



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2026 – 12:32 AM UTC

PDB ID : 22GI / pdb\_000022gi  
Title : 3D1 Fab in complex with pepAVVNQN  
Authors : Lei, Y.  
Deposited on : 2026-01-09  
Resolution : 2.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : **FAILED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

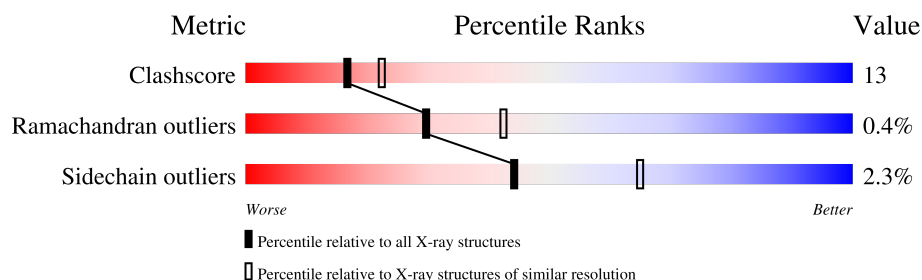
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	211	
1	B	211	
1	G	211	
1	J	211	
2	C	220	
2	D	220	
2	H	220	
2	K	220	

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Mol	Chain	Length	Quality of chain
3	E	6	 33% 50% 17%
3	F	6	 83% 17%
3	I	6	 83% 17%
3	L	6	 67% 33%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12883 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 Light chain of 3D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1548	968	255	321	4			
1	B	210	Total	C	N	O	S	0	0	0
			1548	968	255	321	4			
1	G	209	Total	C	N	O	S	0	0	0
			1542	965	254	319	4			
1	J	209	Total	C	N	O	S	0	0	0
			1543	965	254	320	4			

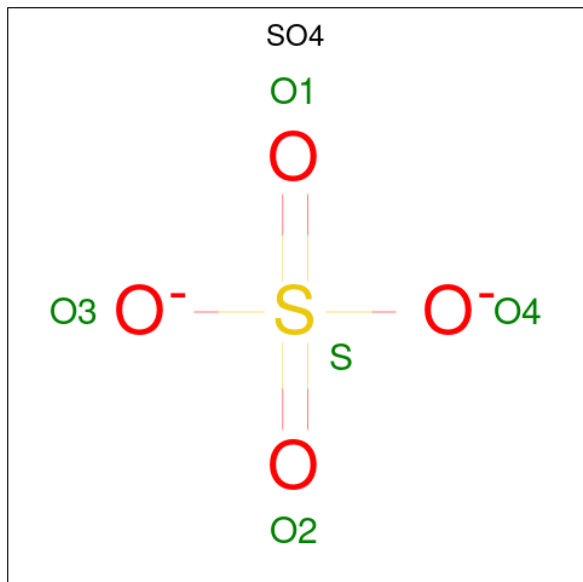
- Molecule 2 is a protein called Heavy chain of 3D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1596	1015	263	312	6			
2	D	214	Total	C	N	O	S	0	0	0
			1596	1015	263	312	6			
2	H	214	Total	C	N	O	S	0	0	0
			1596	1015	263	312	6			
2	K	213	Total	C	N	O	S	0	0	0
			1590	1012	262	310	6			

- Molecule 3 is a protein called ALA-VAL-VAL-ASN-GLN-ASN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			44	26	9	9			
3	F	6	Total	C	N	O	0	0	0
			44	26	9	9			
3	I	6	Total	C	N	O	0	0	0
			44	26	9	9			
3	L	6	Total	C	N	O	0	0	0
			44	26	9	9			

- Molecule 4 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
4	C	1	Total	O	S	5	0
			5	4	1		
4	H	1	Total	O	S	5	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	14	Total	O	0	0
			14	14		
5	C	15	Total	O	0	0
			15	15		
5	D	19	Total	O	0	0
			19	19		
5	G	23	Total	O	0	0
			23	23		
5	H	18	Total	O	0	0
			18	18		
5	J	15	Total	O	0	0
			15	15		
5	K	9	Total	O	0	0
			9	9		

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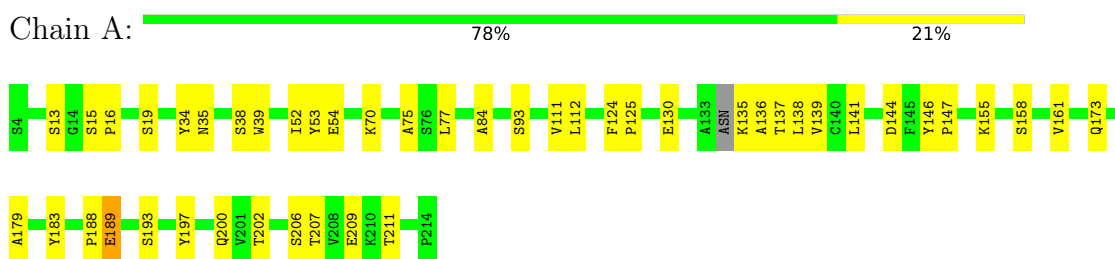
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	O	0	0
			1	1		

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

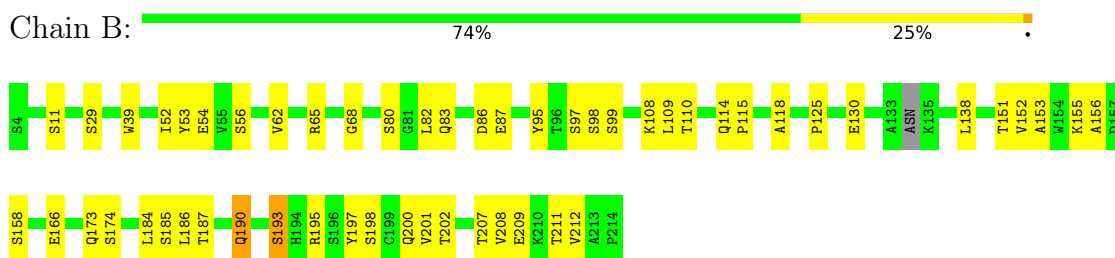
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

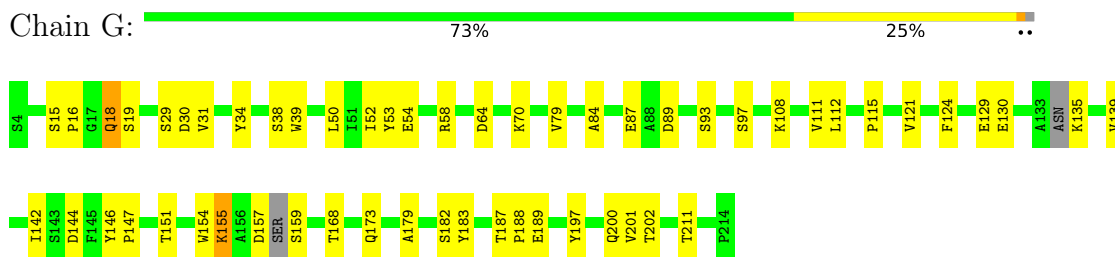
- Molecule 1: Light chain of 3D1



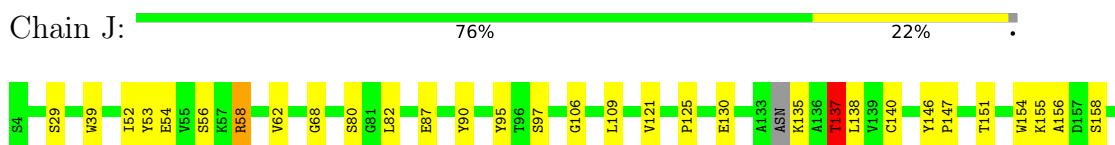
- Molecule 1: Light chain of 3D1



- Molecule 1: Light chain of 3D1



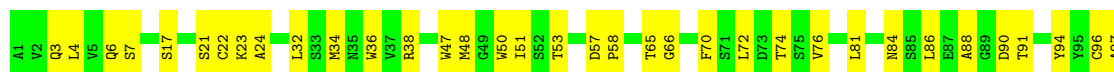
- Molecule 1: Light chain of 3D1





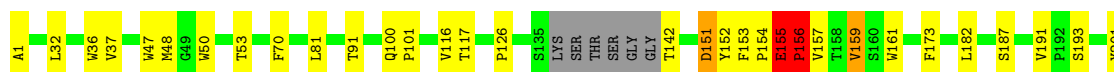
• Molecule 2: Heavy chain of 3D1

Chain C: 69% 27% ..



• Molecule 2: Heavy chain of 3D1

Chain D: 79% 16% ..



• Molecule 2: Heavy chain of 3D1

Chain H: 73% 21% ..



• Molecule 2: Heavy chain of 3D1

Chain K: 69% 26% ..




• Molecule 3: ALA-VAL-VAL-ASN-GLN-ASN

Chain E: 33% 50% 17%




- Molecule 3: ALA-VAL-VAL-ASN-GLN-ASN

Chain F:  83% 17%



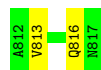
- Molecule 3: ALA-VAL-VAL-ASN-GLN-ASN

Chain I:  83% 17%



- Molecule 3: ALA-VAL-VAL-ASN-GLN-ASN

Chain L:  67% 33%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.50Å 58.62Å 128.44Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	2.73 – 2.64	Depositor
% Data completeness (in resolution range)	97.7 (2.73-2.64)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.63Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.212 , 0.296	Depositor
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.677	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
Total number of atoms	12883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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

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	0/1586	0.81	2/2164 (0.1%)
1	B	0.59	0/1586	0.81	1/2164 (0.0%)
1	G	0.60	1/1579 (0.1%)	0.77	3/2153 (0.1%)
1	J	0.58	1/1580 (0.1%)	0.85	4/2154 (0.2%)
2	C	0.53	1/1639 (0.1%)	0.79	7/2239 (0.3%)
2	D	0.70	2/1639 (0.1%)	0.99	6/2239 (0.3%)
2	H	0.92	4/1639 (0.2%)	1.09	7/2239 (0.3%)
2	K	0.61	1/1633 (0.1%)	0.83	1/2231 (0.0%)
3	E	1.00	0/43	1.56	0/58
3	F	0.53	0/43	1.10	0/58
3	I	0.42	0/43	0.76	0/58
3	L	0.48	0/43	0.92	0/58
All	All	0.65	10/13053 (0.1%)	0.88	31/17815 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	58	ARG	C-N	12.26	1.50	1.33
2	C	219	GLU	C-N	10.53	1.51	1.34
2	K	153	PHE	C-N	8.00	1.49	1.34
2	H	153	PHE	C-O	-6.05	1.17	1.24
2	D	153	PHE	C-O	-5.96	1.17	1.24

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	156	PRO	CA-N-CD	-18.85	85.61	112.00
2	H	156	PRO	CA-N-CD	-18.31	86.36	112.00
1	J	137	THR	CB-CA-C	-12.45	81.92	109.56
1	J	58	ARG	CA-C-N	11.37	131.49	119.78
1	J	58	ARG	C-N-CA	11.37	131.49	119.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	155	GLU	Mainchain

## 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	1548	0	1494	35	0
1	B	1548	0	1494	42	1
1	G	1542	0	1488	37	0
1	J	1543	0	1488	38	0
2	C	1596	0	1548	59	2
2	D	1596	0	1548	32	1
2	H	1596	0	1548	40	1
2	K	1590	0	1543	52	1
3	E	44	0	42	6	0
3	F	44	0	42	2	0
3	I	44	0	42	1	0
3	L	44	0	42	5	0
4	C	5	0	0	0	0
4	H	5	0	0	0	0
5	A	24	0	0	3	0
5	B	14	0	0	7	0
5	C	15	0	0	4	0
5	D	19	0	0	3	0
5	G	23	0	0	2	0
5	H	18	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	15	0	0	2	0
5	K	9	0	0	2	0
5	L	1	0	0	0	0
All	All	12883	0	12319	321	3

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 13.

The worst 5 of 321 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)
2:C:51:ILE:HD13	2:C:58:PRO:HB3	1.37	1.02
1:G:155:LYS:HE2	1:G:200:GLN:OE1	1.65	0.96
1:J:173:GLN:HG3	1:J:174:SER:H	1.31	0.94
2:K:91:THR:HG22	2:K:118:VAL:H	1.32	0.94
1:B:186:LEU:HB3	1:B:190:GLN:HG3	1.51	0.92

All (3) 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)
2:H:217:LYS:NZ	2:K:211:ASN:O[1_655]	1.91	0.29
1:B:83:GLN:OE1	2:C:23:LYS:NZ[2_455]	2.10	0.10
2:C:212:THR:CG2	2:D:216:LYS:NZ[2_555]	2.17	0.03

## 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	206/211 (98%)	190 (92%)	16 (8%)	0	100	100
1	B	206/211 (98%)	199 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	203/211 (96%)	190 (94%)	13 (6%)	0	100	100
1	J	203/211 (96%)	193 (95%)	10 (5%)	0	100	100
2	C	210/220 (96%)	198 (94%)	11 (5%)	1 (0%)	24	36
2	D	210/220 (96%)	204 (97%)	4 (2%)	2 (1%)	12	18
2	H	210/220 (96%)	201 (96%)	7 (3%)	2 (1%)	12	18
2	K	209/220 (95%)	199 (95%)	8 (4%)	2 (1%)	12	18
3	E	4/6 (67%)	2 (50%)	2 (50%)	0	100	100
3	F	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
3	I	4/6 (67%)	4 (100%)	0	0	100	100
3	L	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	1673/1748 (96%)	1586 (95%)	80 (5%)	7 (0%)	30	42

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	156	PRO
2	H	156	PRO
2	D	151	ASP
2	K	156	PRO
2	C	219	GLU

### 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	176/177 (99%)	170 (97%)	6 (3%)	32	52
1	B	176/177 (99%)	172 (98%)	4 (2%)	44	65
1	G	175/177 (99%)	171 (98%)	4 (2%)	44	65
1	J	176/177 (99%)	174 (99%)	2 (1%)	65	79
2	C	178/183 (97%)	178 (100%)	0	100	100
2	D	178/183 (97%)	177 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	178/183 (97%)	167 (94%)	11 (6%)	16	28
2	K	177/183 (97%)	174 (98%)	3 (2%)	53	72
3	E	5/5 (100%)	3 (60%)	2 (40%)	0	0
3	F	5/5 (100%)	5 (100%)	0	100	100
3	I	5/5 (100%)	5 (100%)	0	100	100
3	L	5/5 (100%)	5 (100%)	0	100	100
All	All	1434/1460 (98%)	1401 (98%)	33 (2%)	44	65

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	135	LYS
1	J	137	THR
2	K	158	THR
3	E	814	VAL
3	E	813	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	82	GLN
2	H	206	ASN
2	K	100	GLN
1	J	132	GLN
2	C	206	ASN

### 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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	C	301	-	4,4,4	0.22	0	6,6,6	0.09	0
4	SO4	H	301	-	4,4,4	0.22	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

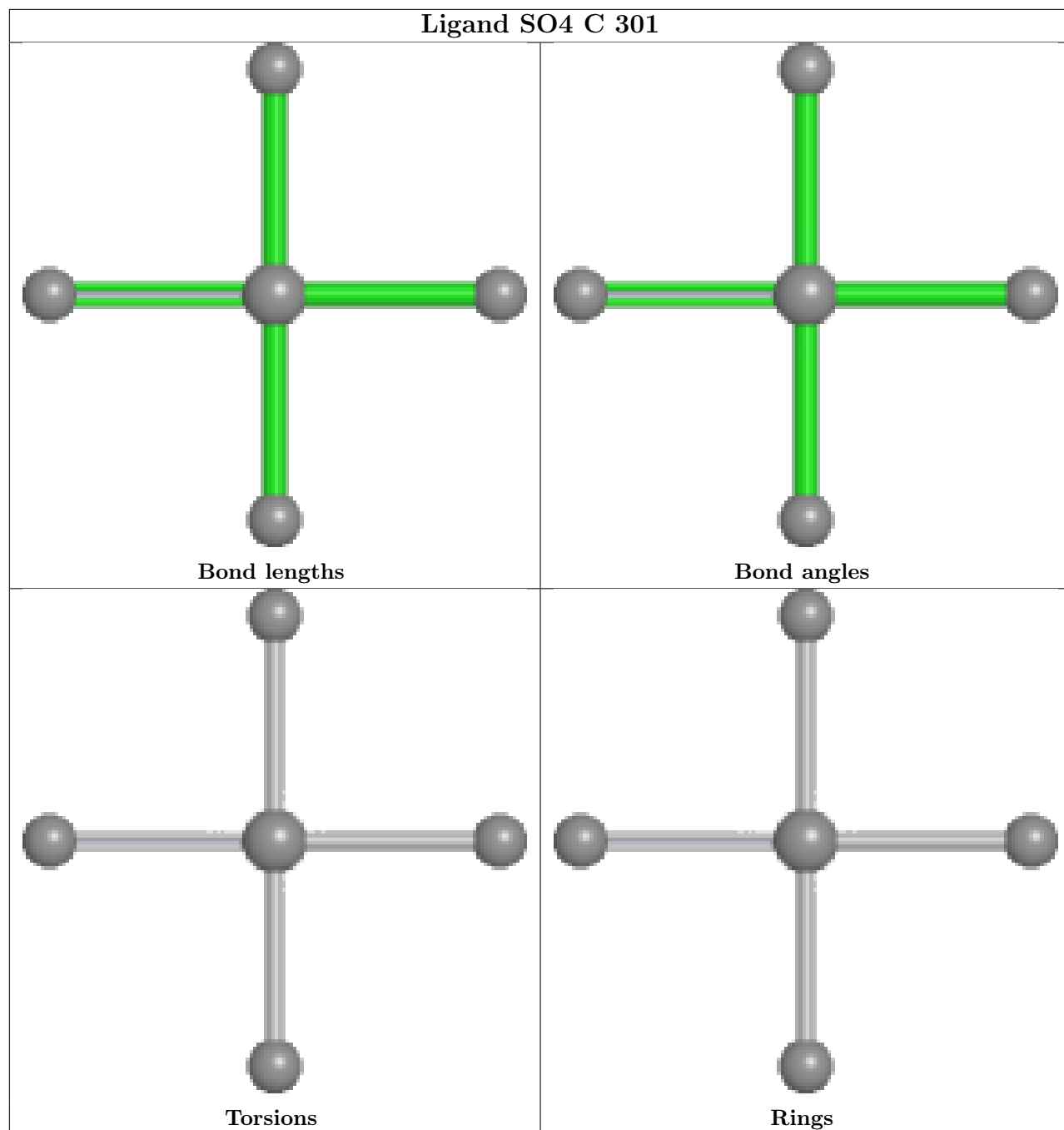
There are no chirality outliers.

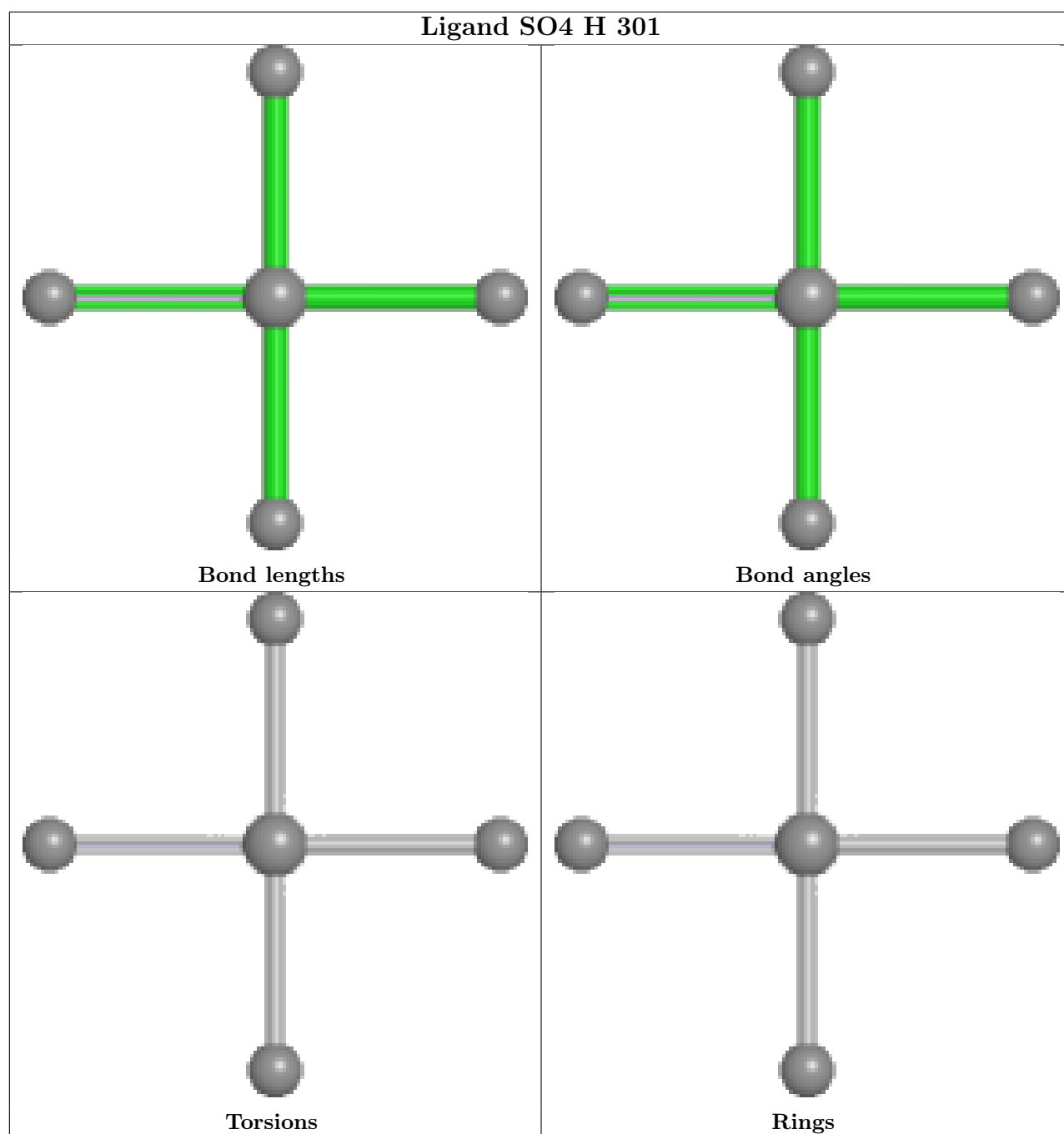
There are no torsion outliers.

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

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.