



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2026 – 12:32 PM JST

PDB ID : 9WEE / pdb_00009wee
Title : Plasmodium vivax aspartyl-tRNA synthetase in complex with Asp-AMP and SO₄
Authors : Sharma, V.K.; Manickam, Y.; Sharma, A.
Deposited on : 2025-08-19
Resolution : 2.32 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

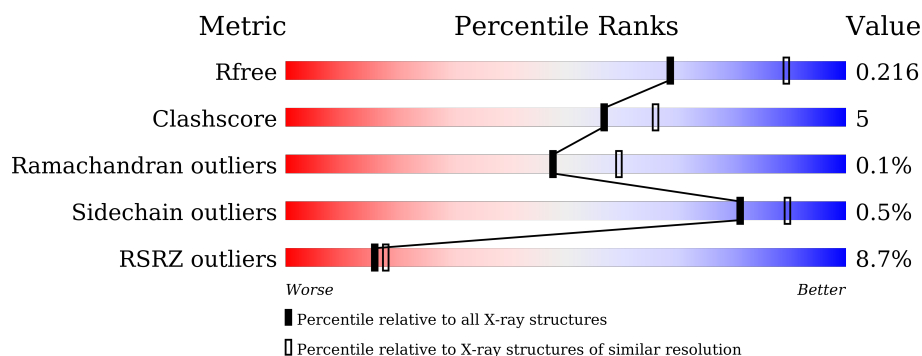
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	536	7% 85% 9% 6%
1	B	536	10% 81% 12% 7%

2 Entry composition [i](#)

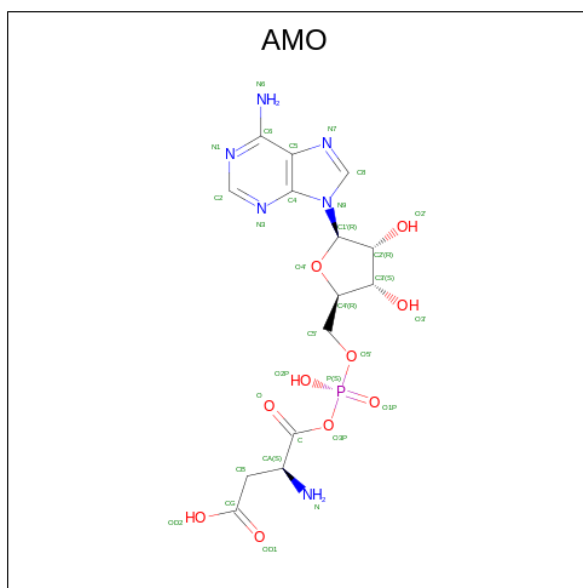
There are 5 unique types of molecules in this entry. The entry contains 8558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 aspartate-tRNA ligase.

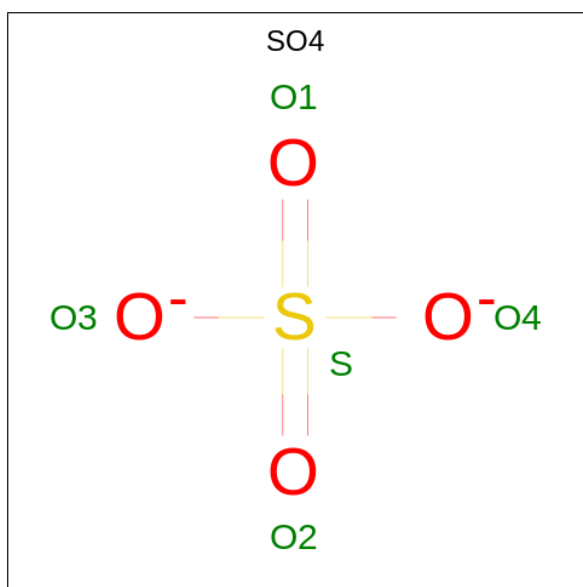
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	2	0
			4059	2603	675	754	27			
1	B	501	Total	C	N	O	S	0	1	0
			4005	2570	664	744	27			

- Molecule 2 is ASPARTYL-ADENOSINE-5'-MONOPHOSPHATE (CCD ID: AMO) (formula: C₁₄H₁₉N₆O₁₀P) (labeled as "Ligand of Interest" by depositor).



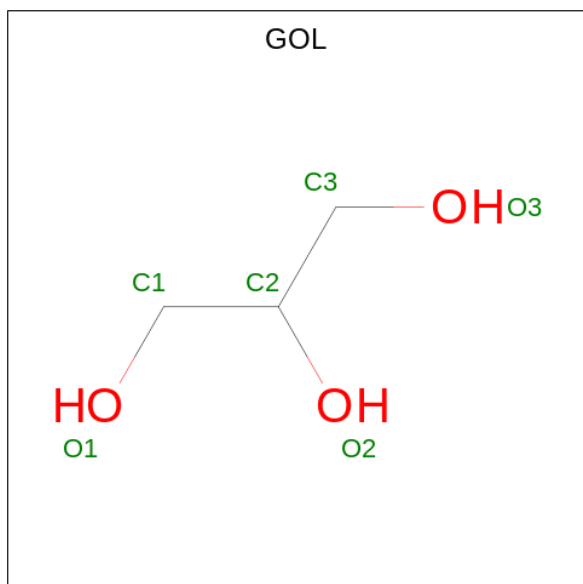
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	14	6	10	1		
2	B	1	Total	C	N	O	P	0	0
			31	14	6	10	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (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		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

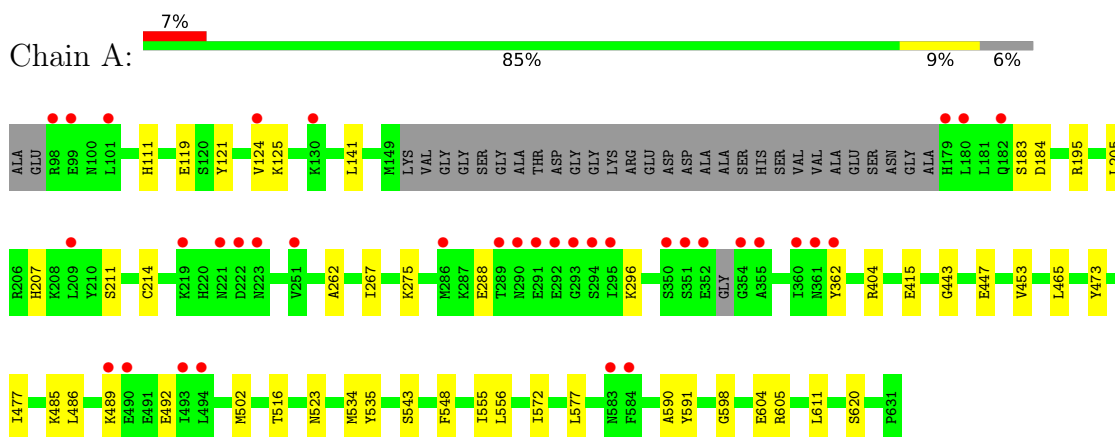
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total	O	0	11
			197	197		
5	B	192	Total	O	0	17
			207	207		

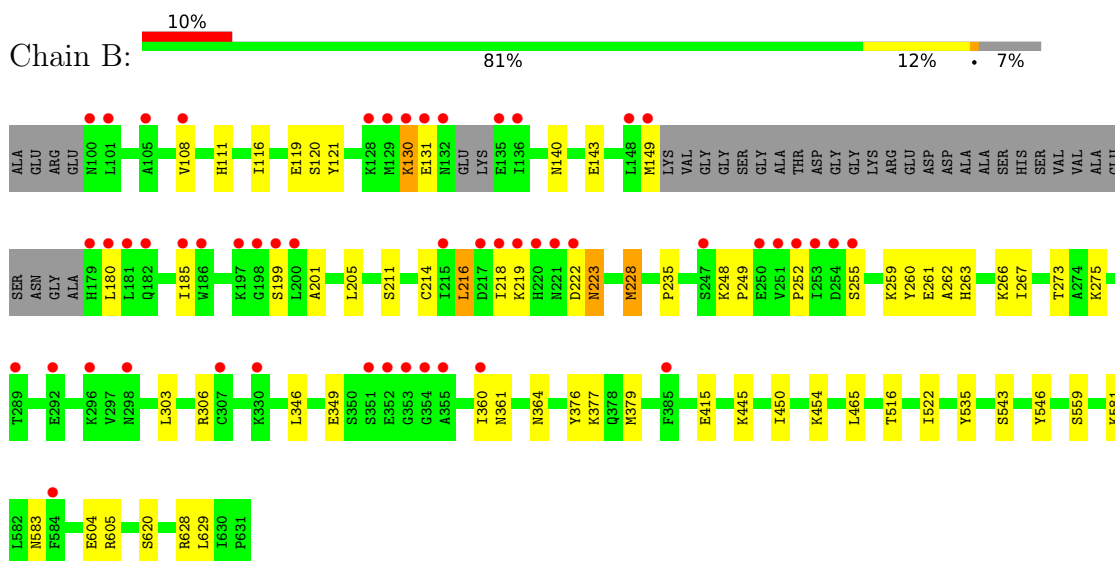
3 Residue-property plots [i](#)

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: aspartate-tRNA ligase



- Molecule 1: aspartate-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.99Å 139.99Å 274.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	121.23 – 2.32 121.23 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (121.23-2.32) 99.9 (121.23-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.15rc1_3423: ???)	Depositor
R, R_{free}	0.190 , 0.217 0.192 , 0.216	Depositor DCC
R_{free} test set	3503 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.3	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	0.95	EDS
Total number of atoms	8558	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, AMO, GOL

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	0.20	0/4153	0.43	0/5604
1	B	0.35	0/4095	0.52	0/5530
All	All	0.28	0/8248	0.47	0/11134

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4059	0	3928	32	0
1	B	4005	0	3853	48	0
2	A	31	0	17	0	0
2	B	31	0	17	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	12	0	16	0	0
4	B	6	0	8	1	0
5	A	197	0	0	2	0
5	B	207	0	0	2	0
All	All	8558	0	7839	74	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 (74) 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:B:120:SER:HA	1:B:266:LYS:HD3	1.74	0.70
1:B:255:SER:O	4:B:703:GOL:H32	1.94	0.66
1:B:361:ASN:HD21	1:B:364:ASN:HA	1.63	0.64
1:A:195:ARG:NH2	5:A:801:HOH:O	2.32	0.62
1:B:349:GLU:HG3	1:B:581:LYS:HB3	1.80	0.62
1:B:180:LEU:HD11	1:B:185:ILE:HD13	1.83	0.61
1:B:180:LEU:HD12	1:B:185:ILE:HG21	1.81	0.61
1:B:111:HIS:NE2	1:B:119:GLU:OE2	2.30	0.60
1:B:249:PRO:HD3	1:B:261:GLU:HG2	1.83	0.60
1:B:216:LEU:O	1:B:216:LEU:HG	2.02	0.59
1:A:591:TYR:HA	1:B:273:THR:HG23	1.85	0.58
1:B:108:VAL:HA	1:B:111:HIS:HB2	1.85	0.58
1:A:572:ILE:HG23	1:A:577:LEU:HB2	1.84	0.58
1:B:120:SER:HB3	1:B:266:LYS:HE2	1.86	0.58
1:A:604:GLU:HG2	1:A:620:SER:HB2	1.84	0.57
1:A:486:LEU:HD13	1:A:502:MET:HE3	1.87	0.57
1:B:445:LYS:NZ	5:B:802:HOH:O	2.38	0.56
1:A:548:PHE:HB2	1:A:556:LEU:HB3	1.87	0.56
1:A:535:TYR:HA	1:A:543:SER:HA	1.90	0.53
1:A:362:TYR:CE2	1:B:629:LEU:HB2	2.44	0.52
1:A:362:TYR:CD1	1:B:629:LEU:HD13	2.44	0.52
1:B:346:LEU:HD22	1:B:360:ILE:HD11	1.91	0.52
1:B:149:MET:CE	1:B:259:LYS:H	2.23	0.52
1:A:489:LYS:HB2	1:A:492:GLU:HG3	1.92	0.52
1:A:453:VAL:HG11	1:A:611:LEU:HD13	1.92	0.52
1:B:604:GLU:HG2	1:B:620:SER:HB2	1.93	0.51
1:A:590:ALA:HB1	1:B:275:LYS:HG3	1.93	0.51
1:B:252:PRO:HB2	1:B:259:LYS:HD2	1.93	0.50
1:B:522:ILE:HG22	1:B:546:TYR:HB3	1.93	0.50
1:B:605:ARG:NH2	3:B:702:SO4:O3	2.40	0.50
1:A:205:LEU:O	1:A:211:SER:HA	2.12	0.49
1:A:362:TYR:OH	1:B:628:ARG:O	2.29	0.49
1:A:534:MET:HE3	1:A:535:TYR:H	1.77	0.49
1:B:199:SER:CB	1:B:218:ILE:CB	2.90	0.49
1:A:465:LEU:HG	1:A:516:THR:HB	1.94	0.48
1:A:124:VAL:HG22	1:A:125:LYS:O	2.14	0.48
1:B:214:CYS:HA	1:B:262:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:HG	1:B:516:THR:HB	1.95	0.47
1:B:205:LEU:O	1:B:211:SER:HA	2.14	0.47
1:B:219:LYS:HA	1:B:223:ASN:ND2	2.29	0.47
1:A:183:SER:OG	1:A:184:ASP:N	2.48	0.46
1:B:130:LYS:HD3	1:B:130:LYS:HA	1.68	0.46
1:A:362:TYR:CE1	1:B:629:LEU:HD13	2.51	0.45
1:B:361:ASN:ND2	1:B:364:ASN:HA	2.29	0.45
1:A:121:TYR:HA	1:A:267:ILE:O	2.17	0.45
1:B:121:TYR:HA	1:B:267:ILE:O	2.17	0.45
1:B:235:PRO:HB2	1:B:273:THR:HB	1.98	0.45
1:B:450:ILE:O	1:B:454:LYS:HG2	2.17	0.45
1:B:216:LEU:C	1:B:216:LEU:HD12	2.42	0.44
1:B:116:ILE:HD11	1:B:131:GLU:HB2	1.99	0.44
1:A:443:GLY:O	1:A:447:GLU:HB2	2.17	0.44
1:B:377:LYS:HD2	1:B:415:GLU:HB2	1.99	0.44
1:B:116:ILE:HD11	1:B:131:GLU:CA	2.47	0.44
1:B:201:ALA:HB2	1:B:228:MET:SD	2.58	0.43
1:A:111:HIS:NE2	1:A:119:GLU:OE2	2.29	0.43
1:B:583:ASN:ND2	5:B:809:HOH:O	2.51	0.43
1:B:116:ILE:O	1:B:266:LYS:NZ	2.51	0.43
1:A:415:GLU:OE1	1:A:598:GLY:HA3	2.19	0.43
1:B:535:TYR:HA	1:B:543:SER:HA	2.00	0.43
1:B:248:LYS:HB2	1:B:260:TYR:CE2	2.54	0.42
1:B:140:ASN:OD1	1:B:143:GLU:HG2	2.19	0.42
1:A:404:ARG:O	1:A:605:ARG:NH2	2.51	0.41
1:A:214:CYS:HA	1:A:262:ALA:O	2.19	0.41
1:A:485:LYS:O	1:A:502:MET:HE1	2.20	0.41
1:B:303:LEU:HD23	1:B:306:ARG:HD3	2.01	0.41
1:B:376:TYR:HA	1:B:379:MET:HE3	2.02	0.41
1:A:275:LYS:HG2	5:A:896:HOH:O	2.20	0.41
1:A:473:TYR:O	1:A:477:ILE:HG12	2.20	0.41
1:A:523:ASN:HA	1:A:543:SER:O	2.20	0.41
1:B:546:TYR:CE1	1:B:559:SER:HA	2.55	0.41
1:A:141:LEU:HB2	1:A:207:HIS:HB3	2.04	0.40
1:A:288:GLU:CD	1:A:296:LYS:HD3	2.46	0.40
1:A:555:ILE:HG13	1:A:556:LEU:N	2.36	0.40
1:B:261:GLU:OE2	1:B:263:HIS:NE2	2.54	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	500/536 (93%)	480 (96%)	20 (4%)	0	100	100
1	B	496/536 (92%)	484 (98%)	11 (2%)	1 (0%)	43	53
All	All	996/1072 (93%)	964 (97%)	31 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	ASP

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	439/485 (90%)	439 (100%)	0	100	100
1	B	429/485 (88%)	425 (99%)	4 (1%)	70	83
All	All	868/970 (90%)	864 (100%)	4 (0%)	81	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	130	LYS
1	B	216	LEU
1	B	223	ASN
1	B	228	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	HIS
1	A	221	ASN
1	A	223	ASN
1	A	299	GLN
1	A	371	GLN
1	A	374	GLN
1	A	487	HIS
1	A	583	ASN
1	B	223	ASN
1	B	233	ASN
1	B	299	GLN
1	B	322	GLN
1	B	361	ASN
1	B	401	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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
3	SO4	B	702	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	B	703	-	5,5,5	0.26	0	5,5,5	0.29	0
2	AMO	A	701	-	31,33,33	0.28	0	44,49,49	0.57	1 (2%)
3	SO4	A	702	-	4,4,4	0.17	0	6,6,6	0.07	0
4	GOL	A	703	-	5,5,5	0.26	0	5,5,5	0.28	0
2	AMO	B	701	-	31,33,33	0.32	0	44,49,49	0.61	1 (2%)
4	GOL	A	704	-	5,5,5	0.26	0	5,5,5	0.27	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
4	GOL	B	703	-	-	0/4/4/4	-
2	AMO	A	701	-	-	1/21/39/39	0/3/3/3
4	GOL	A	703	-	-	0/4/4/4	-
2	AMO	B	701	-	-	1/21/39/39	0/3/3/3
4	GOL	A	704	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	AMO	O-C-CA	2.66	129.71	120.95
2	A	701	AMO	O-C-CA	2.56	129.39	120.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

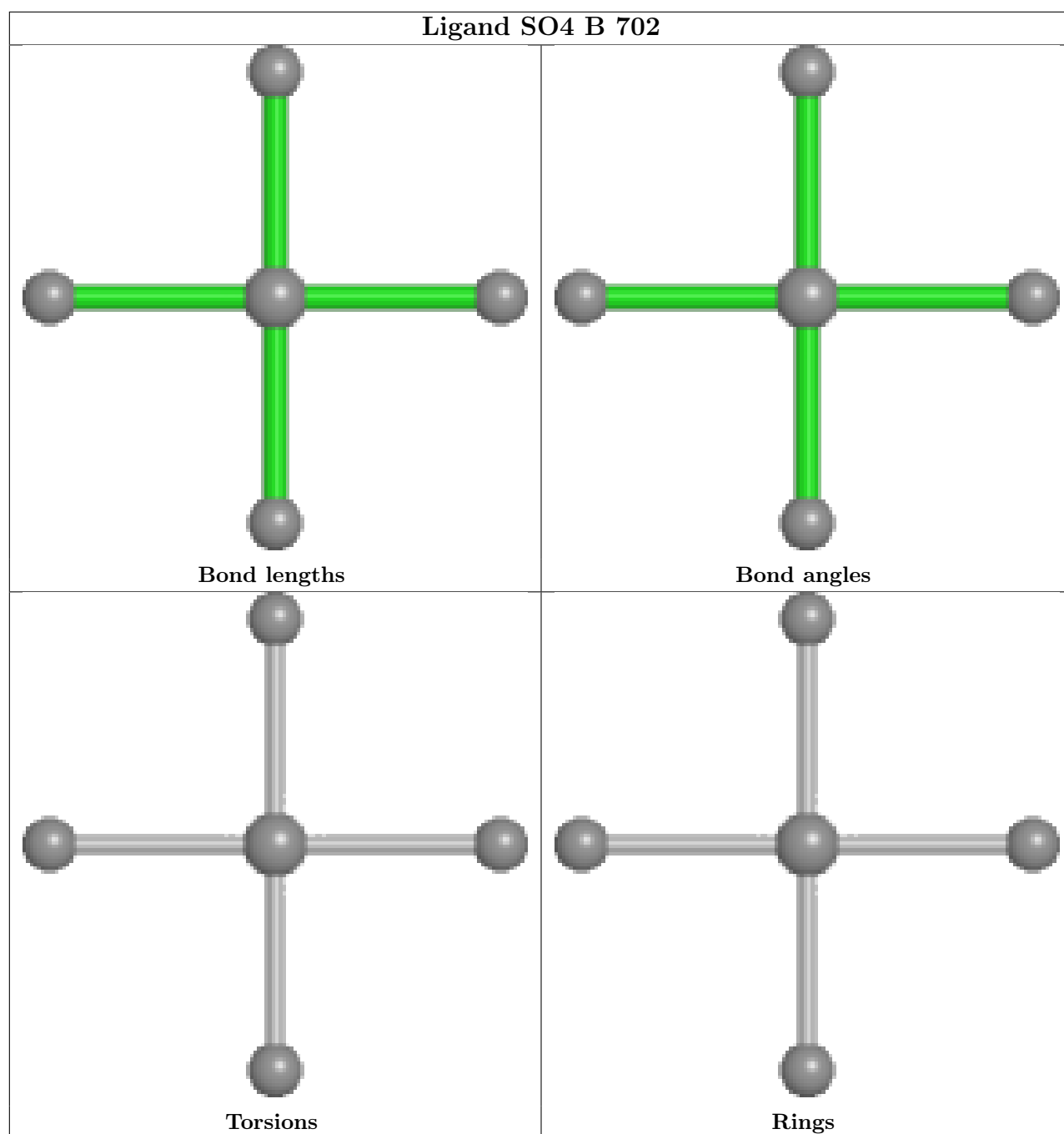
Mol	Chain	Res	Type	Atoms
2	A	701	AMO	CA-CB-CG-OD1
2	B	701	AMO	CA-CB-CG-OD1

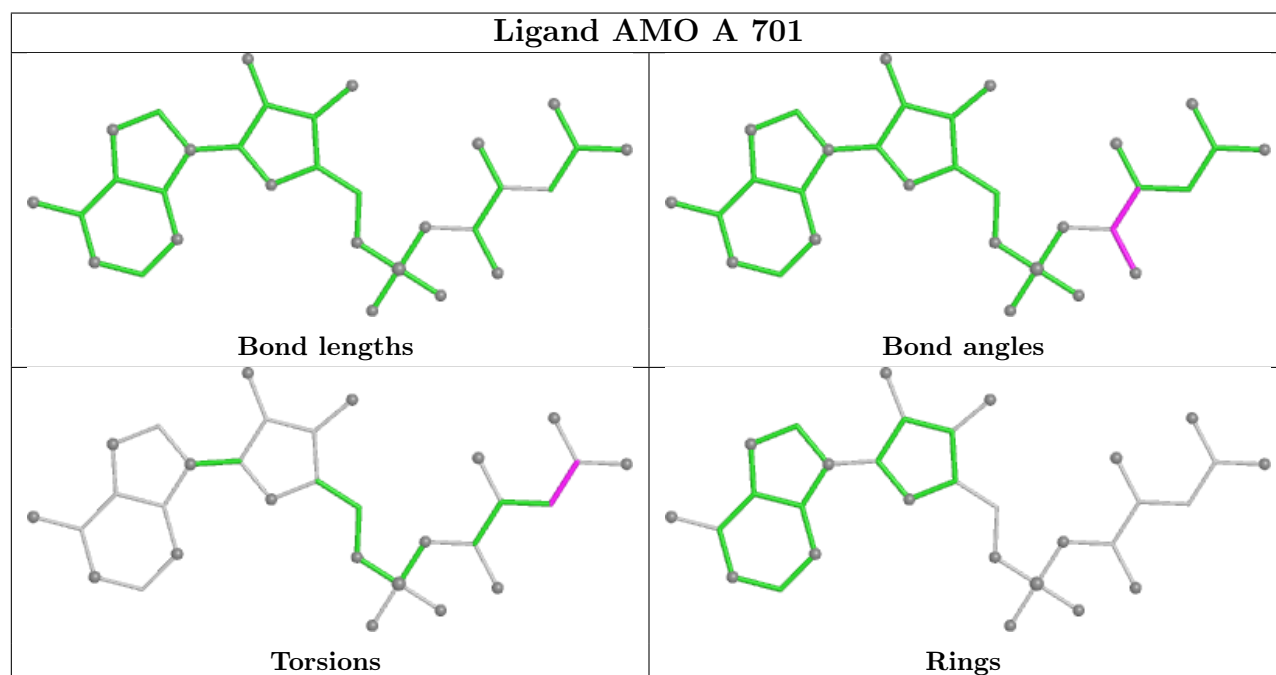
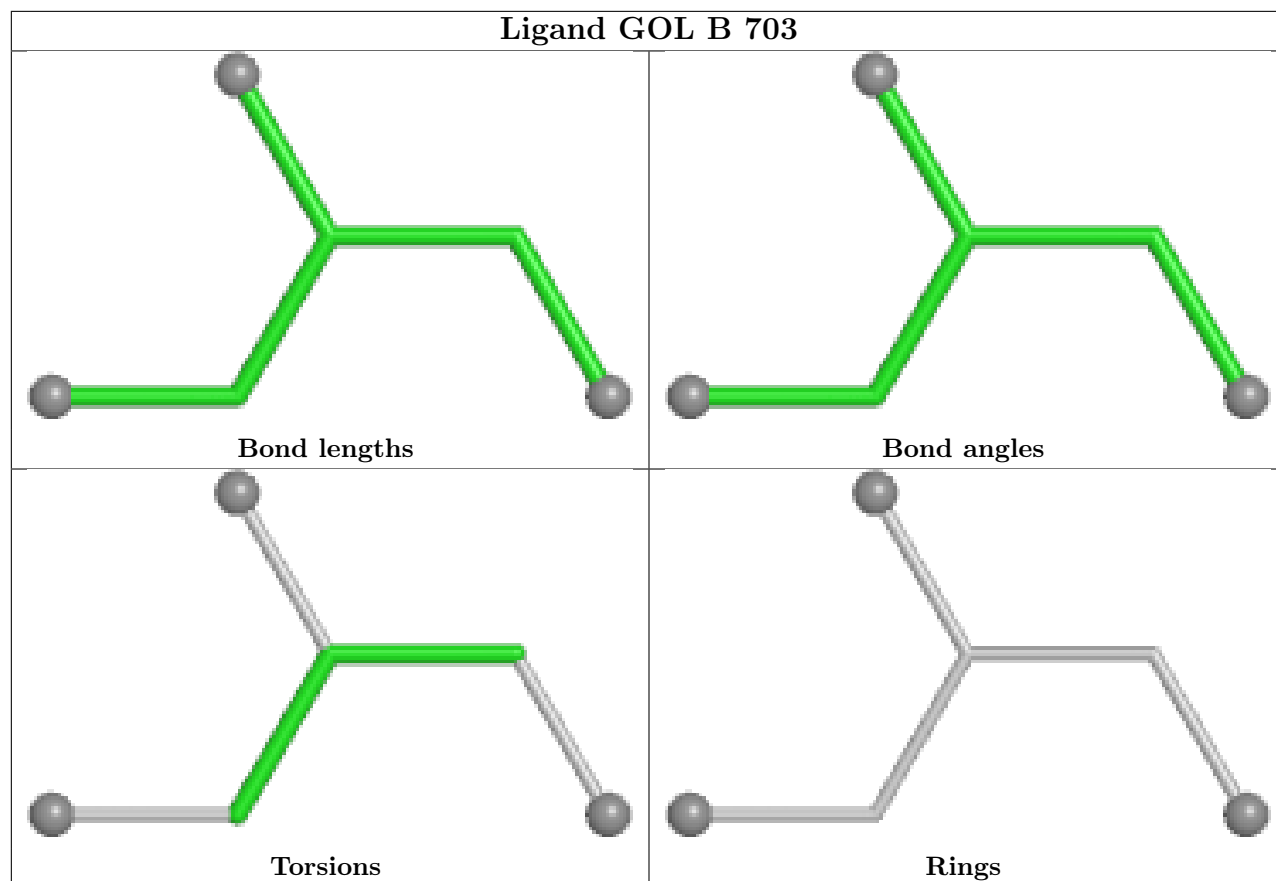
There are no ring outliers.

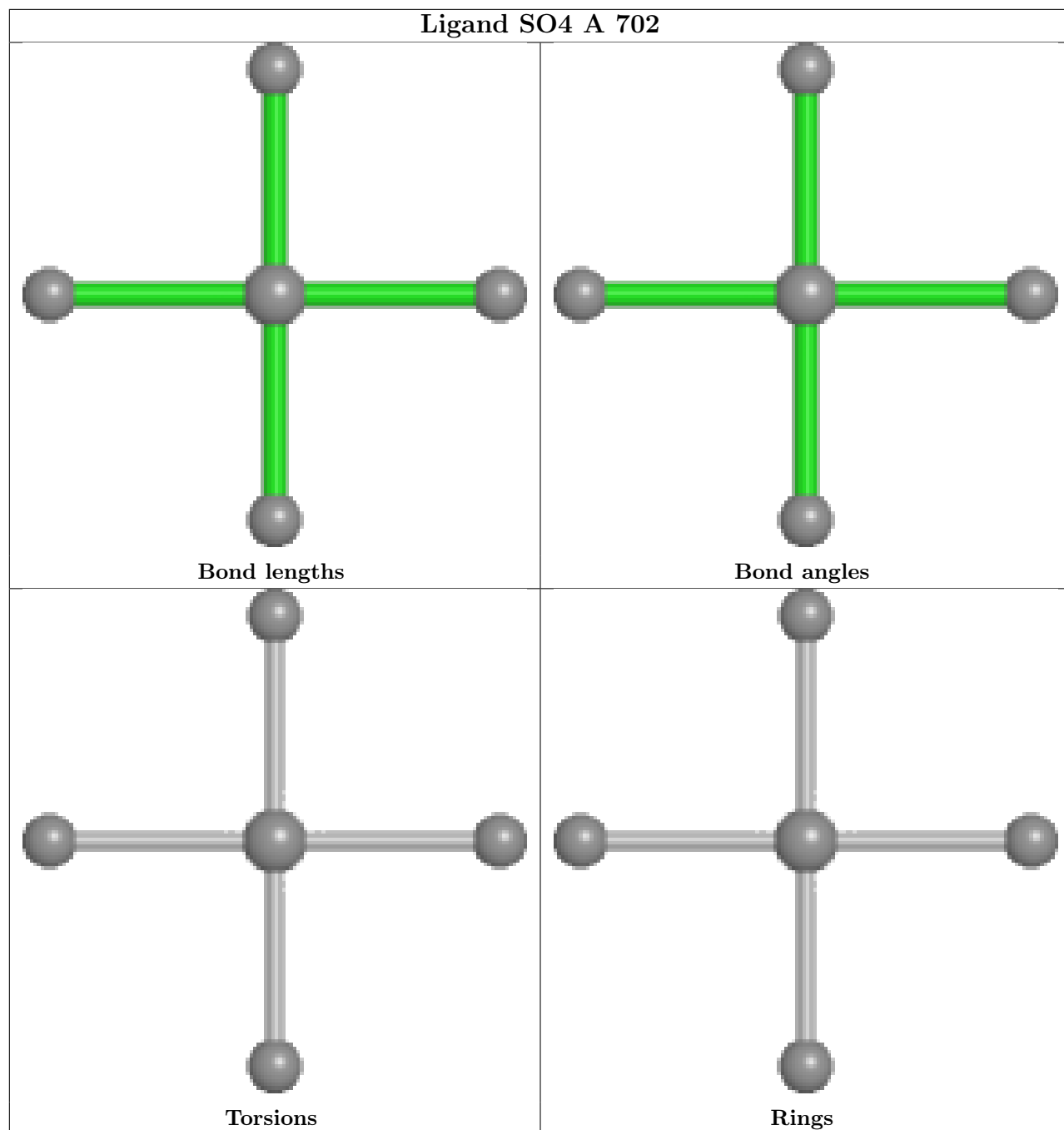
2 monomers are involved in 2 short contacts:

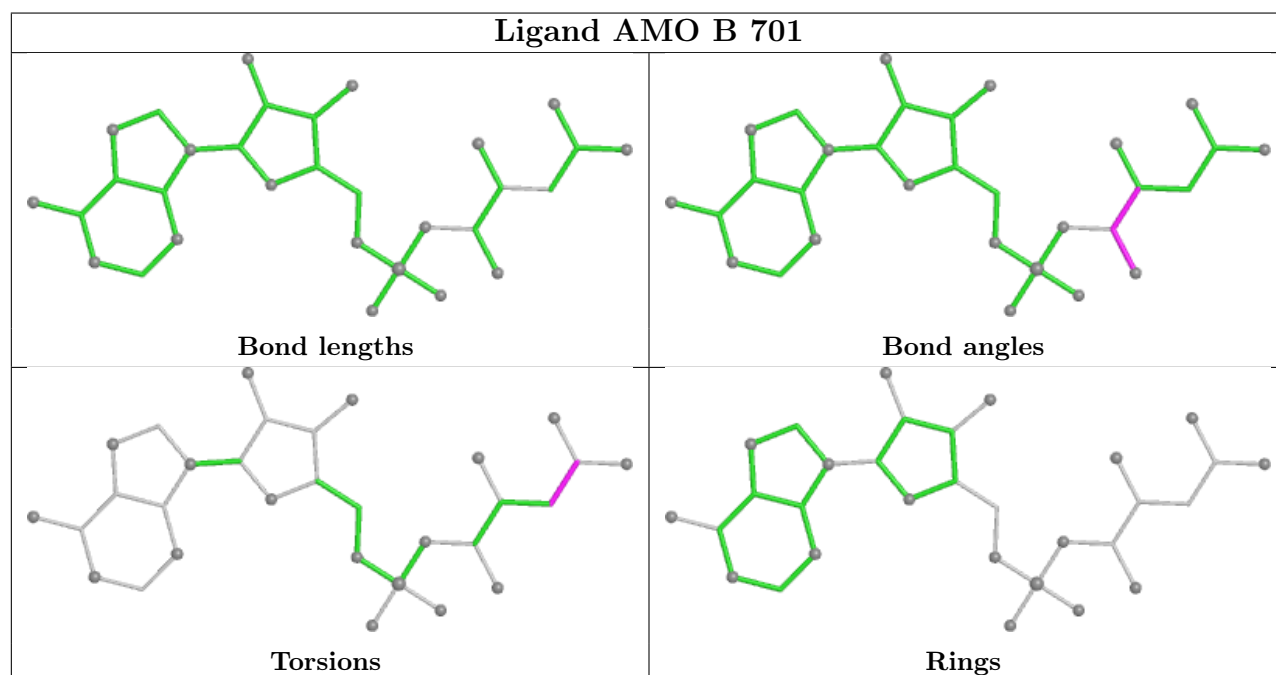
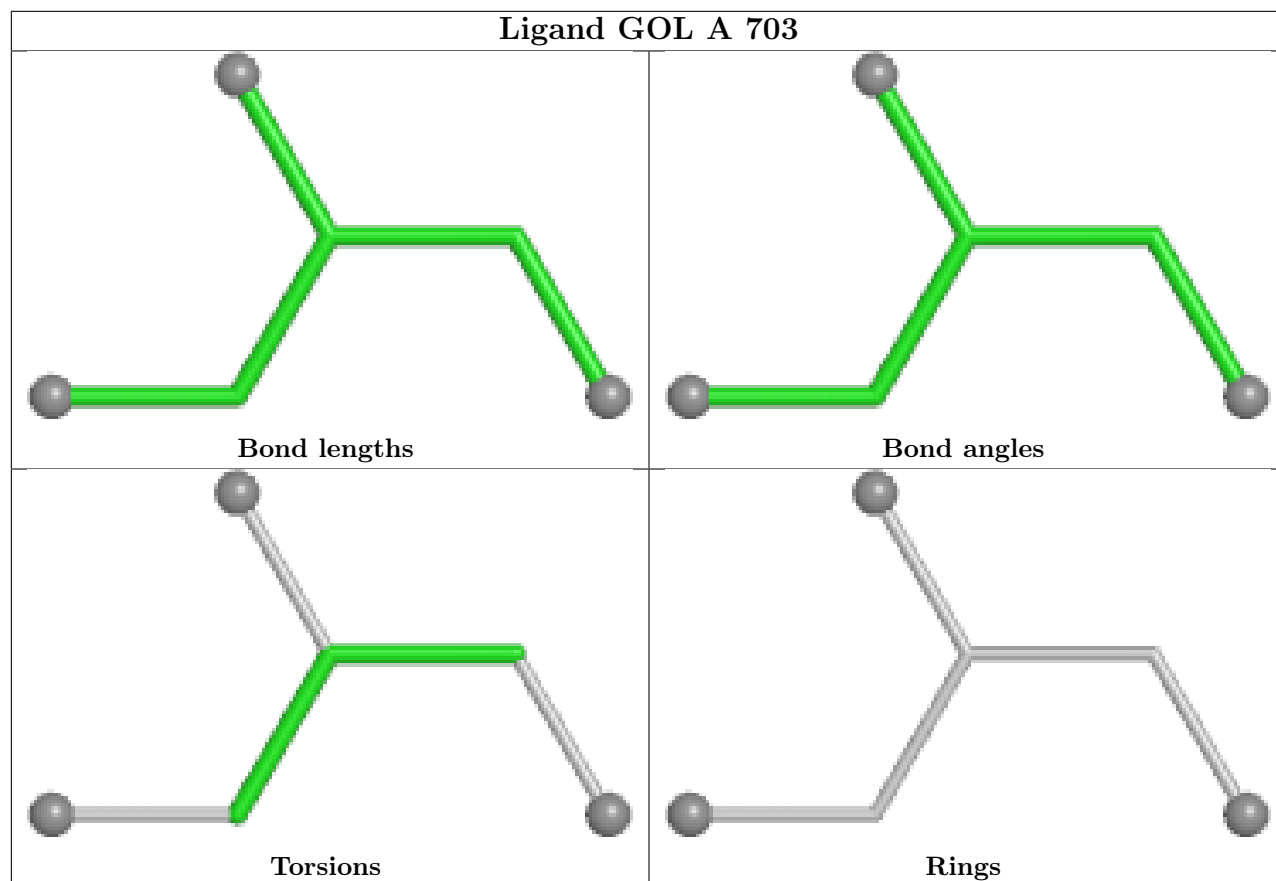
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	SO4	1	0
4	B	703	GOL	1	0

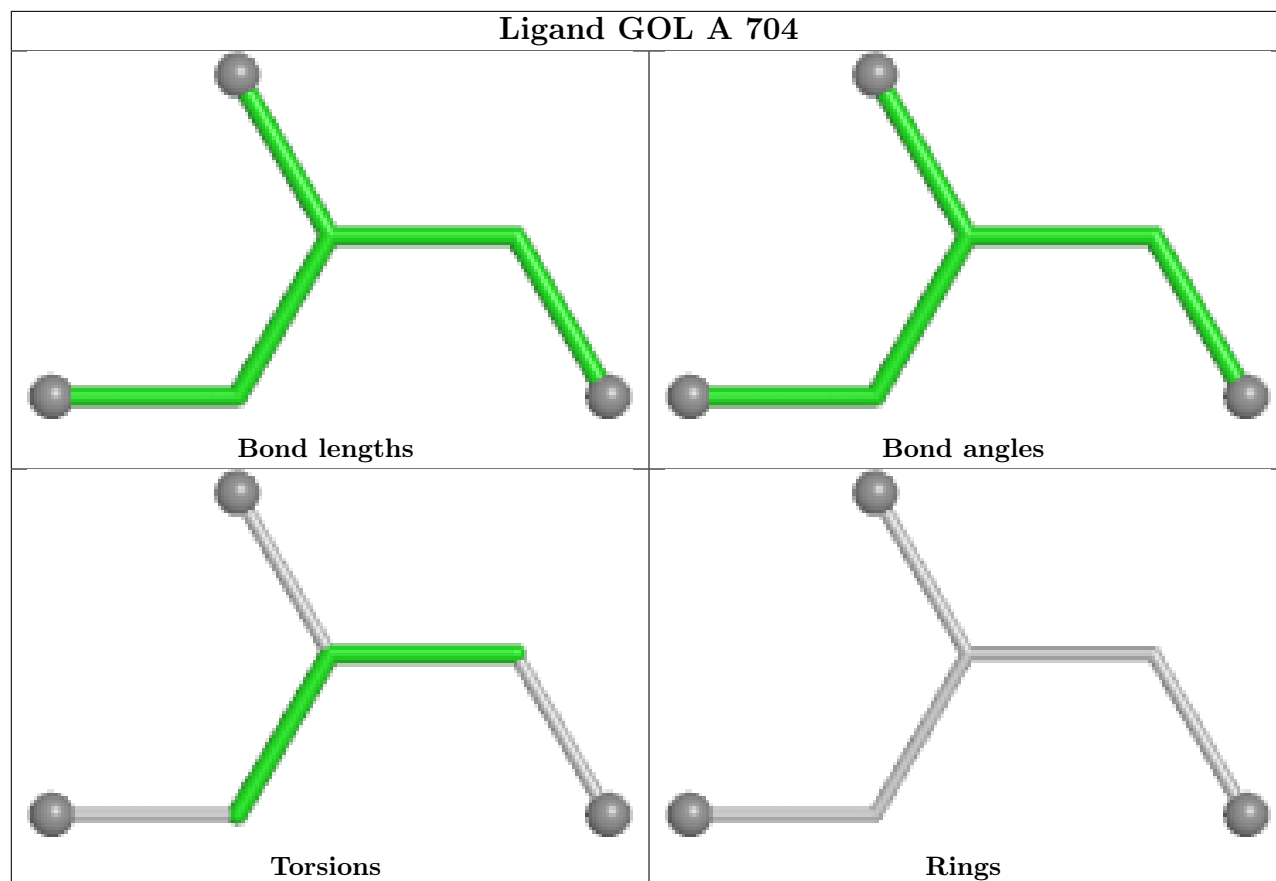
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	504/536 (94%)	0.31	36 (7%)	22	24	31, 57, 107, 144	3 (0%)
1	B	501/536 (93%)	0.44	51 (10%)	12	14	31, 57, 119, 156	2 (0%)
All	All	1005/1072 (93%)	0.38	87 (8%)	16	18	31, 57, 115, 156	5 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	ASN	7.0
1	B	132	ASN	6.5
1	B	253	ILE	6.3
1	A	179	HIS	6.1
1	B	101	LEU	6.1
1	A	362	TYR	5.8
1	A	360	ILE	4.9
1	B	100	ASN	4.5
1	B	353	GLY	4.5
1	B	217	ASP	4.3
1	B	220	HIS	4.3
1	A	350	SER	4.1
1	A	361	ASN	4.0
1	B	219	LYS	3.9
1	B	307	CYS	3.9
1	A	219	LYS	3.9
1	B	254	ASP	3.8
1	B	199	SER	3.8
1	A	98	ARG	3.8
1	A	494	LEU	3.8
1	B	185	ILE	3.8
1	A	490	GLU	3.6
1	B	179	HIS	3.6
1	A	352	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	354	GLY	3.6
1	B	180	LEU	3.6
1	A	290	ASN	3.6
1	B	130	LYS	3.6
1	A	222	ASP	3.5
1	B	250	GLU	3.5
1	B	255	SER	3.4
1	A	292	GLU	3.4
1	B	218	ILE	3.4
1	B	251	VAL	3.4
1	B	149	MET	3.4
1	B	105	ALA	3.3
1	A	291	GLU	3.3
1	B	135	GLU	3.3
1	B	200	LEU	3.3
1	B	128	LYS	3.2
1	A	493	ILE	3.2
1	B	360	ILE	3.1
1	A	351	SER	3.1
1	B	252	PRO	3.0
1	B	182	GLN	3.0
1	A	221	ASN	3.0
1	A	99	GLU	2.9
1	B	222	ASP	2.8
1	A	223	ASN	2.7
1	B	289	THR	2.7
1	B	352	GLU	2.7
1	B	129	MET	2.6
1	B	351	SER	2.6
1	B	136	ILE	2.5
1	B	198	GLY	2.5
1	B	385	PHE	2.5
1	A	101	LEU	2.5
1	A	584	PHE	2.4
1	A	286	MET	2.4
1	B	355	ALA	2.4
1	A	489	LYS	2.4
1	B	197	LYS	2.4
1	B	247	SER	2.4
1	A	251	VAL	2.4
1	A	293	GLY	2.3
1	B	131	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	180	LEU	2.3
1	A	583	ASN	2.3
1	B	215	ILE	2.3
1	B	330	LYS	2.3
1	A	289	THR	2.2
1	B	354	GLY	2.2
1	A	355	ALA	2.2
1	A	209	LEU	2.2
1	B	298	ASN	2.2
1	A	130	LYS	2.2
1	B	181	LEU	2.1
1	B	186	TRP	2.1
1	B	296	LYS	2.1
1	A	124	VAL	2.1
1	B	108	VAL	2.1
1	A	182	GLN	2.1
1	A	295	ILE	2.1
1	B	148	LEU	2.1
1	B	584	PHE	2.1
1	A	294	SER	2.0
1	B	292	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.

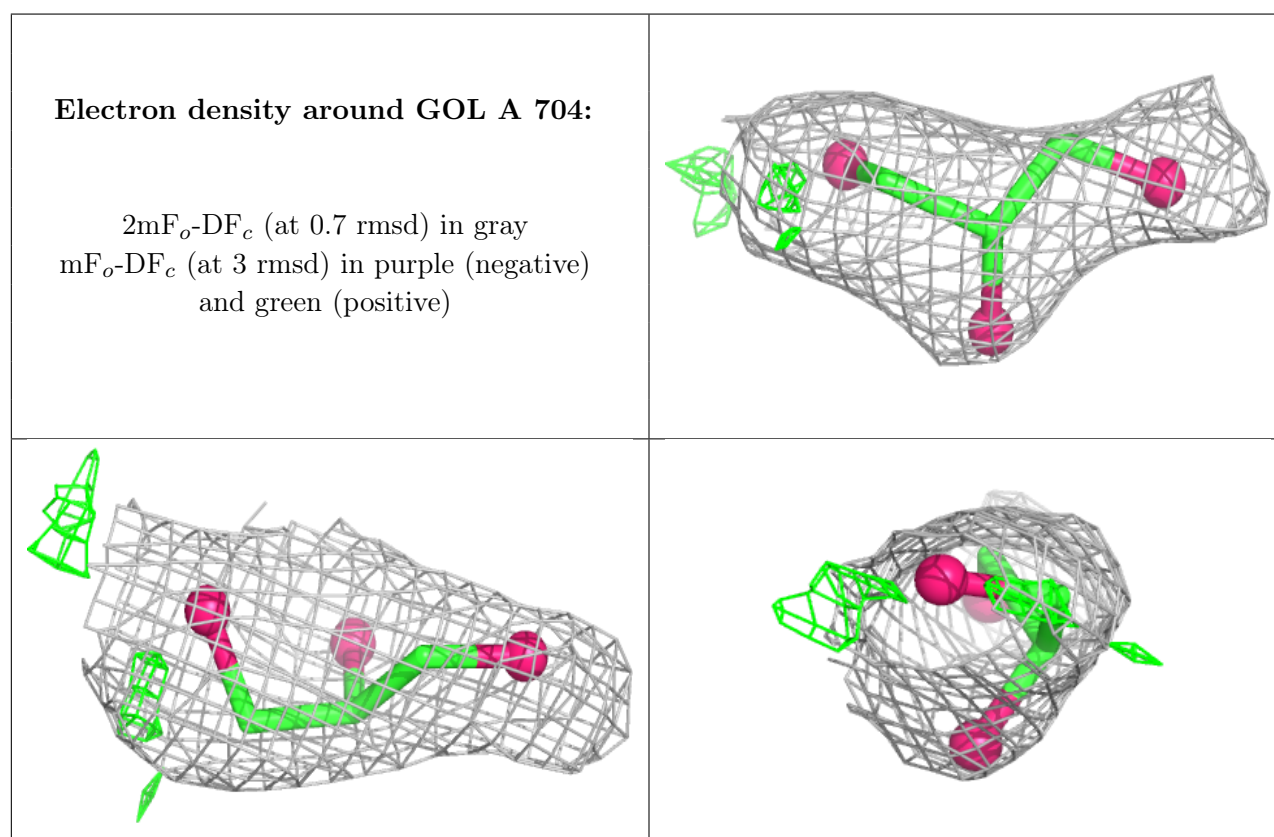
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	704	6/6	0.83	0.17	100,102,102,103	0
4	GOL	A	703	6/6	0.85	0.19	79,81,82,82	0

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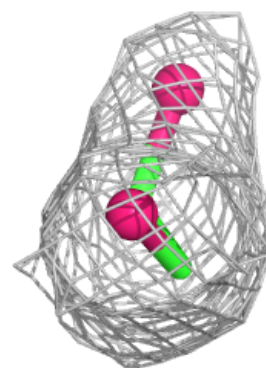
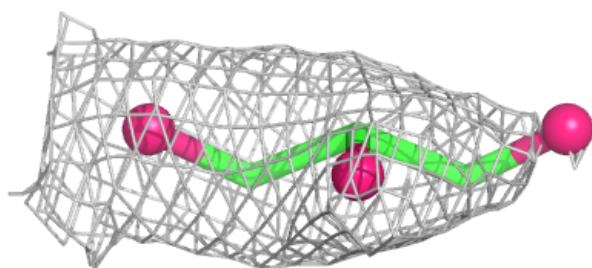
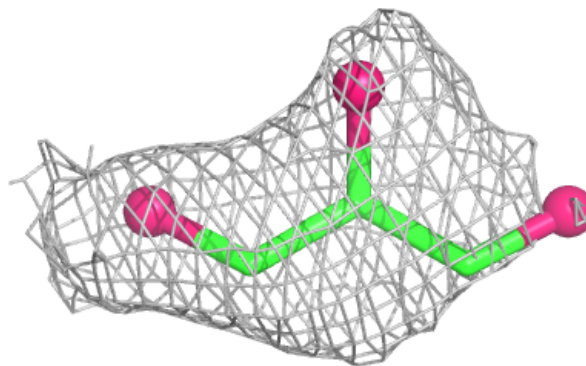
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	703	6/6	0.89	0.12	97,98,99,100	0
3	SO4	A	702	5/5	0.96	0.07	60,60,61,62	5
2	AMO	A	701	31/31	0.96	0.07	43,52,66,68	0
2	AMO	B	701	31/31	0.97	0.07	40,44,59,60	0
3	SO4	B	702	5/5	0.98	0.05	55,55,56,56	5

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.



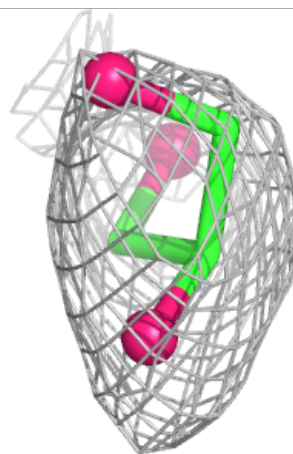
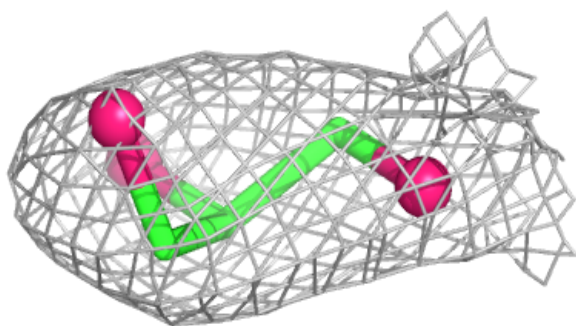
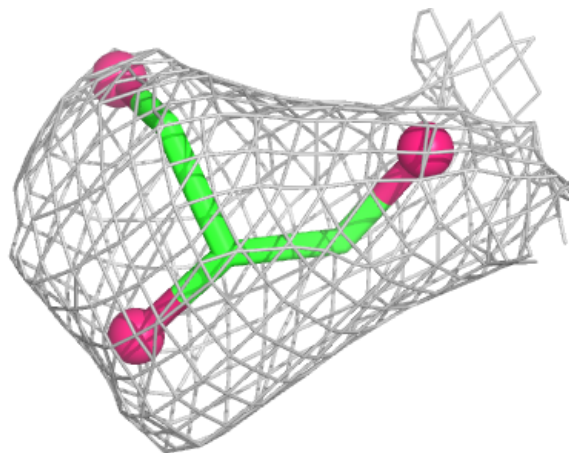
Electron density around GOL A 703:

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



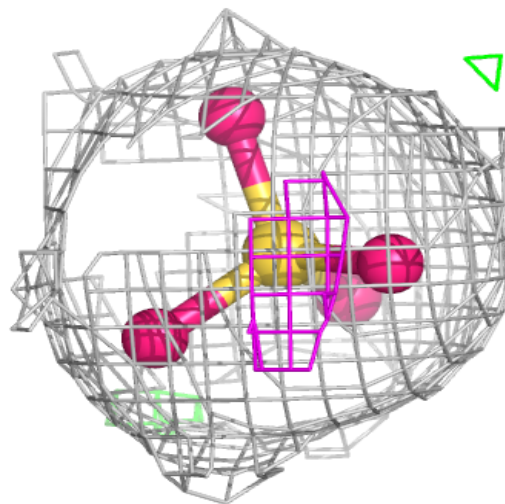
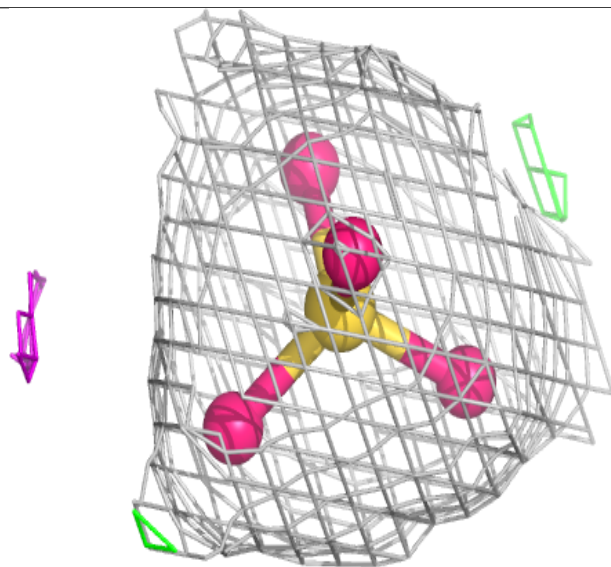
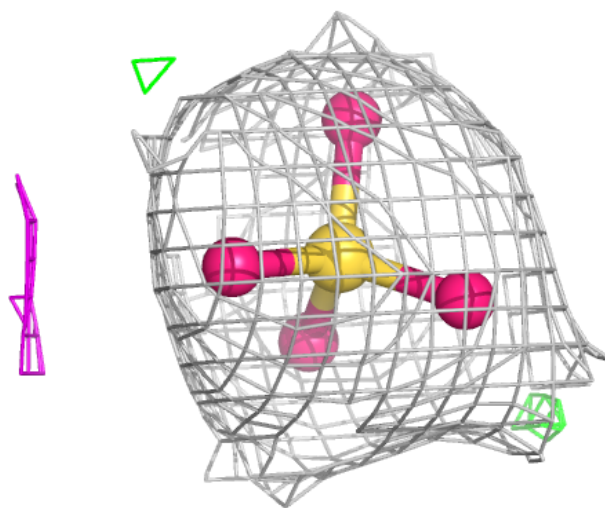
Electron density around GOL B 703:

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



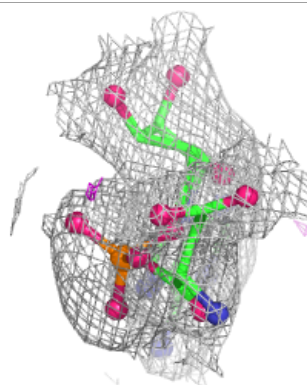
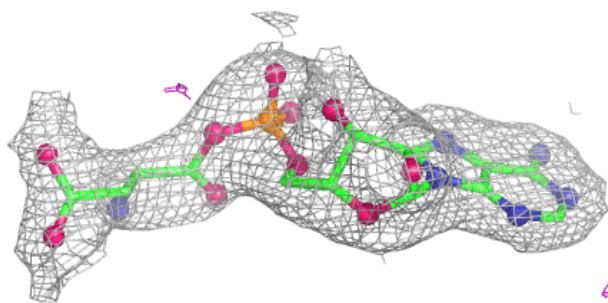
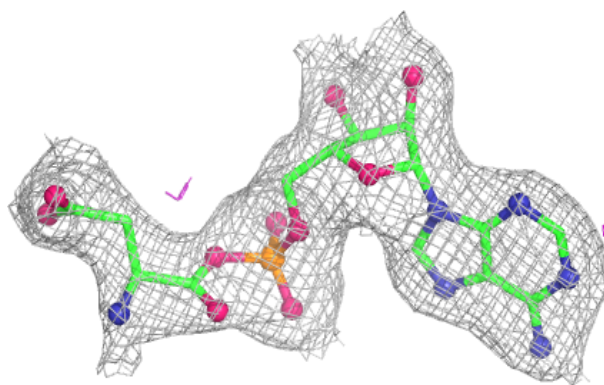
Electron density around SO4 A 702:

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

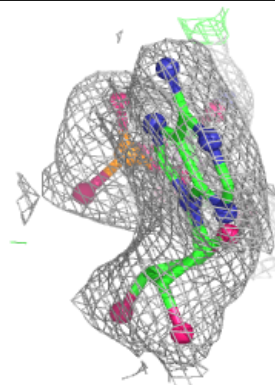
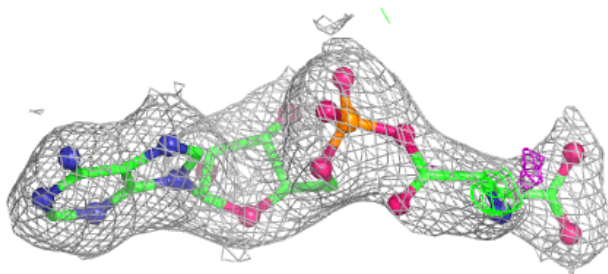
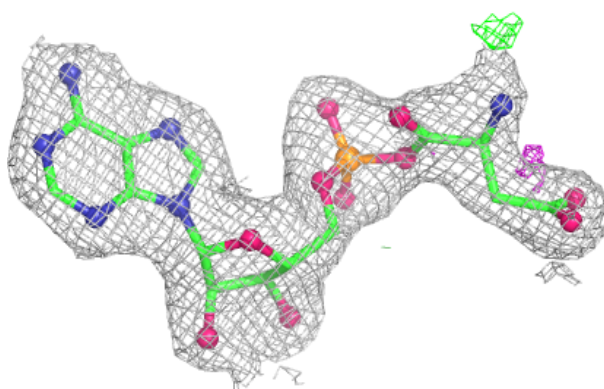


Electron density around AMO A 701:

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

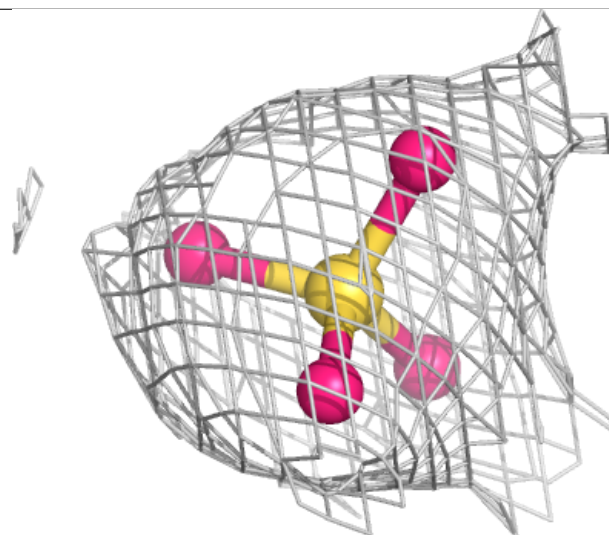
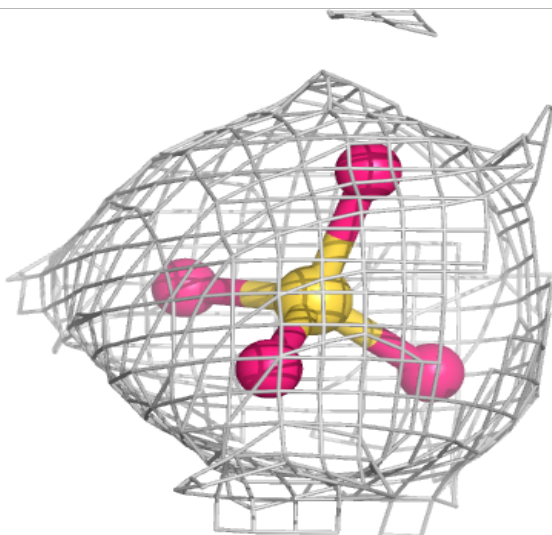
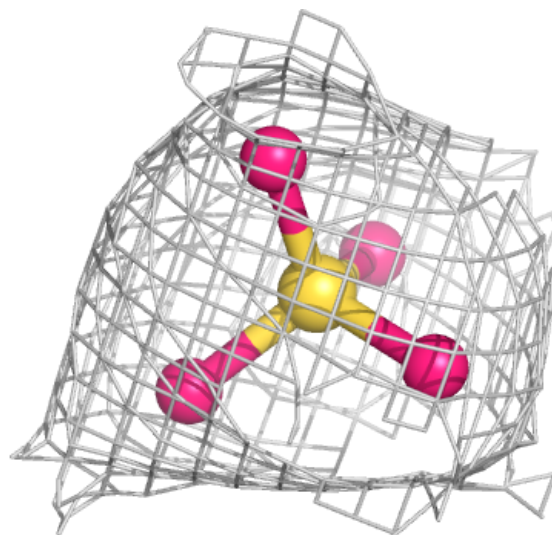
**Electron density around AMO B 701:**

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



Electron density around SO4 B 702:

$2mF_o-DF_c$ (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.