



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 11:35 AM EDT

PDB ID : 8BJI / pdb_00008bj
Title : chimera of ExoY Nucleotidyl Cyclase domain from *Vibrio nigrripulchritudo* fused to a proline-Rich-Domain (PRD) and profilin, bound to ADP-Mg-actin and a sulfate ion
Authors : Teixeira-Nunes, M.; Renault, L.; Retailleau, P.
Deposited on : 2022-11-04
Resolution : 1.75 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

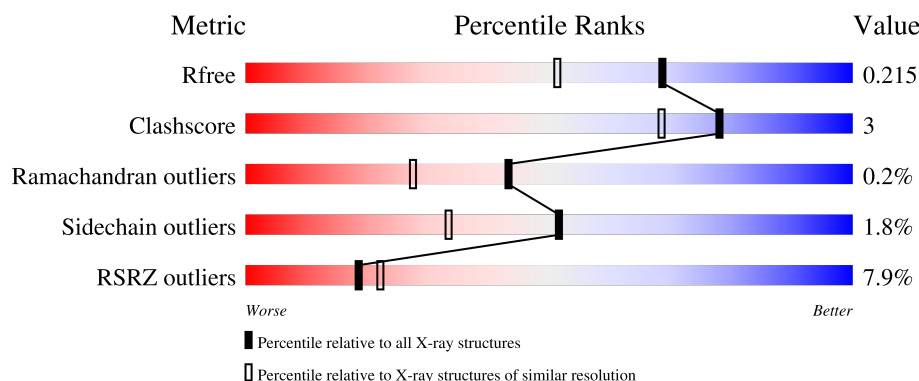
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

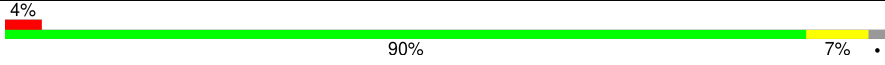
The reported resolution of this entry is 1.75 Å.

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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	375	
2	B	591	

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
7	PEG	A	407	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7926 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 Actin, alpha skeletal muscle, intermediate form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	9	0
			2925	1863	490	551	21			

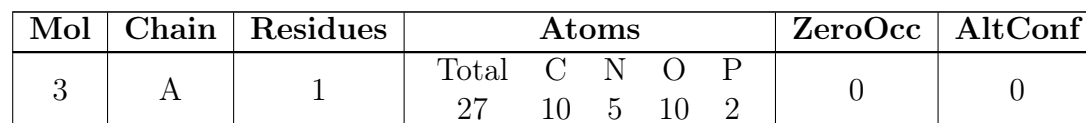
- Molecule 2 is a protein called Putative Adenylate cyclase, Profilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	498	Total	C	N	O	S	0	12	0
			3932	2486	661	770	15			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	451	GLY	-	expression tag	UNP A0A6N3LUE9
B	452	PRO	-	expression tag	UNP A0A6N3LUE9
B	453	GLY	-	expression tag	UNP A0A6N3LUE9
B	454	SER	-	expression tag	UNP A0A6N3LUE9
B	896	PRO	-	linker	UNP A0A6N3LUE9
B	897	PRO	-	linker	UNP A0A6N3LUE9
B	898	PRO	-	linker	UNP A0A6N3LUE9
B	899	PRO	-	linker	UNP A0A6N3LUE9
B	900	PRO	-	linker	UNP A0A6N3LUE9
B	901	GLY	-	linker	UNP A0A6N3LUE9
B	902	GLY	-	linker	UNP A0A6N3LUE9

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

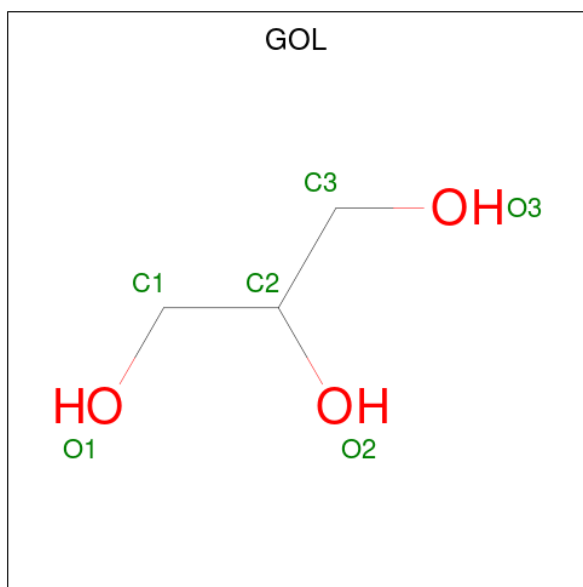


- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4 | A | 1 | Total Mg
1 1 | 0 | 0 |

-
- Chemical structure of TRS (2,3,4-trihydroxy-5-(iminomethyl)pentanoate) showing the following atoms and labels:
- Central carbon: C
 - Left carbon: C1
 - Right carbon: C2
 - Bottom carbon: C3
 - Top oxygen: O2
 - Bottom-left oxygen: O1
 - Bottom-right oxygen: O3
 - Right nitrogen: NH₃⁺N
- The structure is a 5-carbon chain with a central carbon (C) bonded to a left carbon (C1), a right carbon (C2), and a bottom carbon (C3). The left carbon (C1) is bonded to a top oxygen (O2) and a bottom-left oxygen (O1). The right carbon (C2) is bonded to a top oxygen (O2) and a bottom-right oxygen (O3). The bottom carbon (C3) is bonded to a right nitrogen (NH₃⁺N).

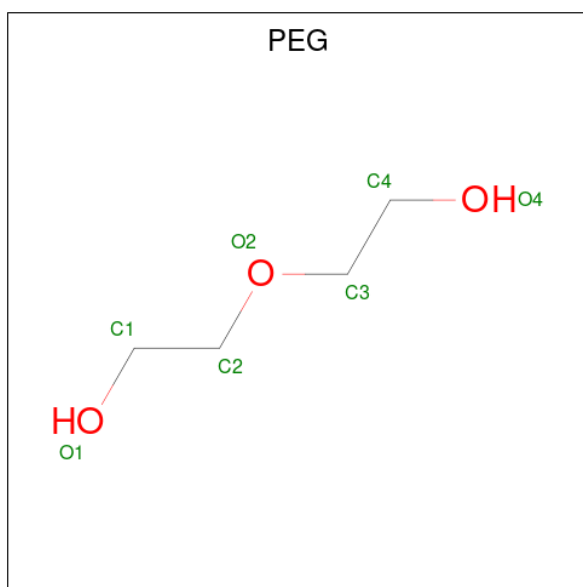
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



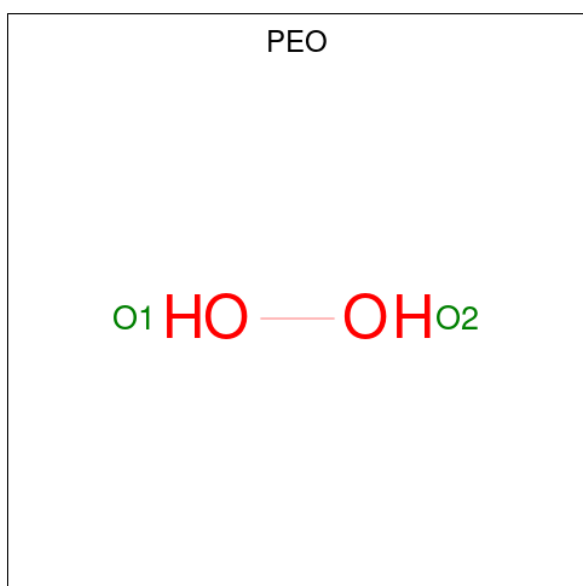
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



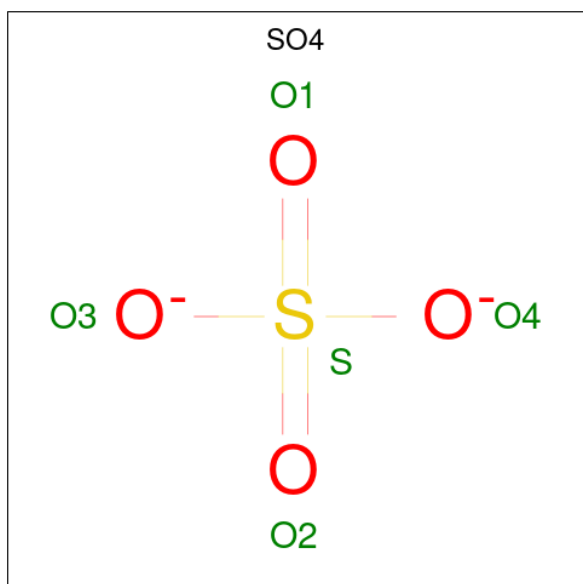
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			2	2		
8	A	1	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

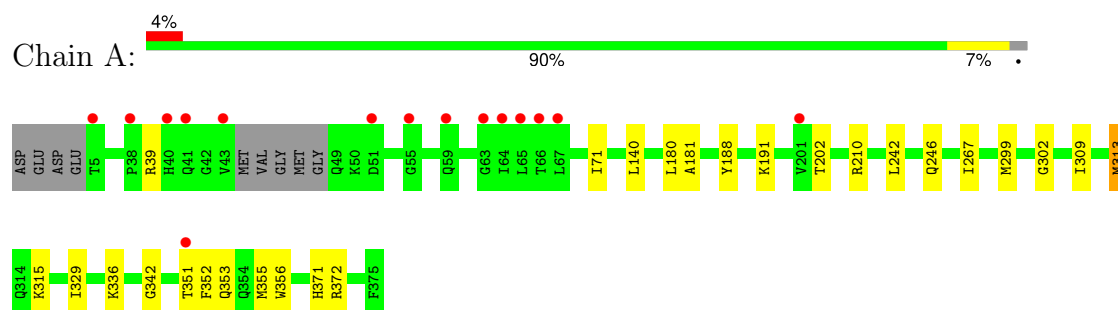
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	382	Total	O	0	0
			382	382		
10	B	562	Total	O	0	0
			562	562		

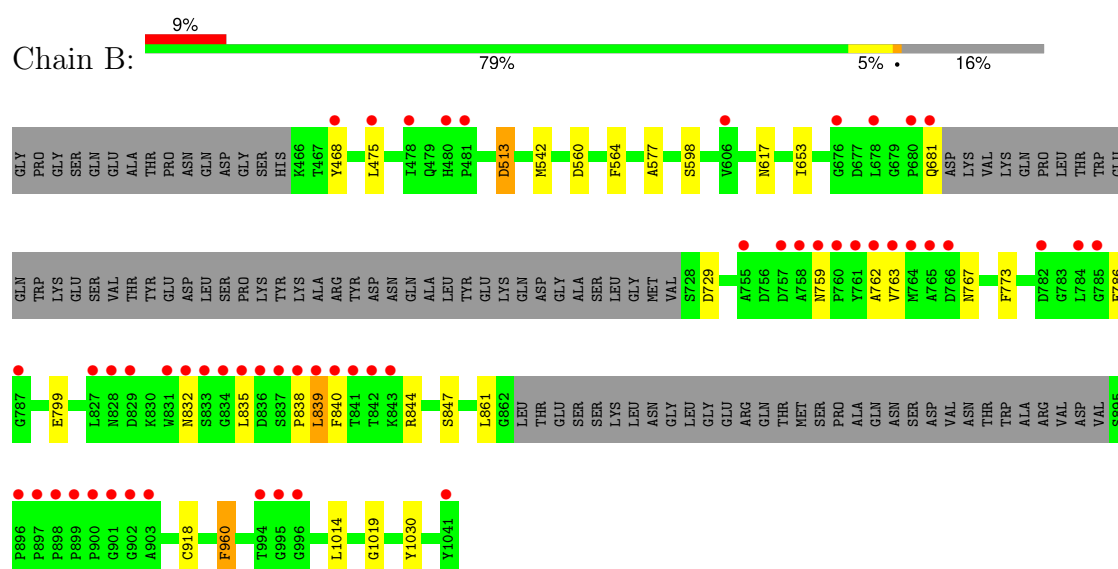
3 Residue-property plots [i](#)

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: Actin, alpha skeletal muscle, intermediate form



- Molecule 2: Putative Adenylate cyclase, Profilin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.97Å 62.85Å 93.59Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	25.06 – 1.75 25.06 – 1.75	Depositor EDS
% Data completeness (in resolution range)	85.4 (25.06-1.75) 85.4 (25.06-1.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.175 , 0.212 0.178 , 0.215	Depositor DCC
R_{free} test set	4141 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7926	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: PEO, GOL, PEG, MG, ADP, SO4, TRS

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	0.76	2/3017 (0.1%)	0.96	0/4085
2	B	0.67	1/4041 (0.0%)	0.93	4/5470 (0.1%)
All	All	0.71	3/7058 (0.0%)	0.94	4/9555 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	MET	SD-CE	-8.99	1.57	1.79
1	A	181	ALA	CA-C	6.38	1.59	1.53
2	B	762	ALA	CA-C	5.71	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	564	PHE	CA-CB-CG	-6.30	107.50	113.80
2	B	773	PHE	CA-CB-CG	-5.29	108.52	113.80
2	B	513	ASP	CA-CB-CG	5.13	117.73	112.60
2	B	960	PHE	CA-CB-CG	5.12	118.92	113.80

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	2925	0	2919	22	0
2	B	3932	0	3882	13	0
3	A	27	0	12	0	0
4	A	1	0	0	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
6	A	18	0	24	2	0
6	B	6	0	8	2	0
7	A	7	0	10	6	0
7	B	7	0	10	0	0
8	A	14	0	0	3	0
8	B	14	0	0	3	0
9	B	15	0	0	0	0
10	A	382	0	0	1	0
10	B	562	0	0	1	0
All	All	7926	0	6889	39	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 3.

All (39) 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)
8:B:1111:PEO:O1	8:B:1111:PEO:O2	1.56	1.24
8:A:412:PEO:O1	8:A:412:PEO:O2	1.53	1.21
8:B:1110:PEO:O1	8:B:1110:PEO:O2	1.54	1.21
8:B:1107:PEO:O2	8:B:1107:PEO:O1	1.55	1.21
8:A:414:PEO:O1	8:A:414:PEO:O2	1.59	1.17
8:A:410:PEO:O1	8:A:410:PEO:O2	1.63	1.17
1:A:267:ILE:HA	7:A:407:PEG:H41	1.53	0.88
1:A:202:THR:HB	6:A:406:GOL:H12	1.57	0.86
1:A:315:LYS:HD2	6:A:404:GOL:H2	1.64	0.78
1:A:188:TYR:HA	7:A:407:PEG:H22	1.68	0.74
2:B:799[A]:GLU:H	2:B:799[A]:GLU:CD	2.01	0.69
2:B:617:ASN:HB2	6:B:1106:GOL:H11	1.77	0.67
1:A:267:ILE:HA	7:A:407:PEG:C4	2.27	0.65
1:A:267:ILE:CA	7:A:407:PEG:H41	2.27	0.61
1:A:353:GLN:HA	1:A:356[B]:TRP:HD1	1.66	0.60
1:A:191:LYS:HD2	7:A:407:PEG:H21	1.86	0.57
1:A:353:GLN:HA	1:A:356[B]:TRP:CD1	2.39	0.57
2:B:839:LEU:HB2	2:B:844:ARG:HB3	1.86	0.56
2:B:598:SER:HB3	10:B:1312:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HH22	2:B:681:GLN:HB3	1.74	0.53
2:B:767:ASN:HB2	2:B:835:LEU:HD22	1.92	0.52
1:A:299[B]:MET:HE3	1:A:309:ILE:HG23	1.93	0.49
1:A:352[B]:PHE:HD1	1:A:355:MET:SD	2.34	0.49
1:A:242:LEU:HD12	1:A:246:GLN:CG	2.44	0.47
2:B:918:CYS:SG	2:B:1014:LEU:HG	2.55	0.46
1:A:140:LEU:O	1:A:342:GLY:HA3	2.17	0.45
2:B:617:ASN:HB2	6:B:1106:GOL:C1	2.45	0.45
1:A:299[B]:MET:HE1	1:A:313:MET:HG3	1.98	0.45
1:A:299[A]:MET:HE3	1:A:329:ILE:HG23	1.98	0.44
1:A:302:GLY:HA2	1:A:336:LYS:HG3	2.02	0.42
1:A:372[A]:ARG:HD3	2:B:1030:TYR:CG	2.55	0.42
2:B:838:PRO:HD2	2:B:840:PHE:CD2	2.55	0.42
1:A:242:LEU:HD12	1:A:246:GLN:HG2	2.02	0.42
1:A:352[B]:PHE:CD1	1:A:355:MET:SD	3.13	0.41
1:A:188:TYR:CA	7:A:407:PEG:H22	2.44	0.41
2:B:577:ALA:HB1	2:B:653:ILE:HG23	2.02	0.41
2:B:861:LEU:O	2:B:1019:GLY:HA2	2.21	0.41
2:B:468:TYR:HB3	2:B:475:LEU:HB2	2.03	0.40
1:A:371:HIS:HB2	10:A:510:HOH:O	2.21	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	371/375 (99%)	363 (98%)	8 (2%)	0	100	100
2	B	504/591 (85%)	480 (95%)	22 (4%)	2 (0%)	30	15
All	All	875/966 (91%)	843 (96%)	30 (3%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	763	VAL
2	B	759	ASN

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	320/318 (101%)	316 (99%)	4 (1%)	61	46
2	B	436/504 (86%)	427 (98%)	9 (2%)	47	27
All	All	756/822 (92%)	743 (98%)	13 (2%)	51	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	71	ILE
1	A	180	LEU
1	A	351	THR
2	B	513	ASP
2	B	542	MET
2	B	560	ASP
2	B	729	ASP
2	B	786	GLU
2	B	832	ASN
2	B	839	LEU
2	B	847	SER
2	B	960	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
2	B	620	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	$\# Z > 2$
9	SO4	B	1101	-	4,4,4	0.17	0	6,6,6	0.14	0
8	PEO	A	408	-	1,1,1	0.60	0	-		
8	PEO	A	412	-	1,1,1	0.75	0	-		
6	GOL	A	404	-	5,5,5	0.05	0	5,5,5	0.21	0
8	PEO	B	1113	-	1,1,1	0.34	0	-		
8	PEO	B	1111	-	1,1,1	0.95	0	-		
8	PEO	B	1107	-	1,1,1	0.92	0	-		
9	SO4	B	1103	-	4,4,4	0.38	0	6,6,6	0.30	0
5	TRS	A	403	-	7,7,7	0.21	0	9,9,9	0.37	0
8	PEO	A	410	-	1,1,1	1.45	0	-		
8	PEO	B	1110	-	1,1,1	0.85	0	-		
6	GOL	A	405	-	5,5,5	0.10	0	5,5,5	0.25	0
5	TRS	B	1104	-	7,7,7	0.18	0	9,9,9	0.23	0
8	PEO	A	414	-	1,1,1	1.16	0	-		
8	PEO	B	1108	-	1,1,1	0.64	0	-		
8	PEO	A	411	-	1,1,1	0.28	0	-		
3	ADP	A	401	4	28,29,29	0.29	0	43,45,45	0.54	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEG	A	407	-	6,6,6	0.19	0	5,5,5	0.10	0
6	GOL	B	1106	-	5,5,5	0.07	0	5,5,5	0.19	0
9	SO4	B	1102	-	4,4,4	0.26	0	6,6,6	0.18	0
8	PEO	A	413	-	1,1,1	0.46	0	-		
8	PEO	B	1109	-	1,1,1	0.43	0	-		
8	PEO	B	1112	-	1,1,1	0.60	0	-		
7	PEG	B	1105	-	6,6,6	0.13	0	5,5,5	0.12	0
6	GOL	A	406	-	5,5,5	0.05	0	5,5,5	0.21	0
8	PEO	A	409	-	1,1,1	0.49	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
6	GOL	A	406	-	-	1/4/4/4	-
5	TRS	B	1104	-	-	0/9/9/9	-
7	PEG	B	1105	-	-	0/4/4/4	-
6	GOL	A	404	-	-	2/4/4/4	-
3	ADP	A	401	4	-	0/16/32/32	0/3/3/3
7	PEG	A	407	-	-	2/4/4/4	-
6	GOL	B	1106	-	-	0/4/4/4	-
6	GOL	A	405	-	-	2/4/4/4	-
5	TRS	A	403	-	-	1/9/9/9	-

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	ADP	O2A-PA-O3A	2.08	112.90	107.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	405	GOL	O1-C1-C2-C3
7	A	407	PEG	O1-C1-C2-O2
6	A	404	GOL	O1-C1-C2-C3
6	A	405	GOL	O1-C1-C2-O2

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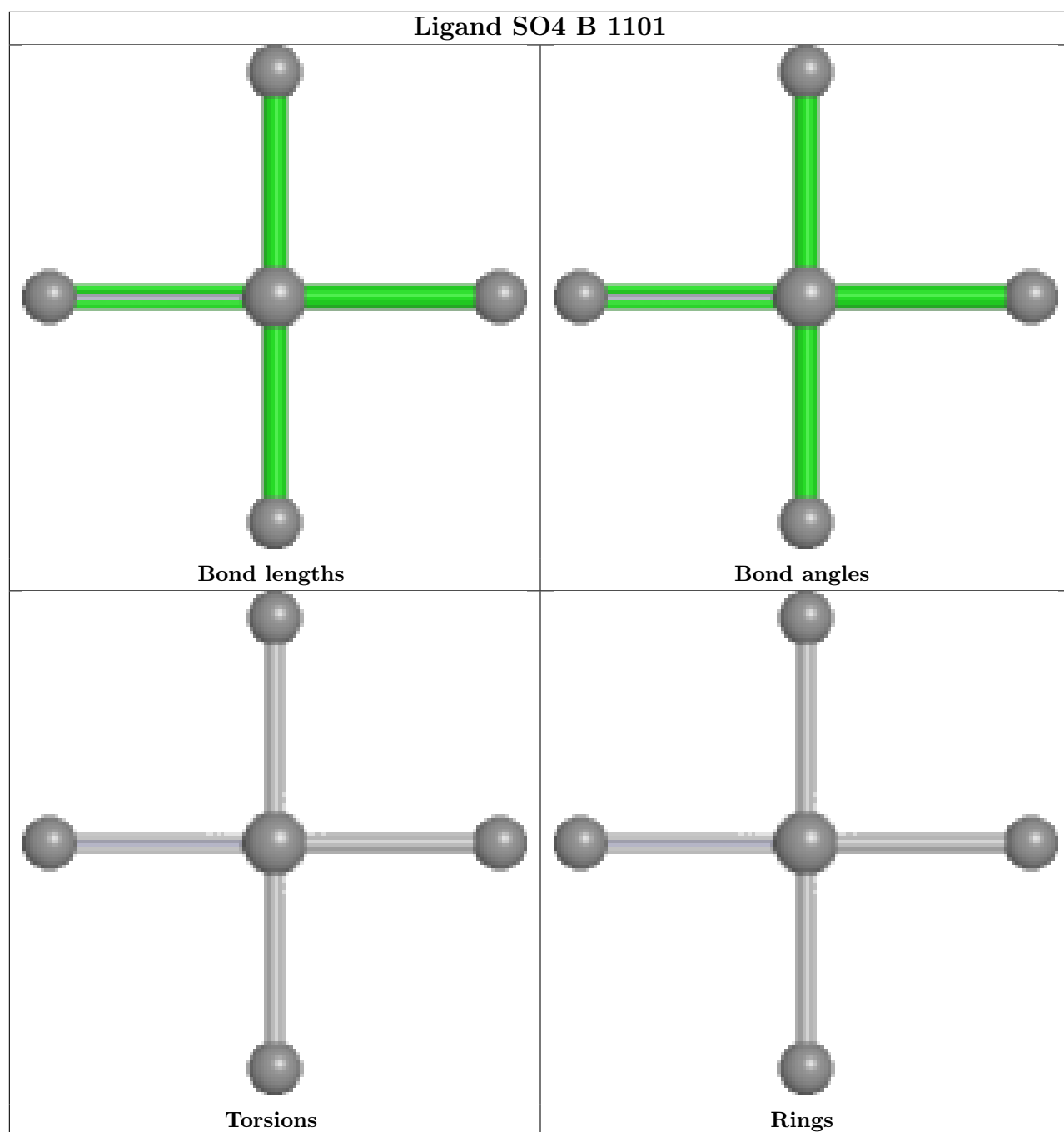
Mol	Chain	Res	Type	Atoms
6	A	404	GOL	O1-C1-C2-O2
6	A	406	GOL	O1-C1-C2-C3
7	A	407	PEG	C4-C3-O2-C2
5	A	403	TRS	C3-C-C1-O1

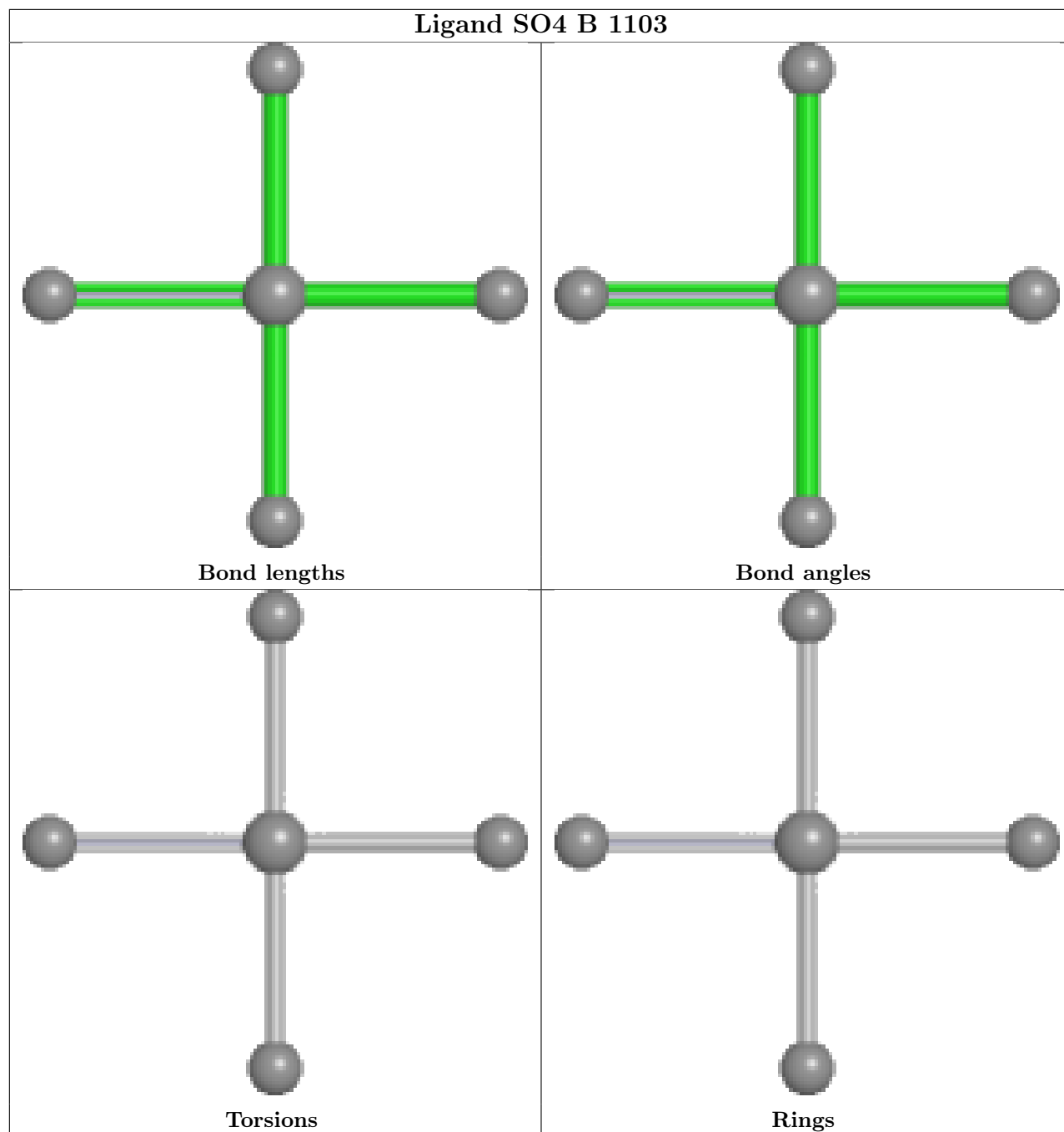
There are no ring outliers.

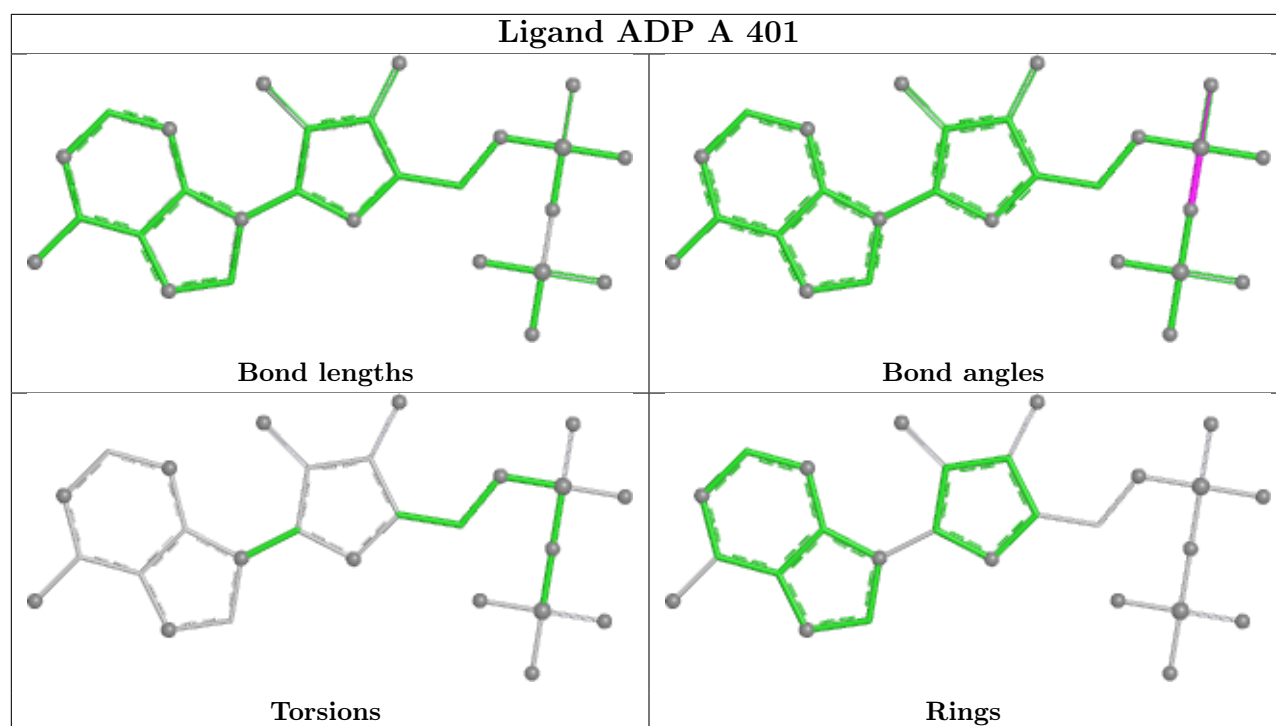
10 monomers are involved in 16 short contacts:

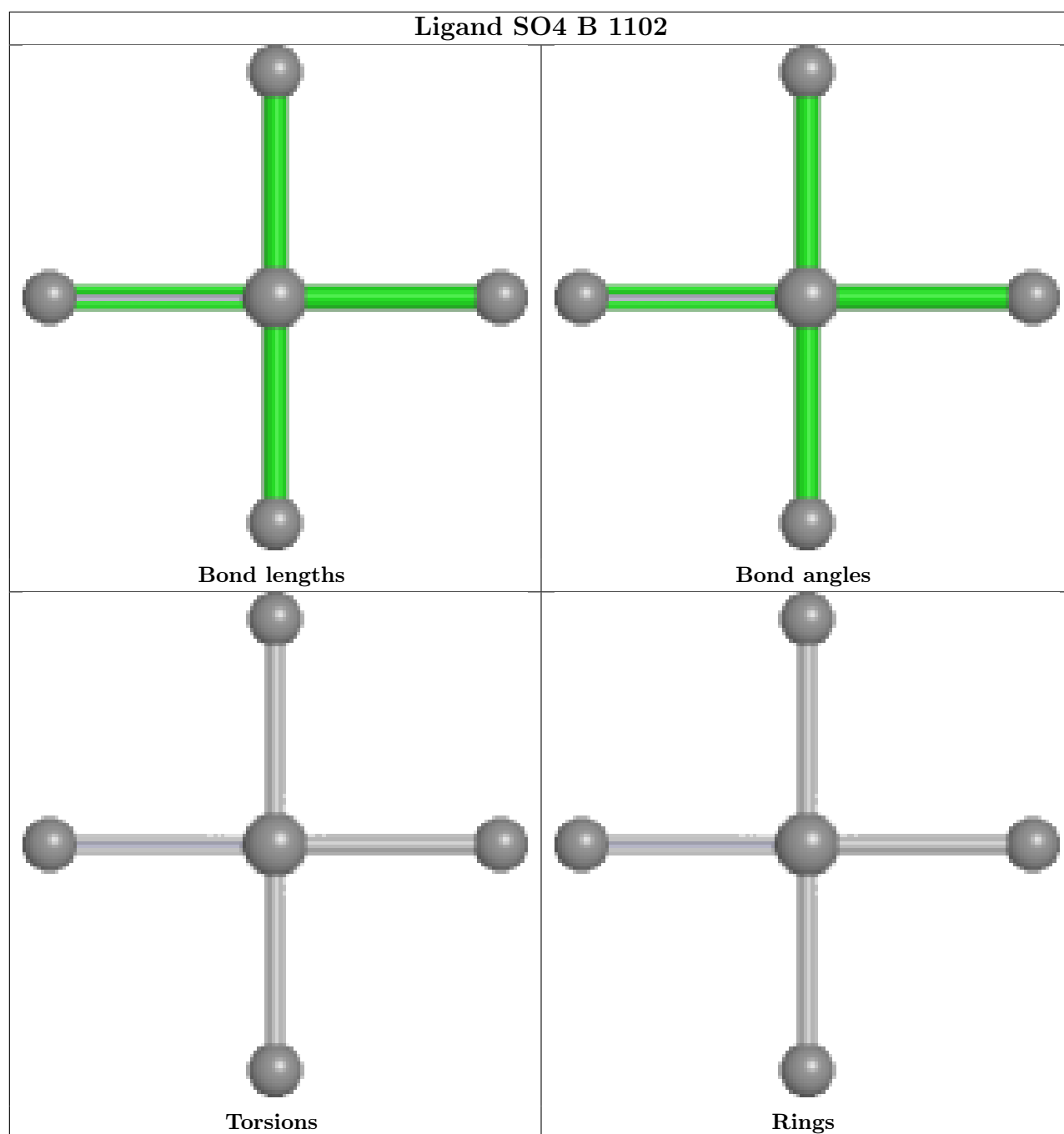
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	412	PEO	1	0
6	A	404	GOL	1	0
8	B	1111	PEO	1	0
8	B	1107	PEO	1	0
8	A	410	PEO	1	0
8	B	1110	PEO	1	0
8	A	414	PEO	1	0
7	A	407	PEG	6	0
6	B	1106	GOL	2	0
6	A	406	GOL	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	366/375 (97%)	-0.07	15 (4%)	41 47	11, 21, 45, 76	9 (2%)
2	B	498/591 (84%)	0.39	53 (10%)	11 13	10, 26, 69, 87	12 (2%)
All	All	864/966 (89%)	0.19	68 (7%)	18 22	10, 24, 63, 87	21 (2%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	835	LEU	8.2
2	B	763	VAL	7.6
2	B	839	LEU	6.6
1	A	43	VAL	6.3
2	B	838	PRO	6.0
2	B	836	ASP	5.6
2	B	762	ALA	5.0
2	B	760	PRO	4.8
2	B	761	TYR	4.7
2	B	827	LEU	4.7
2	B	785	GLY	4.7
2	B	995	GLY	4.6
2	B	840	PHE	4.6
2	B	480[A]	HIS	4.3
2	B	842	THR	4.1
2	B	765	ALA	3.9
2	B	902	GLY	3.9
2	B	903	ALA	3.8
2	B	759	ASN	3.8
2	B	831	TRP	3.8
2	B	837	SER	3.8
1	A	64	ILE	3.6
2	B	897	PRO	3.6
2	B	901	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	787	GLY	3.5
2	B	680	PRO	3.4
2	B	757	ASP	3.3
2	B	994	THR	3.2
2	B	834	GLY	3.2
2	B	764	MET	3.2
1	A	5	THR	3.1
2	B	841	THR	2.9
2	B	996	GLY	2.9
2	B	481	PRO	2.9
2	B	758	ALA	2.8
2	B	900	PRO	2.8
1	A	63	GLY	2.8
1	A	51	ASP	2.8
2	B	896	PRO	2.7
1	A	67	LEU	2.7
1	A	38	PRO	2.7
1	A	59[A]	GLN	2.6
2	B	678	LEU	2.6
2	B	676	GLY	2.5
2	B	681	GLN	2.5
1	A	351	THR	2.5
1	A	41	GLN	2.5
2	B	784	LEU	2.5
2	B	829	ASP	2.5
2	B	899	PRO	2.5
1	A	66	THR	2.4
2	B	468	TYR	2.4
1	A	65	LEU	2.4
1	A	40	HIS	2.4
2	B	832	ASN	2.3
2	B	833	SER	2.3
2	B	898	PRO	2.2
2	B	828	ASN	2.2
2	B	843	LYS	2.2
2	B	478	ILE	2.2
2	B	755	ALA	2.2
2	B	1041	TYR	2.2
2	B	606	VAL	2.1
1	A	55	GLY	2.1
1	A	201	VAL	2.1
2	B	766	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	782	ASP	2.1
2	B	475	LEU	2.1

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
8	PEO	B	1113	2/2	0.55	0.23	52,52,52,52	0
6	GOL	A	406	6/6	0.63	0.20	64,64,64,64	0
6	GOL	A	405	6/6	0.72	0.17	47,48,48,48	0
8	PEO	B	1108	2/2	0.76	0.17	50,50,50,50	0
8	PEO	B	1109	2/2	0.76	0.18	47,47,47,47	0
8	PEO	A	411	2/2	0.76	0.24	47,47,47,47	0
6	GOL	B	1106	6/6	0.78	0.16	50,50,50,50	0
8	PEO	A	414	2/2	0.79	0.29	42,42,42,42	0
7	PEG	B	1105	7/7	0.79	0.13	68,68,68,68	0
6	GOL	A	404	6/6	0.80	0.13	62,62,63,63	0
7	PEG	A	407	7/7	0.80	0.14	41,41,42,42	0
9	SO4	B	1102	5/5	0.80	0.13	76,76,76,76	0
8	PEO	A	413	2/2	0.81	0.24	56,56,56,56	0
8	PEO	B	1112	2/2	0.81	0.20	49,49,49,49	0
8	PEO	A	412	2/2	0.82	0.12	49,49,49,50	0
8	PEO	A	408	2/2	0.82	0.11	54,54,54,54	0
8	PEO	B	1111	2/2	0.85	0.16	41,41,41,42	0
8	PEO	A	410	2/2	0.86	0.21	38,38,38,38	0
8	PEO	B	1110	2/2	0.86	0.16	41,41,41,41	0
8	PEO	A	409	2/2	0.89	0.12	47,47,47,47	0
8	PEO	B	1107	2/2	0.90	0.20	36,36,36,36	0

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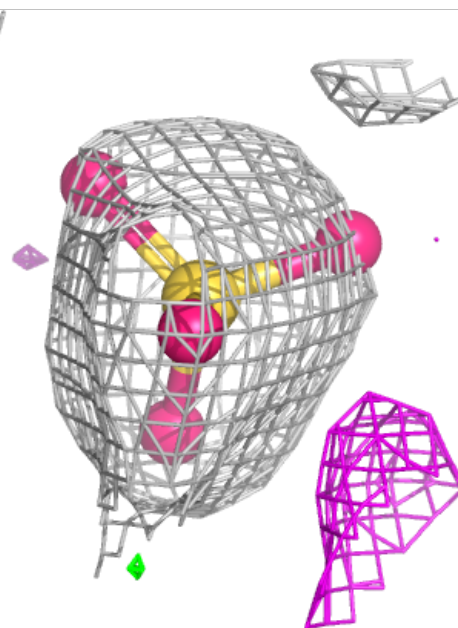
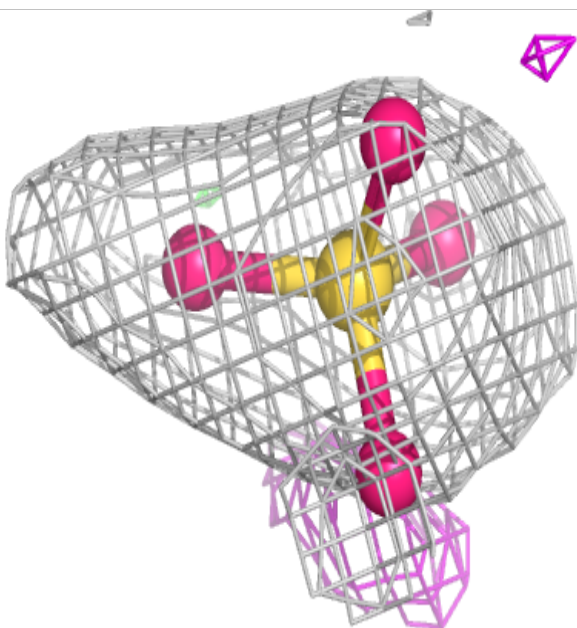
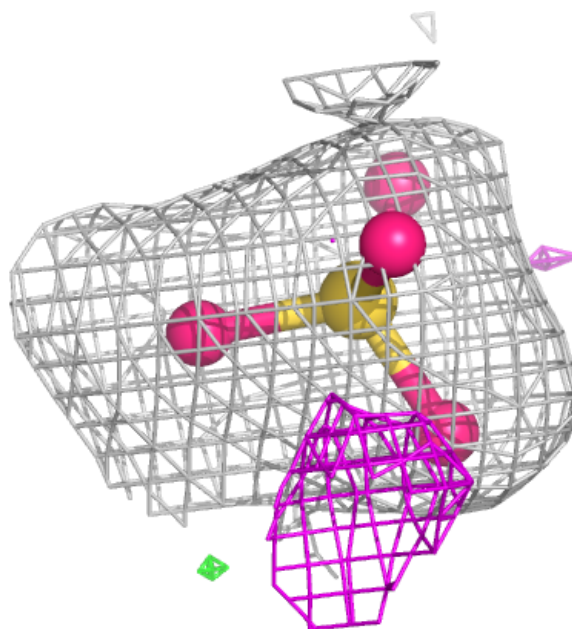
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TRS	A	403	8/8	0.91	0.08	31,32,32,33	0
5	TRS	B	1104	8/8	0.92	0.08	28,29,29,29	0
9	SO4	B	1101	5/5	0.93	0.08	59,60,60,60	0
9	SO4	B	1103	5/5	0.97	0.11	30,30,30,30	0
4	MG	A	402	1/1	0.99	0.05	18,18,18,18	0
3	ADP	A	401	27/27	0.99	0.04	15,17,18,19	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.

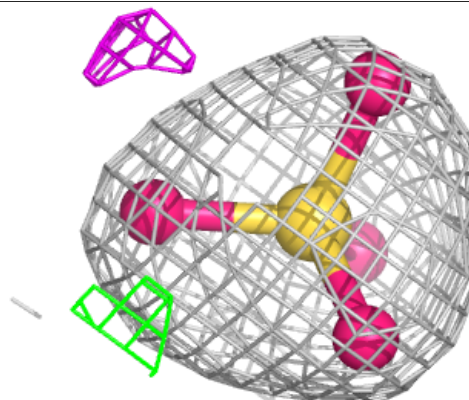
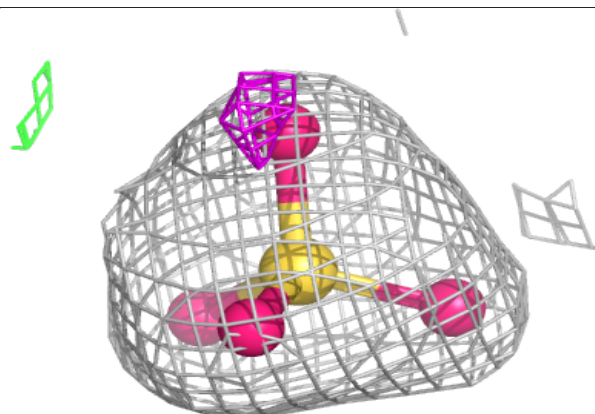
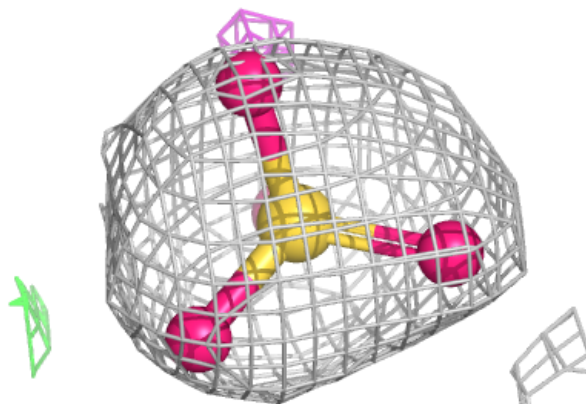
Electron density around SO4 B 1102:

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



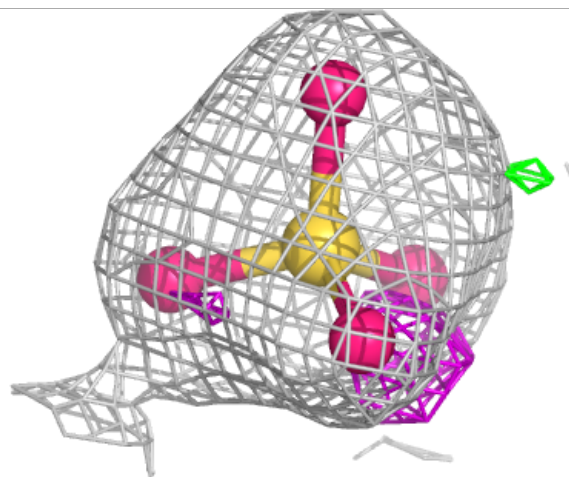
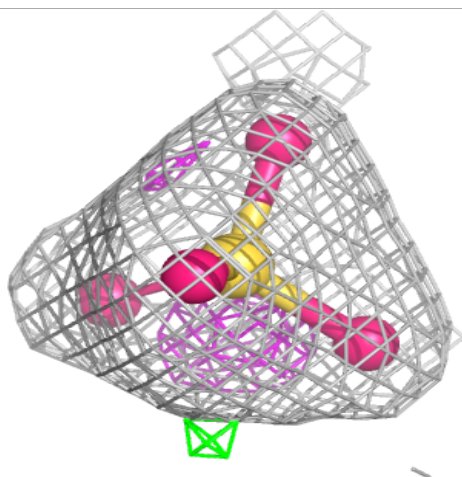
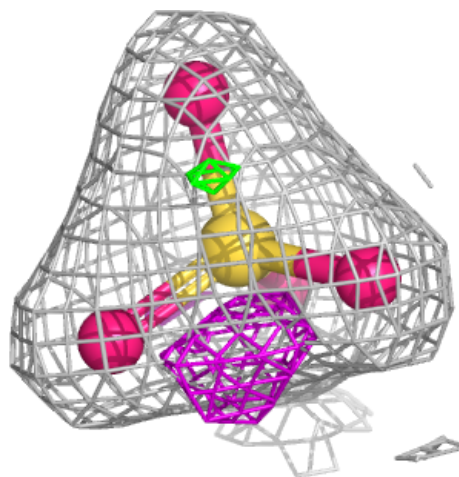
Electron density around SO4 B 1101:

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



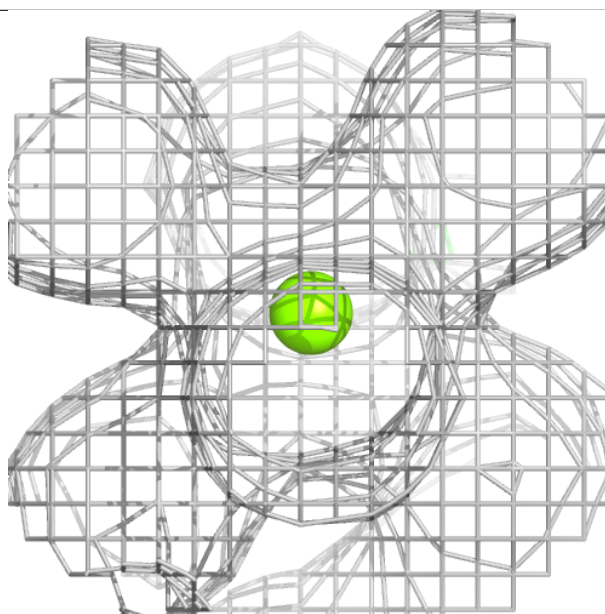
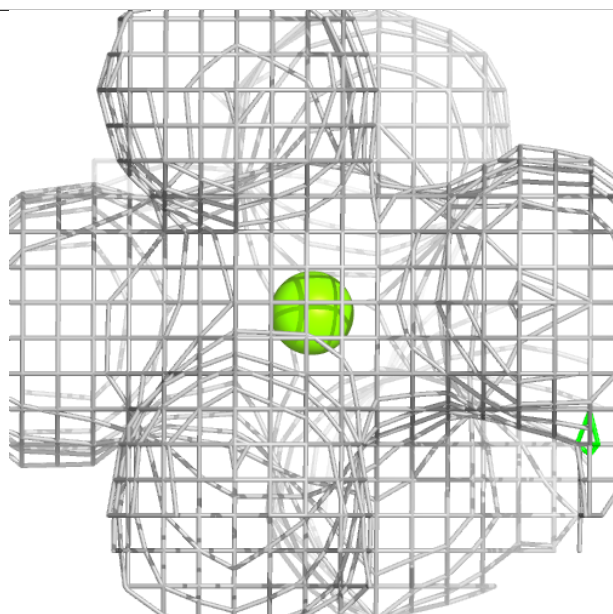
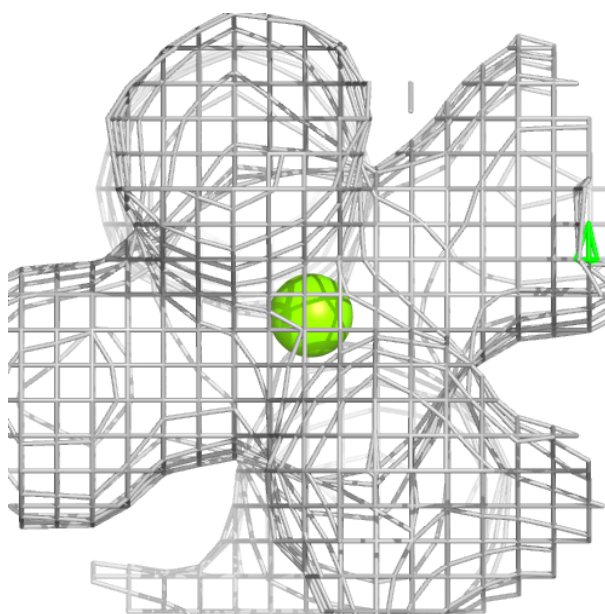
Electron density around SO4 B 1103:

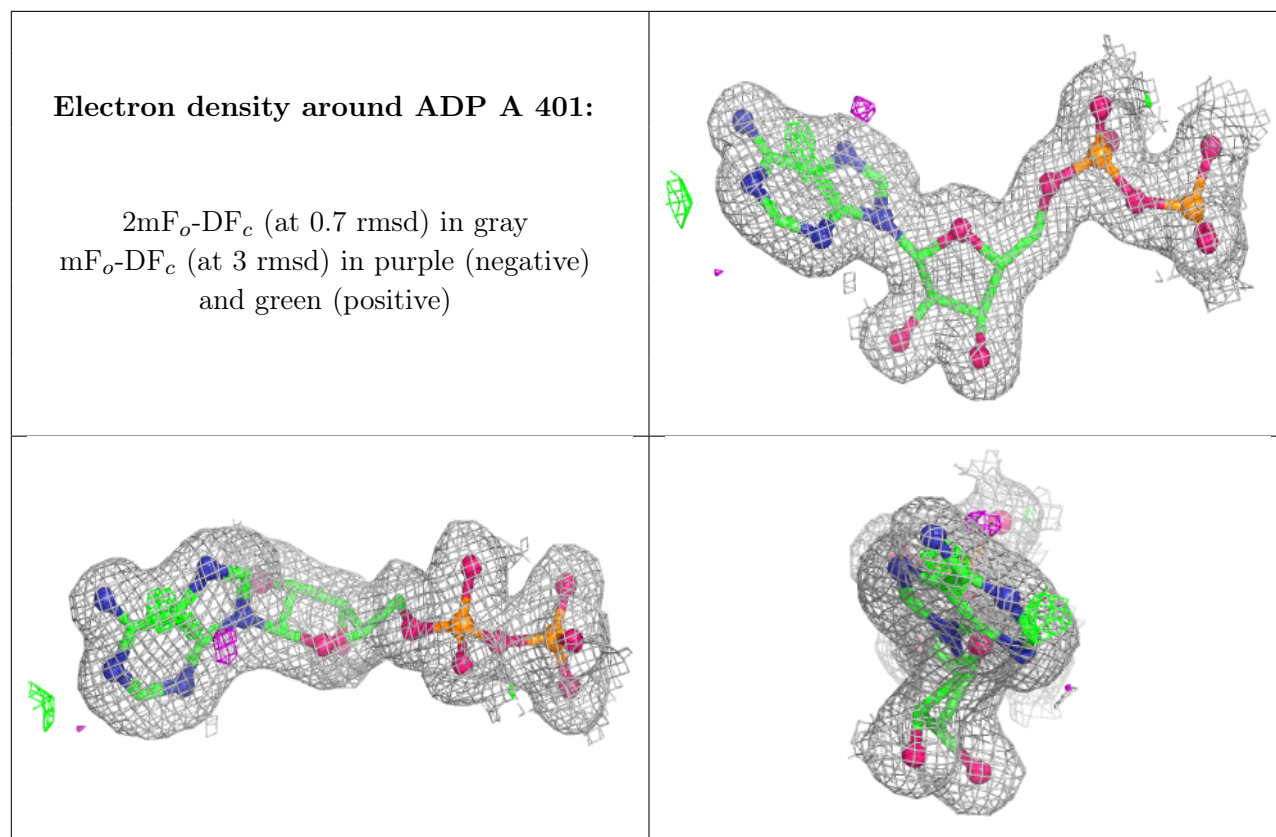
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 402:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.