WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2020 – 09:21 AM BST

PDB ID	:	6TZL
Title	:	The structure of the Streptococcus gordonii surface protein SspB in complex with TEV peptide provides clues to the adherence of oral streptococcal adherence to salivary agglutinin
Authors	:	Schormann, N.; Deivanayagam, C.
Deposited on	:	2019-08-12
Resolution	:	1.60 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.13
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)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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.
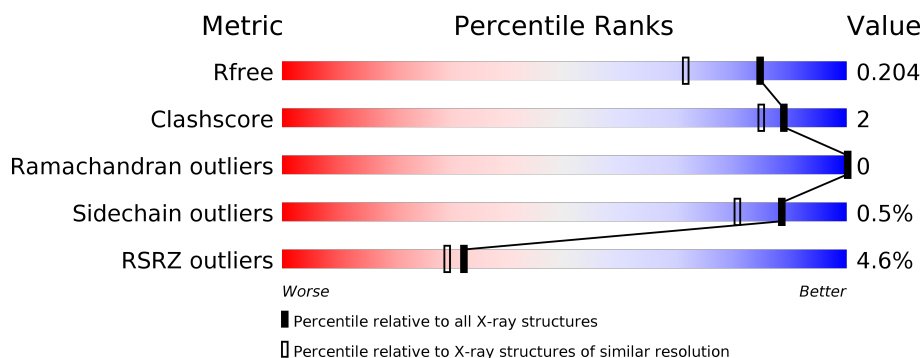
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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 <=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	425	4% / 88% / • / 9%
1	B	425	4% / 85% / 5% / 10%
1	C	425	4% / 92% / • / 5%
1	D	425	5% / 89% / • / 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14201 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 Surface protein adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	4	0
			3023	1900	501	614	8			
1	B	384	Total	C	N	O	S	0	6	0
			3007	1888	498	613	8			
1	C	404	Total	C	N	O	S	0	2	0
			3135	1973	521	633	8			
1	D	399	Total	C	N	O	S	0	2	0
			3092	1948	511	625	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	433	MET	-	expression tag	UNP C9E3B4
A	434	ALA	-	expression tag	UNP C9E3B4
A	435	SER	-	expression tag	UNP C9E3B4
A	436	MET	-	expression tag	UNP C9E3B4
A	437	THR	-	expression tag	UNP C9E3B4
A	438	GLY	-	expression tag	UNP C9E3B4
A	439	GLY	-	expression tag	UNP C9E3B4
A	440	GLN	-	expression tag	UNP C9E3B4
A	441	GLN	-	expression tag	UNP C9E3B4
A	442	MET	-	expression tag	UNP C9E3B4
A	443	GLY	-	expression tag	UNP C9E3B4
A	444	ARG	-	expression tag	UNP C9E3B4
A	445	ILE	-	expression tag	UNP C9E3B4
A	446	GLN	-	expression tag	UNP C9E3B4
A	850	LEU	-	expression tag	UNP C9E3B4
A	851	GLU	-	expression tag	UNP C9E3B4
A	852	HIS	-	expression tag	UNP C9E3B4
A	853	HIS	-	expression tag	UNP C9E3B4
A	854	HIS	-	expression tag	UNP C9E3B4
A	855	HIS	-	expression tag	UNP C9E3B4
A	856	HIS	-	expression tag	UNP C9E3B4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	857	HIS	-	expression tag	UNP C9E3B4
B	433	MET	-	expression tag	UNP C9E3B4
B	434	ALA	-	expression tag	UNP C9E3B4
B	435	SER	-	expression tag	UNP C9E3B4
B	436	MET	-	expression tag	UNP C9E3B4
B	437	THR	-	expression tag	UNP C9E3B4
B	438	GLY	-	expression tag	UNP C9E3B4
B	439	GLY	-	expression tag	UNP C9E3B4
B	440	GLN	-	expression tag	UNP C9E3B4
B	441	GLN	-	expression tag	UNP C9E3B4
B	442	MET	-	expression tag	UNP C9E3B4
B	443	GLY	-	expression tag	UNP C9E3B4
B	444	ARG	-	expression tag	UNP C9E3B4
B	445	ILE	-	expression tag	UNP C9E3B4
B	446	GLN	-	expression tag	UNP C9E3B4
B	850	LEU	-	expression tag	UNP C9E3B4
B	851	GLU	-	expression tag	UNP C9E3B4
B	852	HIS	-	expression tag	UNP C9E3B4
B	853	HIS	-	expression tag	UNP C9E3B4
B	854	HIS	-	expression tag	UNP C9E3B4
B	855	HIS	-	expression tag	UNP C9E3B4
B	856	HIS	-	expression tag	UNP C9E3B4
B	857	HIS	-	expression tag	UNP C9E3B4
C	433	MET	-	expression tag	UNP C9E3B4
C	434	ALA	-	expression tag	UNP C9E3B4
C	435	SER	-	expression tag	UNP C9E3B4
C	436	MET	-	expression tag	UNP C9E3B4
C	437	THR	-	expression tag	UNP C9E3B4
C	438	GLY	-	expression tag	UNP C9E3B4
C	439	GLY	-	expression tag	UNP C9E3B4
C	440	GLN	-	expression tag	UNP C9E3B4
C	441	GLN	-	expression tag	UNP C9E3B4
C	442	MET	-	expression tag	UNP C9E3B4
C	443	GLY	-	expression tag	UNP C9E3B4
C	444	ARG	-	expression tag	UNP C9E3B4
C	445	ILE	-	expression tag	UNP C9E3B4
C	446	GLN	-	expression tag	UNP C9E3B4
C	850	LEU	-	expression tag	UNP C9E3B4
C	851	GLU	-	expression tag	UNP C9E3B4
C	852	HIS	-	expression tag	UNP C9E3B4
C	853	HIS	-	expression tag	UNP C9E3B4
C	854	HIS	-	expression tag	UNP C9E3B4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	855	HIS	-	expression tag	UNP C9E3B4
C	856	HIS	-	expression tag	UNP C9E3B4
C	857	HIS	-	expression tag	UNP C9E3B4
D	433	MET	-	expression tag	UNP C9E3B4
D	434	ALA	-	expression tag	UNP C9E3B4
D	435	SER	-	expression tag	UNP C9E3B4
D	436	MET	-	expression tag	UNP C9E3B4
D	437	THR	-	expression tag	UNP C9E3B4
D	438	GLY	-	expression tag	UNP C9E3B4
D	439	GLY	-	expression tag	UNP C9E3B4
D	440	GLN	-	expression tag	UNP C9E3B4
D	441	GLN	-	expression tag	UNP C9E3B4
D	442	MET	-	expression tag	UNP C9E3B4
D	443	GLY	-	expression tag	UNP C9E3B4
D	444	ARG	-	expression tag	UNP C9E3B4
D	445	ILE	-	expression tag	UNP C9E3B4
D	446	GLN	-	expression tag	UNP C9E3B4
D	850	LEU	-	expression tag	UNP C9E3B4
D	851	GLU	-	expression tag	UNP C9E3B4
D	852	HIS	-	expression tag	UNP C9E3B4
D	853	HIS	-	expression tag	UNP C9E3B4
D	854	HIS	-	expression tag	UNP C9E3B4
D	855	HIS	-	expression tag	UNP C9E3B4
D	856	HIS	-	expression tag	UNP C9E3B4
D	857	HIS	-	expression tag	UNP C9E3B4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by author).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	499	Total O 499 499	0	0
3	B	457	Total O 457 457	0	0
3	C	510	Total O 510 510	0	0
3	D	448	Total O 448 448	0	0

3 Residue-property plots ⓘ

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: Surface protein adhesin
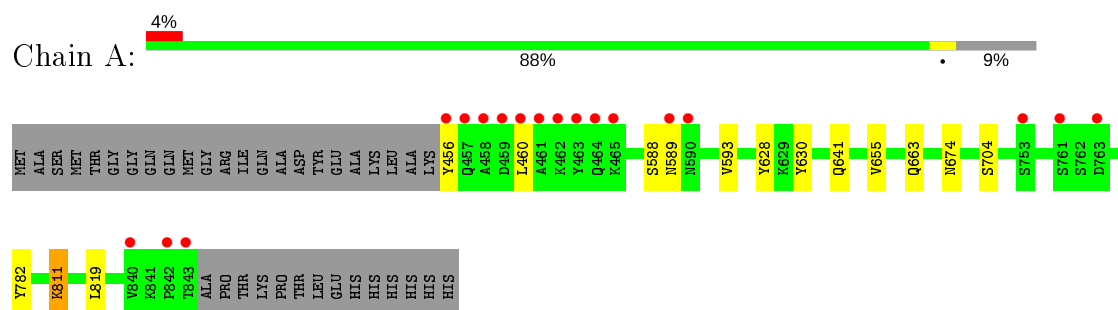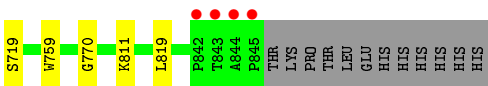

- Molecule 1: Surface protein adhesin
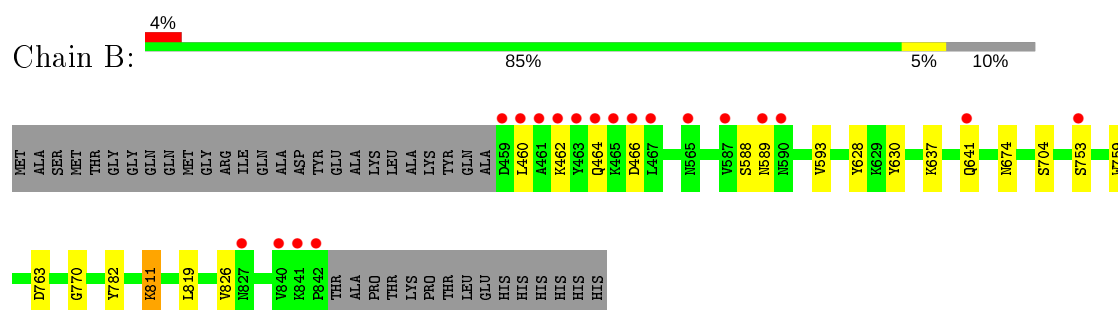
- Molecule 1: Surface protein adhesin
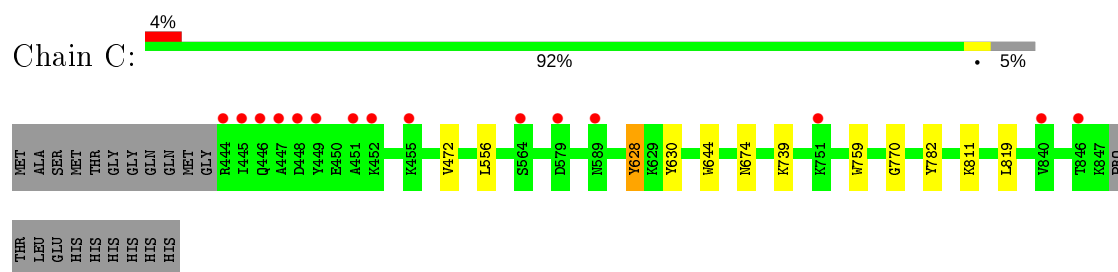
- Molecule 1: Surface protein adhesin
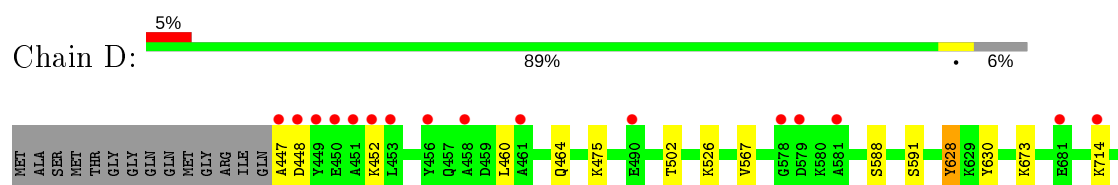
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.97Å 133.33Å 246.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 1.60 34.93 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.96-1.60) 99.9 (34.93-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.180 , 0.193 0.190 , 0.204	Depositor DCC
R_{free} test set	14429 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14201	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.62	0/3086	0.71	0/4181
1	B	0.62	0/3069	0.73	1/4157 (0.0%)
1	C	0.63	0/3200	0.73	0/4334
1	D	0.62	0/3157	0.71	0/4278
All	All	0.62	0/12512	0.72	1/16950 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	589	ASN	CB-CA-C	7.89	126.18	110.40

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	3023	0	2943	14	0
1	B	3007	0	2922	16	0
1	C	3135	0	3069	7	0
1	D	3092	0	3021	14	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	0	0	0
3	A	499	0	0	0	0
3	B	457	0	0	2	0
3	C	510	0	0	2	0
3	D	448	0	0	5	0
All	All	14201	0	11955	46	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 2.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:LYS:HE2	3:D:1002:HOH:O	1.21	1.30
1:D:714:LYS:CE	3:D:1002:HOH:O	1.97	0.79
1:B:704:SER:OG	1:B:811:LYS:HE2	1.84	0.78
1:D:588:SER:HB3	1:D:591:SER:OG	1.92	0.69
1:A:641:GLN:OE1	1:B:641:GLN:HB3	1.95	0.67
1:A:628:TYR:CE1	1:A:630:TYR:CE1	2.82	0.67
1:D:673:LYS:NZ	3:D:1001:HOH:O	2.26	0.67
1:B:628:TYR:CE1	1:B:630:TYR:CE1	2.82	0.67
1:C:472:VAL:HG23	3:C:901:HOH:O	1.99	0.63
1:A:588:SER:O	1:A:589:ASN:CG	2.38	0.62
1:D:502:THR:HG22	1:D:719:SER:OG	2.00	0.62
1:A:641:GLN:HG3	1:B:641:GLN:HG2	1.82	0.61
1:A:630:TYR:CE1	1:A:655:VAL:HG11	2.37	0.59
1:A:704:SER:OG	1:A:811:LYS:HE2	2.02	0.58
1:A:641:GLN:CD	1:B:641:GLN:HB3	2.26	0.56
1:A:456:TYR:OH	1:A:460:LEU:HD11	2.06	0.55
1:B:637:LYS:HE2	3:B:1404:HOH:O	2.08	0.53
1:D:714:LYS:NZ	3:D:1002:HOH:O	2.26	0.53
1:A:628:TYR:OH	1:A:819:LEU:HD12	2.09	0.52
1:B:628:TYR:OH	1:B:819:LEU:HD12	2.11	0.50
1:D:447:ALA:HB3	3:D:1298:HOH:O	2.11	0.50
1:B:460:LEU:O	1:B:464:GLN:HG2	2.11	0.50
1:B:462:LYS:NZ	1:B:466:ASP:OD2	2.45	0.47
1:B:588:SER:HB3	1:B:593:VAL:CG1	2.46	0.46
1:B:826:VAL:O	3:B:1001:HOH:O	2.20	0.46
1:D:628:TYR:CE1	1:D:630:TYR:CE2	3.03	0.46
1:C:628:TYR:CE1	1:C:630:TYR:CE2	3.04	0.46
1:D:628:TYR:OH	1:D:819:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:LEU:O	1:D:464:GLN:HG2	2.17	0.45
1:B:753:SER:O	1:D:475:LYS:HE3	2.17	0.45
1:D:448:ASP:O	1:D:452:LYS:HD2	2.18	0.44
1:A:641:GLN:OE1	1:B:641:GLN:CB	2.65	0.43
1:C:739:LYS:HE2	3:C:922:HOH:O	2.19	0.43
1:C:628:TYR:OH	1:C:819:LEU:HD12	2.18	0.43
1:D:526:LYS:HD3	1:D:567:VAL:CG2	2.49	0.43
1:A:630:TYR:CE1	1:A:655:VAL:CG1	3.02	0.42
1:C:759:TRP:CZ3	1:C:770:GLY:HA3	2.55	0.41
1:A:588:SER:HB3	1:A:593:VAL:CG1	2.50	0.41
1:B:759:TRP:CZ3	1:B:770:GLY:HA3	2.56	0.41
1:B:763[B]:ASP:N	1:B:763[B]:ASP:OD1	2.52	0.41
1:D:759:TRP:CZ3	1:D:770:GLY:HA3	2.55	0.41
1:B:674:ASN:O	1:B:782:TYR:HA	2.21	0.41
1:C:556:LEU:HD23	1:C:644:TRP:CE3	2.56	0.41
1:C:674:ASN:O	1:C:782:TYR:HA	2.20	0.41
1:A:674:ASN:O	1:A:782:TYR:HA	2.21	0.41
1:A:588:SER:HB3	1:A:593:VAL:HG11	2.02	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	390/425 (92%)	382 (98%)	8 (2%)	0	100	100
1	B	388/425 (91%)	382 (98%)	6 (2%)	0	100	100
1	C	404/425 (95%)	397 (98%)	7 (2%)	0	100	100
1	D	399/425 (94%)	392 (98%)	7 (2%)	0	100	100
All	All	1581/1700 (93%)	1553 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	333/358 (93%)	331 (99%)	2 (1%)	86	77
1	B	332/358 (93%)	331 (100%)	1 (0%)	92	87
1	C	343/358 (96%)	341 (99%)	2 (1%)	86	77
1	D	338/358 (94%)	336 (99%)	2 (1%)	86	77
All	All	1346/1432 (94%)	1339 (100%)	7 (0%)	88	80

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

Mol	Chain	Res	Type
1	A	663	GLN
1	A	811	LYS
1	B	811	LYS
1	C	628	TYR
1	C	811	LYS
1	D	628	TYR
1	D	811	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	590	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)

6 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	$\#|Z| > 2$
2	SO4	A	1002	-	4,4,4	0.38	0	6,6,6	0.04	0
2	SO4	B	901	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	D	902	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	1001	-	4,4,4	0.40	0	6,6,6	0.07	0
2	SO4	D	901	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	D	903	-	4,4,4	0.38	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 then 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.
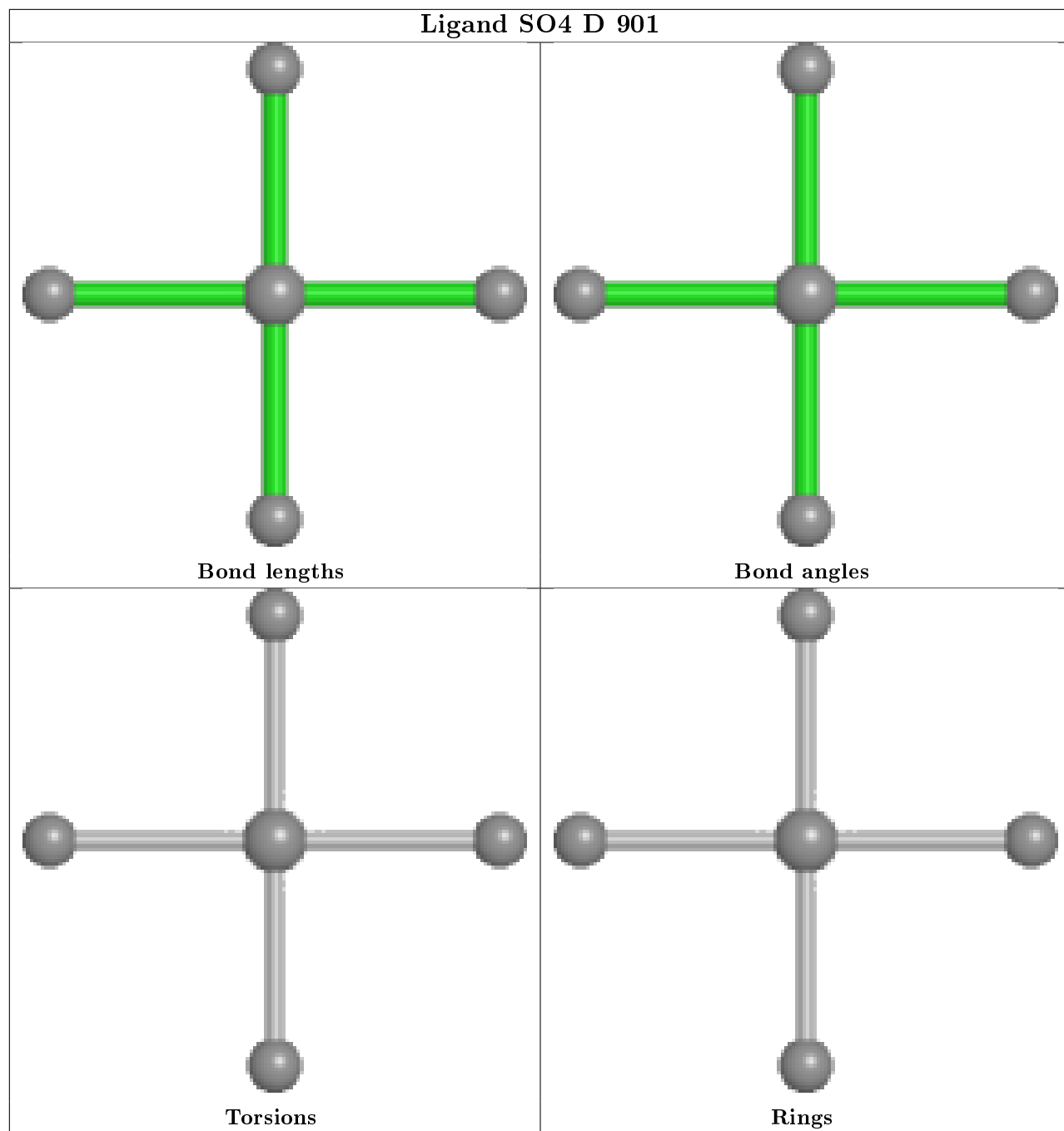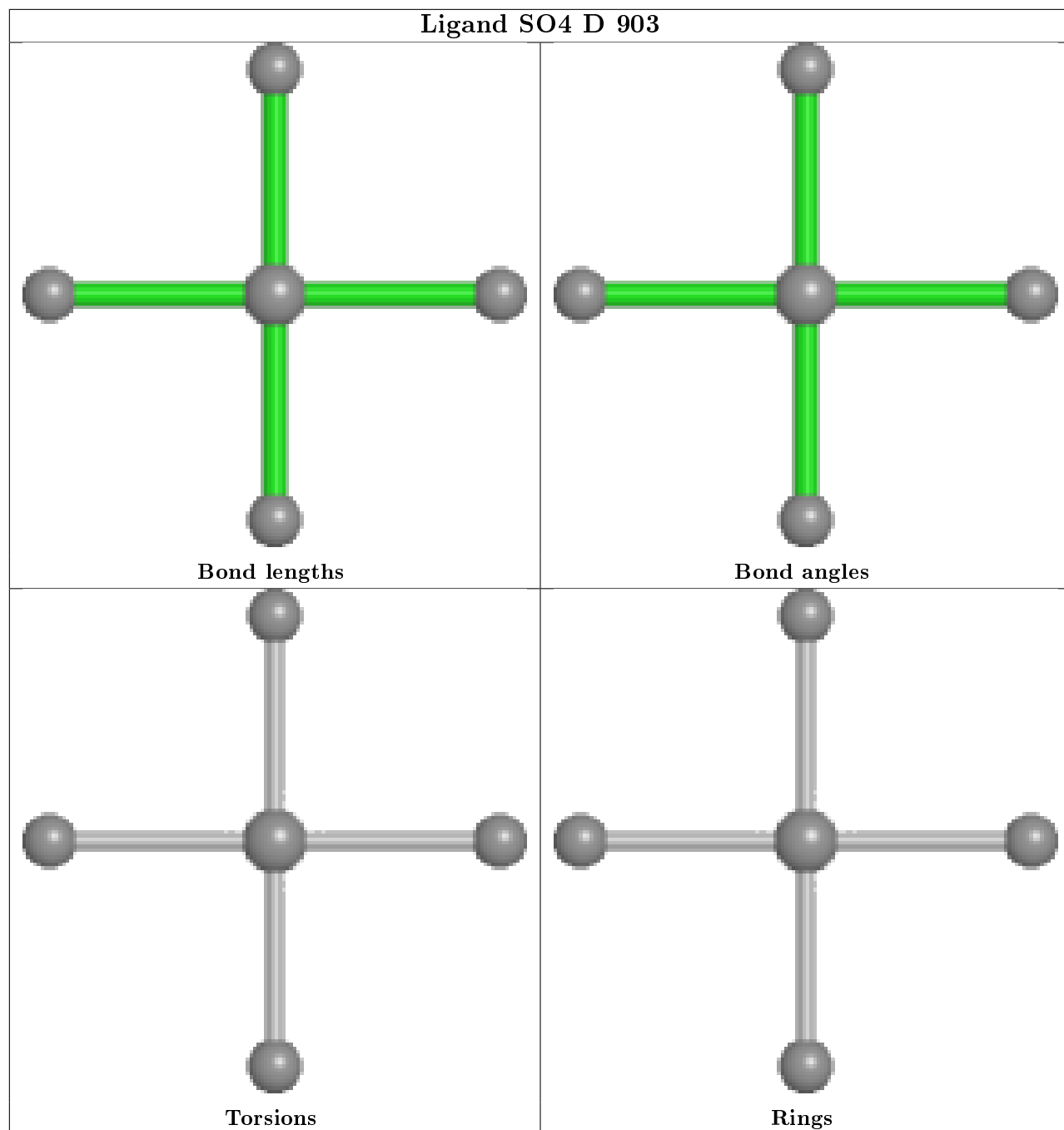
Ligand SO4 A 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 902

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 901

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 903

Bond lengths

Bond angles

Torsions

Rings
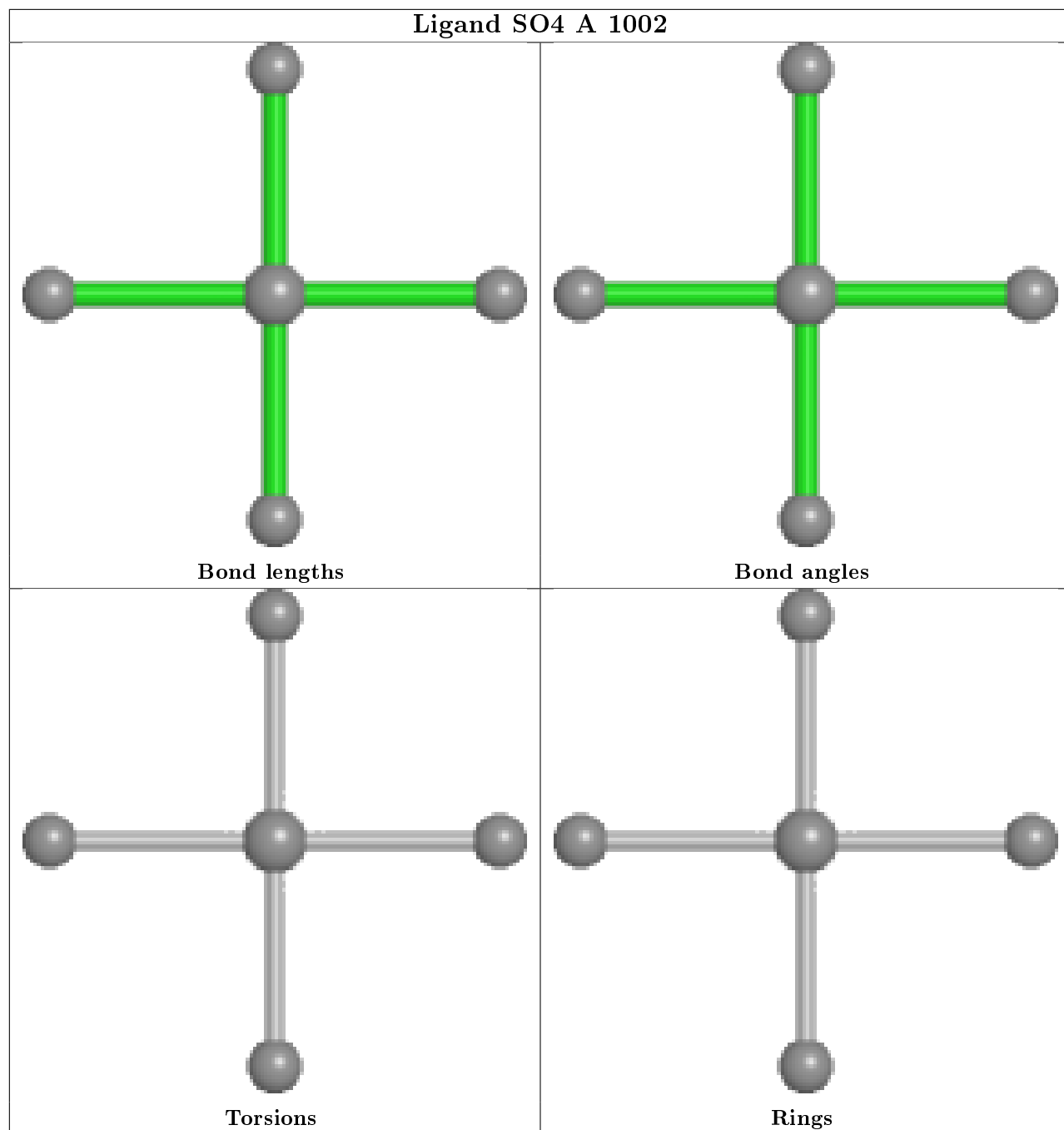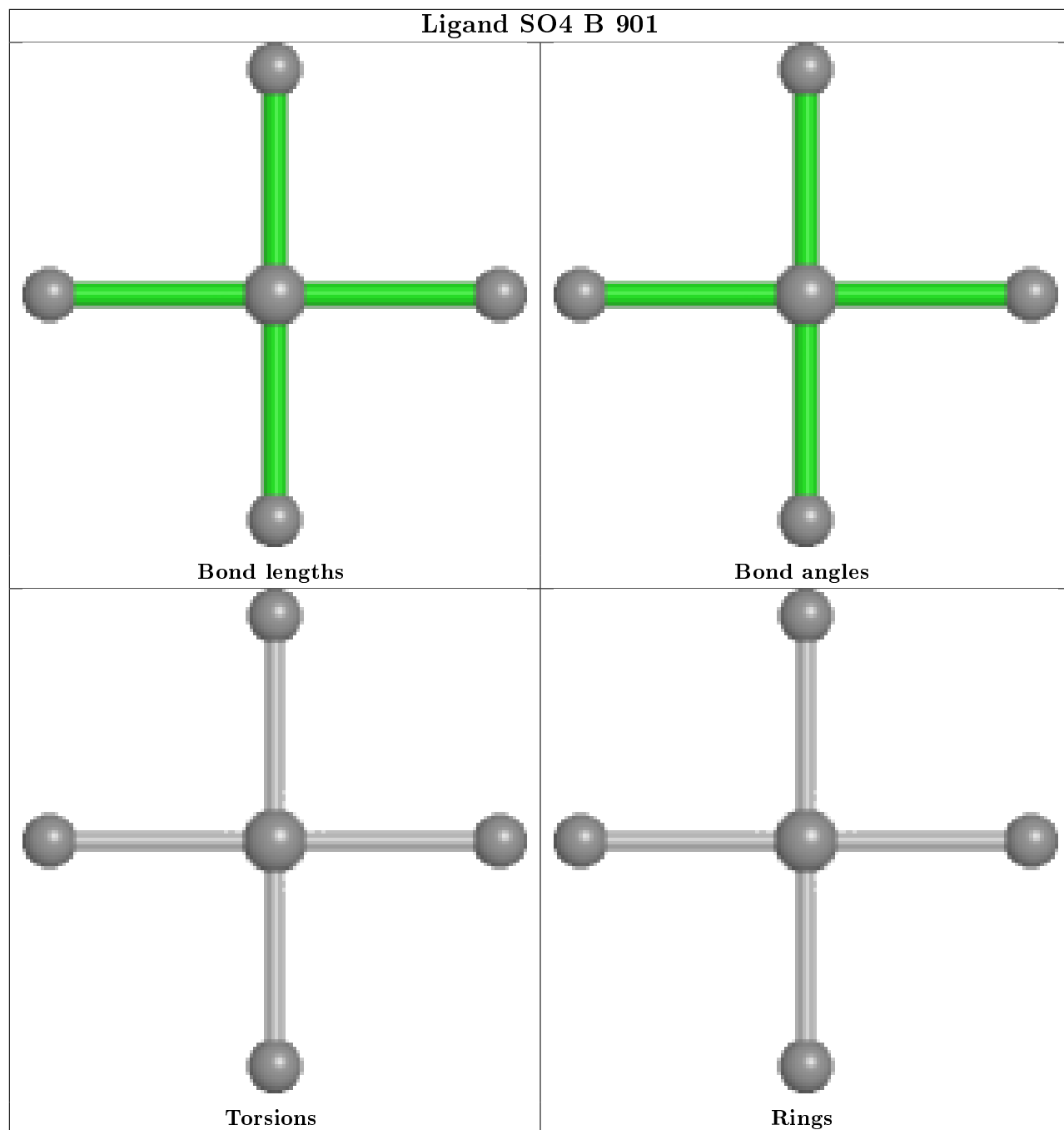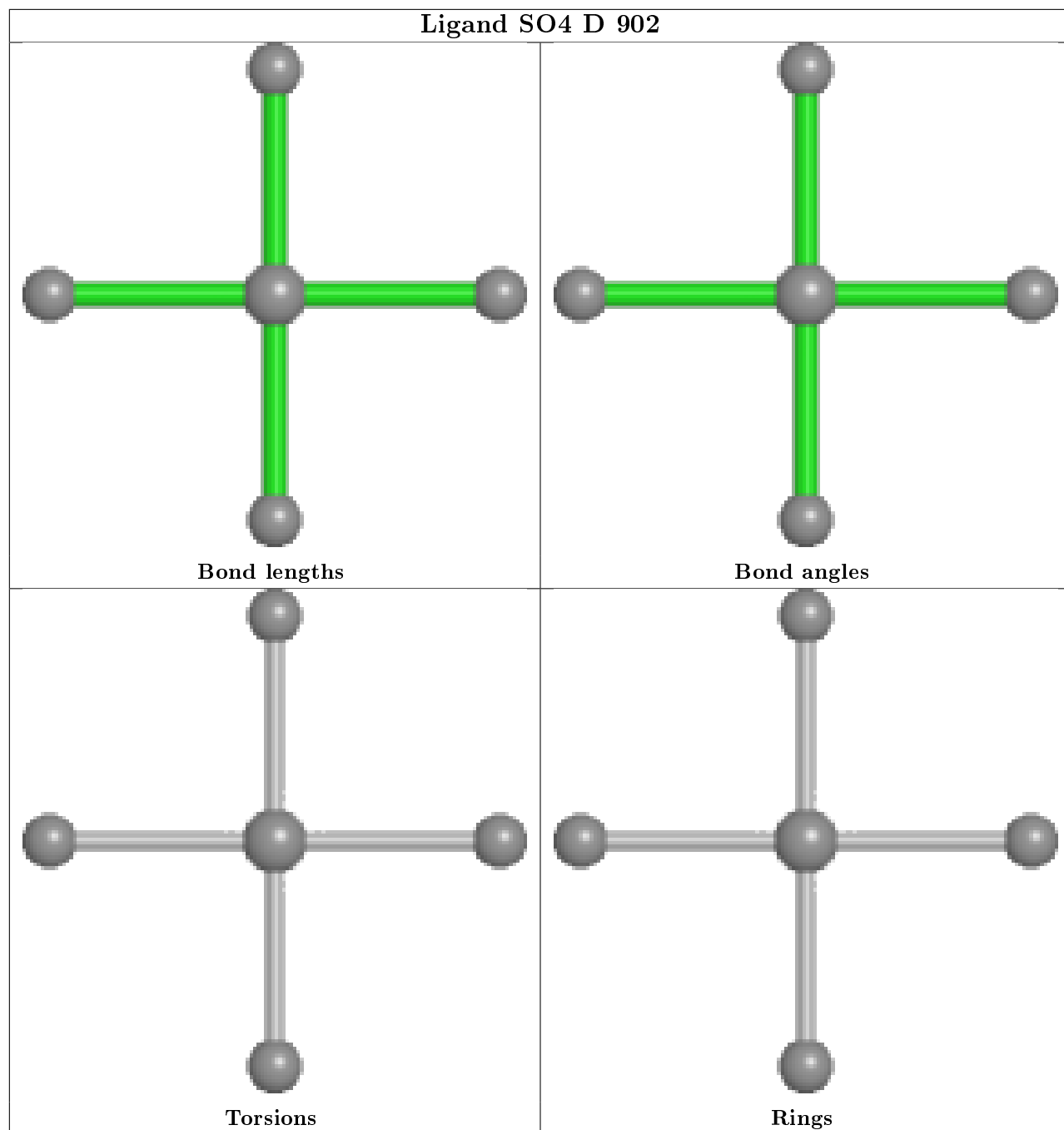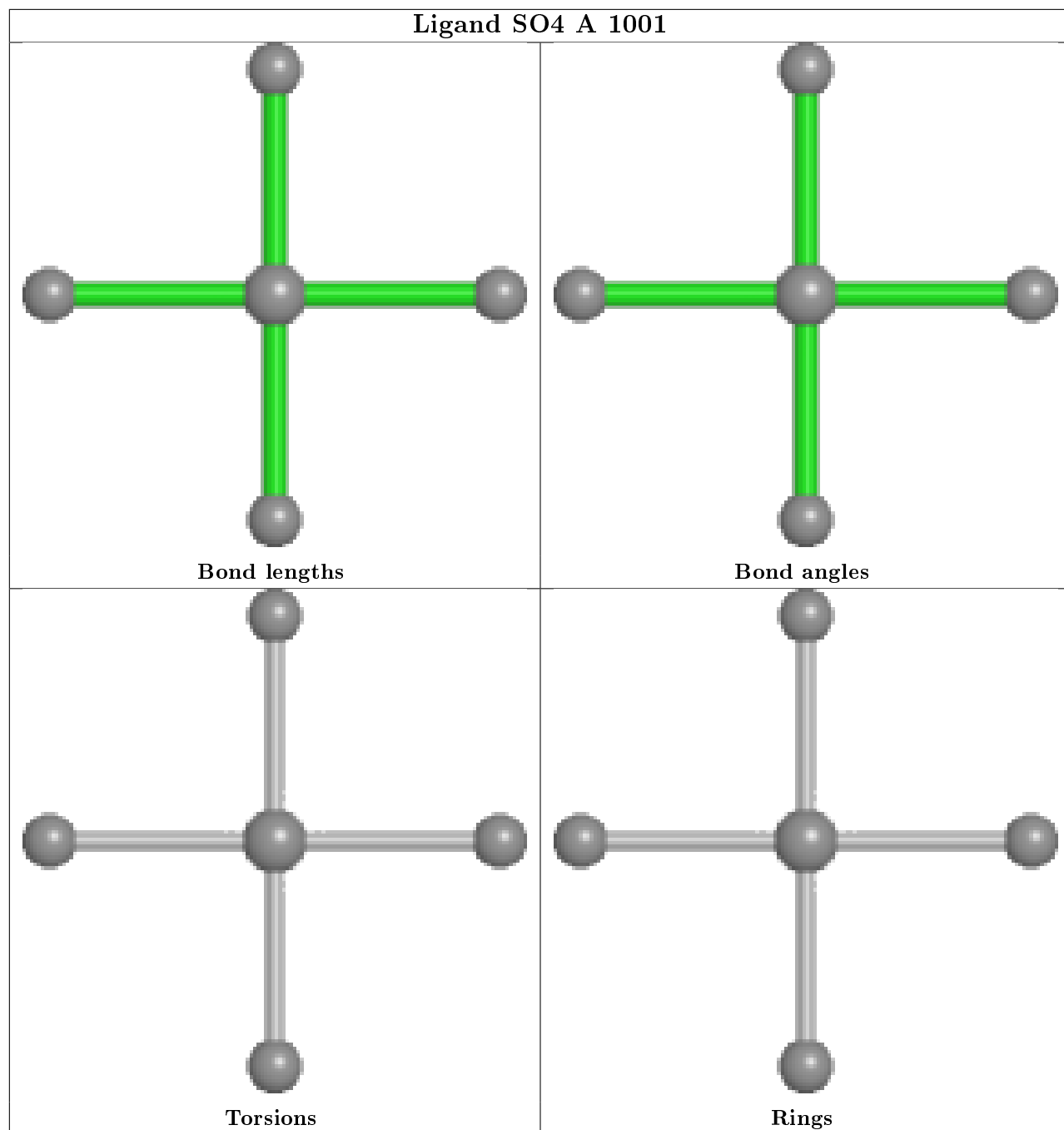
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	388/425 (91%)	0.11	18 (4%)	32	29	12, 21, 42, 92	0
1	B	384/425 (90%)	0.15	19 (4%)	29	27	13, 22, 39, 84	0
1	C	404/425 (95%)	0.06	15 (3%)	41	39	12, 20, 45, 85	0
1	D	399/425 (93%)	0.10	20 (5%)	28	26	15, 26, 50, 86	0
All	All	1575/1700 (92%)	0.10	72 (4%)	32	29	12, 22, 45, 92	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	TYR	7.6
1	B	460	LEU	7.6
1	A	460	LEU	7.0
1	D	449	TYR	6.8
1	C	445	ILE	6.8
1	B	461	ALA	6.5
1	D	448	ASP	5.8
1	A	458	ALA	5.8
1	C	447	ALA	5.5
1	A	590	ASN	5.4
1	D	461	ALA	5.3
1	A	843	THR	5.0
1	C	846	THR	4.8
1	C	444	ARG	4.8
1	B	842	PRO	4.6
1	D	447	ALA	4.6
1	B	459	ASP	4.5
1	A	842	PRO	4.5
1	D	458	ALA	4.2
1	A	461	ALA	4.0
1	C	448	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	452	LYS	3.8
1	C	451	ALA	3.8
1	B	590	ASN	3.8
1	B	462	LYS	3.8
1	B	589	ASN	3.6
1	A	457	GLN	3.6
1	B	463	TYR	3.6
1	B	827	ASN	3.4
1	C	589	ASN	3.4
1	D	579	ASP	3.3
1	A	840	VAL	3.3
1	D	578	GLY	3.3
1	B	753	SER	3.2
1	C	455	LYS	3.1
1	B	840	VAL	3.1
1	B	841	LYS	3.0
1	D	844	ALA	3.0
1	A	753	SER	2.9
1	D	451	ALA	2.9
1	D	490	GLU	2.9
1	B	464	GLN	2.9
1	D	450	GLU	2.9
1	C	449	TYR	2.9
1	A	589	ASN	2.9
1	D	681	GLU	2.9
1	A	464	GLN	2.8
1	A	465	LYS	2.8
1	A	463	TYR	2.8
1	A	459	ASP	2.8
1	C	751	LYS	2.7
1	D	845	PRO	2.7
1	D	843	THR	2.7
1	A	763	ASP	2.6
1	D	581	ALA	2.6
1	C	452	LYS	2.5
1	B	466	ASP	2.5
1	D	453	LEU	2.4
1	C	446	GLN	2.4
1	B	565	ASN	2.4
1	B	467	LEU	2.3
1	A	462	LYS	2.3
1	D	456	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	714	LYS	2.3
1	A	761	SER	2.2
1	C	564	SER	2.2
1	B	465	LYS	2.2
1	B	641	GLN	2.2
1	C	579	ASP	2.1
1	B	587	VAL	2.1
1	C	840	VAL	2.1
1	D	842	PRO	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(Å²)	Q<0.9
2	SO4	B	901	5/5	0.84	0.26	72,72,74,74	0
2	SO4	D	902	5/5	0.91	0.20	77,79,80,80	0
2	SO4	D	901	5/5	0.92	0.28	78,79,80,80	0
2	SO4	D	903	5/5	0.94	0.22	77,78,80,80	0
2	SO4	A	1002	5/5	0.95	0.10	61,62,63,64	0
2	SO4	A	1001	5/5	0.98	0.11	48,48,50,50	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 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
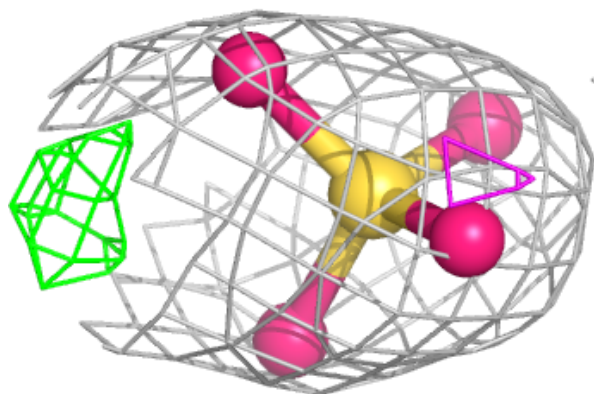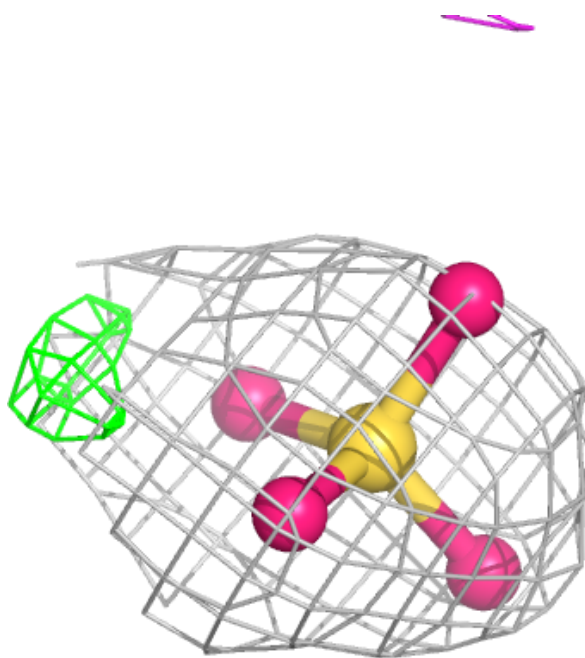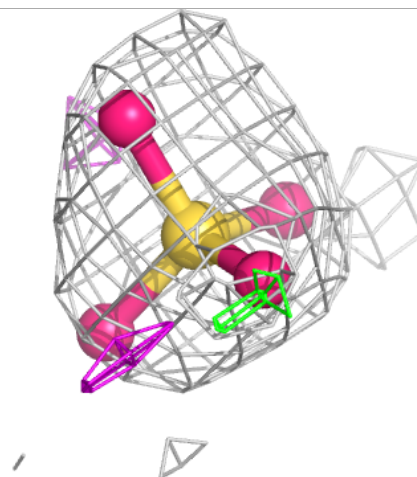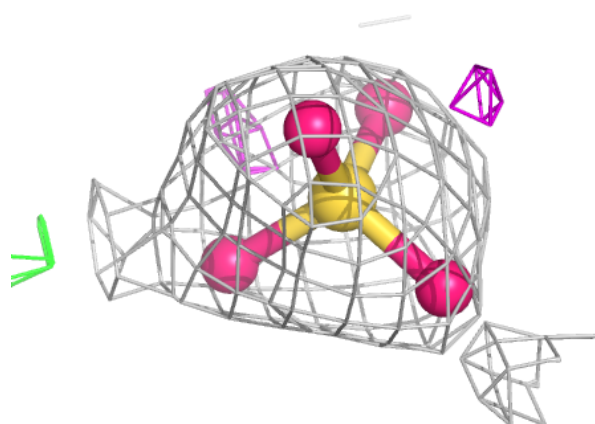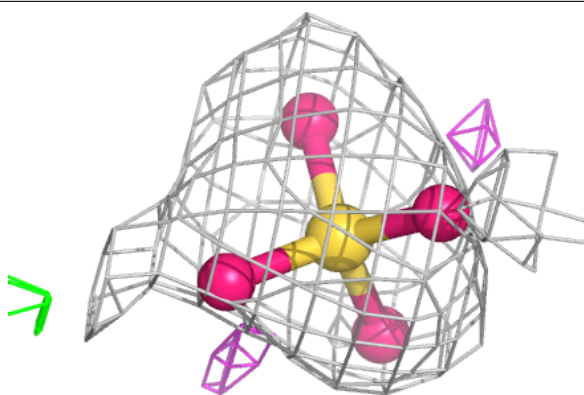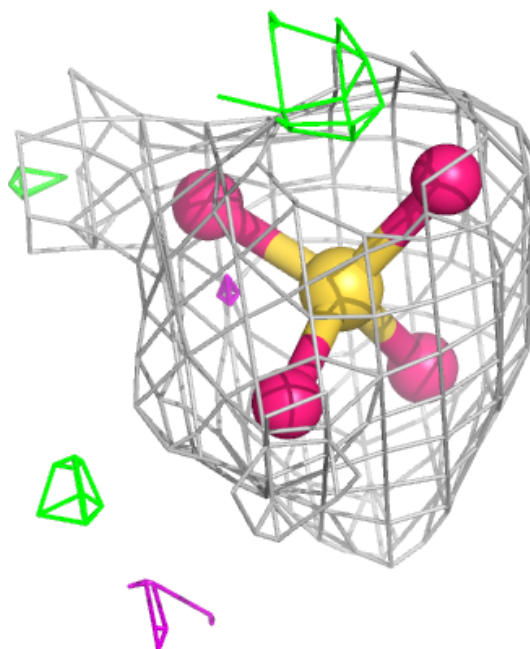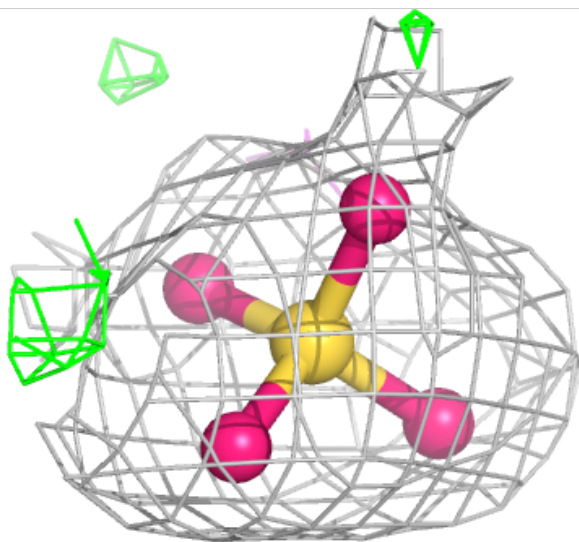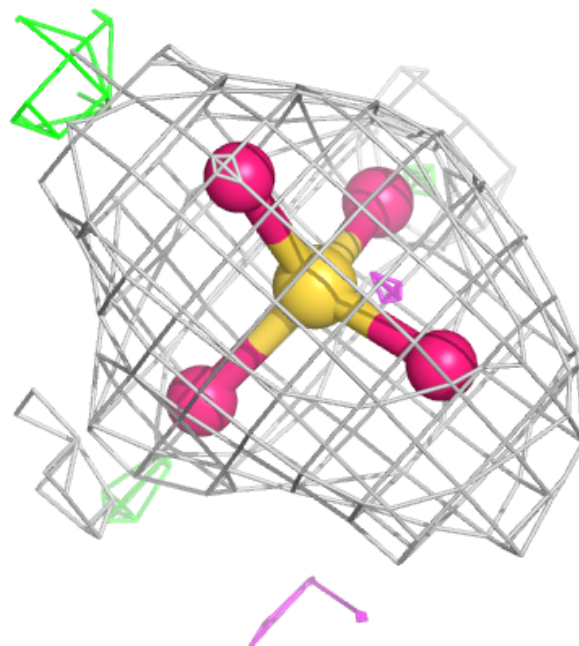and green (positive)
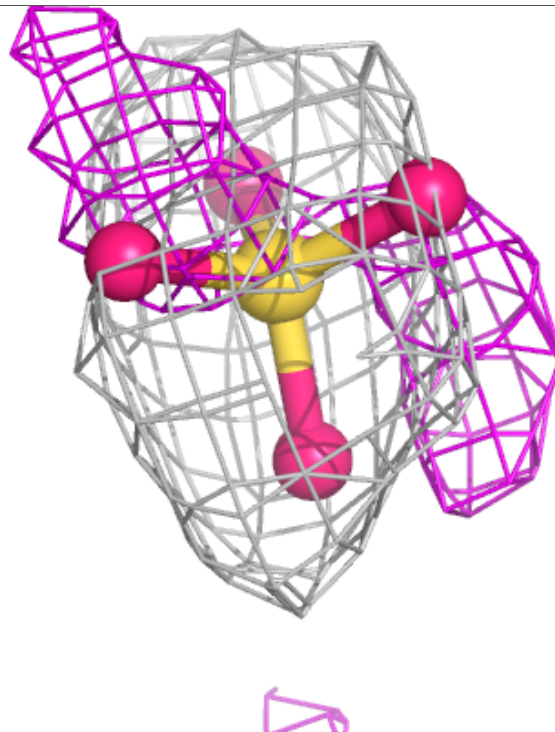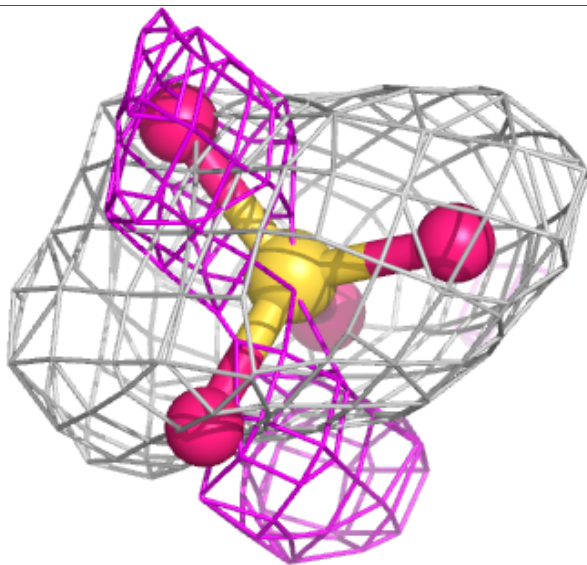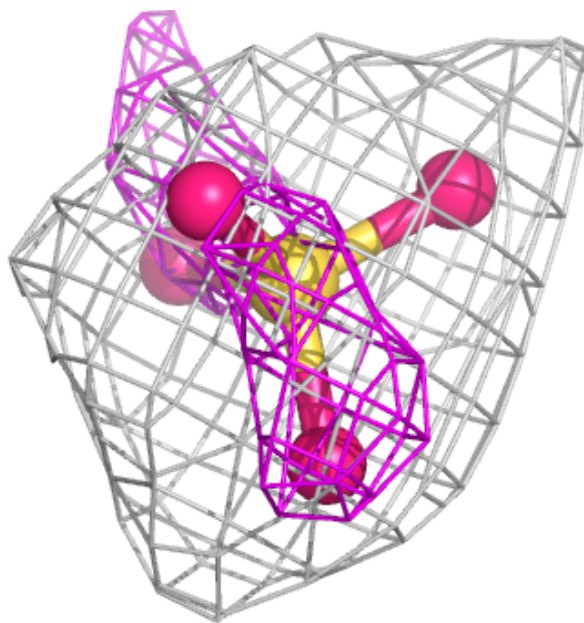
Electron density around SO4 D 902:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
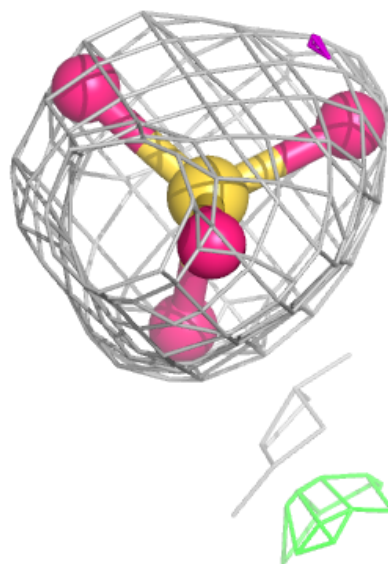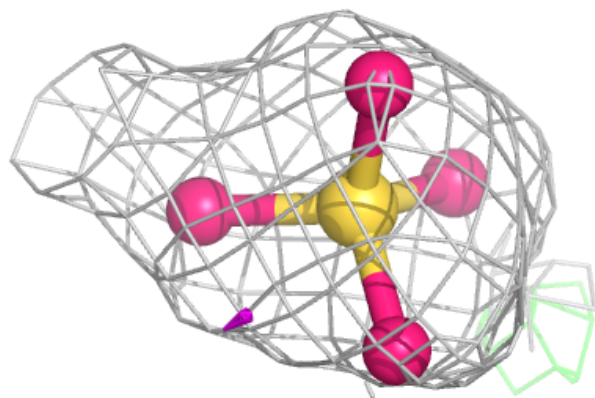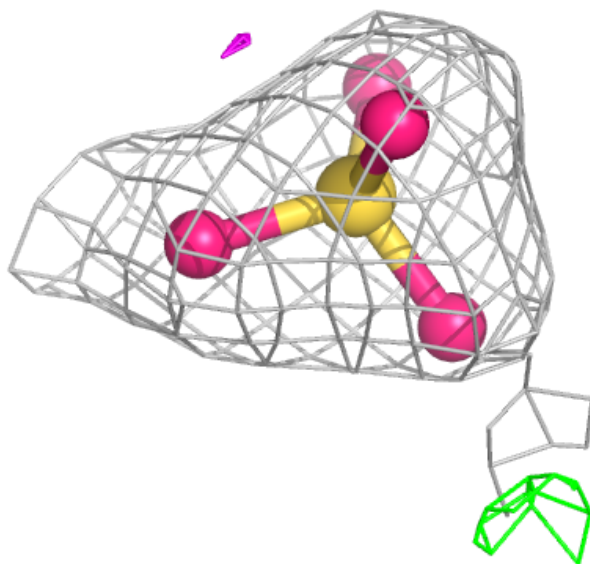
Electron density around SO4 D 901:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
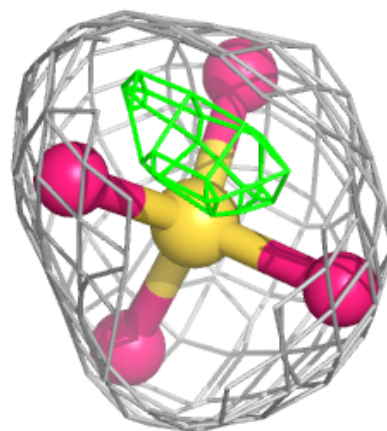
Electron density around SO4 D 903:

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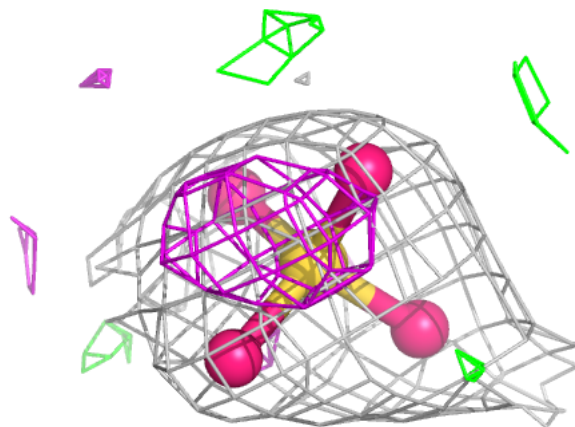mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SO4 A 1002:

$2mF_o$-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 1001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
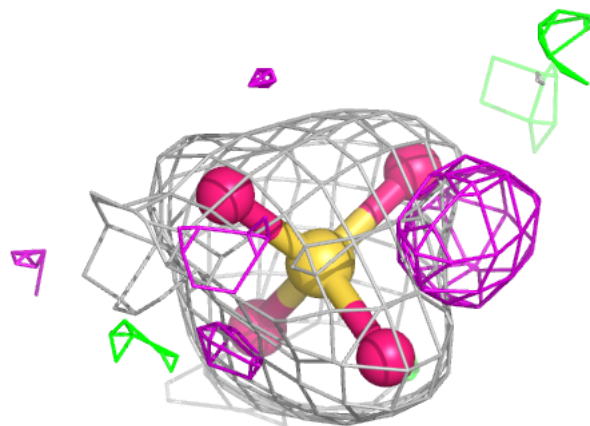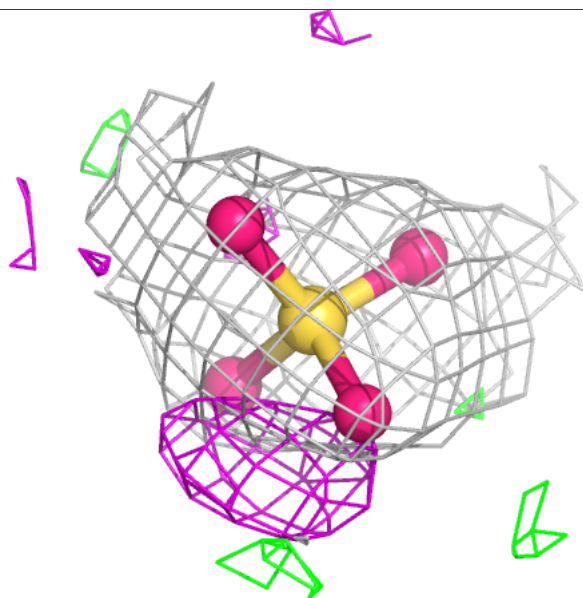
6.5 Other polymers ⓘ

There are no such residues in this entry.