



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2025 – 01:13 PM JST

PDB ID : 9LJ9 / pdb\_00009lj9  
Title : Crystal structure of a bifunctional 3-hexulose-6-phosphate synthase/6-phospho-3-hexuloisomerase  
Authors : Wang, H.; Feng, Y.; Liu, L.; Li, Y.X.; Ji, Y.  
Deposited on : 2025-01-14  
Resolution : 2.64 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](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

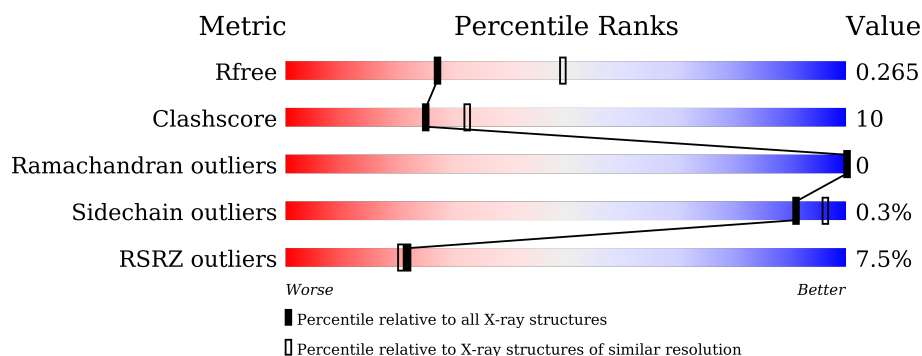
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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))
$R_{free}$	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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  $\geq 3$ , 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	426	<div> <div>6%</div> <div>69%</div> <div>16%</div> <div>15%</div> </div>
1	B	426	<div> <div>7%</div> <div>70%</div> <div>15%</div> <div>15%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5662 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 3-hexulose-6-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	362	Total	C	N	O	S	0	0	0
			2743	1753	464	512	14			
1	A	362	Total	C	N	O	S	0	0	0
			2743	1753	464	512	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	407	PRO	-	expression tag	UNP O59601
B	408	ASN	-	expression tag	UNP O59601
B	409	SER	-	expression tag	UNP O59601
B	410	SER	-	expression tag	UNP O59601
B	411	SER	-	expression tag	UNP O59601
B	412	VAL	-	expression tag	UNP O59601
B	413	ASP	-	expression tag	UNP O59601
B	414	LYS	-	expression tag	UNP O59601
B	415	LEU	-	expression tag	UNP O59601
B	416	ALA	-	expression tag	UNP O59601
B	417	ALA	-	expression tag	UNP O59601
B	418	ALA	-	expression tag	UNP O59601
B	419	LEU	-	expression tag	UNP O59601
B	420	GLU	-	expression tag	UNP O59601
B	421	HIS	-	expression tag	UNP O59601
B	422	HIS	-	expression tag	UNP O59601
B	423	HIS	-	expression tag	UNP O59601
B	424	HIS	-	expression tag	UNP O59601
B	425	HIS	-	expression tag	UNP O59601
B	426	HIS	-	expression tag	UNP O59601
A	407	PRO	-	expression tag	UNP O59601
A	408	ASN	-	expression tag	UNP O59601
A	409	SER	-	expression tag	UNP O59601
A	410	SER	-	expression tag	UNP O59601
A	411	SER	-	expression tag	UNP O59601

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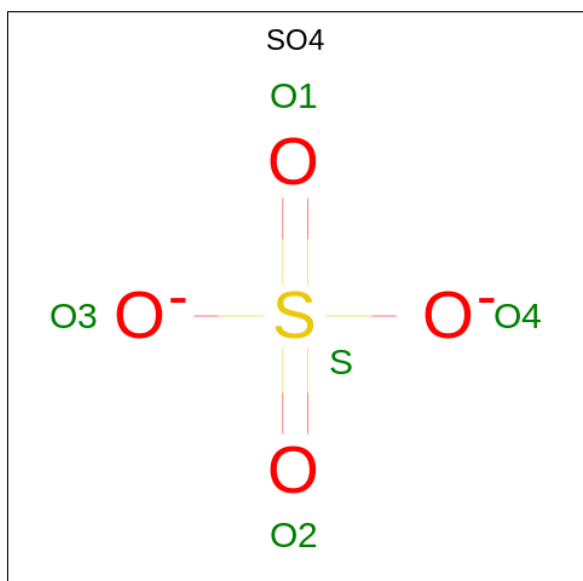
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Chain	Residue	Modelled	Actual	Comment	Reference
A	412	VAL	-	expression tag	UNP O59601
A	413	ASP	-	expression tag	UNP O59601
A	414	LYS	-	expression tag	UNP O59601
A	415	LEU	-	expression tag	UNP O59601
A	416	ALA	-	expression tag	UNP O59601
A	417	ALA	-	expression tag	UNP O59601
A	418	ALA	-	expression tag	UNP O59601
A	419	LEU	-	expression tag	UNP O59601
A	420	GLU	-	expression tag	UNP O59601
A	421	HIS	-	expression tag	UNP O59601
A	422	HIS	-	expression tag	UNP O59601
A	423	HIS	-	expression tag	UNP O59601
A	424	HIS	-	expression tag	UNP O59601
A	425	HIS	-	expression tag	UNP O59601
A	426	HIS	-	expression tag	UNP O59601

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



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

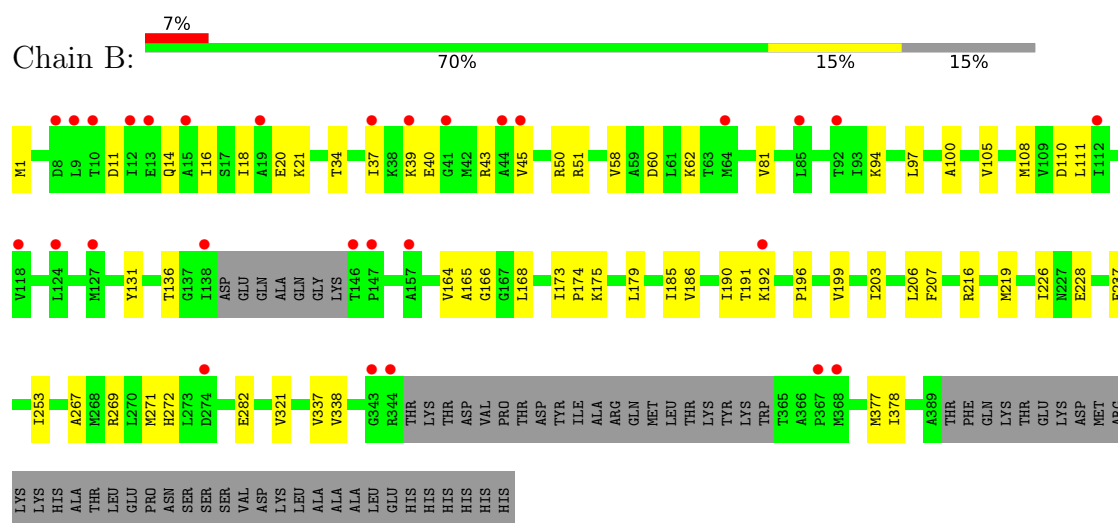
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	72	Total	O	0	0
			72	72		
4	A	92	Total	O	0	0
			92	92		

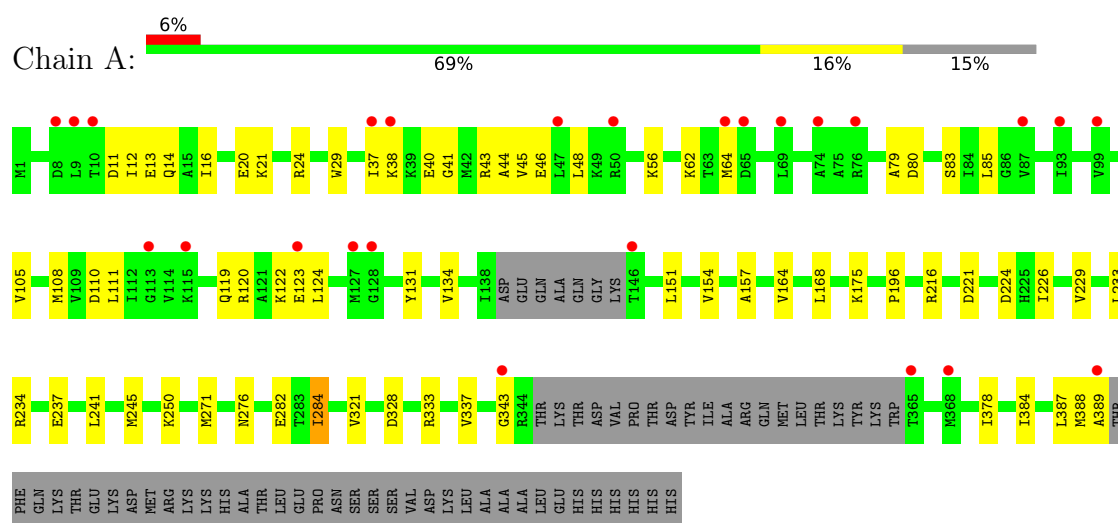
### 3 Residue-property plots [i](#)

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: 3-hexulose-6-phosphate synthase



#### • Molecule 1: 3-hexulose-6-phosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.92Å 205.70Å 143.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.59 – 2.64 32.59 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.59-2.64) 99.7 (32.59-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.221 , 0.265 0.221 , 0.265	Depositor DCC
$R_{free}$ test set	1459 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.18	0/2773	0.36	0/3739
1	B	0.21	0/2773	0.35	0/3739
All	All	0.20	0/5546	0.35	0/7478

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	2743	0	2897	55	1
1	B	2743	0	2897	55	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	92	0	0	9	1
4	B	72	0	0	8	1
All	All	5662	0	5794	108	2

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 10.



All (108) 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:186:VAL:CG2	1:B:190:ILE:HD12	1.67	1.23
1:B:186:VAL:CG2	1:B:190:ILE:CD1	2.22	1.16
1:B:186:VAL:HG23	1:B:190:ILE:HD12	1.19	1.14
1:A:282:GLU:OE1	4:A:601:HOH:O	1.67	1.11
1:B:20:GLU:O	1:B:20:GLU:OE1	1.77	1.01
1:B:186:VAL:HG21	1:B:190:ILE:HD11	1.41	0.99
1:A:389:ALA:O	4:A:602:HOH:O	1.85	0.94
1:B:186:VAL:HG21	1:B:190:ILE:CD1	1.94	0.91
1:A:224:ASP:OD2	4:A:604:HOH:O	1.87	0.90
1:B:40:GLU:OE2	1:B:43:ARG:NH2	2.07	0.86
1:A:40:GLU:HA	4:A:603:HOH:O	1.75	0.86
1:B:186:VAL:CG2	1:B:190:ILE:HD11	2.02	0.84
1:A:41:GLY:N	4:A:603:HOH:O	1.87	0.81
1:B:282:GLU:OE1	4:B:602:HOH:O	1.98	0.80
1:A:328:ASP:OD2	1:A:333:ARG:NH2	2.14	0.80
1:A:37:ILE:HD11	1:A:38:LYS:HE2	1.62	0.79
1:A:40:GLU:CA	4:A:603:HOH:O	2.29	0.79
1:B:338:VAL:O	4:B:603:HOH:O	2.02	0.77
1:B:40:GLU:CD	1:B:43:ARG:HH21	1.93	0.76
1:B:60:ASP:OD1	1:B:62:LYS:NZ	2.14	0.75
1:A:122:LYS:HE2	1:A:157:ALA:O	1.87	0.75
1:B:228:GLU:OE2	4:B:604:HOH:O	2.06	0.73
1:B:18:ILE:HD12	1:B:191:THR:HA	1.72	0.71
1:A:44:ALA:O	1:A:48:LEU:HD23	1.90	0.70
1:B:186:VAL:HG23	1:B:190:ILE:CD1	2.04	0.69
1:B:40:GLU:OE2	1:B:43:ARG:NE	2.27	0.68
1:A:343:GLY:HA2	4:A:635:HOH:O	1.93	0.68
1:A:234:ARG:HB2	1:A:237:GLU:HG3	1.74	0.67
1:B:18:ILE:HG21	1:B:191:THR:HG22	1.77	0.66
1:A:62:LYS:C	1:A:85:LEU:HD11	2.23	0.64
1:B:237:GLU:OE2	4:B:605:HOH:O	2.15	0.64
1:B:34:THR:HA	1:B:37:ILE:HG12	1.79	0.63
1:B:136:THR:HG21	1:B:168:LEU:HD21	1.79	0.63
1:B:226:ILE:HD13	1:B:378:ILE:HD12	1.80	0.62
1:B:97:LEU:HD23	4:B:609:HOH:O	1.99	0.61
1:B:40:GLU:OE2	1:B:43:ARG:CZ	2.49	0.61
1:A:122:LYS:HE2	1:A:157:ALA:HB1	1.83	0.61
1:A:37:ILE:HD12	1:A:38:LYS:HD3	1.81	0.61
1:A:384:ILE:O	1:A:388:MET:HG3	2.01	0.61
1:B:175:LYS:O	1:B:179:LEU:HD12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:CD1	1:A:38:LYS:HE2	2.32	0.59
1:B:199:VAL:O	1:B:203:ILE:HG13	2.02	0.59
1:A:64:MET:HE3	1:A:64:MET:HA	1.86	0.58
1:B:20:GLU:OE1	1:B:20:GLU:C	2.45	0.58
1:A:62:LYS:HA	1:A:85:LEU:CD1	2.34	0.58
1:B:175:LYS:HE3	1:B:179:LEU:HD11	1.86	0.58
1:A:43:ARG:HA	1:A:46:GLU:HG2	1.86	0.58
1:A:221:ASP:OD2	4:A:605:HOH:O	2.17	0.57
1:A:108:MET:HG3	1:A:131:TYR:HB2	1.88	0.56
1:B:11:ASP:HB3	1:B:14:GLN:HB2	1.89	0.55
1:B:216:ARG:NH2	1:A:233:LEU:O	2.40	0.55
1:A:12:ILE:O	1:A:16:ILE:HG22	2.07	0.55
1:B:253:ILE:HD12	1:B:267:ALA:HB2	1.90	0.54
1:A:226:ILE:HD13	1:A:378:ILE:HD12	1.89	0.53
1:B:108:MET:HG3	1:B:131:TYR:HB2	1.90	0.52
1:A:37:ILE:CD1	1:A:38:LYS:CE	2.88	0.51
1:B:216:ARG:NH1	4:B:611:HOH:O	2.31	0.51
1:B:203:ILE:HA	1:B:206:LEU:HD12	1.93	0.50
1:A:120:ARG:O	1:A:124:LEU:HG	2.11	0.50
1:B:321:VAL:HG22	1:B:337:VAL:HB	1.94	0.50
1:A:62:LYS:CA	1:A:85:LEU:HD11	2.42	0.49
1:A:11:ASP:HB3	1:A:14:GLN:HB2	1.93	0.49
1:A:119:GLN:OE1	1:A:123:GLU:OE1	2.31	0.49
1:B:271:MET:CE	1:B:272:HIS:CE1	2.97	0.48
1:A:122:LYS:CE	1:A:157:ALA:O	2.61	0.48
1:A:20:GLU:CD	1:A:24:ARG:HH12	2.20	0.48
1:B:219:MET:HG2	1:A:378:ILE:HG22	1.96	0.48
1:B:21:LYS:HD3	1:B:196:PRO:HG2	1.96	0.48
1:B:100:ALA:HB1	1:B:105:VAL:O	2.14	0.47
1:B:50:ARG:HE	1:B:50:ARG:HB2	1.43	0.47
1:A:62:LYS:CA	1:A:85:LEU:CD1	2.93	0.47
1:A:21:LYS:HD3	1:A:196:PRO:HG2	1.96	0.46
1:A:64:MET:HE3	1:A:64:MET:CA	2.45	0.46
1:B:39:LYS:N	4:B:601:HOH:O	1.96	0.46
1:B:1:MET:HB2	1:B:1:MET:HE2	1.78	0.45
1:A:164:VAL:HG13	1:A:168:LEU:HD11	1.98	0.45
1:B:271:MET:HE2	1:B:271:MET:HB3	1.85	0.45
1:A:45:VAL:HG11	1:A:79:ALA:HB2	1.97	0.45
1:B:173:ILE:N	1:B:174:PRO:HD2	2.32	0.45
1:B:58:VAL:HG22	1:B:81:VAL:HB	2.00	0.44
1:B:165:ALA:HB2	1:B:185:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HD13	1:B:203:ILE:HG23	2.00	0.44
1:A:284:ILE:HD13	1:A:284:ILE:HA	1.71	0.44
1:A:250:LYS:HG2	1:A:276:ASN:ND2	2.33	0.44
1:A:175:LYS:HD2	1:A:175:LYS:HA	1.74	0.44
1:A:271:MET:HE2	1:A:271:MET:HB3	1.90	0.44
1:B:110:ASP:OD1	1:B:111:LEU:N	2.51	0.43
1:A:229:VAL:O	1:A:233:LEU:HG	2.19	0.43
1:B:136:THR:OG1	1:B:166:GLY:O	2.33	0.43
1:B:164:VAL:HG13	1:B:168:LEU:HD11	2.00	0.42
1:B:16:ILE:HD11	1:B:51:ARG:HG2	2.00	0.42
1:A:110:ASP:OD1	1:A:111:LEU:N	2.53	0.42
1:A:321:VAL:HG22	1:A:337:VAL:HB	2.01	0.42
1:A:245:MET:HE1	1:A:387:LEU:HD11	2.01	0.42
1:B:377:MET:HE3	1:B:377:MET:HA	2.02	0.41
1:A:37:ILE:HD12	1:A:38:LYS:CE	2.50	0.41
1:A:134:VAL:HG11	1:A:154:VAL:HG21	2.02	0.41
1:B:269:ARG:NH2	4:B:617:HOH:O	2.53	0.41
1:A:83:SER:HA	1:A:108:MET:O	2.20	0.41
1:A:241:LEU:HD13	1:A:321:VAL:HG11	2.02	0.41
1:A:80:ASP:O	1:A:105:VAL:HG13	2.21	0.41
1:B:271:MET:HE3	1:B:272:HIS:ND1	2.36	0.41
1:A:151:LEU:HD22	1:A:164:VAL:HG21	2.03	0.41
1:B:94:LYS:HE2	1:B:94:LYS:HB3	1.79	0.40
1:A:29:TRP:CE2	1:A:56:LYS:HE2	2.55	0.40
1:B:1:MET:HB3	1:B:207:PHE:CD2	2.56	0.40
1:A:12:ILE:HB	1:A:40:GLU:HG3	2.03	0.40
1:A:216:ARG:HD3	4:A:610:HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:NZ	1:A:13:GLU:OE1[5_555]	1.51	0.69
4:B:657:HOH:O	4:A:661:HOH:O[3_554]	2.19	0.01

## 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	356/426 (84%)	348 (98%)	8 (2%)	0	100	100
1	B	356/426 (84%)	348 (98%)	8 (2%)	0	100	100
All	All	712/852 (84%)	696 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	291/348 (84%)	290 (100%)	1 (0%)	91	96
1	B	291/348 (84%)	290 (100%)	1 (0%)	91	96
All	All	582/696 (84%)	580 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	VAL
1	A	284	ILE

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

Mol	Chain	Res	Type
1	B	77	HIS

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Mol	Chain	Res	Type
1	A	77	HIS
1	A	276	ASN
1	A	315	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	SO4	B	502	-	4,4,4	0.42	0	6,6,6	0.05	0
3	SO4	A	502	-	4,4,4	0.41	0	6,6,6	0.04	0

There are no bond length outliers.

There are no bond angle outliers.

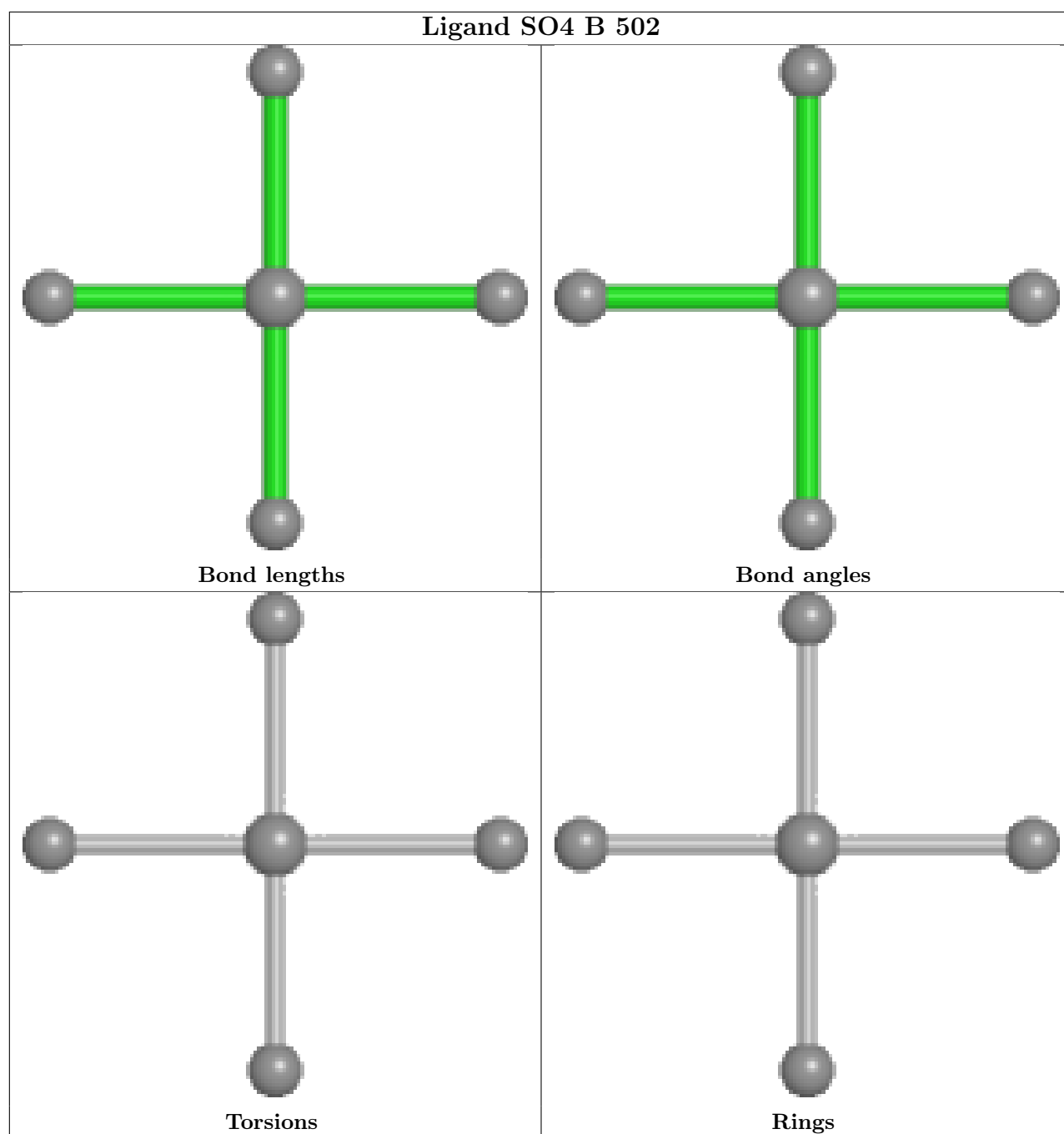
There are no chirality outliers.

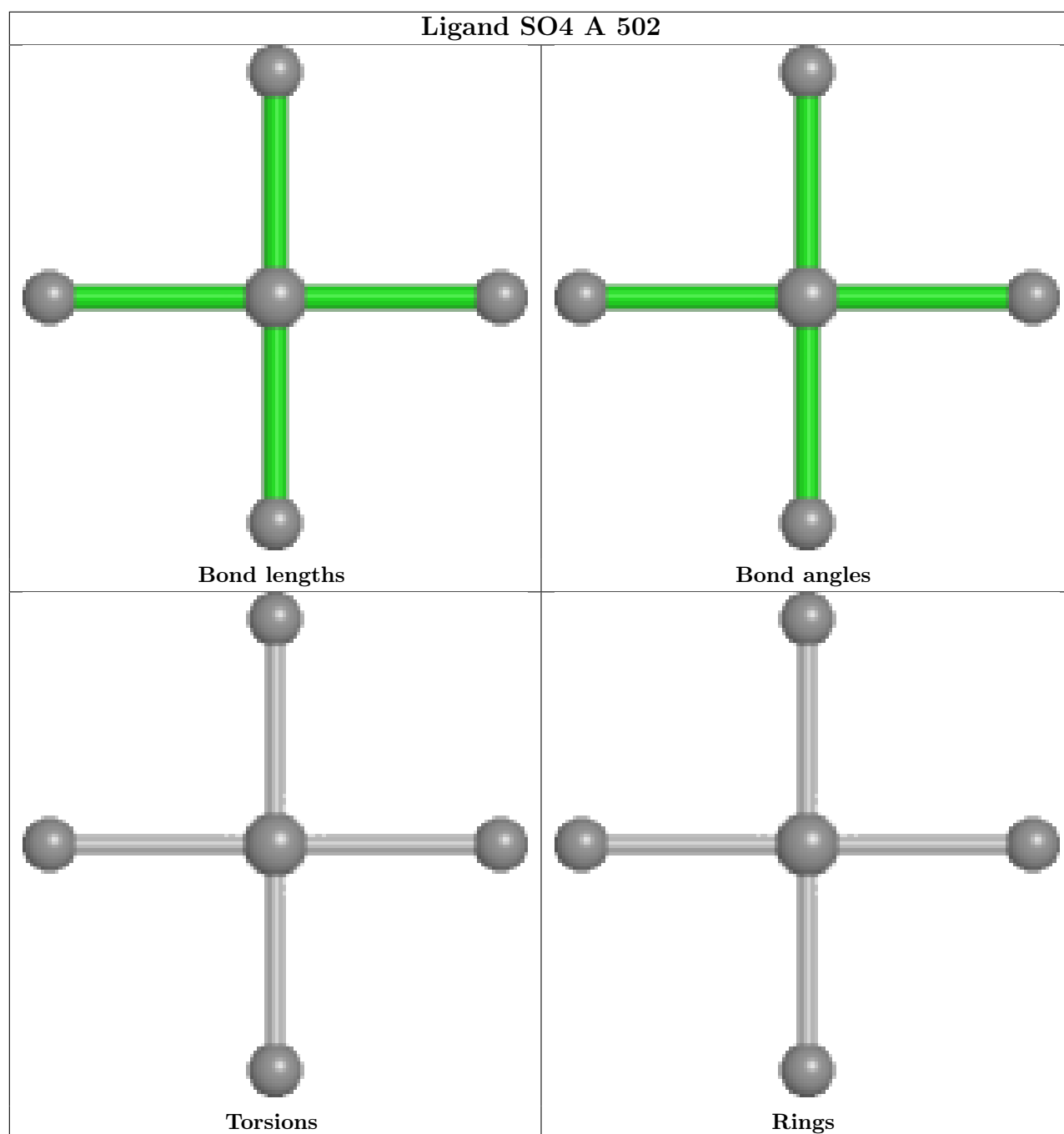
There are no torsion outliers.

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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	362/426 (84%)	0.21	25 (6%) 24 23	25, 47, 90, 106	0
1	B	362/426 (84%)	0.40	29 (8%) 20 19	26, 58, 106, 123	0
All	All	724/852 (84%)	0.30	54 (7%) 22 20	25, 53, 98, 123	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	LEU	4.0
1	A	365	THR	3.9
1	B	15	ALA	3.7
1	B	368	MET	3.7
1	A	115	LYS	3.6
1	A	74	ALA	3.5
1	A	37	ILE	3.4
1	A	343	GLY	3.4
1	B	37	ILE	3.3
1	B	343	GLY	3.3
1	A	10	THR	3.2
1	B	157	ALA	3.2
1	B	9	LEU	3.0
1	B	39	LYS	2.9
1	B	10	THR	2.8
1	A	87	VAL	2.7
1	A	368	MET	2.7
1	A	389	ALA	2.7
1	B	138	ILE	2.7
1	B	8	ASP	2.7
1	A	146	THR	2.7
1	B	12	ILE	2.6
1	A	93	ILE	2.5
1	A	99	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	127	MET	2.4
1	B	19	ALA	2.4
1	A	38	LYS	2.4
1	A	50	ARG	2.4
1	B	367	PRO	2.4
1	B	344	ARG	2.3
1	B	127	MET	2.3
1	A	64	MET	2.3
1	B	124	LEU	2.3
1	B	112	ILE	2.3
1	B	147	PRO	2.3
1	A	128	GLY	2.3
1	A	76	ARG	2.3
1	B	274	ASP	2.2
1	A	47	LEU	2.2
1	B	146	THR	2.2
1	B	45	VAL	2.2
1	B	192	LYS	2.2
1	B	41	GLY	2.2
1	A	113	GLY	2.2
1	B	92	THR	2.1
1	A	8	ASP	2.1
1	B	118	VAL	2.1
1	B	44	ALA	2.1
1	A	65	ASP	2.1
1	A	123	GLU	2.0
1	B	64	MET	2.0
1	A	69	LEU	2.0
1	B	13	GLU	2.0
1	B	85	LEU	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

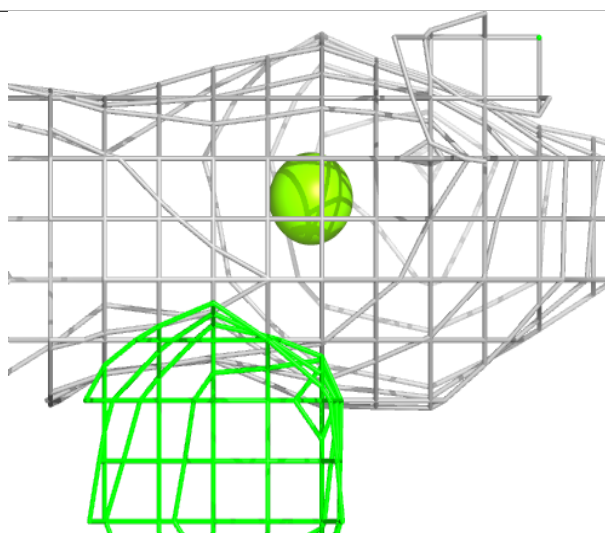
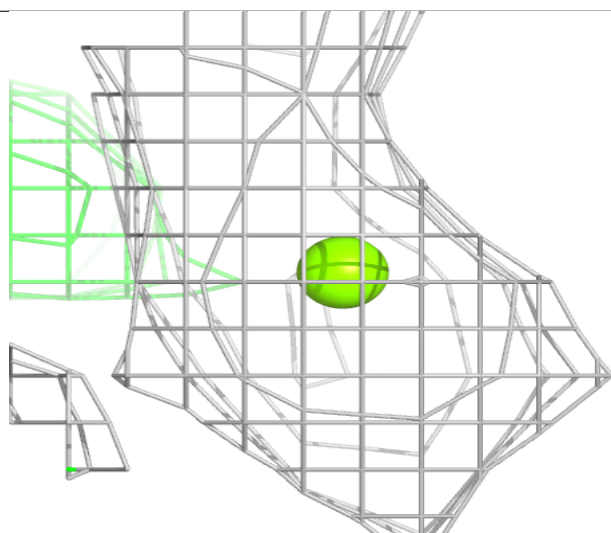
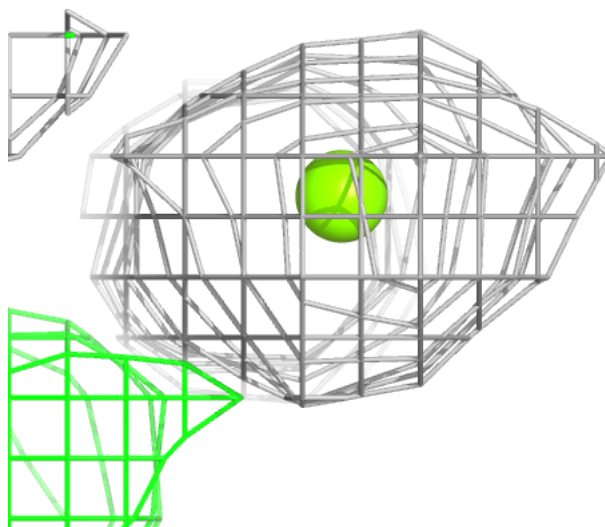
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	501	1/1	0.66	0.24	74,74,74,74	0
2	MG	A	501	1/1	0.76	0.29	65,65,65,65	0
3	SO4	A	502	5/5	0.80	0.23	55,70,73,96	5
3	SO4	B	502	5/5	0.86	0.25	79,79,90,95	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.

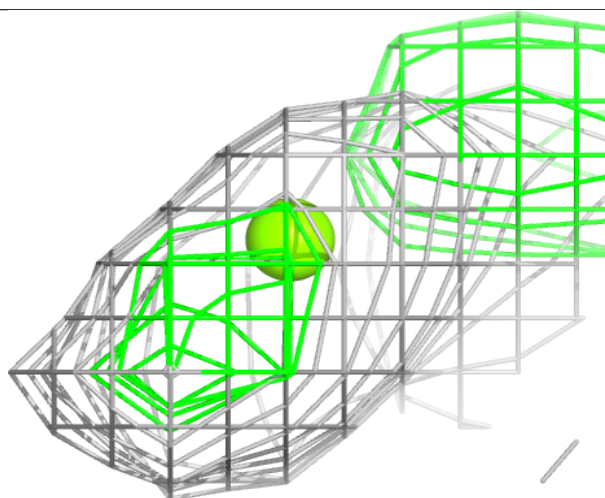
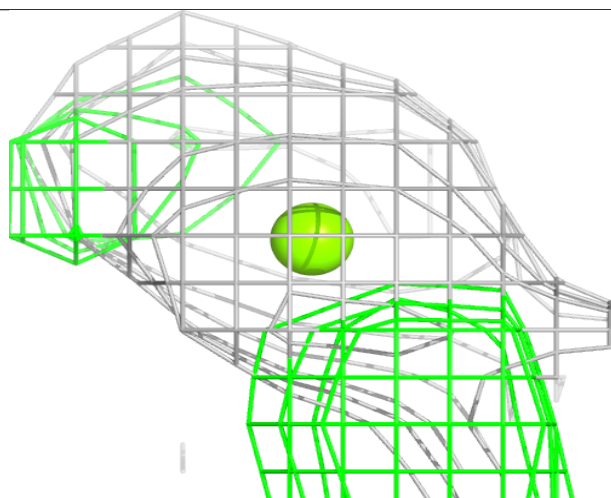
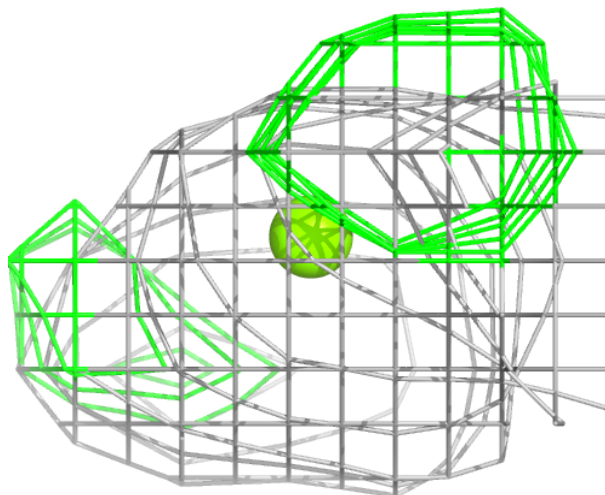
**Electron density around MG B 501:**

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



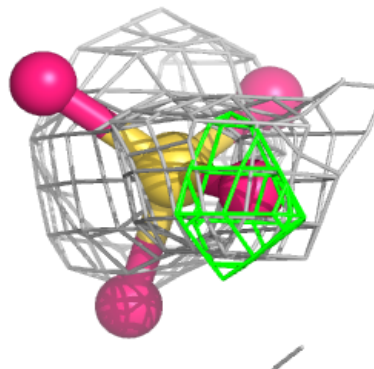
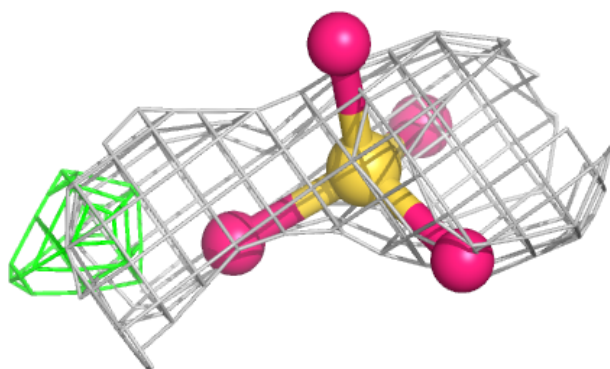
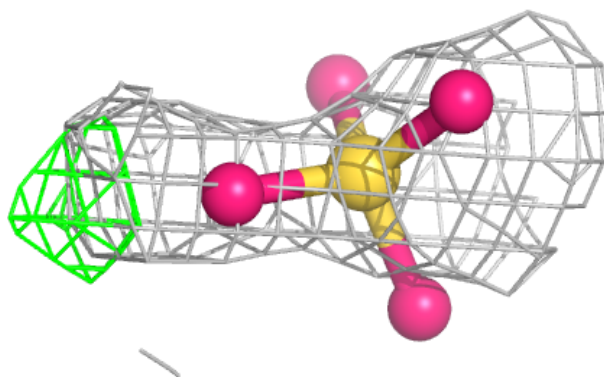
**Electron density around MG A 501:**

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

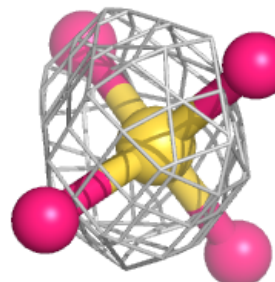
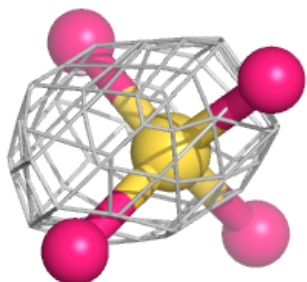
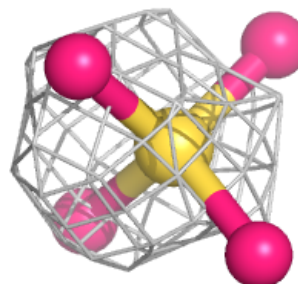


**Electron density around SO4 A 502:**

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

**Electron density around SO4 B 502:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.