C1-O5-C5	2.51	115.56	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	402	NAG	C1
3	B	401	NAG	C1

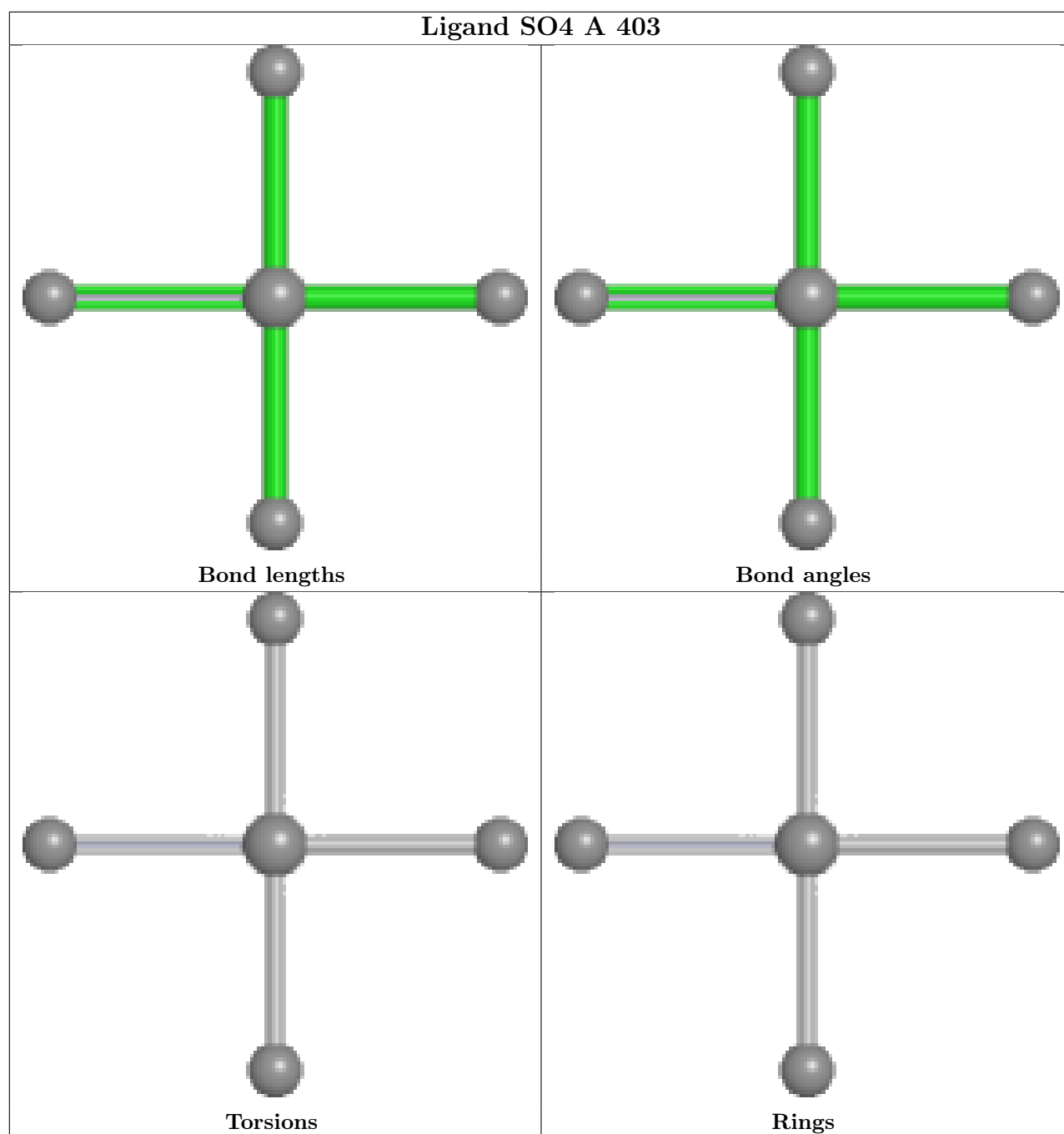
All (6) torsion outliers are listed below:

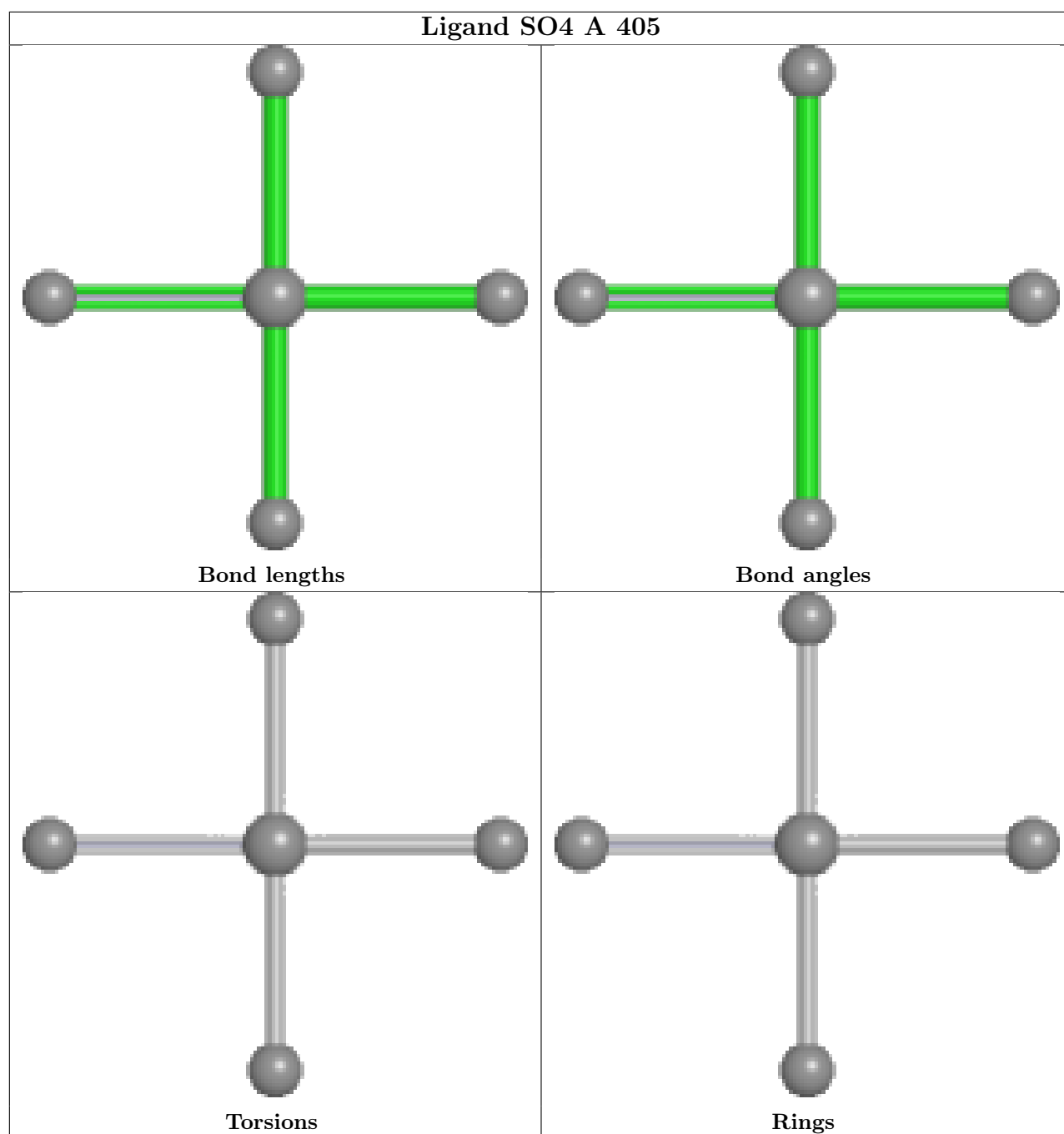
Mol	Chain	Res	Type	Atoms
3	B	401	NAG	C3-C2-N2-C7
3	B	401	NAG	C8-C7-N2-C2
3	B	401	NAG	O7-C7-N2-C2
3	A	401	NAG	C8-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2
3	B	401	NAG	C1-C2-N2-C7

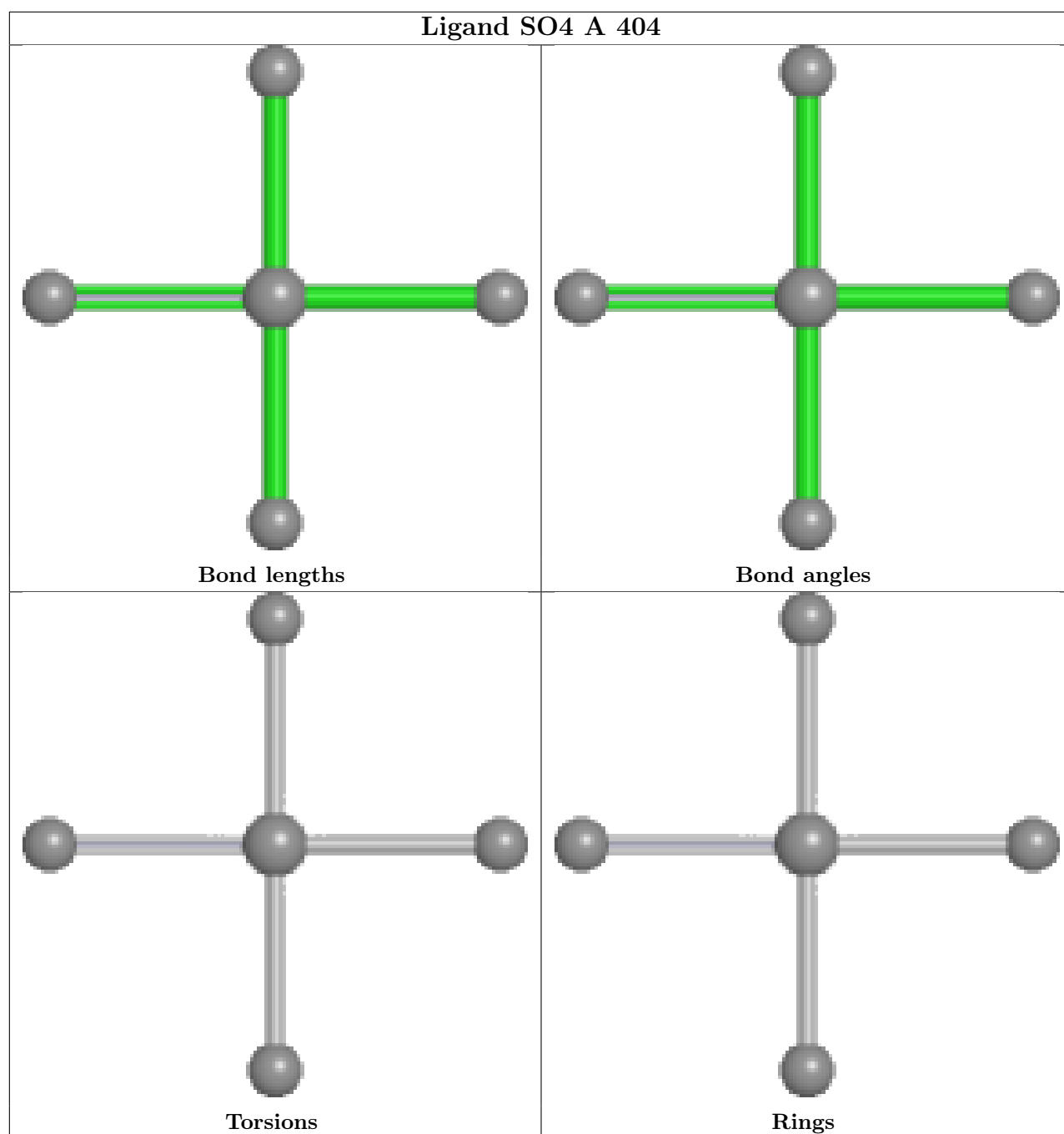
There are no ring outliers.

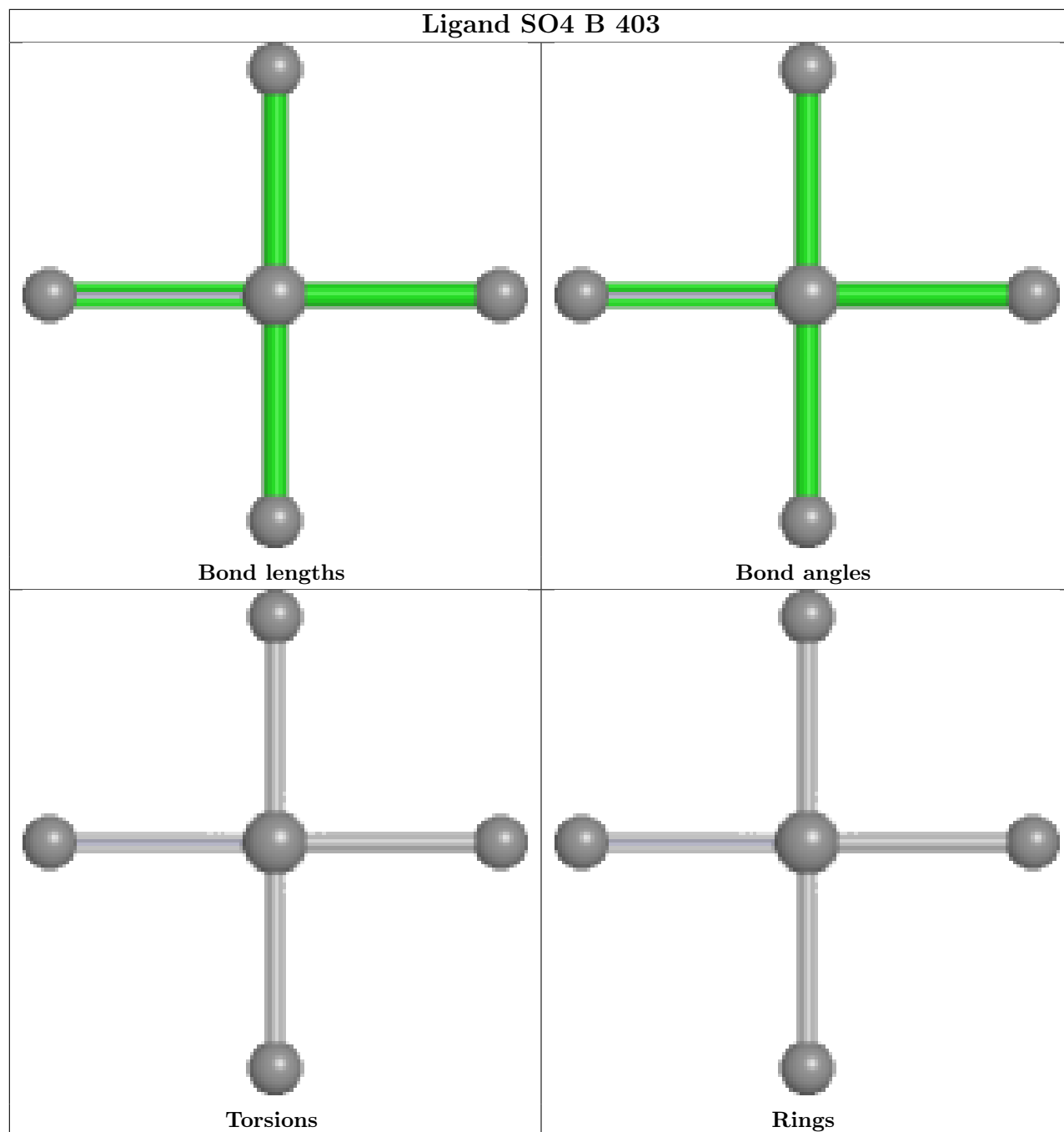
No monomer is involved in short contacts.

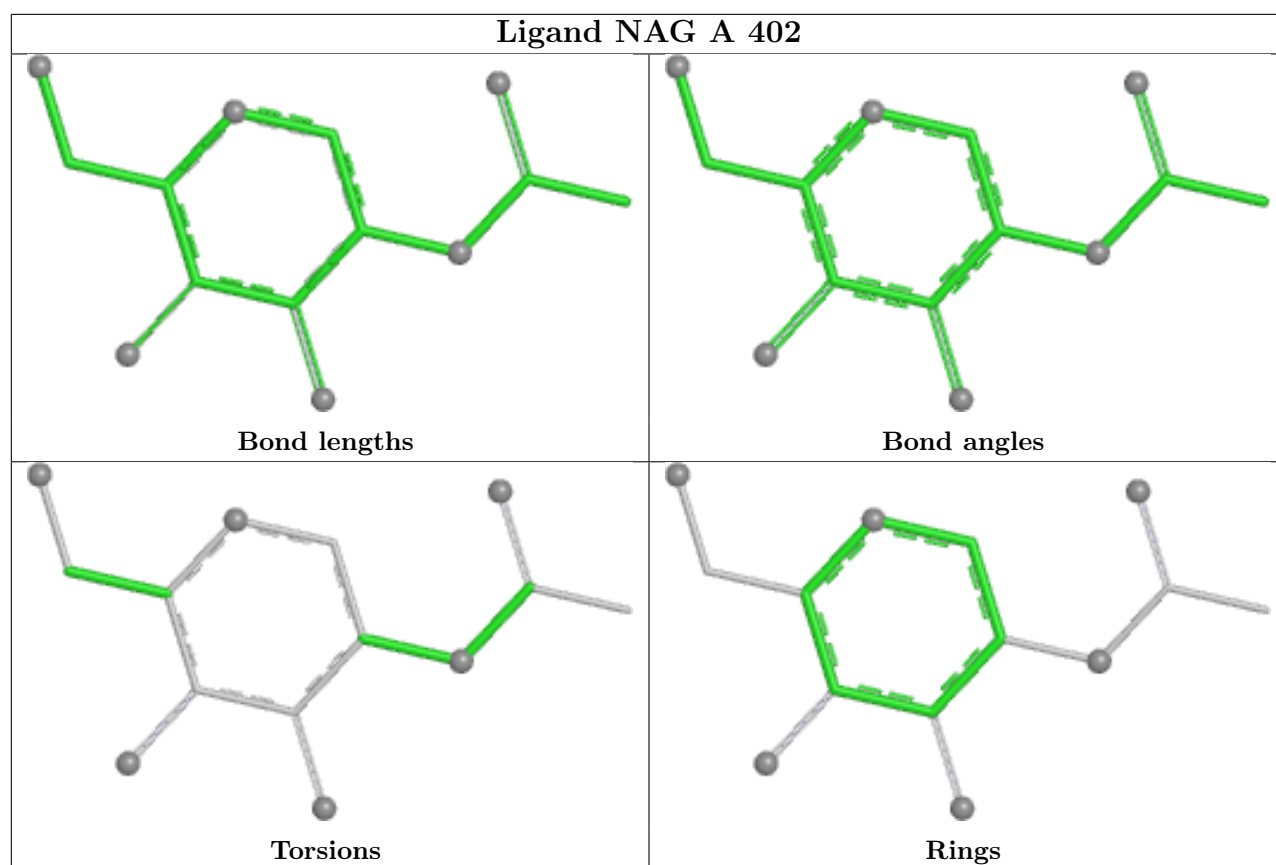
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

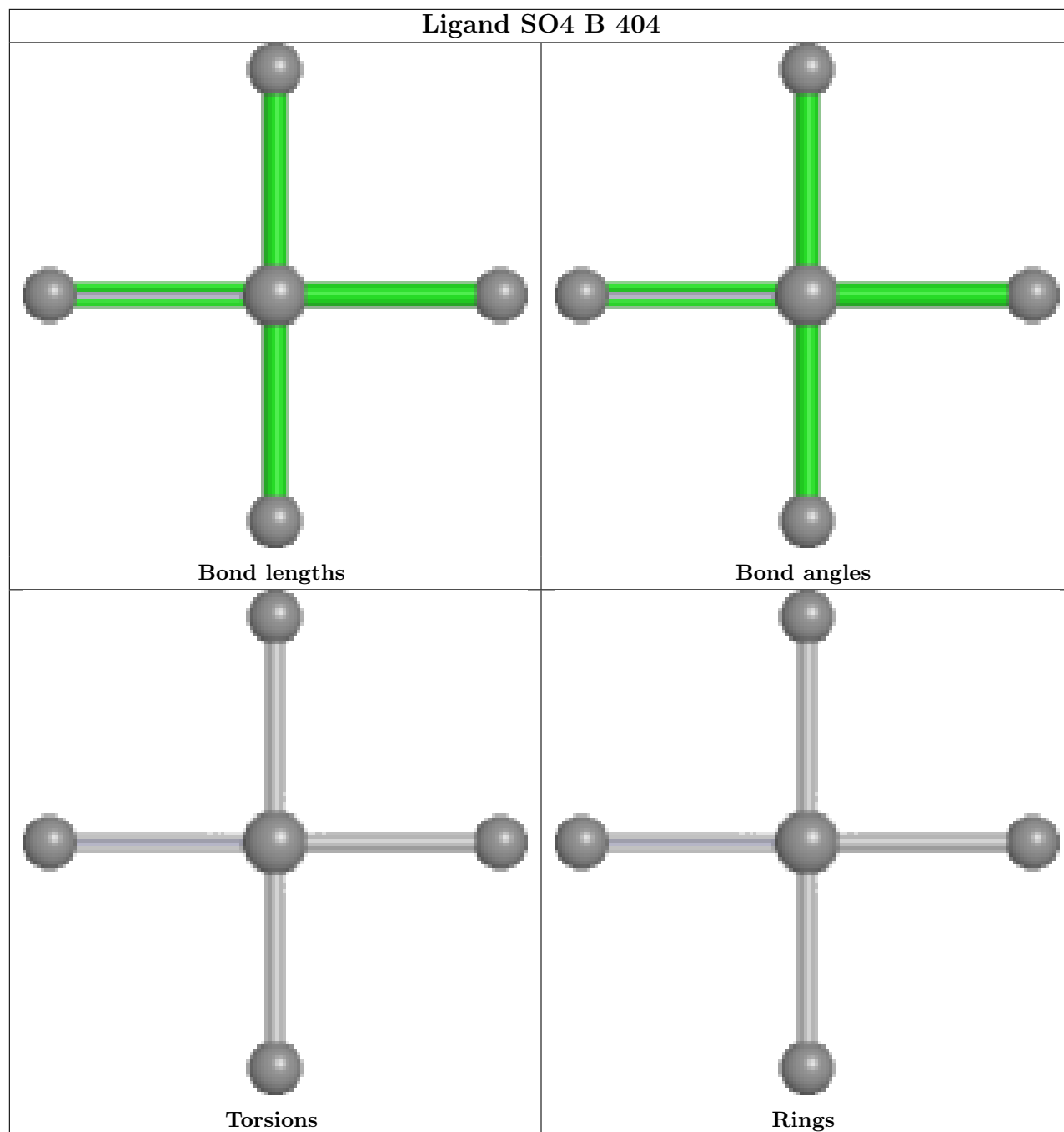


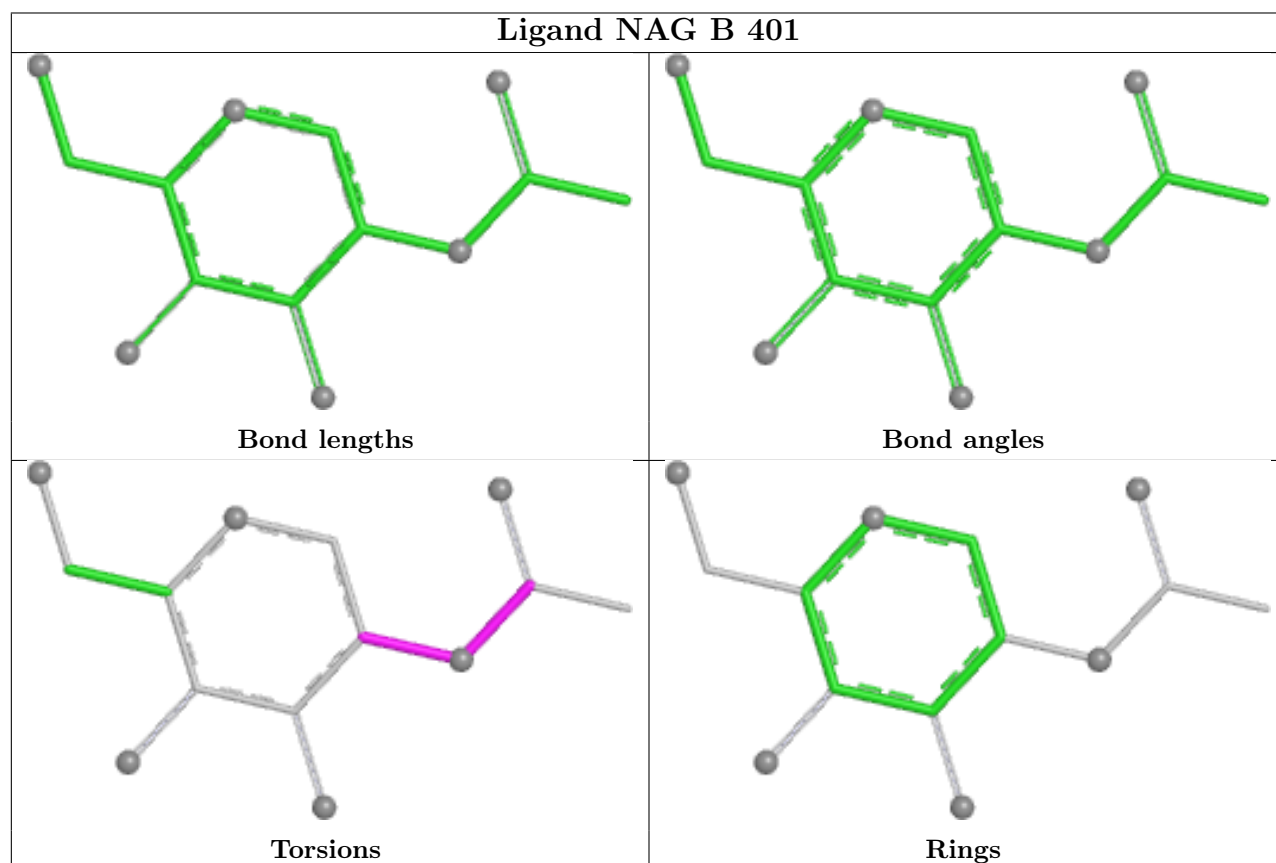
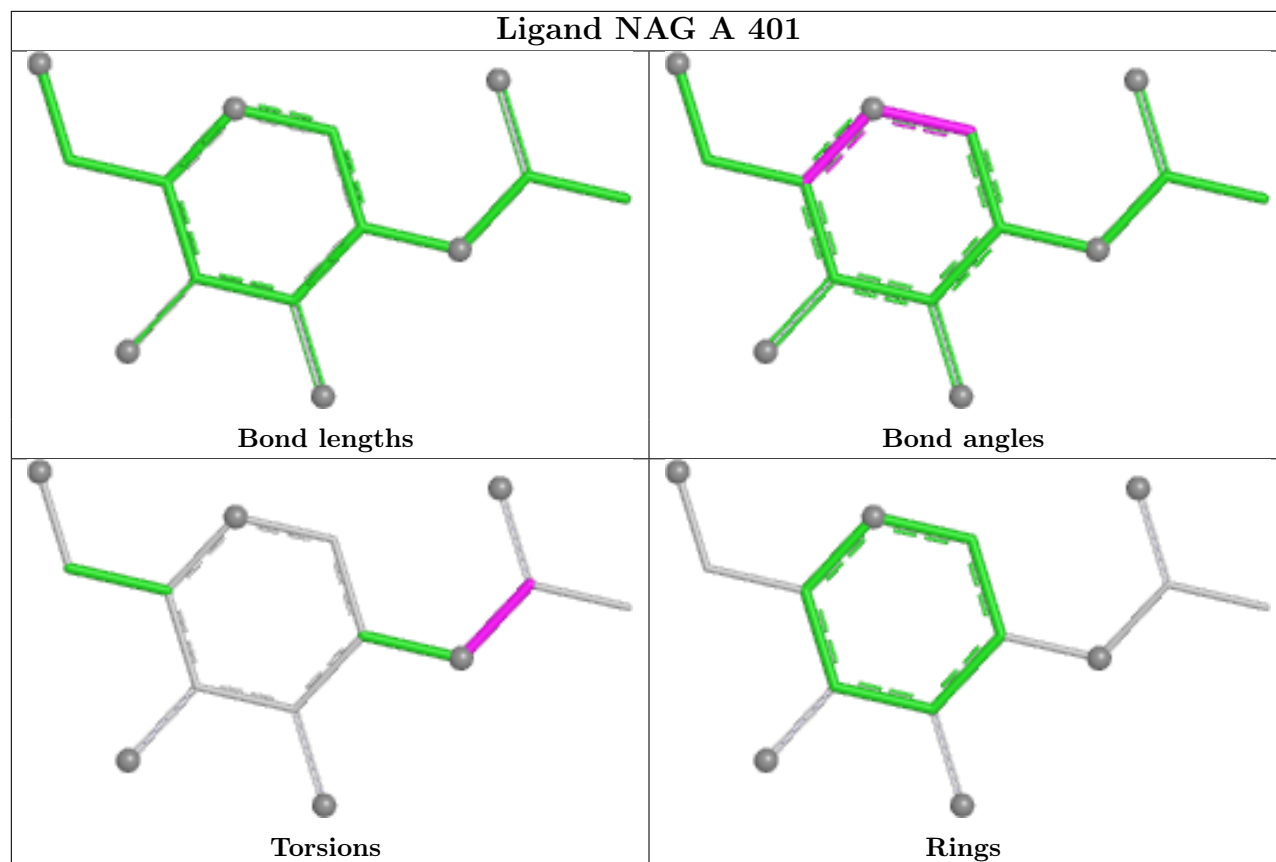


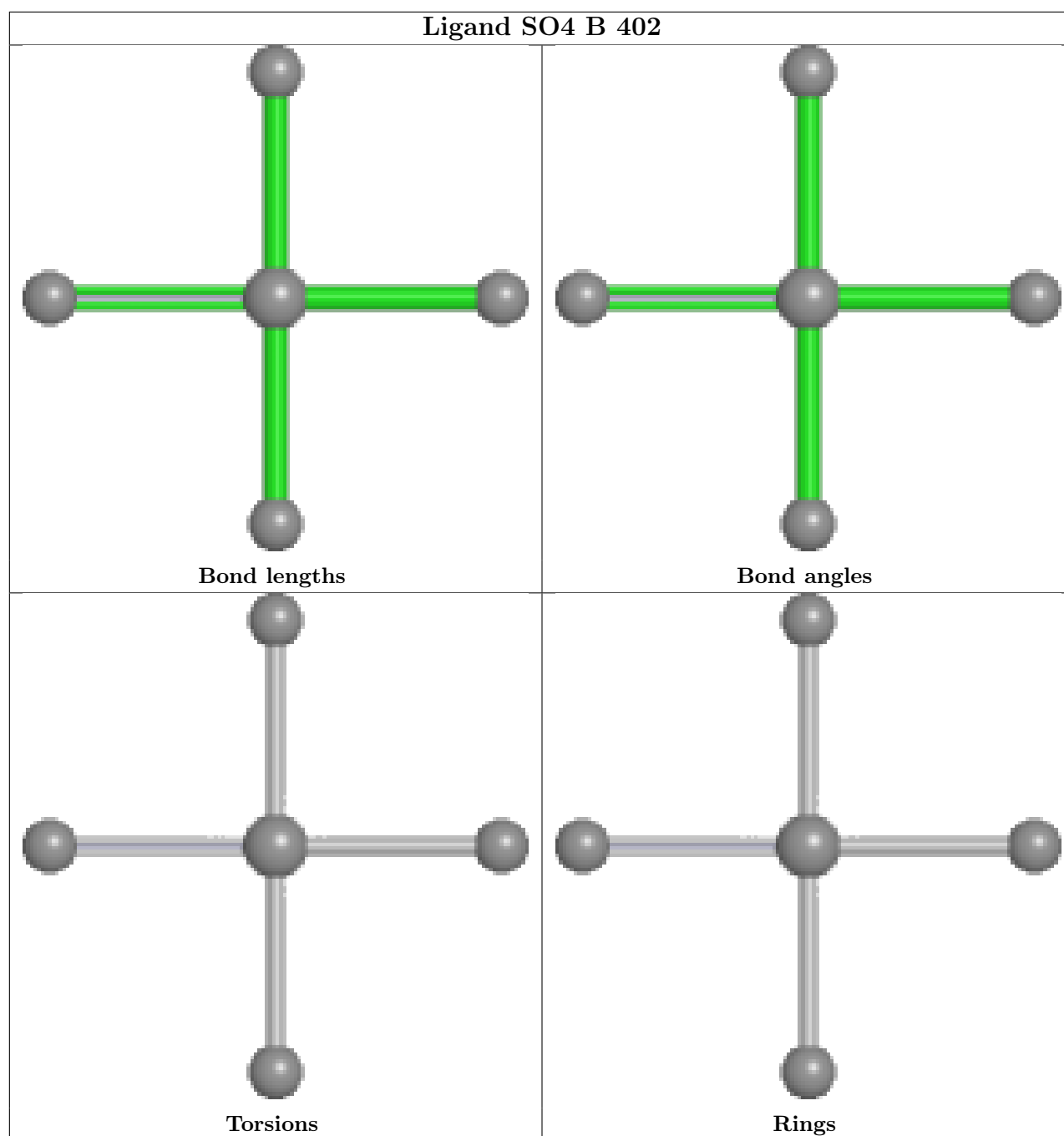












5.7 Other polymers [i](#)

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	355/358 (99%)	0.81	38 (10%) 11 8	15, 47, 95, 139	10 (2%)
1	B	355/358 (99%)	1.17	70 (19%) 3 2	16, 63, 110, 141	12 (3%)
2	C	20/31 (64%)	3.10	15 (75%) 0 0	44, 75, 120, 162	6 (30%)
2	D	14/31 (45%)	2.55	9 (64%) 0 0	47, 98, 111, 122	3 (21%)
All	All	744/778 (95%)	1.07	132 (17%) 4 3	15, 55, 108, 162	31 (4%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ALA	9.7
2	C	576	ASP	6.6
1	A	270	PRO	6.0
1	A	318	GLN	5.9
1	A	267	HIS	5.9
2	C	577	PRO	5.8
1	B	182	CYS	5.4
1	A	275	SER	5.1
1	B	181	ALA	4.9
2	C	582	PHE	4.9
2	C	575	ILE	4.9
2	D	579	GLY	4.8
1	B	267	HIS	4.8
1	B	268	SER	4.8
1	B	89	ILE	4.7
1	B	269	ILE	4.4
1	B	180	LEU	4.4
1	B	93	ASN	4.4
2	C	574	GLN	4.4
1	B	320	SER	4.4
1	B	319	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	573	ILE	4.3
2	D	582	PHE	4.2
2	D	588	PHE	4.1
1	B	271	VAL	4.0
2	C	590	ASP	4.0
1	A	75	ALA	3.9
1	B	178	SER	3.9
1	B	270	PRO	3.9
1	A	269	ILE	3.8
1	B	185	ASP	3.7
2	C	578	ASN	3.7
1	B	105	ILE	3.7
1	A	356	CYS	3.6
1	A	268	SER	3.6
1	B	266	ARG	3.5
1	B	139	PRO	3.5
2	C	579	GLY	3.5
1	B	177	LEU	3.4
1	A	271	VAL	3.3
2	C	571	PRO	3.3
1	B	214	HIS	3.3
1	B	217	GLY	3.3
1	A	214	HIS	3.2
1	B	275	SER	3.2
1	B	56	PHE	3.2
1	B	274	HIS	3.2
1	A	324	GLY	3.2
2	C	589	PRO	3.1
1	B	75	ALA	3.1
1	A	206	PHE	3.1
1	B	324	GLY	3.1
1	B	23	PRO	3.1
1	B	48	PRO	3.0
1	B	179	ASN	3.0
2	C	588	PHE	3.0
1	B	106	ASN	3.0
1	B	356	CYS	3.0
1	A	3	VAL	2.9
1	B	264	SER	2.9
1	B	148	LEU	2.9
2	D	589	PRO	2.9
1	B	317	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	184	ARG	2.9
1	B	117	GLU	2.8
1	A	89	ILE	2.8
2	C	580	LEU	2.8
1	A	320	SER	2.8
1	A	266	ARG	2.8
1	A	316	PRO	2.8
1	A	272	PHE	2.7
1	B	146	ILE	2.8
1	A	90	SER	2.7
1	B	97	TYR	2.7
1	B	193	ALA	2.7
1	B	49	SER	2.7
1	B	249	THR	2.6
1	B	163	LEU	2.6
1	B	94	LYS	2.6
1	B	44	THR	2.6
1	A	87	HIS	2.5
1	B	4	THR	2.5
1	A	273	CYS	2.5
1	B	3	VAL	2.5
1	A	116	GLN	2.5
1	B	98	VAL	2.5
1	B	91	ALA	2.4
1	A	2	CYS	2.4
1	B	265	CYS	2.4
1	A	249	THR	2.4
1	B	104	GLY	2.4
1	A	260	PHE	2.4
1	B	74	THR	2.4
1	B	143	HIS	2.4
2	D	580	LEU	2.4
2	D	583	ASN	2.4
1	B	172	LEU	2.4
1	B	261	SER	2.4
1	B	111	VAL	2.4
1	A	263	GLN	2.3
1	A	91	ALA	2.3
1	A	14	GLY	2.3
1	A	4	THR	2.3
2	C	572	ASP	2.3
2	D	586	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	584	PRO	2.3
1	B	183	ILE	2.2
1	B	114	SER	2.2
1	B	151	HIS	2.2
2	D	581	SER	2.2
1	A	322	ASN	2.2
1	A	180	LEU	2.2
1	B	99	ASP	2.2
1	B	167	VAL	2.2
1	B	120	GLU	2.2
1	A	74	THR	2.1
1	B	165	LYS	2.1
1	B	149	LEU	2.1
1	B	134	ALA	2.1
1	A	189	ASN	2.1
1	B	57	THR	2.1
1	A	45	ALA	2.1
1	B	206	PHE	2.1
2	C	581	SER	2.1
1	B	321	CYS	2.1
1	B	43	PHE	2.1
1	B	325	LYS	2.0
1	A	183	ILE	2.0
1	A	274	HIS	2.0
1	B	107	TYR	2.0
1	A	151	HIS	2.0
1	B	137	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

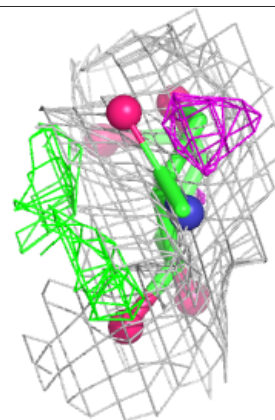
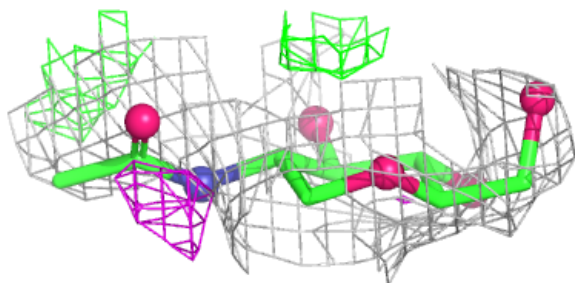
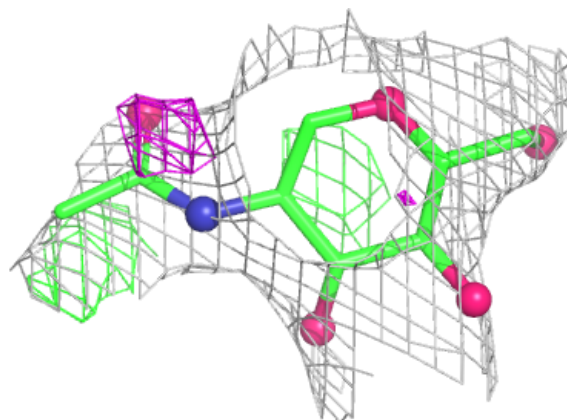
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	402	14/15	0.51	0.20	65,85,93,95	0
3	NAG	B	401	14/15	0.51	0.18	88,102,111,112	0
3	NAG	A	401	14/15	0.64	0.20	73,93,105,117	0
4	SO4	A	405	5/5	0.64	0.34	90,104,119,261	0
4	SO4	A	404	5/5	0.77	0.17	85,94,104,144	0
4	SO4	B	403	5/5	0.82	0.18	86,88,97,133	0
4	SO4	A	403	5/5	0.84	0.45	66,69,74,107	0
4	SO4	B	404	5/5	0.86	0.35	74,83,110,209	0
4	SO4	B	402	5/5	0.87	0.27	55,64,75,112	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.

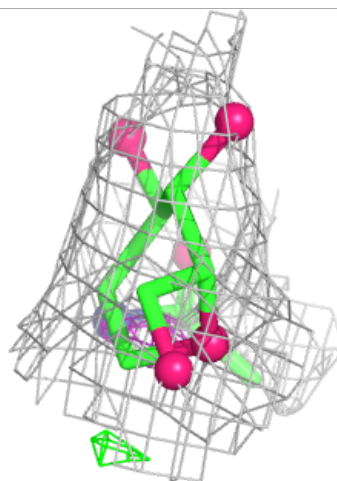
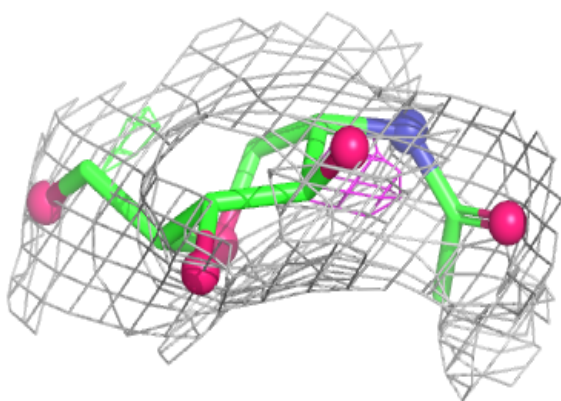
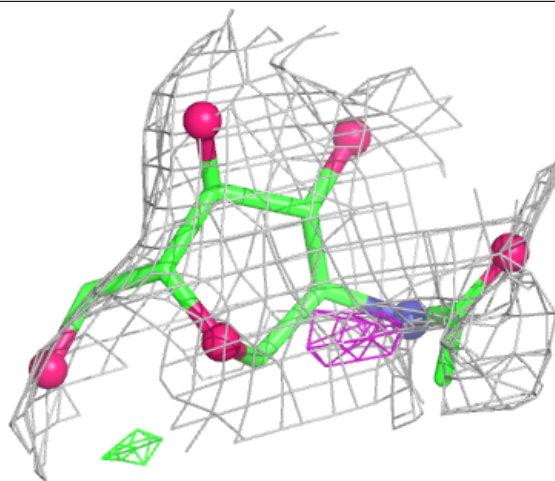
Electron density around NAG A 402:

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



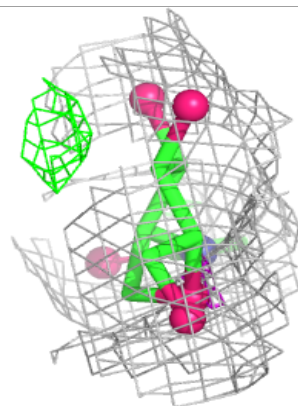
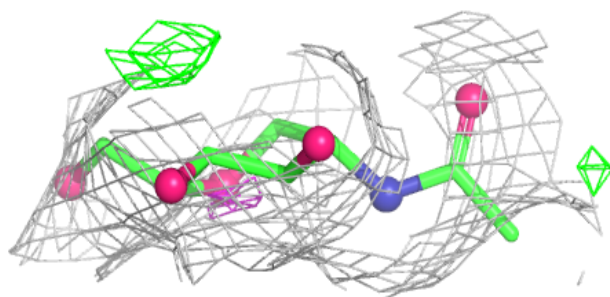
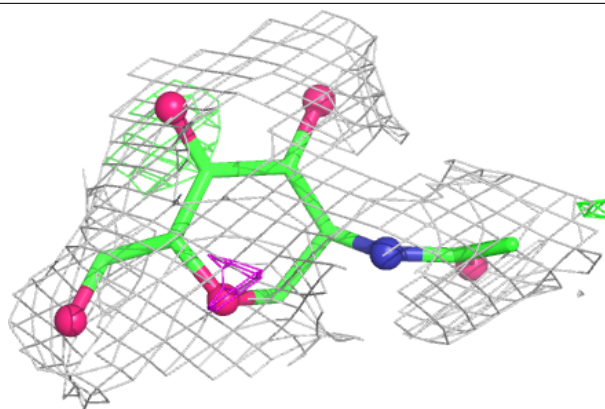
Electron density around NAG B 401:

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



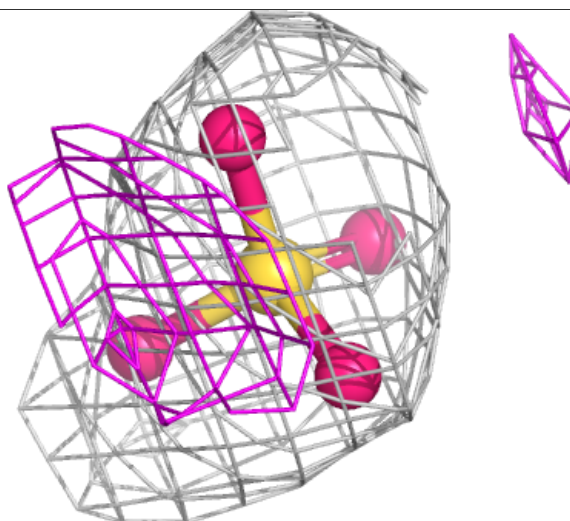
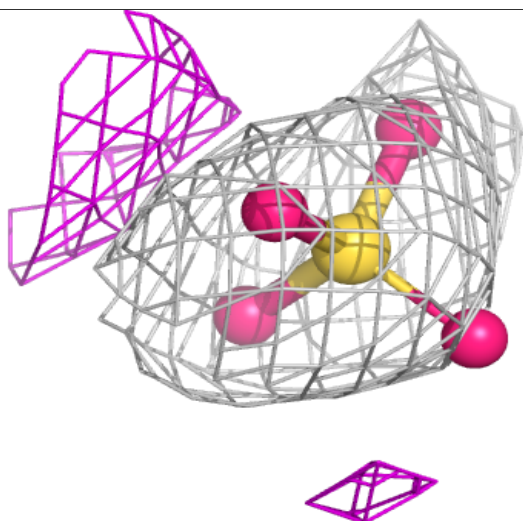
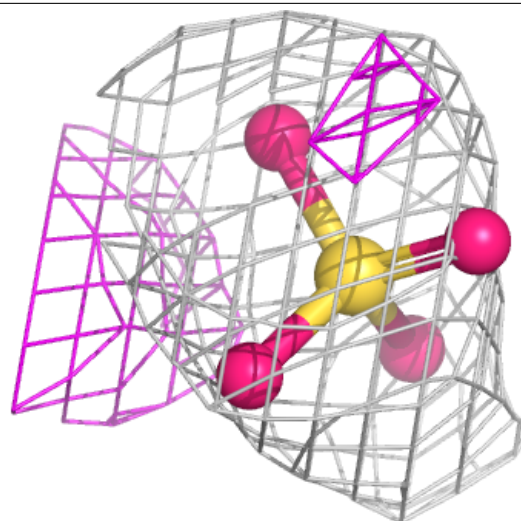
Electron density around NAG A 401:

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



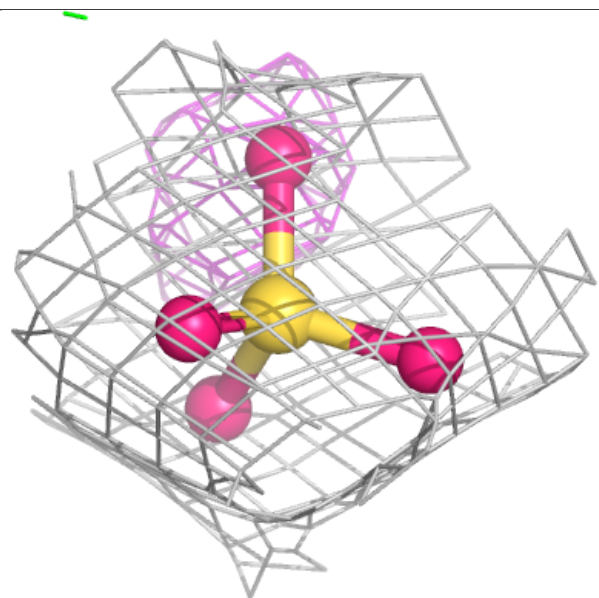
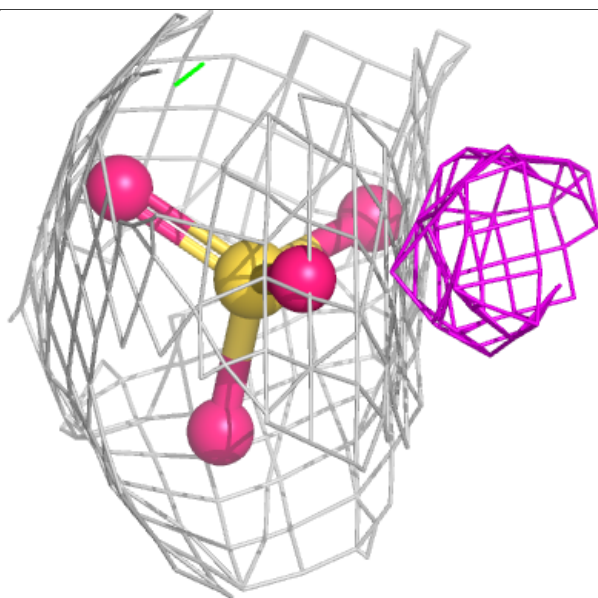
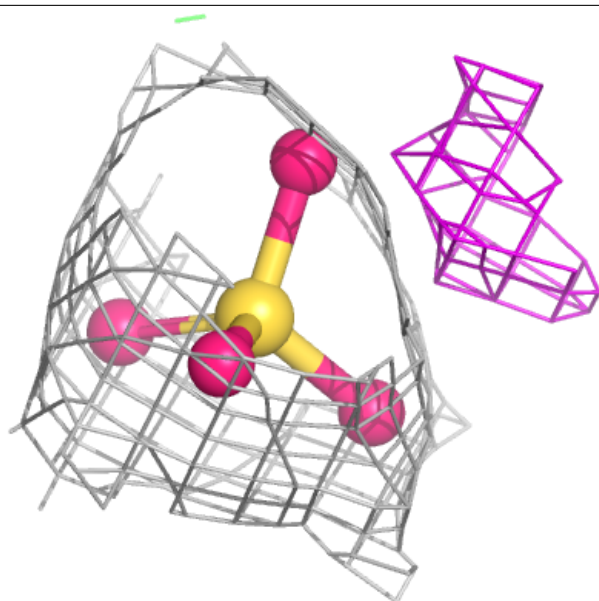
Electron density around SO4 A 405:

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



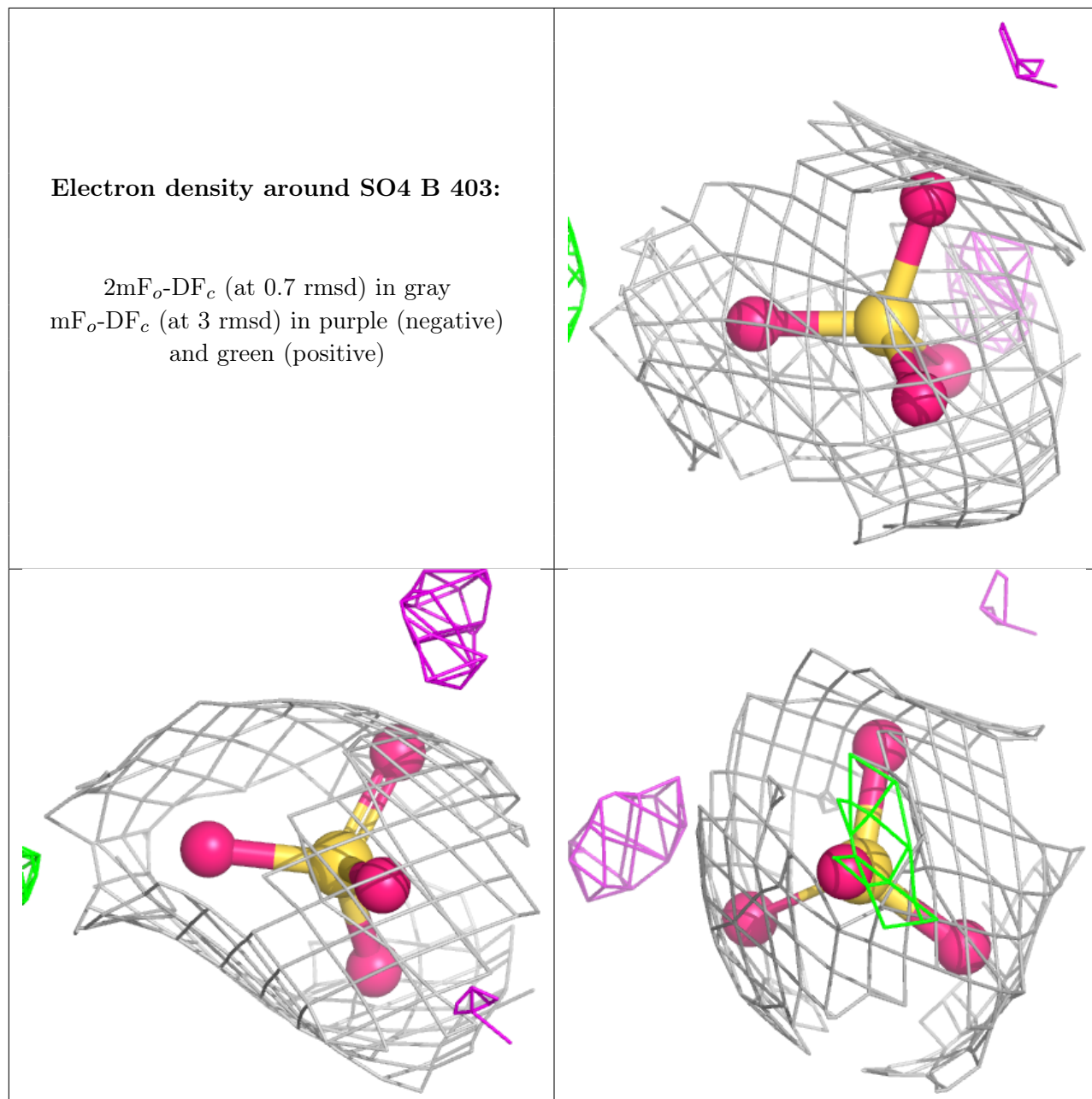
Electron density around SO4 A 404:

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



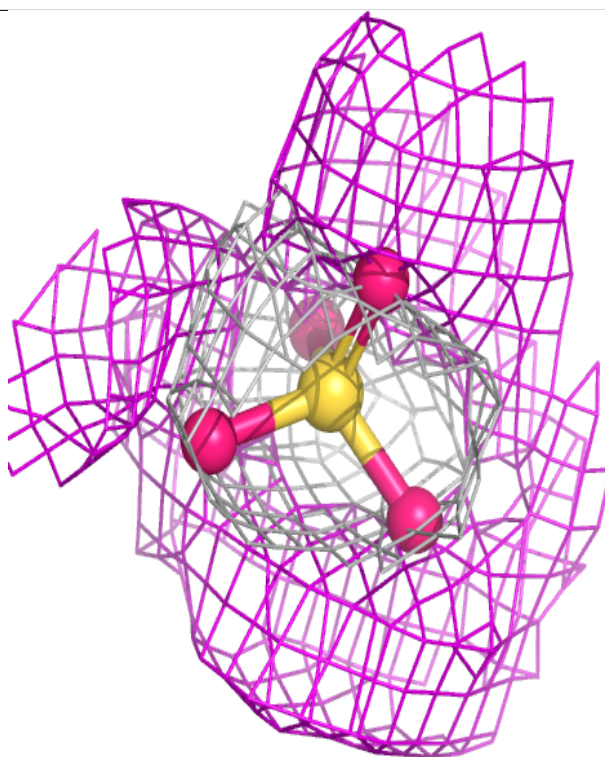
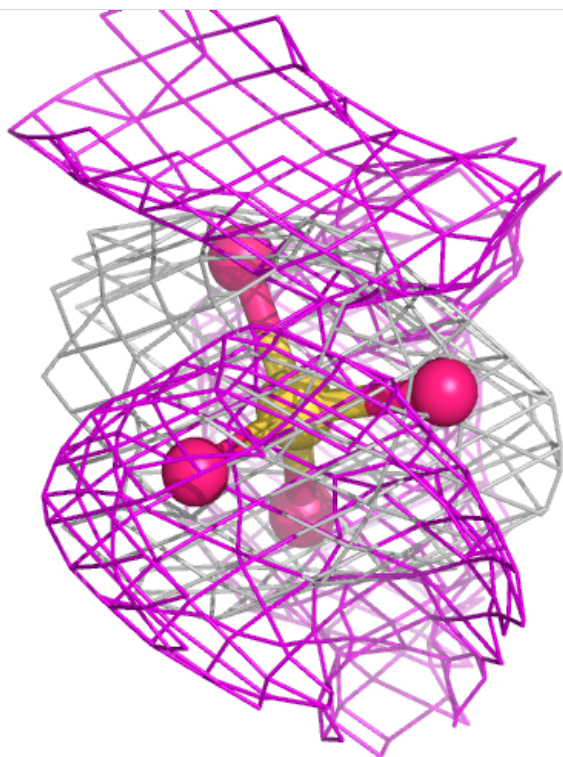
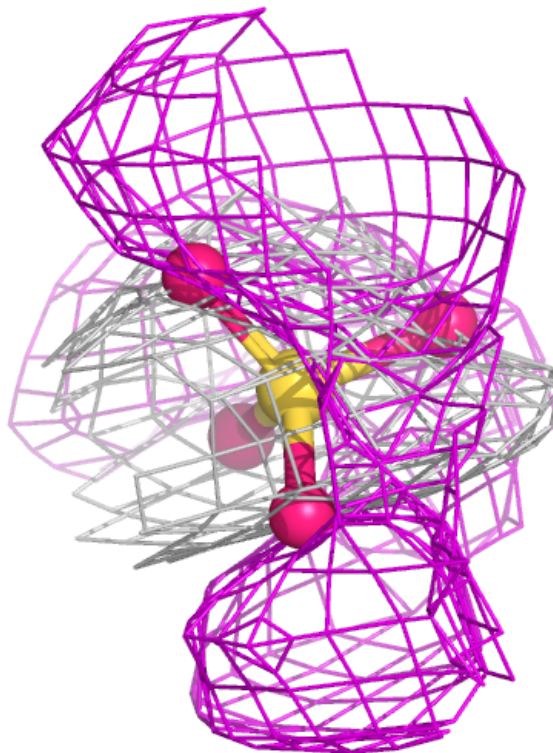
Electron density around SO4 B 403:

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



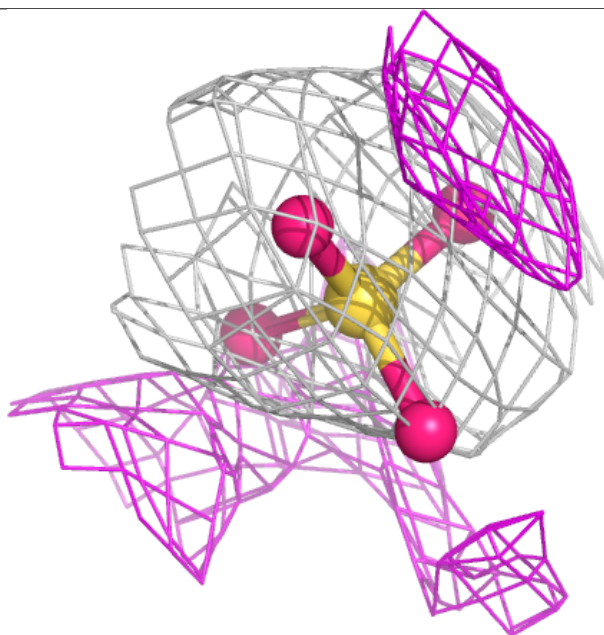
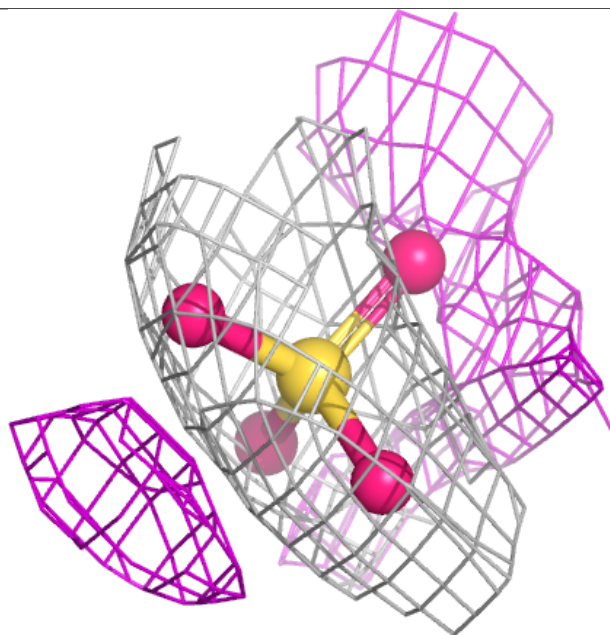
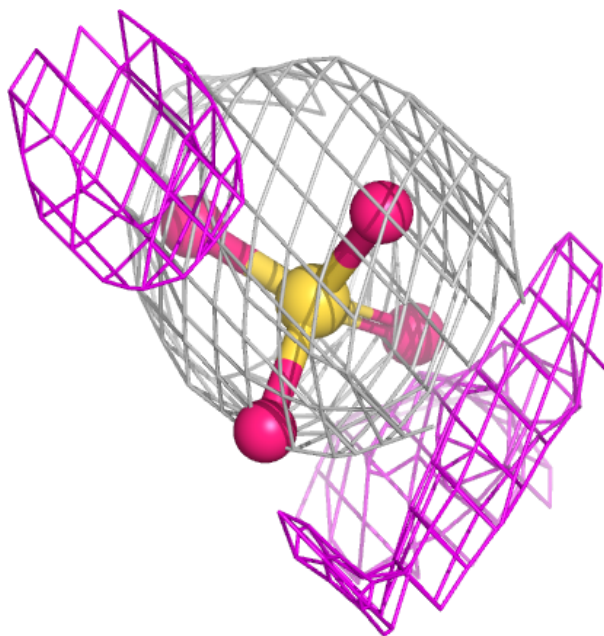
Electron density around SO4 A 403:

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



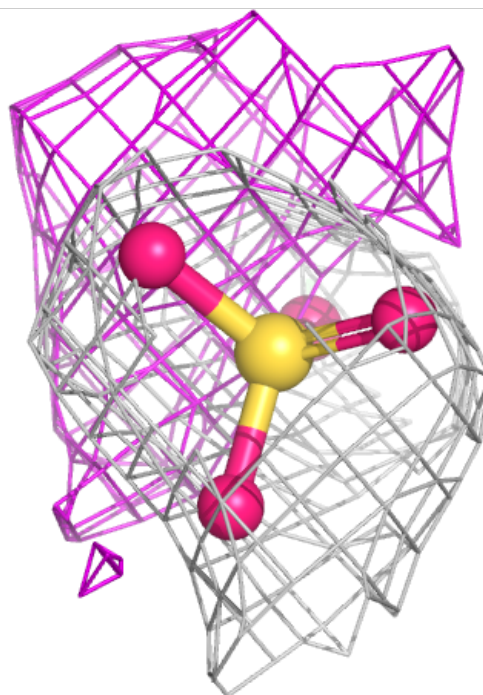
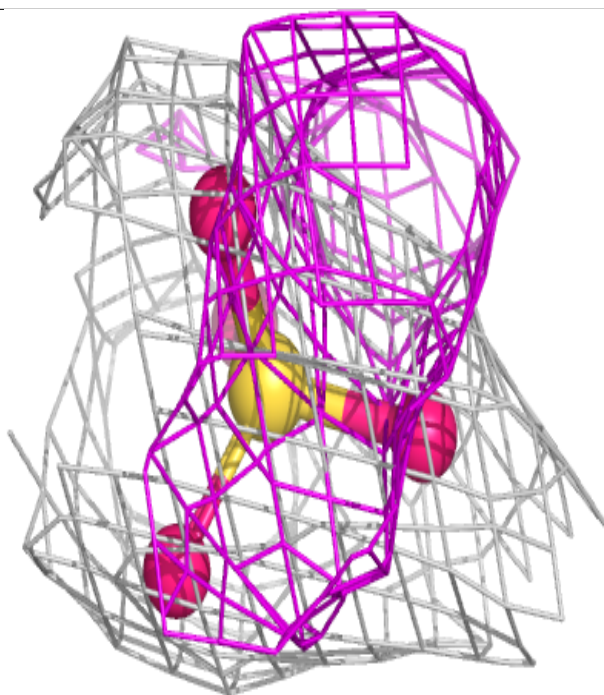
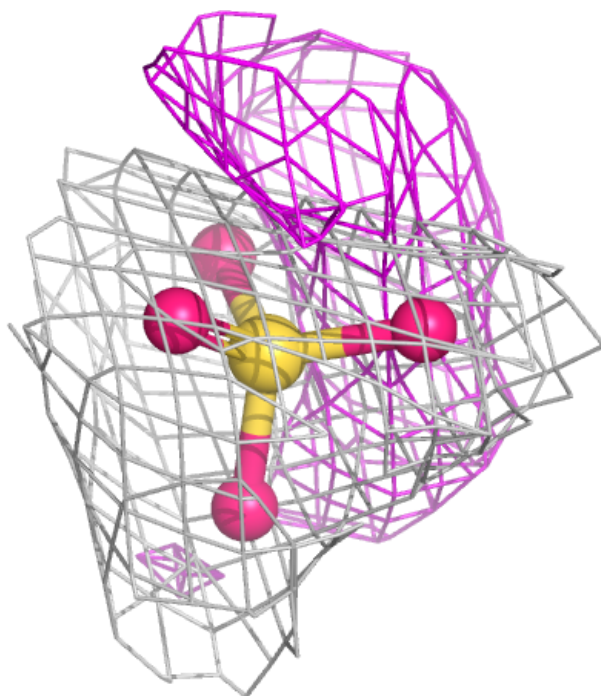
Electron density around SO4 B 404:

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



Electron density around SO4 B 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.