



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:28 AM UTC

PDB ID : 9GAL / pdb\_00009gal  
Title : 3-methylbenzoyl-CoA reductase from *Thauera chlorobenzoica* (subunits Mb-dON) + ADP  
Authors : Ermler, U.; Boll, M.; Demmer, U.; Fuchs, J.  
Deposited on : 2024-07-29  
Resolution : 2.15 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 : 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

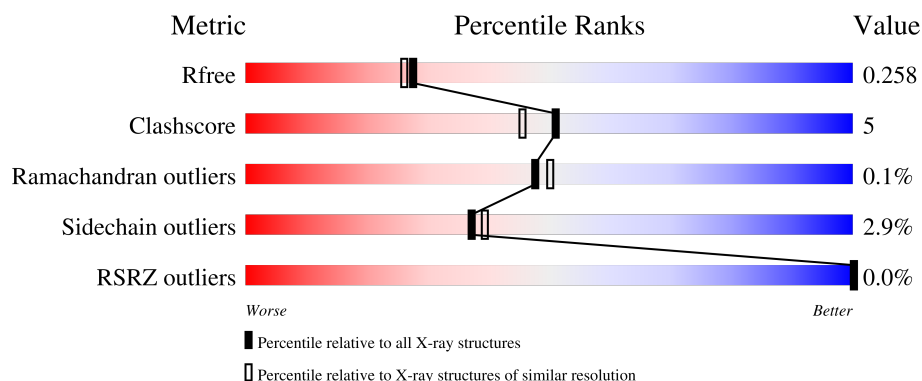
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	445	 83% 15% .
1	E	445	 84% 12% ..
1	I	445	 86% 10% ..
1	M	445	 84% 14% ..
2	B	388	 89% 10% .

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Mol	Chain	Length	Quality of chain
2	F	388	 89% 11%
2	J	388	 89% 11%
2	N	388	 89% 10%
3	C	273	 84% 11% ..
3	G	273	 78% 18% ..
3	K	273	 84% 12% ..
3	O	273	 81% 15% ..
4	D	269	 81% 14% ..
4	H	269	 84% 12% ..
4	L	269	 80% 15% ..
4	P	269	 79% 17% ..

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 42682 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-methylbenzoyl-CoA reductase beta subunit MbdO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	2	0
			3471	2200	602	651	18			
1	E	436	Total	C	N	O	S	0	2	0
			3464	2196	597	653	18			
1	I	436	Total	C	N	O	S	0	3	0
			3473	2202	599	654	18			
1	M	437	Total	C	N	O	S	0	2	0
			3468	2198	599	653	18			

- Molecule 2 is a protein called 3-methylbenzoyl-CoA reductase gamma subunit MbdN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S	0	0	0
			3093	1965	525	588	15			
2	F	387	Total	C	N	O	S	0	0	0
			3093	1965	525	588	15			
2	J	387	Total	C	N	O	S	0	0	0
			3093	1965	525	588	15			
2	N	387	Total	C	N	O	S	0	0	0
			3093	1965	525	588	15			

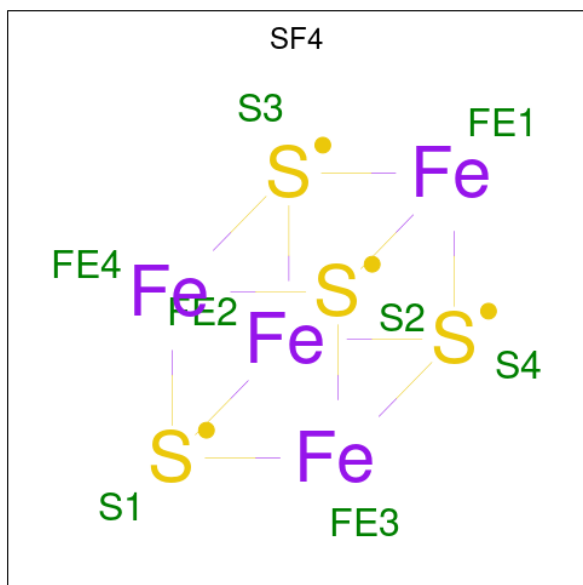
- Molecule 3 is a protein called 3-methylbenzoyl-CoA reductase delta subunit MbdP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	264	Total	C	N	O	S	0	3	0
			2023	1264	360	385	14			
3	G	264	Total	C	N	O	S	0	3	0
			2026	1266	363	383	14			
3	K	264	Total	C	N	O	S	0	1	0
			2004	1254	355	381	14			
3	O	264	Total	C	N	O	S	0	2	0
			2015	1260	359	382	14			

- Molecule 4 is a protein called 3-methylbenzoyl-CoA reductase alpha subunit MbdQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	261	Total	C	N	O	S	0	1	0
			1934	1215	345	363	11			
4	H	261	Total	C	N	O	S	0	0	0
			1928	1212	344	361	11			
4	L	261	Total	C	N	O	S	0	1	0
			1939	1218	348	362	11			
4	P	261	Total	C	N	O	S	0	1	0
			1939	1218	348	362	11			

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



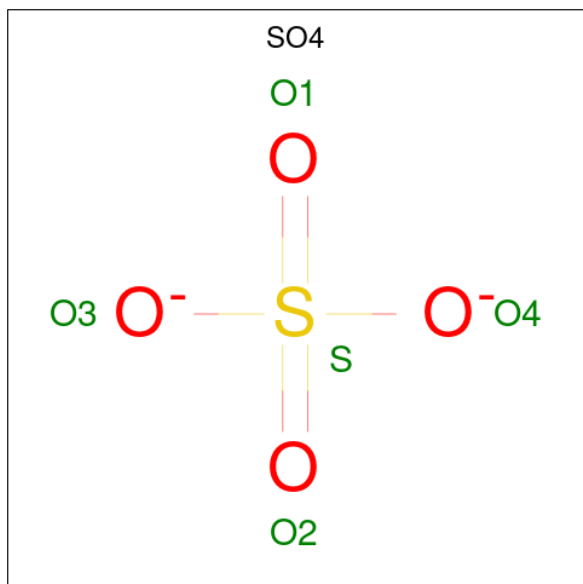
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	D	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		
5	F	1	Total	Fe	S	0	0
			8	4	4		
5	G	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	Fe	S	0	0
			8	4	4		
5	J	1	Total	Fe	S	0	0
			8	4	4		
5	L	1	Total	Fe	S	0	0
			8	4	4		
5	M	1	Total	Fe	S	0	0
			8	4	4		
5	N	1	Total	Fe	S	0	0
			8	4	4		
5	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



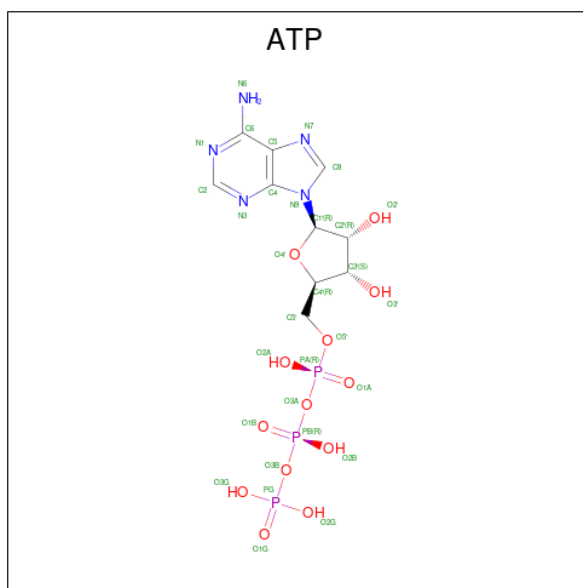
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	N	1	Total	O	S	0	0
			5	4	1		
6	O	1	Total	O	S	0	0
			5	4	1		
6	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

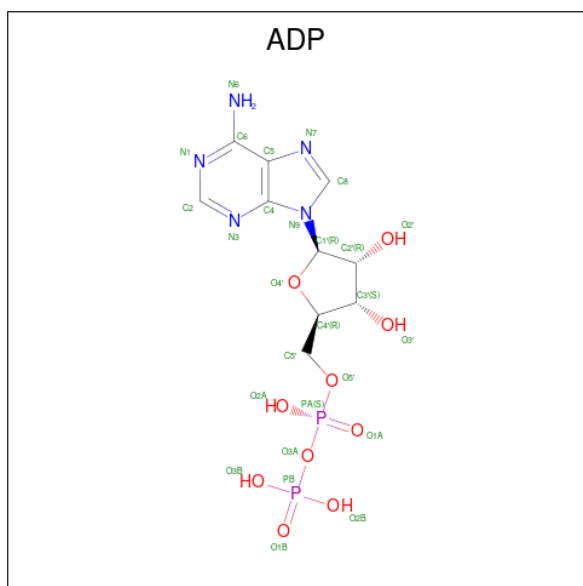


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	
			31	10	5	13	3	0
7	G	1	Total	C	N	O	P	
			31	10	5	13	3	0
7	K	1	Total	C	N	O	P	
			31	10	5	13	3	0
7	O	1	Total	C	N	O	P	
			31	10	5	13	3	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0
8	G	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0
8	K	1	Total Mg 1 1	0	0
8	L	1	Total Mg 1 1	0	0
8	O	1	Total Mg 1 1	0	0
8	P	1	Total Mg 1 1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C N O P 27 10 5 10 2	0	0
9	H	1	Total C N O P 27 10 5 10 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	P	
			27	10	5	10	2	
9	P	1	Total	C	N	O	P	
			27	10	5	10	2	

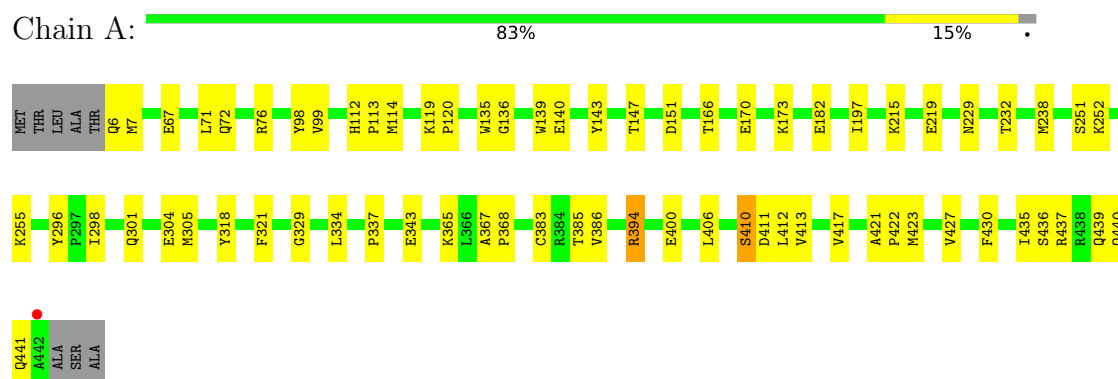
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	13	Total	O		
			13	13	0	0
10	B	17	Total	O		
			17	17	0	0
10	C	8	Total	O		
			8	8	0	0
10	D	7	Total	O		
			7	7	0	0
10	E	18	Total	O		
			18	18	0	0
10	F	25	Total	O		
			26	26	0	1
10	G	14	Total	O		
			14	14	0	0
10	H	9	Total	O		
			9	9	0	0
10	I	15	Total	O		
			15	15	0	0
10	J	36	Total	O		
			36	36	0	0
10	K	12	Total	O		
			12	12	0	0
10	L	12	Total	O		
			12	12	0	0
10	M	9	Total	O		
			9	9	0	0
10	N	10	Total	O		
			10	10	0	0
10	O	14	Total	O		
			14	14	0	0
10	P	10	Total	O		
			10	10	0	0

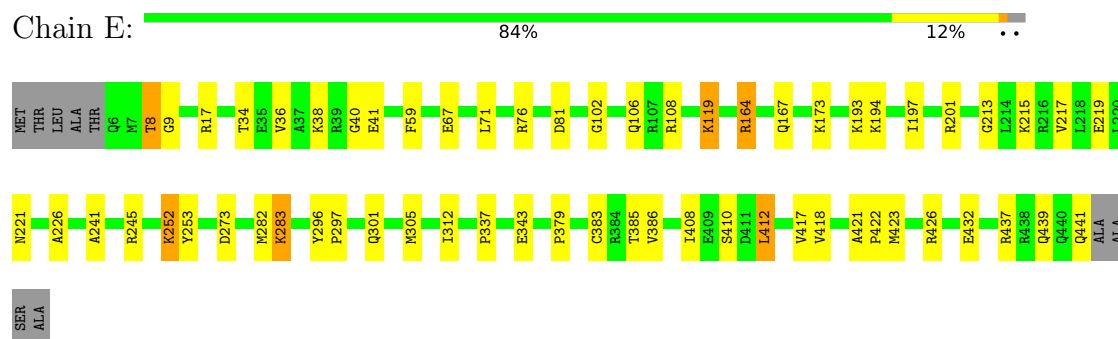
### 3 Residue-property plots

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.

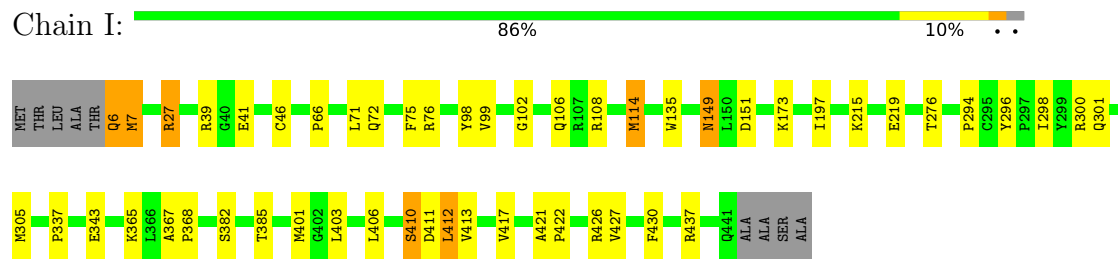
- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO




- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO



- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO



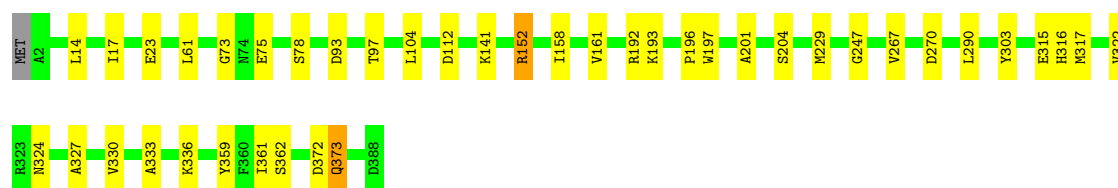
- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO

Chain M:  84% 14% ..




• Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN

Chain B:  89% 10% .




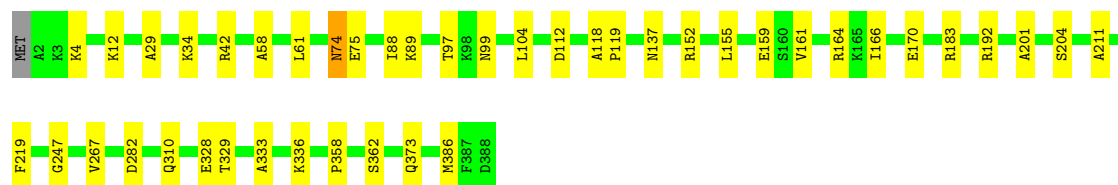
• Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN

Chain F:  89% 11%



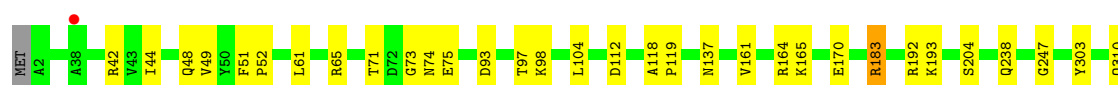
• Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN

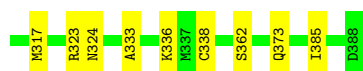
Chain J:  89% 11%



• Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN

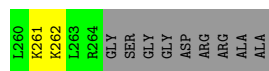
Chain N:  89% 10%





- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain C: 84% 11% ..



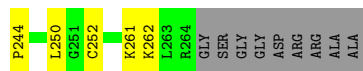
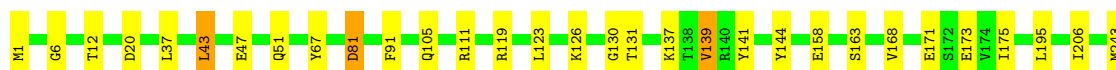
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain G: 78% 18% ..



- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain K: 84% 12% ..



- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

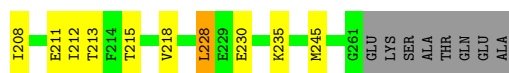
Chain O: 81% 15% ..



- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

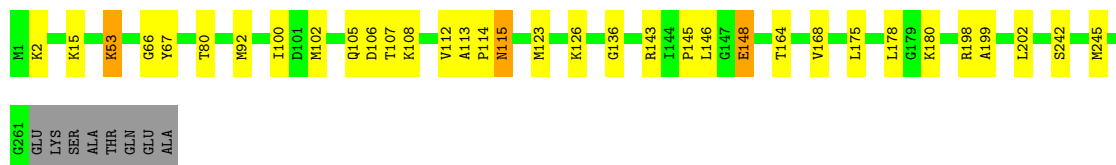
Chain D: 81% 14% ..





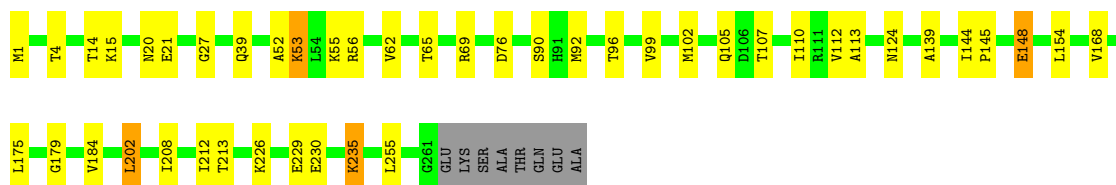
- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain H: 84% 12% ..



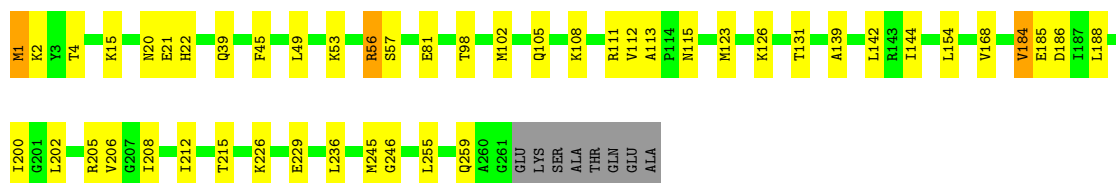
- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain L: 80% 15% ..



- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain P: 79% 17% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.92Å 157.90Å 165.15Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	47.81 – 2.15 47.81 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.81-2.15) 97.4 (47.81-2.15)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.238 , 0.260 0.239 , 0.258	Depositor DCC
$R_{free}$ test set	16470 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 25.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.097 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: ATP, ADP, SF4, 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	0.20	0/3546	0.36	0/4792
1	E	0.17	0/3539	0.35	0/4783
1	I	0.20	0/3548	0.36	0/4794
1	M	0.19	0/3543	0.37	0/4789
2	B	0.16	0/3159	0.36	0/4281
2	F	0.18	0/3159	0.35	0/4281
2	J	0.17	0/3159	0.36	0/4281
2	N	0.19	0/3159	0.37	2/4281 (0.0%)
3	C	0.16	0/2050	0.32	0/2765
3	G	0.18	0/2053	0.33	0/2768
3	K	0.16	0/2031	0.32	0/2740
3	O	0.19	0/2042	0.35	0/2754
4	D	0.16	0/1962	0.33	0/2642
4	H	0.18	0/1956	0.36	0/2634
4	L	0.16	0/1967	0.35	0/2648
4	P	0.16	0/1967	0.36	0/2648
All	All	0.18	0/42840	0.35	2/57881 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	48	GLN	CA-C-N	5.03	130.76	121.70
2	N	48	GLN	C-N-CA	5.03	130.76	121.70

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	3471	0	3404	36	0
1	E	3464	0	3390	40	0
1	I	3473	0	3402	30	0
1	M	3468	0	3395	41	0
2	B	3093	0	3036	30	0
2	F	3093	0	3036	28	0
2	J	3093	0	3036	24	0
2	N	3093	0	3036	26	0
3	C	2023	0	2047	19	0
3	G	2026	0	2056	31	0
3	K	2004	0	2032	23	0
3	O	2015	0	2044	25	0
4	D	1934	0	1966	32	0
4	H	1928	0	1962	27	0
4	L	1939	0	1974	29	0
4	P	1939	0	1974	34	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
5	D	8	0	0	0	0
5	E	8	0	0	0	0
5	F	8	0	0	0	0
5	G	8	0	0	0	0
5	I	8	0	0	0	0
5	J	8	0	0	0	0
5	L	8	0	0	0	0
5	M	8	0	0	0	0
5	N	8	0	0	1	0
5	O	8	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
6	G	5	0	0	0	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
6	M	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	5	0	0	0	0
6	O	5	0	0	0	0
6	P	5	0	0	0	0
7	C	31	0	12	0	0
7	G	31	0	12	1	0
7	K	31	0	12	0	0
7	O	31	0	12	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	D	27	0	12	1	0
9	H	27	0	12	0	0
9	L	27	0	12	0	0
9	P	27	0	12	1	0
10	A	13	0	0	0	0
10	B	17	0	0	0	0
10	C	8	0	0	1	0
10	D	7	0	0	0	0
10	E	18	0	0	1	0
10	F	26	0	0	0	0
10	G	14	0	0	0	0
10	H	9	0	0	0	0
10	I	15	0	0	0	0
10	J	36	0	0	0	0
10	K	12	0	0	0	0
10	L	12	0	0	0	0
10	M	9	0	0	0	0
10	N	10	0	0	0	0
10	O	14	0	0	2	0
10	P	10	0	0	1	0
All	All	42682	0	41886	438	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (438) 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:F:71:THR:HG22	2:F:73:GLY:H	1.30	0.94
2:N:71:THR:HG22	2:N:73:GLY:H	1.34	0.90
4:D:102:MET:HE3	4:D:131:THR:HG21	1.56	0.87
4:D:208:ILE:HG23	4:D:212:ILE:HD11	1.59	0.85
1:A:197:ILE:HD11	1:A:337:PRO:HG2	1.61	0.81
4:P:208:ILE:HG23	4:P:212:ILE:HD11	1.61	0.80
3:C:108:LYS:HG2	3:C:123:LEU:HD22	1.64	0.79
1:E:8:THR:HG22	1:E:252:LYS:HE3	1.66	0.77
4:H:242:SER:HA	4:H:245:MET:HE2	1.67	0.77
4:P:1:MET:HG3	4:P:2:LYS:H	1.48	0.77
2:N:183:ARG:HH11	2:N:183:ARG:HB2	1.50	0.77
3:C:139:VAL:HG22	3:C:144:TYR:HB2	1.69	0.75
4:L:208:ILE:HG23	4:L:212:ILE:HD11	1.68	0.74
2:F:71:THR:HG21	2:F:93:ASP:OD2	1.87	0.74
1:A:72:GLN:OE1	1:A:114:MET:HE1	1.89	0.73
2:B:152:ARG:HD3	2:B:290:LEU:HD12	1.72	0.71
2:N:71:THR:HG21	2:N:93:ASP:OD2	1.90	0.71
3:O:139:VAL:HG22	3:O:144:TYR:HB2	1.73	0.71
1:A:436:SER:O	1:A:440:GLN:N	2.23	0.71
4:D:92:MET:HA	4:D:92:MET:HE2	1.73	0.70
2:F:373:GLN:HG2	3:G:123:LEU:HD12	1.72	0.70
1:I:71:LEU:HD11	1:I:296:TYR:CG	2.27	0.69
4:P:45:PHE:HE2	4:P:56:ARG:HD2	1.57	0.69
1:I:197:ILE:HD11	1:I:337:PRO:HG2	1.73	0.68
2:J:42:ARG:HB2	2:J:61:LEU:CD2	2.23	0.67
4:D:98:THR:HB	4:D:212:ILE:HG12	1.77	0.67
4:D:191:VAL:O	4:D:195:ILE:HD12	1.95	0.67
1:M:262:GLU:O	1:M:266:VAL:HG23	1.94	0.66
4:P:229:GLU:HG2	4:P:236:LEU:HD13	1.78	0.66
1:M:71:LEU:HD11	1:M:296:TYR:CG	2.32	0.65
1:E:426:ARG:NH1	4:H:123:MET:HE2	2.11	0.65
2:F:34:LYS:NZ	2:F:99:ASN:O	2.28	0.65
4:P:1:MET:HE1	4:P:22:HIS:NE2	2.12	0.65
1:M:364:LYS:HG2	1:M:401:MET:HE3	1.79	0.64
3:K:139:VAL:HG22	3:K:144:TYR:HB2	1.78	0.64
1:E:432:GLU:OE1	4:H:80:THR:HG21	1.98	0.64
2:F:234:GLN:OE1	2:F:234:GLN:N	2.25	0.64
1:I:71:LEU:HD11	1:I:296:TYR:CD2	2.33	0.63
1:M:197:ILE:HD11	1:M:337:PRO:HG2	1.79	0.63
3:G:139:VAL:HG22	3:G:144:TYR:HB2	1.81	0.63
1:M:364:LYS:CG	1:M:401:MET:HE3	2.28	0.62
2:F:373:GLN:CG	3:G:123:LEU:HD12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:255:LEU:HD23	3:O:258:LEU:HD12	1.81	0.62
3:C:87:ARG:HG3	3:C:255:LEU:HD21	1.81	0.62
1:I:27:ARG:HD2	1:I:27:ARG:O	2.00	0.62
2:N:164:ARG:NH1	2:N:165:LYS:O	2.34	0.60
2:J:159:GLU:HG2	2:J:166:ILE:HG12	1.83	0.60
2:F:312:LYS:HA	2:F:317:MET:HE3	1.84	0.60
2:B:361:ILE:HD12	3:C:122[B]:ARG:CZ	2.31	0.60
3:K:91:PHE:HD2	3:K:250:LEU:HD21	1.66	0.60
2:N:164:ARG:HH22	2:N:170:GLU:CD	2.10	0.60
3:K:1:MET:SD	3:K:20:ASP:HB2	2.41	0.59
4:H:92:MET:HE2	4:H:92:MET:HA	1.85	0.59
4:P:1:MET:HE1	4:P:22:HIS:CE1	2.37	0.59
1:A:410:SER:OG	1:A:411:ASP:N	2.35	0.59
3:K:43:LEU:O	3:K:47:GLU:HG3	2.02	0.59
4:P:202:LEU:HD12	4:P:205:ARG:HH11	1.67	0.59
1:E:164:ARG:HG2	1:E:164:ARG:HH11	1.68	0.59
4:D:102:MET:CE	4:D:131:THR:HG21	2.31	0.58
3:G:168:VAL:HG23	4:H:168:VAL:HG23	1.85	0.58
2:B:247:GLY:HA3	2:B:333:ALA:O	2.02	0.58
1:E:197:ILE:HD11	1:E:337:PRO:HG2	1.86	0.58
1:E:282:MET:CE	1:E:312:ILE:HD12	2.33	0.58
1:E:385:THR:HA	2:F:112:ASP:HB3	1.85	0.58
3:G:197:LYS:NZ	3:G:231:GLU:OE2	2.32	0.58
2:J:74:ASN:C	2:J:74:ASN:OD1	2.47	0.58
3:C:138:THR:HG22	3:C:142:MET:HE2	1.86	0.58
3:C:168:VAL:HG23	4:D:168:VAL:HG23	1.86	0.58
3:O:111:ARG:HG2	3:O:206:ILE:HD12	1.86	0.57
2:N:247:GLY:HA3	2:N:333:ALA:O	2.05	0.57
3:O:97[B]:ARG:HD2	3:O:210:SER:O	2.04	0.57
4:P:1:MET:CG	4:P:2:LYS:H	2.18	0.57
2:B:75:GLU:HG3	2:B:97:THR:HG22	1.85	0.57
1:I:298:ILE:O	1:I:298:ILE:HG13	2.04	0.56
2:N:193:LYS:HE2	2:N:324:ASN:O	2.05	0.56
4:P:144:ILE:HD11	4:P:184:VAL:HG21	1.85	0.56
1:I:385:THR:HA	2:J:112:ASP:HB3	1.86	0.56
3:O:122[A]:ARG:C	3:O:123:LEU:HD23	2.31	0.56
2:J:336:LYS:HE2	3:K:126:LYS:HB3	1.86	0.56
1:M:274:LYS:HD3	1:M:274:LYS:N	2.20	0.56
2:F:247:GLY:HA3	2:F:333:ALA:O	2.05	0.56
1:A:140:GLU:CG	1:A:147:THR:HG21	2.36	0.55
2:B:104:LEU:HG	2:B:161:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:GLY:O	1:E:217:VAL:HG23	2.07	0.55
3:K:137:LYS:NZ	3:K:171:GLU:OE1	2.40	0.55
1:A:383:CYS:SG	1:A:386:VAL:HG22	2.47	0.55
4:D:19:LEU:HD12	4:D:24:GLU:O	2.07	0.55
1:A:296:TYR:HB2	1:A:412:LEU:O	2.07	0.55
1:E:164:ARG:HH11	1:E:164:ARG:CG	2.19	0.55
4:H:53:LYS:HD2	4:H:53:LYS:O	2.07	0.55
1:E:426:ARG:HH11	4:H:123:MET:HE2	1.71	0.54
1:M:385:THR:HA	2:N:112:ASP:HB3	1.88	0.54
4:L:144:ILE:HD11	4:L:184:VAL:HG21	1.88	0.54
3:G:97[B]:ARG:HD2	3:G:210:SER:O	2.08	0.54
1:A:385:THR:HA	2:B:112:ASP:HB3	1.88	0.54
2:J:29:ALA:HB1	2:J:34:LYS:NZ	2.22	0.54
1:A:67:GLU:OE2	1:A:98:TYR:HD2	1.91	0.54
3:K:91:PHE:CD2	3:K:250:LEU:HD21	2.42	0.53
4:L:96:THR:OG1	4:L:213:THR:OG1	2.24	0.53
1:E:296:TYR:HB2	1:E:412:LEU:O	2.09	0.53
2:F:386:MET:HE3	3:G:77:LEU:HD21	1.89	0.53
1:I:76:ARG:NH1	1:I:114:MET:SD	2.81	0.53
3:G:111:ARG:HG2	3:G:206:ILE:HD12	1.89	0.53
1:E:173:LYS:HD2	1:E:343:GLU:HG2	1.89	0.53
2:B:336:LYS:HE2	3:C:126:LYS:HB3	1.91	0.53
4:L:102:MET:HG2	4:L:107:THR:HG23	1.90	0.53
3:O:168:VAL:HG23	4:P:168:VAL:HG23	1.89	0.53
1:E:71:LEU:HD11	1:E:296:TYR:CZ	2.44	0.53
1:M:294:PRO:HG2	1:M:296:TYR:CZ	2.44	0.53
1:I:27:ARG:HH12	1:I:114:MET:HB3	1.74	0.53
1:I:421:ALA:HB3	1:I:422:PRO:HD3	1.90	0.53
4:D:92:MET:HG3	4:D:245:MET:HE1	1.90	0.53
1:A:71:LEU:HD11	1:A:296:TYR:CG	2.44	0.52
2:F:87:ILE:HD12	2:F:251:GLU:HA	1.90	0.52
2:B:14:LEU:HA	2:B:17:ILE:HD12	1.91	0.52
3:O:246:PHE:HA	10:O:412:HOH:O	2.10	0.52
3:C:111:ARG:HG2	3:C:206:ILE:HD12	1.90	0.52
4:D:139:ALA:HB1	4:D:144:ILE:O	2.10	0.52
2:N:183:ARG:HH11	2:N:183:ARG:CB	2.21	0.52
2:J:247:GLY:HA3	2:J:333:ALA:O	2.10	0.52
3:O:163:SER:N	3:O:173:GLU:OE1	2.43	0.52
2:B:61:LEU:CD1	2:B:158:ILE:HG23	2.40	0.52
1:E:102:GLY:O	1:E:106:GLN:HG3	2.10	0.52
2:J:201:ALA:HB2	2:J:267:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:333:ALA:HA	2:J:362:SER:O	2.10	0.52
2:J:373:GLN:HG3	3:K:123:LEU:HD12	1.92	0.52
4:P:4:THR:HG21	4:P:255:LEU:HA	1.91	0.51
3:C:163:SER:N	3:C:173:GLU:OE1	2.41	0.51
4:D:102:MET:HE1	4:D:195:ILE:CG2	2.40	0.51
1:E:297:PRO:HD3	1:E:412:LEU:O	2.10	0.51
3:O:122[B]:ARG:C	3:O:123:LEU:HD23	2.36	0.51
2:B:78:SER:HB2	4:D:205:ARG:HG2	1.92	0.51
4:P:81:GLU:OE2	4:P:108:LYS:NZ	2.29	0.51
4:P:102:MET:HE3	4:P:131:THR:HG21	1.92	0.51
4:P:108:LYS:HG2	4:P:123:MET:HG3	1.93	0.51
3:C:196:THR:OG1	3:C:224:MET:HE1	2.11	0.51
1:M:422:PRO:O	1:M:426:ARG:HD2	2.10	0.51
3:G:1:MET:SD	3:G:20:ASP:HB2	2.51	0.51
3:G:87:ARG:HG3	3:G:255:LEU:HD21	1.93	0.51
3:G:214:LEU:HB2	3:G:238:VAL:HG22	1.93	0.51
4:L:208:ILE:CG2	4:L:212:ILE:HD11	2.38	0.51
2:F:75:GLU:HG3	2:F:97:THR:HG22	1.93	0.50
4:P:1:MET:CG	4:P:2:LYS:N	2.72	0.50
4:L:15:LYS:HD3	4:L:15:LYS:N	2.26	0.50
1:M:221:ASN:OD1	1:M:226:ALA:HB1	2.11	0.50
2:B:373:GLN:HG3	3:C:123:LEU:HD12	1.92	0.50
4:D:102:MET:HE1	4:D:195:ILE:HG21	1.93	0.50
4:H:113:ALA:HB1	4:H:114:PRO:CD	2.41	0.50
3:C:81:ASP:OD1	3:C:81:ASP:N	2.44	0.50
2:F:345:GLN:O	2:F:349:SER:OG	2.29	0.50
3:K:175:ILE:CD1	4:L:105:GLN:HG3	2.42	0.50
1:A:120:PRO:HG3	1:A:143:TYR:CD2	2.46	0.50
1:M:78:VAL:HG21	1:M:113:PRO:CG	2.41	0.50
1:M:364:LYS:HA	1:M:401:MET:CE	2.42	0.49
1:I:406:LEU:HD13	1:I:430:PHE:HB2	1.94	0.49
1:A:334:LEU:HD12	1:A:334:LEU:H	1.78	0.49
4:L:124:ASN:HA	4:L:202:LEU:HD21	1.93	0.49
3:K:163:SER:N	3:K:173:GLU:OE1	2.39	0.49
1:E:59:PHE:O	1:E:193:LYS:NZ	2.43	0.49
1:M:149[A]:ASN:OD1	2:N:137:ASN:HB2	2.12	0.49
1:I:401:MET:HE2	1:I:403:LEU:HD12	1.93	0.49
2:J:88:ILE:HG13	2:J:89:LYS:N	2.28	0.49
3:K:37:LEU:CD2	4:L:179:GLY:HA2	2.42	0.49
1:M:410:SER:OG	1:M:411:ASP:N	2.39	0.49
2:F:385:ILE:HD12	2:F:385:ILE:C	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:102:MET:HG2	4:H:107:THR:HG23	1.94	0.48
3:K:105:GLN:HA	3:K:130:GLY:HA2	1.95	0.48
1:M:71:LEU:HD11	1:M:296:TYR:CD2	2.47	0.48
2:B:196:PRO:HD2	2:B:197:TRP:CZ3	2.48	0.48
4:D:96:THR:OG1	4:D:213:THR:OG1	2.23	0.48
1:E:221:ASN:OD1	1:E:226:ALA:HB1	2.12	0.48
1:E:273[B]:ASP:HB2	1:E:282:MET:HG3	1.94	0.48
3:K:168:VAL:HG23	4:L:168:VAL:HG23	1.95	0.48
4:L:55:LYS:HE3	4:L:56:ARG:H	1.77	0.48
3:O:87:ARG:HG3	3:O:255:LEU:HD21	1.95	0.48
2:J:192:ARG:HD2	2:J:204:SER:HB2	1.95	0.48
1:M:332:TYR:OH	1:M:348:MET:HE1	2.13	0.48
3:C:226:LYS:HE3	3:C:230:ASP:OD2	2.13	0.48
2:B:61:LEU:HD12	2:B:158:ILE:HG23	1.96	0.48
1:A:173:LYS:HD2	1:A:343:GLU:HG2	1.95	0.48
4:H:115:ASN:OD1	4:H:115:ASN:N	2.47	0.48
4:D:102:MET:HG2	4:D:218:VAL:HG21	1.95	0.48
4:D:215:THR:HG22	4:D:245:MET:HG3	1.96	0.48
2:F:386:MET:HE2	2:F:387:PHE:CE2	2.48	0.48
4:H:106:ASP:HB3	4:H:108:LYS:HZ3	1.79	0.48
1:M:273[A]:ASP:C	1:M:274:LYS:HD3	2.39	0.48
3:G:6:GLY:HA3	3:G:252:CYS:HB2	1.96	0.47
3:G:30:MET:HB3	3:G:246:PHE:CZ	2.49	0.47
3:G:81:ASP:OD1	3:G:81:ASP:N	2.46	0.47
2:J:164:ARG:HH12	2:J:170:GLU:CD	2.22	0.47
4:L:14:THR:C	4:L:15:LYS:HD3	2.40	0.47
1:A:417:VAL:O	1:A:417:VAL:HG12	2.14	0.47
3:G:113:ASP:HB3	3:G:119[B]:ARG:HE	1.79	0.47
4:H:112:VAL:HG12	4:H:113:ALA:O	2.15	0.47
3:O:19:LEU:HD12	3:O:24:ASN:O	2.14	0.47
3:G:175:ILE:CD1	4:H:105:GLN:HG3	2.44	0.47
1:M:98:TYR:CE2	1:M:412:LEU:HD11	2.49	0.47
4:P:112:VAL:HG12	4:P:113:ALA:O	2.15	0.47
1:A:182:GLU:OE2	2:B:141:LYS:HG2	2.14	0.47
1:A:436:SER:O	1:A:440:GLN:HB2	2.15	0.47
4:H:113:ALA:HB1	4:H:114:PRO:HD2	1.97	0.47
1:I:215:LYS:O	1:I:219:GLU:HG3	2.15	0.47
2:B:17:ILE:HD12	2:B:229:MET:HE1	1.96	0.47
3:G:91:PHE:CD2	3:G:250:LEU:HD21	2.49	0.47
2:B:333:ALA:HA	2:B:362:SER:O	2.14	0.47
2:F:237:ARG:HH11	2:F:237:ARG:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:367:ALA:HB3	1:I:368:PRO:HD3	1.97	0.47
2:N:118:ALA:HB3	2:N:119:PRO:HD3	1.96	0.47
3:K:111:ARG:HG2	3:K:206:ILE:HD12	1.97	0.47
1:M:364:LYS:HA	1:M:401:MET:HE2	1.96	0.47
3:O:81:ASP:OD1	3:O:81:ASP:N	2.48	0.47
2:B:303:TYR:CD1	2:B:317:MET:HB3	2.49	0.47
3:K:137:LYS:HD3	3:K:141:TYR:HE2	1.78	0.47
2:N:385:ILE:C	2:N:385:ILE:HD12	2.39	0.47
3:O:175:ILE:CD1	4:P:105:GLN:HG3	2.45	0.47
1:A:215:LYS:HD2	1:A:329:GLY:HA3	1.97	0.46
3:G:34:GLY:HA2	4:H:143:ARG:HG3	1.97	0.46
1:E:8:THR:HG21	1:E:253:TYR:HA	1.96	0.46
4:L:229:GLU:OE2	4:L:235:LYS:HG3	2.14	0.46
1:A:435:ILE:O	1:A:439:GLN:HG3	2.16	0.46
2:J:183:ARG:HH22	2:J:282:ASP:CG	2.22	0.46
4:L:20:ASN:C	4:L:20:ASN:OD1	2.59	0.46
1:A:367:ALA:HB3	1:A:368:PRO:HD3	1.97	0.46
1:A:421:ALA:HB3	1:A:422:PRO:HD3	1.97	0.46
2:F:333:ALA:HA	2:F:362:SER:O	2.14	0.46
2:J:58:ALA:O	2:J:164:ARG:NH2	2.49	0.46
3:K:243:MET:N	3:K:244:PRO:CD	2.79	0.46
4:L:96:THR:HG1	4:L:213:THR:HG1	1.58	0.46
4:L:145:PRO:HB2	4:L:148:GLU:HG2	1.97	0.46
2:B:141:LYS:HD3	2:B:141:LYS:N	2.30	0.46
3:G:19:LEU:HD12	3:G:24:ASN:O	2.15	0.46
1:I:71:LEU:HD13	1:I:98:TYR:OH	2.16	0.46
1:M:273[A]:ASP:HA	1:M:274:LYS:HD3	1.97	0.46
1:E:421:ALA:HB3	1:E:422:PRO:HD3	1.97	0.46
2:N:75:GLU:HG3	2:N:97:THR:HG22	1.97	0.46
2:N:333:ALA:HA	2:N:362:SER:O	2.15	0.46
2:J:104:LEU:HG	2:J:161:VAL:HG21	1.97	0.46
4:L:1:MET:SD	4:L:21:GLU:HG2	2.56	0.46
4:D:142:LEU:CD1	4:D:188:LEU:HD21	2.45	0.46
1:I:417:VAL:HG12	1:I:417:VAL:O	2.15	0.46
4:P:255:LEU:O	4:P:259:GLN:HG3	2.14	0.46
2:B:372:ASP:OD2	4:D:176[B]:SER:OG	2.27	0.46
1:E:282:MET:HE2	1:E:312:ILE:HD12	1.98	0.46
3:G:18:VAL:HG23	3:G:48:THR:HG22	1.97	0.45
3:G:243:MET:N	3:G:244:PRO:CD	2.79	0.45
2:J:4:LYS:HD2	2:J:4:LYS:N	2.31	0.45
2:J:118:ALA:HB3	2:J:119:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:417:VAL:HG12	1:M:417:VAL:O	2.15	0.45
1:A:301:GLN:O	1:A:305:MET:HG3	2.17	0.45
1:M:437:ARG:HA	1:M:440:GLN:HB2	1.97	0.45
2:B:192:ARG:HD2	2:B:204:SER:HB2	1.98	0.45
4:D:188:LEU:O	4:D:191:VAL:HB	2.17	0.45
4:D:91:HIS:ND1	4:D:92:MET:HE3	2.32	0.45
4:D:215:THR:CG2	4:D:245:MET:HG3	2.45	0.45
1:E:283:LYS:HA	1:E:283:LYS:HD2	1.74	0.45
2:F:42:ARG:HB2	2:F:61:LEU:HD13	1.98	0.45
1:M:73:THR:HB	1:M:78:VAL:HG23	1.98	0.45
2:N:104:LEU:HG	2:N:161:VAL:HG21	1.98	0.45
1:E:9:GLY:HA2	1:E:17:ARG:HD2	1.98	0.45
2:F:303:TYR:CD1	2:F:317:MET:HB3	2.52	0.45
1:I:294:PRO:HG2	1:I:296:TYR:CZ	2.51	0.45
1:M:248:GLU:HG2	1:M:252:LYS:HE3	1.97	0.45
3:O:162:ILE:HA	3:O:173:GLU:OE1	2.17	0.45
4:D:191:VAL:HG13	4:D:195:ILE:HD11	1.97	0.45
4:L:62:VAL:O	4:L:76:ASP:N	2.47	0.45
1:M:273[B]:ASP:C	1:M:274:LYS:HD3	2.41	0.45
1:M:367:ALA:HB3	1:M:368:PRO:HD3	1.98	0.45
2:N:323:ARG:HA	2:N:323:ARG:HD2	1.87	0.45
3:O:243:MET:N	3:O:244:PRO:CD	2.80	0.45
2:B:322:VAL:HG13	2:B:327:ALA:HB3	1.99	0.45
1:E:418:VAL:HG13	1:E:423:MET:HE1	1.98	0.45
2:F:254:PRO:HG3	2:F:366:GLU:O	2.17	0.45
4:L:52:ALA:O	4:L:53:LYS:HD3	2.17	0.45
2:N:49:VAL:O	2:N:65:ARG:NH1	2.50	0.45
4:P:246:GLY:N	10:P:405:HOH:O	2.50	0.45
1:E:252:LYS:HD2	1:E:252:LYS:O	2.17	0.44
1:I:27:ARG:HD2	1:I:27:ARG:C	2.42	0.44
1:M:417:VAL:O	4:P:126:LYS:HE2	2.17	0.44
4:P:15:LYS:HD3	4:P:15:LYS:N	2.31	0.44
1:A:229:ASN:HB3	1:A:232:THR:OG1	2.18	0.44
4:L:65:THR:C	4:L:69:ARG:HB3	2.42	0.44
3:O:108:LYS:HB3	3:O:123:LEU:HD22	1.99	0.44
2:B:193:LYS:NZ	2:B:324:ASN:O	2.40	0.44
2:F:118:ALA:HB3	2:F:119:PRO:HD3	2.00	0.44
2:J:155:LEU:HD11	2:J:166:ILE:CG1	2.48	0.44
3:C:65:THR:C	3:C:69:ARG:HB3	2.43	0.44
4:L:52:ALA:C	4:L:53:LYS:HG3	2.41	0.44
2:B:73:GLY:HA2	2:B:93:ASP:CG	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:VAL:HG22	1:I:135:TRP:CE3	2.52	0.44
4:D:199:ALA:HB3	4:D:228:LEU:HD11	1.99	0.44
2:F:51:PHE:CD1	2:F:52:PRO:HD2	2.53	0.44
1:M:406:LEU:HD13	1:M:430:PHE:HB2	2.00	0.44
2:N:338:CYS:HA	5:N:401:SF4:S1	2.58	0.44
4:P:45:PHE:CE2	4:P:56:ARG:HD2	2.46	0.44
4:P:215:THR:HG22	4:P:245:MET:HG3	1.99	0.44
1:M:430:PHE:CE2	1:M:434:LEU:HD11	2.53	0.44
1:E:76:ARG:HA	1:E:76:ARG:NH1	2.32	0.44
1:E:379:PRO:HD2	1:E:408:ILE:O	2.18	0.44
1:I:382:SER:HB2	1:I:412:LEU:HD11	1.99	0.44
2:J:75:GLU:HG3	2:J:97:THR:HG22	1.99	0.44
1:M:173:LYS:HD2	1:M:343:GLU:HG2	2.00	0.44
1:M:228:PHE:CD1	1:M:228:PHE:C	2.96	0.44
1:M:278:GLY:O	1:M:280:VAL:HG13	2.17	0.44
2:N:42:ARG:CB	2:N:61:LEU:HD22	2.48	0.44
1:A:423:MET:O	1:A:427:VAL:HG23	2.18	0.44
2:B:75:GLU:HG3	2:B:97:THR:CG2	2.48	0.44
4:L:154:LEU:HD22	4:L:226:LYS:HD2	1.99	0.44
1:M:57:ARG:NH2	1:M:243:ALA:O	2.50	0.44
4:D:15:LYS:HD3	4:D:15:LYS:N	2.33	0.43
1:M:438:ARG:O	1:M:442:ALA:HB2	2.18	0.43
2:B:192:ARG:NH1	2:B:270:ASP:OD2	2.47	0.43
3:O:9:ILE:HD12	3:O:69:ARG:HA	2.00	0.43
1:A:136:GLY:HA2	1:A:139:TRP:CE3	2.53	0.43
2:F:234:GLN:H	2:F:234:GLN:CD	2.17	0.43
3:G:136:GLU:OE1	7:G:301:ATP:O3'	2.34	0.43
3:K:81:ASP:N	3:K:81:ASP:OD1	2.50	0.43
3:O:1:MET:SD	3:O:20:ASP:HB2	2.58	0.43
4:P:108:LYS:HG2	4:P:123:MET:CG	2.48	0.43
1:A:251:SER:O	1:A:255:LYS:HG3	2.19	0.43
4:D:146:LEU:HD21	9:D:301:ADP:H2'	1.99	0.43
3:G:131:THR:HG21	3:G:195:LEU:HD13	2.01	0.43
1:M:140:GLU:HG3	1:M:147:THR:HG21	1.99	0.43
2:N:192:ARG:HD2	2:N:204:SER:HB2	1.99	0.43
2:N:303:TYR:CD1	2:N:317:MET:HB3	2.53	0.43
4:P:142:LEU:CD1	4:P:188:LEU:HD21	2.49	0.43
4:D:112:VAL:HG12	4:D:113:ALA:O	2.18	0.43
1:I:173:LYS:HD2	1:I:343:GLU:HG2	1.99	0.43
4:D:99:VAL:HB	4:D:110:ILE:HB	1.99	0.43
4:P:20:ASN:OD1	4:P:20:ASN:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:65:THR:C	3:G:69:ARG:HB3	2.44	0.43
3:G:175:ILE:HD13	4:H:105:GLN:HG3	2.00	0.43
1:I:102:GLY:O	1:I:106:GLN:HG3	2.18	0.43
1:E:40:GLY:O	1:E:119:LYS:NZ	2.52	0.43
3:K:67:TYR:HE2	4:L:175:LEU:O	2.01	0.43
3:C:206:ILE:O	3:C:207:ASN:HB2	2.19	0.43
4:H:2:LYS:HD2	4:H:2:LYS:HA	1.88	0.43
4:D:187:ILE:O	4:D:191:VAL:HG23	2.18	0.42
1:I:72:GLN:HA	1:I:75:PHE:HD2	1.82	0.42
4:L:99:VAL:HB	4:L:110:ILE:HB	2.01	0.42
2:N:74:ASN:HB2	4:P:200:ILE:HG21	2.02	0.42
3:O:167:THR:HG23	10:O:413:HOH:O	2.19	0.42
1:M:152:TYR:HB2	1:M:154:MET:HE2	2.01	0.42
3:O:6:GLY:HA3	3:O:252:CYS:HB2	2.01	0.42
1:A:394:ARG:NH1	4:D:205:ARG:HD2	2.35	0.42
2:F:36:TRP:CE2	2:F:62:LEU:HB2	2.54	0.42
2:J:211:ALA:HB2	2:J:219:PHE:CZ	2.55	0.42
3:K:131:THR:HG21	3:K:195:LEU:HD13	2.02	0.42
3:C:105:GLN:NE2	10:C:403:HOH:O	2.53	0.42
1:I:305:MET:O	1:I:427:VAL:HG11	2.19	0.42
2:N:97:THR:O	2:N:98:LYS:HD2	2.20	0.42
4:P:111:ARG:HG2	4:P:206:VAL:HB	2.01	0.42
3:K:6:GLY:HA3	3:K:252:CYS:HB2	2.02	0.42
3:O:159:ALA:HB1	3:O:190:GLY:HA2	2.02	0.42
3:K:47:GLU:O	3:K:51:GLN:HG3	2.20	0.42
1:E:417:VAL:O	4:H:126:LYS:HE2	2.19	0.42
4:L:112:VAL:HG12	4:L:113:ALA:O	2.18	0.42
3:O:123:LEU:HD23	3:O:123:LEU:N	2.34	0.42
1:E:383:CYS:SG	1:E:386:VAL:HG22	2.60	0.42
4:H:145:PRO:HB2	4:H:148:GLU:HG2	2.02	0.42
2:B:201:ALA:HB2	2:B:267:VAL:HB	2.02	0.42
1:E:241:ALA:O	1:E:245:ARG:HB2	2.19	0.42
2:F:372:ASP:O	2:F:376:ILE:HG12	2.20	0.42
2:F:386:MET:HB3	2:F:387:PHE:CD2	2.54	0.42
1:I:46:CYS:O	1:I:66:PRO:HD2	2.19	0.42
1:I:365:LYS:HB2	1:I:365:LYS:HE2	1.85	0.42
3:K:43:LEU:HD22	3:K:47:GLU:OE2	2.20	0.42
1:M:135:TRP:HA	1:M:138:ILE:HD12	2.00	0.42
2:B:361:ILE:HD12	3:C:122[A]:ARG:NH1	2.35	0.41
4:D:109:ALA:O	4:D:121:PHE:HA	2.20	0.41
2:J:75:GLU:HG3	2:J:97:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:SER:HA	3:C:67:TYR:CE1	2.56	0.41
3:C:259:ARG:HD2	3:C:259:ARG:HA	1.84	0.41
2:F:315:GLU:HG2	2:F:316:HIS:N	2.35	0.41
3:K:175:ILE:HD12	4:L:105:GLN:HG3	2.02	0.41
4:P:98:THR:HB	4:P:212:ILE:HG12	2.01	0.41
4:P:202:LEU:HD12	4:P:205:ARG:NH1	2.34	0.41
1:A:99:VAL:HG22	1:A:135:TRP:CE3	2.54	0.41
2:B:17:ILE:CD1	2:B:229:MET:HE1	2.49	0.41
4:D:55:LYS:HB3	4:D:55:LYS:HE3	1.88	0.41
1:E:252:LYS:HD2	1:E:252:LYS:C	2.45	0.41
1:E:417:VAL:O	1:E:417:VAL:HG12	2.20	0.41
3:O:43:LEU:O	3:O:47:GLU:HG3	2.19	0.41
4:P:154:LEU:HD22	4:P:226:LYS:HD2	2.02	0.41
1:A:406:LEU:HD13	1:A:430:PHE:HB2	2.03	0.41
4:H:136:GLY:HA2	4:H:146:LEU:HD13	2.01	0.41
1:M:188:GLU:O	1:M:192:GLY:N	2.51	0.41
3:G:1:MET:SD	3:G:21:GLU:HG2	2.61	0.41
4:H:15:LYS:HD3	4:H:15:LYS:N	2.35	0.41
1:A:112:HIS:ND1	1:A:113:PRO:HD2	2.35	0.41
1:A:298:ILE:O	1:A:298:ILE:HG13	2.21	0.41
1:A:437:ARG:HA	1:A:440:GLN:HB2	2.02	0.41
2:B:330:VAL:O	2:B:359:TYR:HA	2.21	0.41
3:G:210:SER:HA	3:G:211:GLN:HA	1.86	0.41
1:I:39:ARG:HE	1:I:41:GLU:CD	2.28	0.41
1:M:78:VAL:HG21	1:M:113:PRO:HG3	2.03	0.41
2:N:51:PHE:CD1	2:N:52:PRO:HD2	2.56	0.41
3:O:61:TYR:OH	3:O:259:ARG:HD3	2.21	0.41
1:A:71:LEU:CD1	1:A:296:TYR:CD2	3.04	0.41
1:A:318:TYR:HA	1:A:321:PHE:CZ	2.56	0.41
1:E:67[B]:GLU:HG3	10:E:608:HOH:O	2.20	0.41
1:E:301:GLN:O	1:E:305:MET:HG3	2.21	0.41
3:G:41:ALA:O	3:G:45:VAL:HG23	2.21	0.41
3:G:198:ARG:O	3:G:201:GLN:HB3	2.20	0.41
2:J:329:THR:HG23	2:J:358:PRO:C	2.46	0.41
1:E:81:ASP:OD1	1:E:108:ARG:NH1	2.48	0.41
4:H:164:THR:O	4:H:198:ARG:HD3	2.21	0.41
4:H:175:LEU:O	4:H:178:LEU:HB2	2.20	0.41
1:I:6:GLN:N	1:I:7:MET:HE2	2.36	0.41
1:I:410:SER:OG	1:I:411:ASP:N	2.53	0.41
4:L:4:THR:HG21	4:L:255:LEU:HA	2.02	0.41
1:M:48:ILE:H	1:M:48:ILE:HG13	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:261:LEU:O	1:M:265:VAL:HG23	2.21	0.41
2:N:336:LYS:HA	2:N:336:LYS:HD2	1.93	0.41
4:P:15:LYS:NZ	9:P:301:ADP:O1B	2.54	0.41
4:P:185:GLU:HG2	4:P:186:ASP:N	2.36	0.41
1:A:7:MET:HE3	1:A:7:MET:HB2	1.96	0.41
4:H:102:MET:HE2	4:H:102:MET:HB3	1.99	0.41
1:E:8:THR:CG2	1:E:9:GLY:N	2.84	0.40
1:E:215:LYS:O	1:E:219:GLU:HG3	2.21	0.40
2:F:54:GLU:HG2	2:F:175:VAL:HA	2.04	0.40
4:H:66:GLY:O	4:H:67:TYR:C	2.63	0.40
4:H:100:ILE:HD11	4:H:199:ALA:HB1	2.03	0.40
2:N:44:ILE:HG23	2:N:44:ILE:O	2.21	0.40
4:D:160:VAL:O	4:D:190:GLY:HA3	2.21	0.40
4:H:145:PRO:HG2	4:H:148:GLU:OE2	2.20	0.40
3:O:105:GLN:HA	3:O:130:GLY:HA2	2.03	0.40
1:A:166:THR:O	1:A:170:GLU:HG2	2.22	0.40
1:A:215:LYS:O	1:A:219:GLU:HG3	2.21	0.40
2:B:315:GLU:HG2	2:B:316:HIS:N	2.36	0.40
1:E:34:THR:HG22	1:E:38:LYS:HE3	2.03	0.40
1:E:36:VAL:HG13	1:E:41:GLU:HB2	2.03	0.40
3:G:47:GLU:O	3:G:51:GLN:HG3	2.22	0.40
1:I:300:ARG:HG3	1:I:301:GLN:N	2.36	0.40
4:L:139:ALA:HB1	4:L:144:ILE:O	2.21	0.40
4:P:139:ALA:HB1	4:P:144:ILE:O	2.21	0.40
3:G:31:ARG:HG3	3:G:32:PRO:HD2	2.02	0.40
1:I:149:ASN:HB3	2:J:137:ASN:CG	2.46	0.40
4:L:27:GLY:HA3	4:L:52:ALA:HB2	2.04	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	437/445 (98%)	427 (98%)	9 (2%)	1 (0%)	43	44
1	E	436/445 (98%)	425 (98%)	10 (2%)	1 (0%)	43	44
1	I	437/445 (98%)	425 (97%)	11 (2%)	1 (0%)	43	44
1	M	437/445 (98%)	424 (97%)	13 (3%)	0	100	100
2	B	385/388 (99%)	375 (97%)	10 (3%)	0	100	100
2	F	385/388 (99%)	377 (98%)	8 (2%)	0	100	100
2	J	385/388 (99%)	376 (98%)	9 (2%)	0	100	100
2	N	385/388 (99%)	379 (98%)	6 (2%)	0	100	100
3	C	265/273 (97%)	263 (99%)	1 (0%)	1 (0%)	30	26
3	G	265/273 (97%)	257 (97%)	8 (3%)	0	100	100
3	K	263/273 (96%)	258 (98%)	5 (2%)	0	100	100
3	O	264/273 (97%)	259 (98%)	5 (2%)	0	100	100
4	D	260/269 (97%)	258 (99%)	1 (0%)	1 (0%)	30	26
4	H	259/269 (96%)	257 (99%)	2 (1%)	0	100	100
4	L	260/269 (97%)	259 (100%)	1 (0%)	0	100	100
4	P	260/269 (97%)	259 (100%)	1 (0%)	0	100	100
All	All	5383/5500 (98%)	5278 (98%)	100 (2%)	5 (0%)	48	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	410	SER
1	I	410	SER
1	A	410	SER
3	C	207	ASN
4	D	191	VAL

### 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	368/371 (99%)	356 (97%)	12 (3%)	33	34
1	E	368/371 (99%)	356 (97%)	12 (3%)	33	34
1	I	369/371 (100%)	357 (97%)	12 (3%)	33	34
1	M	368/371 (99%)	356 (97%)	12 (3%)	33	34
2	B	335/336 (100%)	332 (99%)	3 (1%)	70	77
2	F	335/336 (100%)	331 (99%)	4 (1%)	63	70
2	J	335/336 (100%)	328 (98%)	7 (2%)	47	52
2	N	335/336 (100%)	331 (99%)	4 (1%)	63	70
3	C	214/215 (100%)	204 (95%)	10 (5%)	23	21
3	G	214/215 (100%)	209 (98%)	5 (2%)	44	49
3	K	212/215 (99%)	204 (96%)	8 (4%)	29	29
3	O	213/215 (99%)	204 (96%)	9 (4%)	26	25
4	D	198/203 (98%)	189 (96%)	9 (4%)	24	22
4	H	197/203 (97%)	192 (98%)	5 (2%)	42	45
4	L	198/203 (98%)	190 (96%)	8 (4%)	28	27
4	P	198/203 (98%)	189 (96%)	9 (4%)	24	22
All	All	4457/4500 (99%)	4328 (97%)	129 (3%)	37	39

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	76	ARG
1	A	119	LYS
1	A	151	ASP
1	A	238	MET
1	A	252	LYS
1	A	304	GLU
1	A	365	LYS
1	A	394	ARG
1	A	400	GLU
1	A	413	VAL
1	A	441	GLN
2	B	23	GLU
2	B	152	ARG
2	B	373	GLN
3	C	12	THR

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Mol	Chain	Res	Type
3	C	42	GLU
3	C	43	LEU
3	C	50	GLU
3	C	81	ASP
3	C	139	VAL
3	C	226	LYS
3	C	233	ASN
3	C	261	LYS
3	C	262	LYS
4	D	24	GLU
4	D	55	LYS
4	D	56	ARG
4	D	80	THR
4	D	108	LYS
4	D	211	GLU
4	D	228	LEU
4	D	230	GLU
4	D	235	LYS
1	E	8	THR
1	E	119	LYS
1	E	164	ARG
1	E	167	GLN
1	E	194	LYS
1	E	201	ARG
1	E	252	LYS
1	E	283	LYS
1	E	412	LEU
1	E	437	ARG
1	E	439	GLN
1	E	441	GLN
2	F	4	LYS
2	F	61	LEU
2	F	165	LYS
2	F	328	GLU
3	G	55	ASN
3	G	81	ASP
3	G	173	GLU
3	G	210	SER
3	G	262	LYS
4	H	53	LYS
4	H	115	ASN
4	H	148	GLU

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Mol	Chain	Res	Type
4	H	180	LYS
4	H	202	LEU
1	I	6	GLN
1	I	7	MET
1	I	27	ARG
1	I	108	ARG
1	I	114	MET
1	I	149	ASN
1	I	151	ASP
1	I	276	THR
1	I	412	LEU
1	I	413	VAL
1	I	426	ARG
1	I	437	ARG
2	J	12	LYS
2	J	74	ASN
2	J	99	ASN
2	J	152	ARG
2	J	310	GLN
2	J	328	GLU
2	J	386	MET
3	K	12	THR
3	K	43	LEU
3	K	81	ASP
3	K	119	ARG
3	K	139	VAL
3	K	158	GLU
3	K	261	LYS
3	K	262	LYS
4	L	39	GLN
4	L	53	LYS
4	L	90	SER
4	L	92	MET
4	L	148	GLU
4	L	202	LEU
4	L	230	GLU
4	L	235	LYS
1	M	8	THR
1	M	76	ARG
1	M	164	ARG
1	M	167	GLN
1	M	274	LYS

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Mol	Chain	Res	Type
1	M	277	GLU
1	M	283	LYS
1	M	304	GLU
1	M	410	SER
1	M	412	LEU
1	M	436	SER
1	M	439	GLN
2	N	183	ARG
2	N	238	GLN
2	N	310	GLN
2	N	373	GLN
3	O	12	THR
3	O	43	LEU
3	O	67	TYR
3	O	81	ASP
3	O	116	HIS
3	O	119	ARG
3	O	139	VAL
3	O	229	ARG
3	O	261	LYS
4	P	1	MET
4	P	21	GLU
4	P	39	GLN
4	P	49	LEU
4	P	53	LYS
4	P	56	ARG
4	P	57	SER
4	P	115	ASN
4	P	184	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
2	B	238	GLN
2	B	373	GLN
3	C	24	ASN
3	C	29	HIS
3	C	71	GLN
3	C	180	ASN
4	D	105	GLN
4	D	115	ASN

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Mol	Chain	Res	Type
4	D	193	GLN
1	E	130	ASN
1	E	202	GLN
1	E	223	ASN
1	E	439	GLN
2	F	259	GLN
2	F	300	HIS
2	F	373	GLN
3	G	71	GLN
4	H	42	HIS
4	H	58	HIS
1	I	69	ASN
1	I	202	GLN
1	I	335	ASN
2	J	194	ASN
2	J	300	HIS
3	K	24	ASN
3	K	55	ASN
4	L	47	GLN
4	L	193	GLN
1	M	202	GLN
1	M	223	ASN
1	M	235	ASN
1	M	267	HIS
1	M	335	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

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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
6	SO4	P	303	-	4,4,4	0.36	0	6,6,6	0.19	0
5	SF4	G	303	3,4	0,12,12	-	-	-		
7	ATP	O	301	8	32,33,33	0.79	2 (6%)	48,52,52	0.84	2 (4%)
6	SO4	M	502	-	4,4,4	0.36	0	6,6,6	0.10	0
9	ADP	H	301	8	28,29,29	1.43	3 (10%)	43,45,45	1.96	13 (30%)
5	SF4	I	501	1	0,12,12	-	-	-		
5	SF4	J	401	2	0,12,12	-	-	-		
6	SO4	C	303	-	4,4,4	0.37	0	6,6,6	0.09	0
6	SO4	B	402	-	4,4,4	0.25	0	6,6,6	0.09	0
5	SF4	M	501	1	0,12,12	-	-	-		
5	SF4	E	501	1	0,12,12	-	-	-		
6	SO4	G	304	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	F	402	-	4,4,4	0.27	0	6,6,6	0.09	0
6	SO4	K	303	-	4,4,4	0.25	0	6,6,6	0.09	0
6	SO4	J	402	-	4,4,4	0.39	0	6,6,6	0.08	0
5	SF4	O	303	3,4	0,12,12	-	-	-		
6	SO4	E	502	-	4,4,4	0.34	0	6,6,6	0.15	0
5	SF4	B	401	2	0,12,12	-	-	-		
9	ADP	L	302	8	28,29,29	1.41	5 (17%)	43,45,45	2.00	11 (25%)
9	ADP	P	301	8	28,29,29	1.41	5 (17%)	43,45,45	2.00	11 (25%)
5	SF4	L	301	3,4	0,12,12	-	-	-		
7	ATP	G	301	8	32,33,33	0.79	2 (6%)	48,52,52	0.84	1 (2%)
6	SO4	N	402	-	4,4,4	0.26	0	6,6,6	0.07	0
5	SF4	A	501	1	0,12,12	-	-	-		
9	ADP	D	301	8	28,29,29	1.41	3 (10%)	43,45,45	1.87	12 (27%)
5	SF4	D	300	3,4	0,12,12	-	-	-		
6	SO4	L	304	-	4,4,4	0.42	0	6,6,6	0.25	0
5	SF4	F	401	2	0,12,12	-	-	-		
6	SO4	O	304	-	4,4,4	0.36	0	6,6,6	0.11	0
7	ATP	C	301	8	32,33,33	0.87	2 (6%)	48,52,52	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SF4	N	401	2	0,12,12	-	-	-		
7	ATP	K	301	8	32,33,33	0.80	2 (6%)	48,52,52	0.84	1 (2%)

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
5	SF4	G	303	3,4	-	-	0/6/5/5
7	ATP	O	301	8	-	1/22/38/38	0/3/3/3
9	ADP	H	301	8	-	0/16/32/32	0/3/3/3
5	SF4	I	501	1	-	-	0/6/5/5
5	SF4	J	401	2	-	-	0/6/5/5
5	SF4	E	501	1	-	-	0/6/5/5
5	SF4	M	501	1	-	-	0/6/5/5
5	SF4	O	303	3,4	-	-	0/6/5/5
5	SF4	B	401	2	-	-	0/6/5/5
9	ADP	L	302	8	-	0/16/32/32	0/3/3/3
9	ADP	P	301	8	-	0/16/32/32	0/3/3/3
7	ATP	G	301	8	-	2/22/38/38	0/3/3/3
5	SF4	L	301	3,4	-	-	0/6/5/5
9	ADP	D	301	8	-	0/16/32/32	0/3/3/3
5	SF4	A	501	1	-	-	0/6/5/5
5	SF4	D	300	3,4	-	-	0/6/5/5
5	SF4	F	401	2	-	-	0/6/5/5
7	ATP	C	301	8	-	3/22/38/38	0/3/3/3
5	SF4	N	401	2	-	-	0/6/5/5
7	ATP	K	301	8	-	1/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	301	ADP	C5-C4	4.67	1.47	1.39
9	P	301	ADP	C5-C4	4.64	1.47	1.39
9	D	301	ADP	C5-C4	4.60	1.47	1.39
9	L	302	ADP	C5-C4	4.48	1.47	1.39
9	L	302	ADP	C5-C6	2.81	1.48	1.41
9	P	301	ADP	C5-C6	2.70	1.48	1.41
9	H	301	ADP	C8-N7	2.64	1.36	1.31
9	D	301	ADP	C8-N7	2.60	1.36	1.31
9	H	301	ADP	C5-C6	2.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	302	ADP	C8-N7	2.46	1.36	1.31
9	D	301	ADP	C5-C6	2.41	1.47	1.41
9	P	301	ADP	C8-N7	2.34	1.36	1.31
9	P	301	ADP	C5-N7	-2.30	1.34	1.39
7	K	301	ATP	C2-N1	-2.30	1.29	1.33
7	O	301	ATP	C2-N1	-2.27	1.29	1.33
7	C	301	ATP	C2-N1	-2.25	1.29	1.33
7	G	301	ATP	C2-N1	-2.24	1.30	1.33
9	L	302	ADP	C5-N7	-2.23	1.35	1.39
9	L	302	ADP	PA-O3A	2.18	1.61	1.59
7	G	301	ATP	C5-C4	-2.17	1.35	1.39
7	C	301	ATP	C5-C4	-2.16	1.35	1.39
9	P	301	ADP	PA-O3A	2.15	1.61	1.59
7	K	301	ATP	C5-C4	-2.15	1.35	1.39
7	O	301	ATP	C5-C4	-2.12	1.35	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	302	ADP	C5-C4-N3	-6.11	118.30	126.72
9	P	301	ADP	C5-C4-N3	-6.03	118.42	126.72
9	H	301	ADP	C5-C4-N3	-5.17	119.59	126.72
9	P	301	ADP	N3-C4-N9	4.99	135.65	127.17
9	D	301	ADP	C5-C4-N3	-4.91	119.96	126.72
9	L	302	ADP	N3-C4-N9	4.77	135.28	127.17
9	H	301	ADP	C4-C5-N7	-4.29	105.67	110.58
9	L	302	ADP	C2-N3-C4	4.05	121.73	111.83
9	H	301	ADP	N3-C4-N9	4.02	134.01	127.17
9	D	301	ADP	C4-C5-N7	-3.96	106.06	110.58
9	D	301	ADP	N3-C4-N9	3.86	133.73	127.17
9	P	301	ADP	C2-N3-C4	3.85	121.24	111.83
9	L	302	ADP	N3-C2-N1	-3.77	122.87	128.58
9	L	302	ADP	C4-C5-N7	-3.72	106.33	110.58
9	D	301	ADP	C3'-C2'-C1'	3.62	108.31	101.46
9	P	301	ADP	N3-C2-N1	-3.59	123.14	128.58
9	P	301	ADP	C4-C5-N7	-3.50	106.58	110.58
9	D	301	ADP	C4-N9-C8	3.34	109.24	105.74
9	H	301	ADP	C5-N7-C8	3.30	108.64	103.45
9	H	301	ADP	C4-N9-C8	3.25	109.15	105.74
9	H	301	ADP	O4'-C1'-N9	3.18	114.19	108.09
9	L	302	ADP	C3'-C2'-C1'	3.14	107.41	101.46
9	P	301	ADP	C4-N9-C8	3.05	108.94	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	301	ADP	C3'-C2'-C1'	3.02	107.18	101.46
9	D	301	ADP	C5-N7-C8	2.98	108.14	103.45
9	H	301	ADP	C2-N3-C4	2.97	119.09	111.83
9	L	302	ADP	C5-N7-C8	2.87	107.97	103.45
9	H	301	ADP	N3-C2-N1	-2.87	124.24	128.58
9	D	301	ADP	C2-N3-C4	2.86	118.82	111.83
9	P	301	ADP	C5-N7-C8	2.84	107.92	103.45
9	H	301	ADP	C3'-C2'-C1'	2.82	106.79	101.46
9	D	301	ADP	N3-C2-N1	-2.80	124.34	128.58
9	L	302	ADP	C4-N9-C8	2.79	108.67	105.74
9	P	301	ADP	O4'-C1'-N9	2.75	113.37	108.09
9	L	302	ADP	O4'-C1'-N9	2.74	113.35	108.09
9	H	301	ADP	N9-C8-N7	-2.68	110.14	113.94
9	D	301	ADP	N9-C8-N7	-2.60	110.25	113.94
7	G	301	ATP	O4'-C4'-C3'	-2.54	100.11	105.15
9	D	301	ADP	N6-C6-N1	2.46	123.86	118.38
7	K	301	ATP	O4'-C4'-C3'	-2.35	100.50	105.15
9	L	302	ADP	N9-C8-N7	-2.34	110.62	113.94
7	C	301	ATP	O4'-C4'-C3'	-2.34	100.51	105.15
9	P	301	ADP	N9-C8-N7	-2.33	110.62	113.94
9	L	302	ADP	C6-C5-N7	2.31	136.54	132.09
9	H	301	ADP	C6-C5-N7	2.27	136.46	132.09
9	H	301	ADP	C2-N1-C6	2.23	122.40	118.73
7	O	301	ATP	O4'-C4'-C3'	-2.17	100.84	105.15
9	D	301	ADP	C2-N1-C6	2.15	122.26	118.73
9	D	301	ADP	C6-C5-N7	2.13	136.20	132.09
9	H	301	ADP	N6-C6-N1	2.13	123.11	118.38
7	O	301	ATP	O3'-C3'-C2'	-2.04	105.28	111.82
9	P	301	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

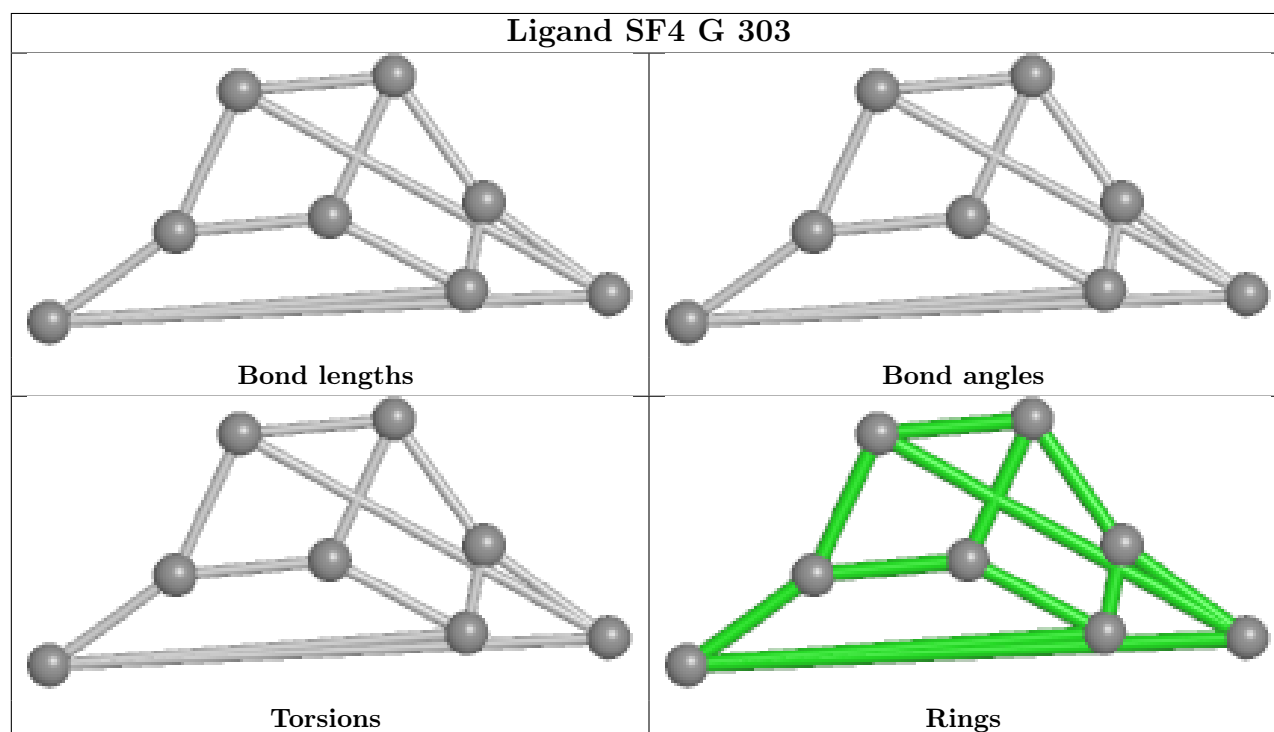
Mol	Chain	Res	Type	Atoms
7	C	301	ATP	PB-O3B-PG-O1G
7	C	301	ATP	PG-O3B-PB-O1B
7	G	301	ATP	C3'-C4'-C5'-O5'
7	C	301	ATP	PG-O3B-PB-O2B
7	G	301	ATP	PG-O3B-PB-O2B
7	K	301	ATP	PG-O3B-PB-O2B
7	O	301	ATP	PG-O3B-PB-O2B

There are no ring outliers.

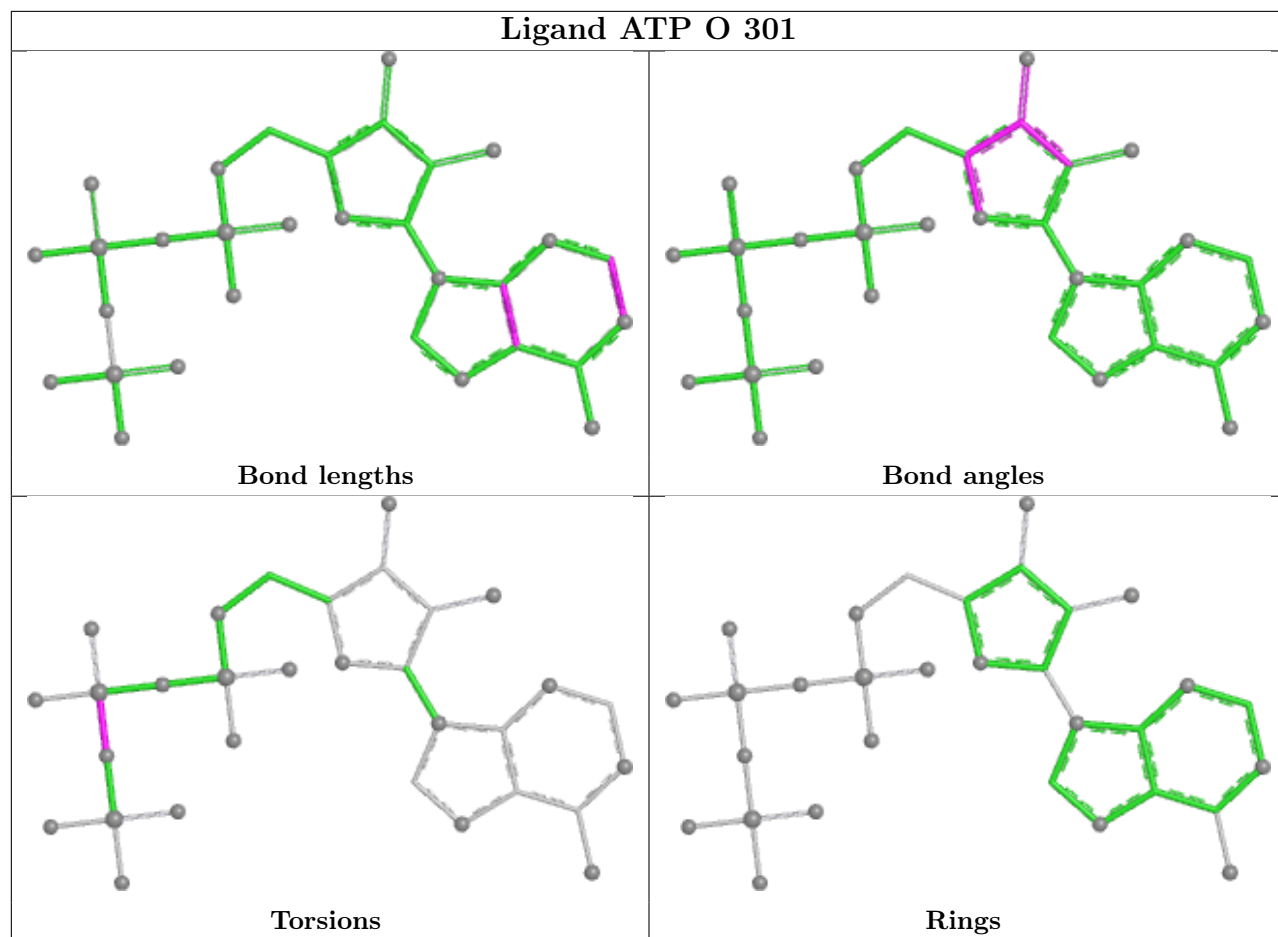
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	301	ADP	1	0
7	G	301	ATP	1	0
9	D	301	ADP	1	0
5	N	401	SF4	1	0

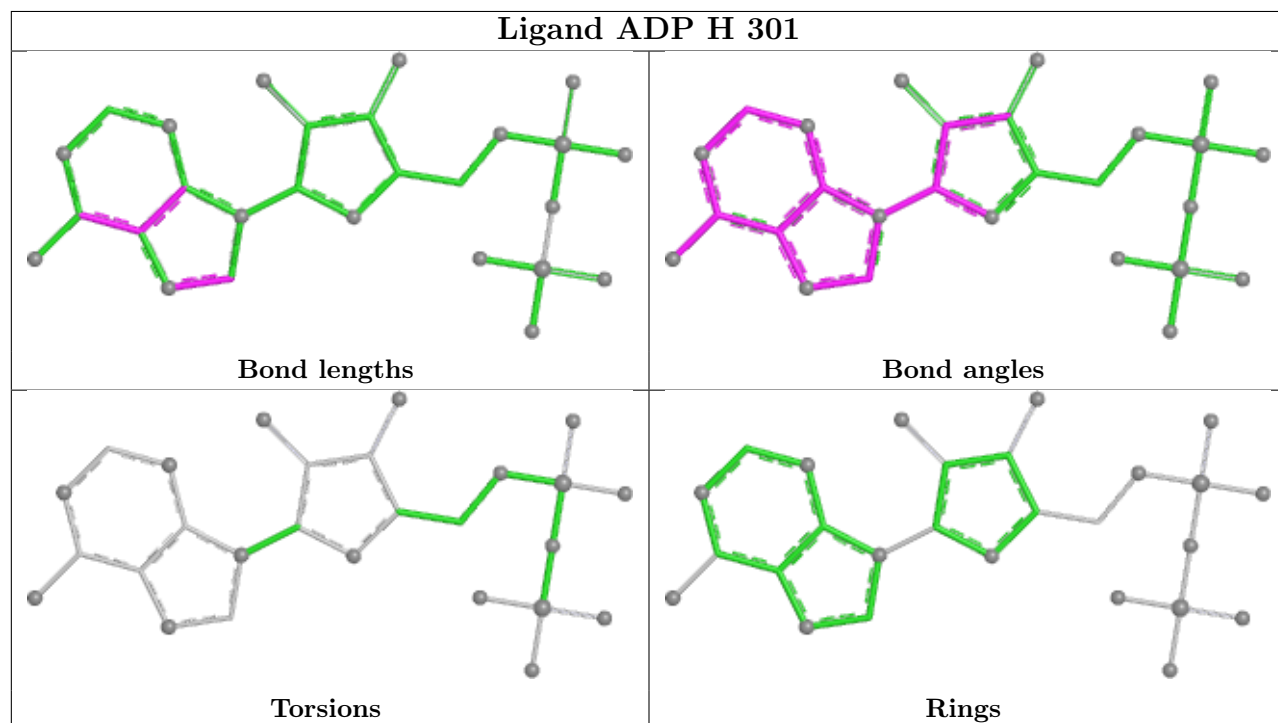
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



## Ligand ATP O 301

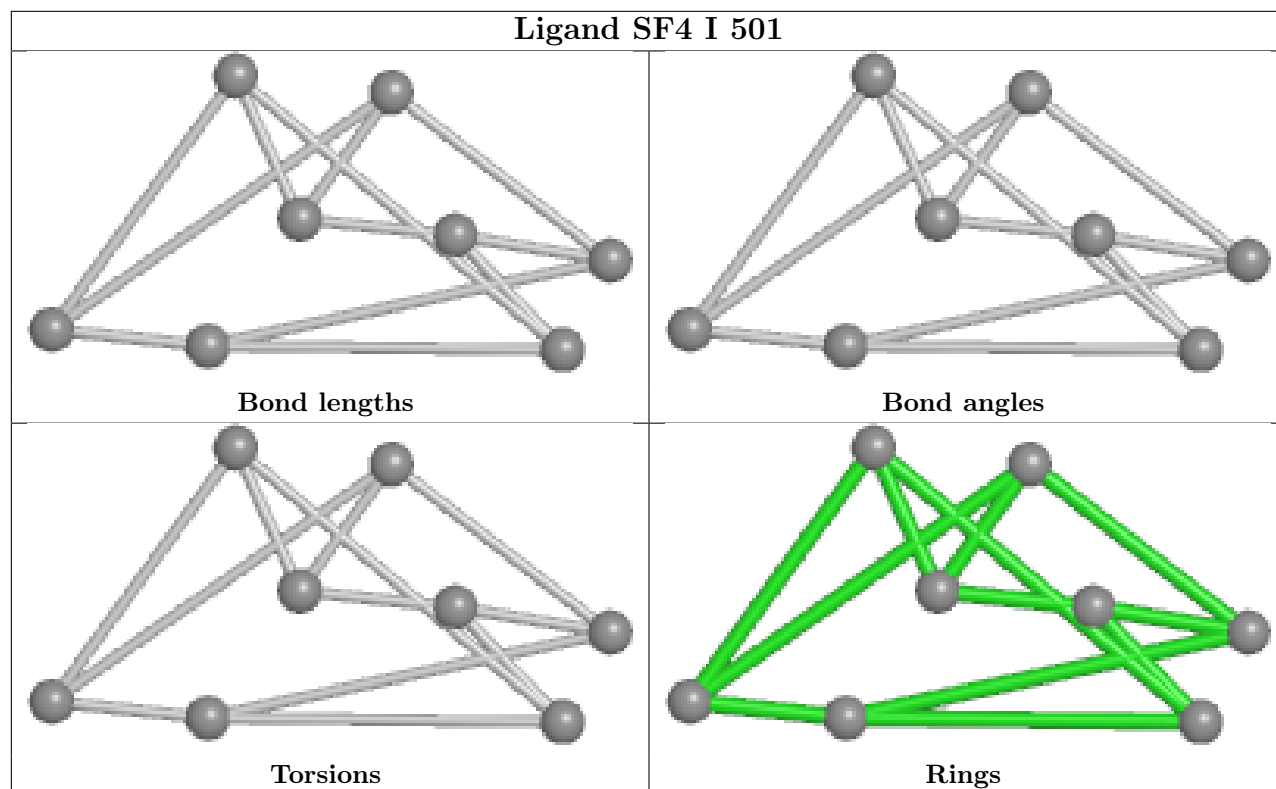


## Ligand ADP H 301

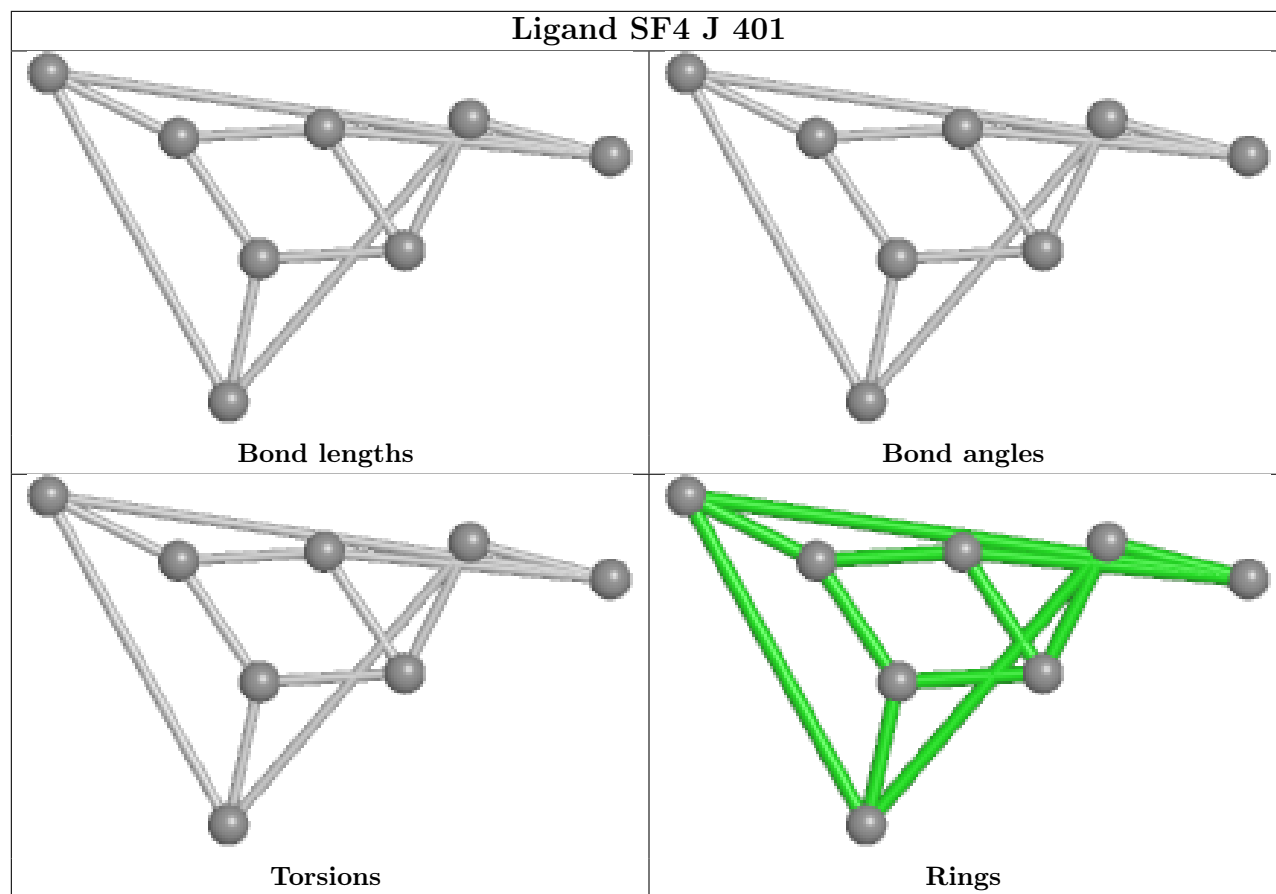




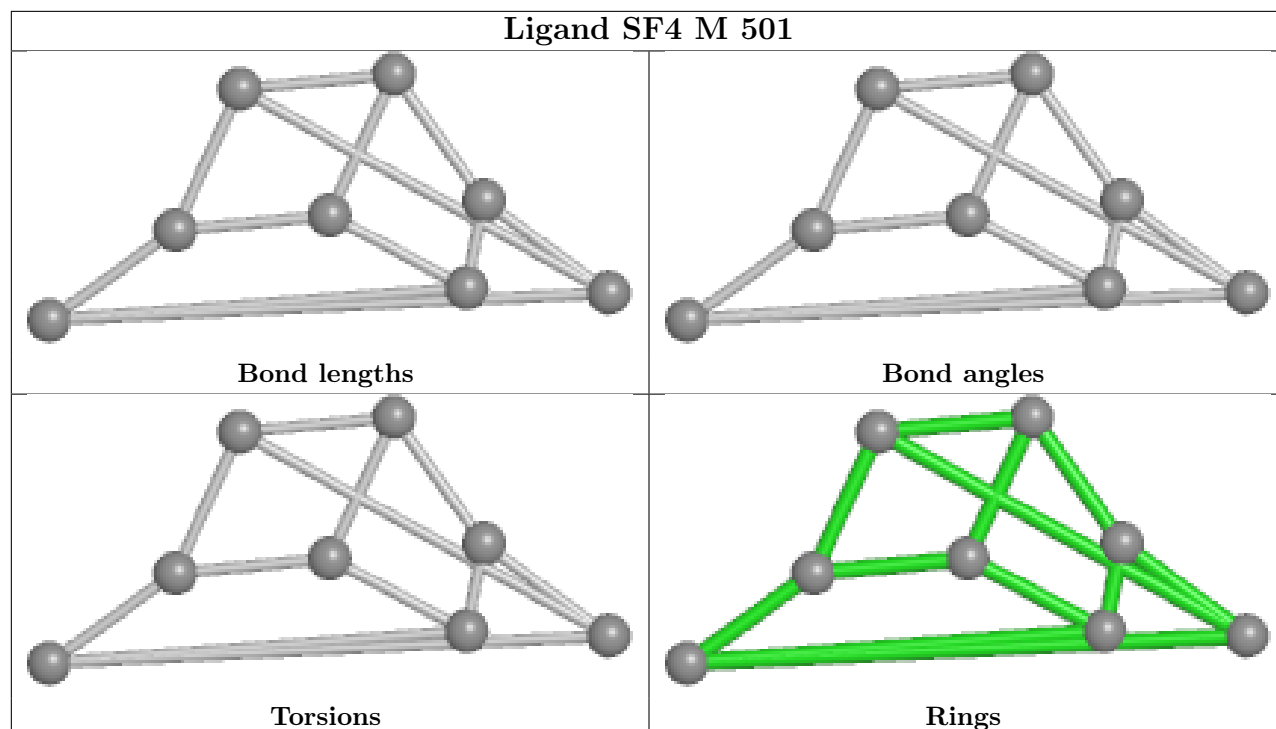
## Ligand SF4 I 501



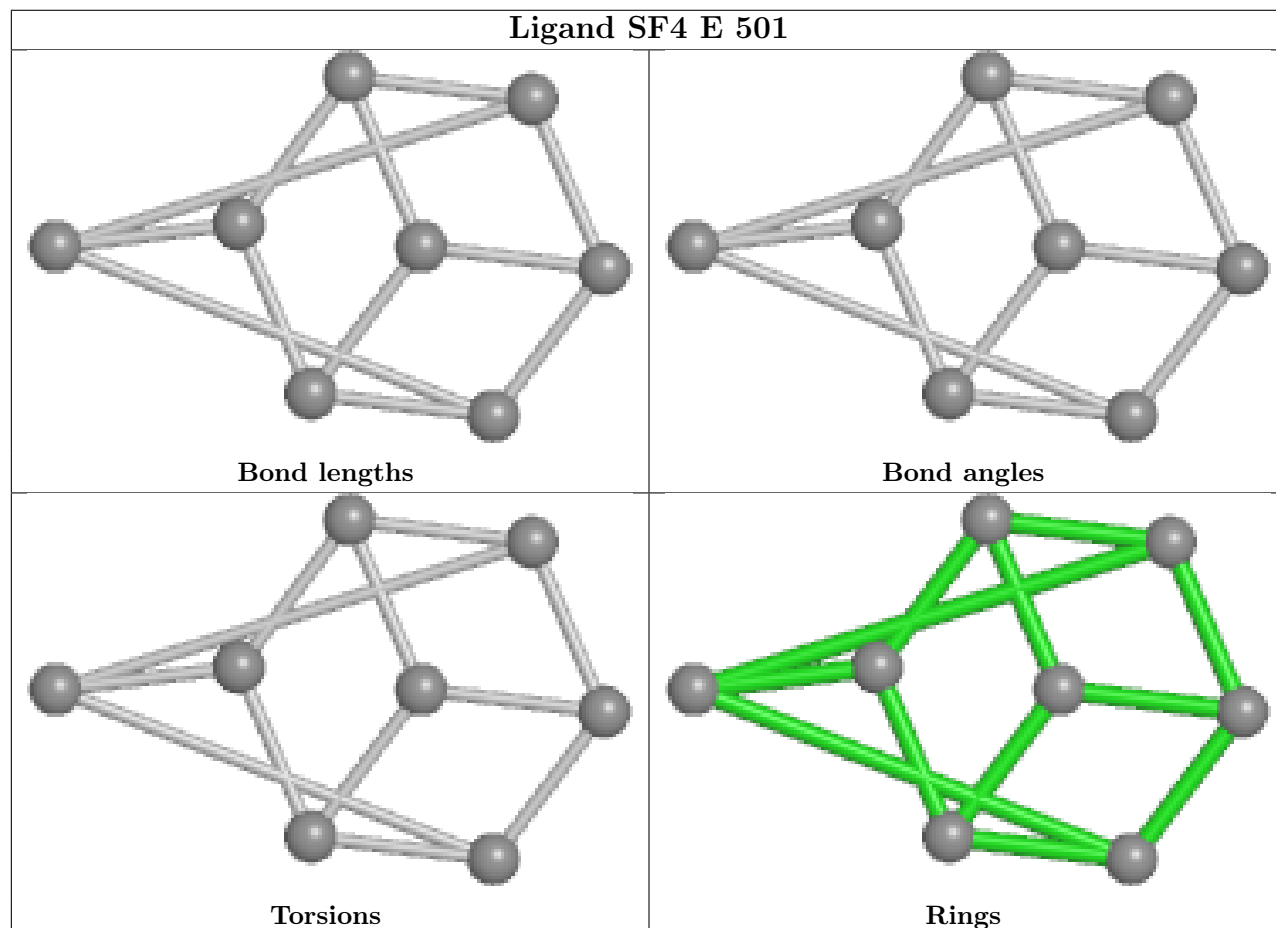
## Ligand SF4 J 401



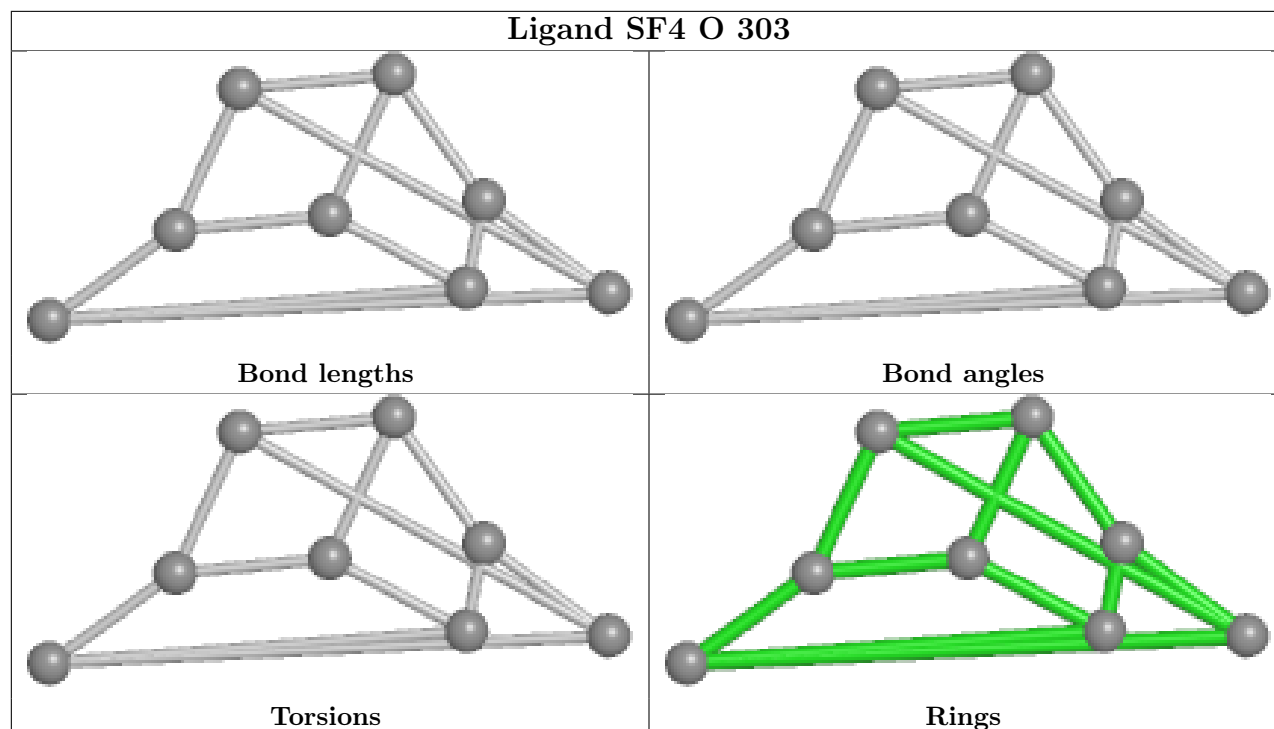
## Ligand SF4 M 501



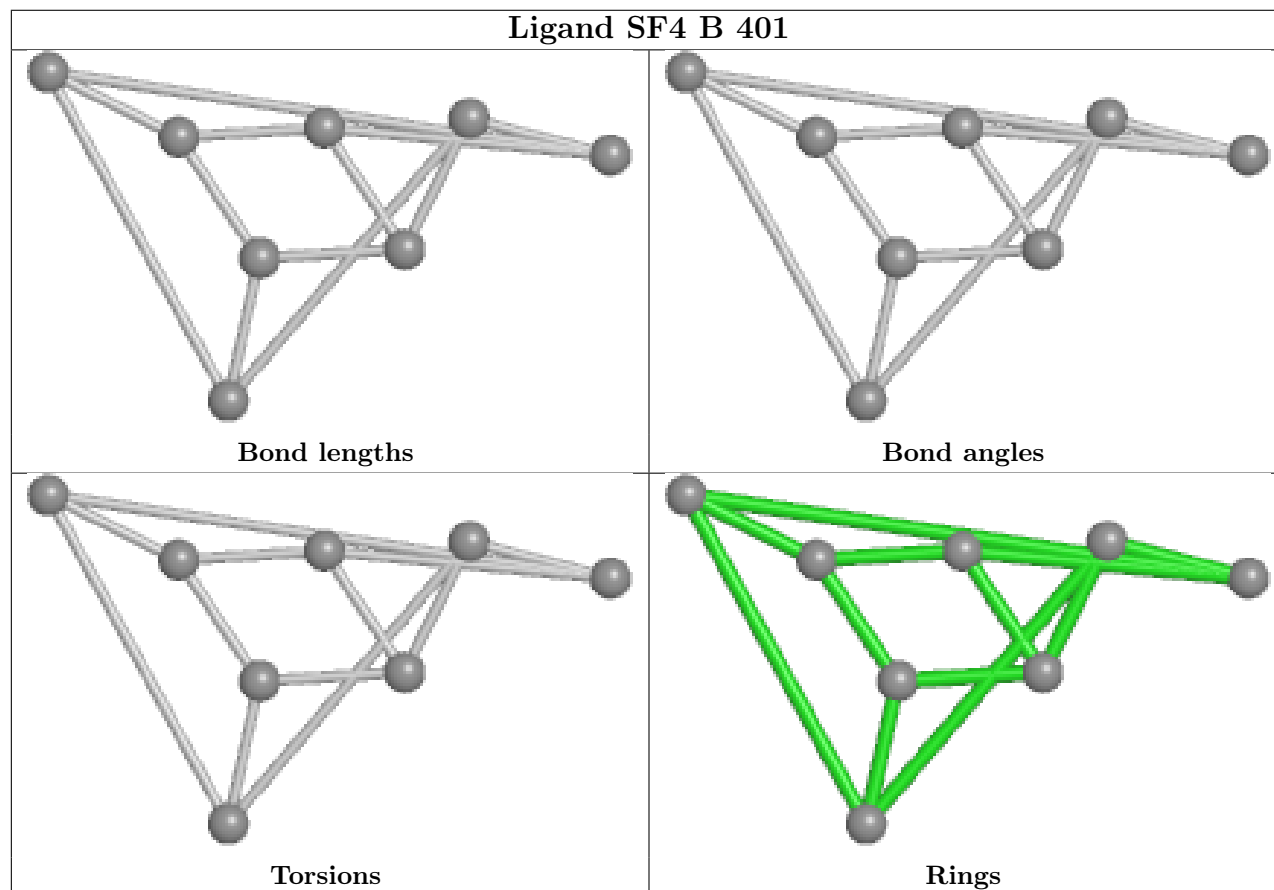
## Ligand SF4 E 501

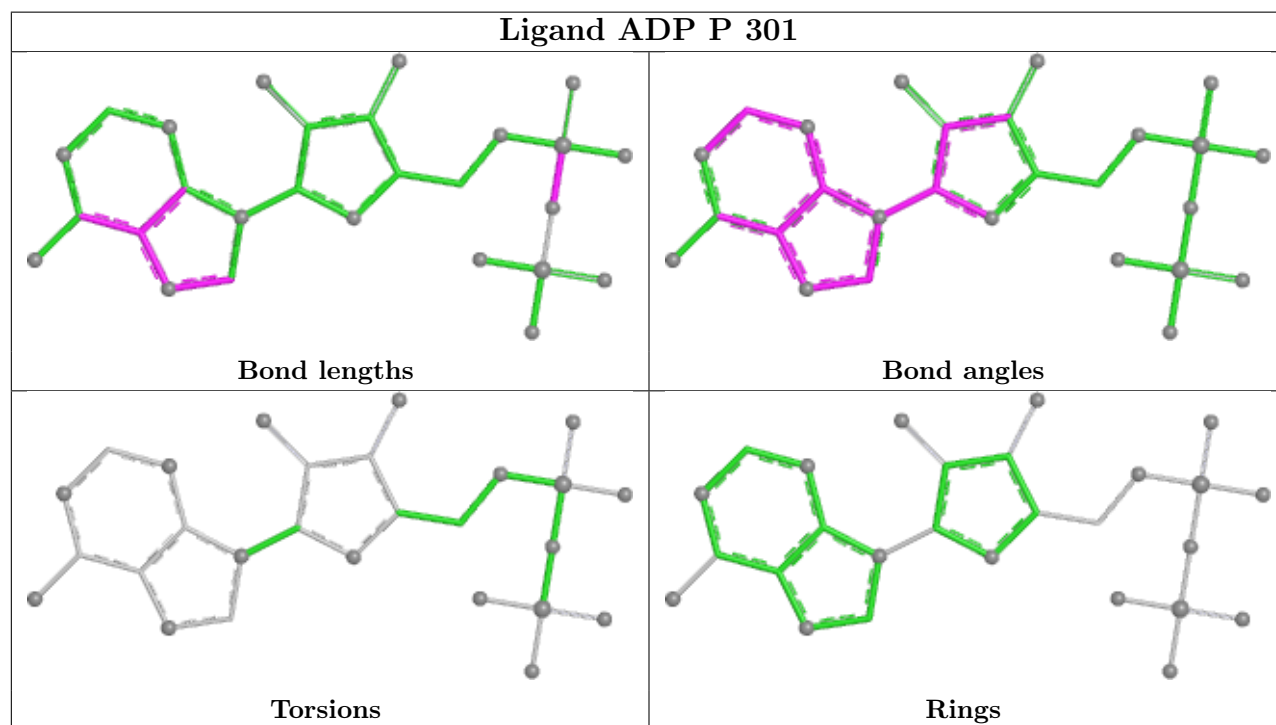
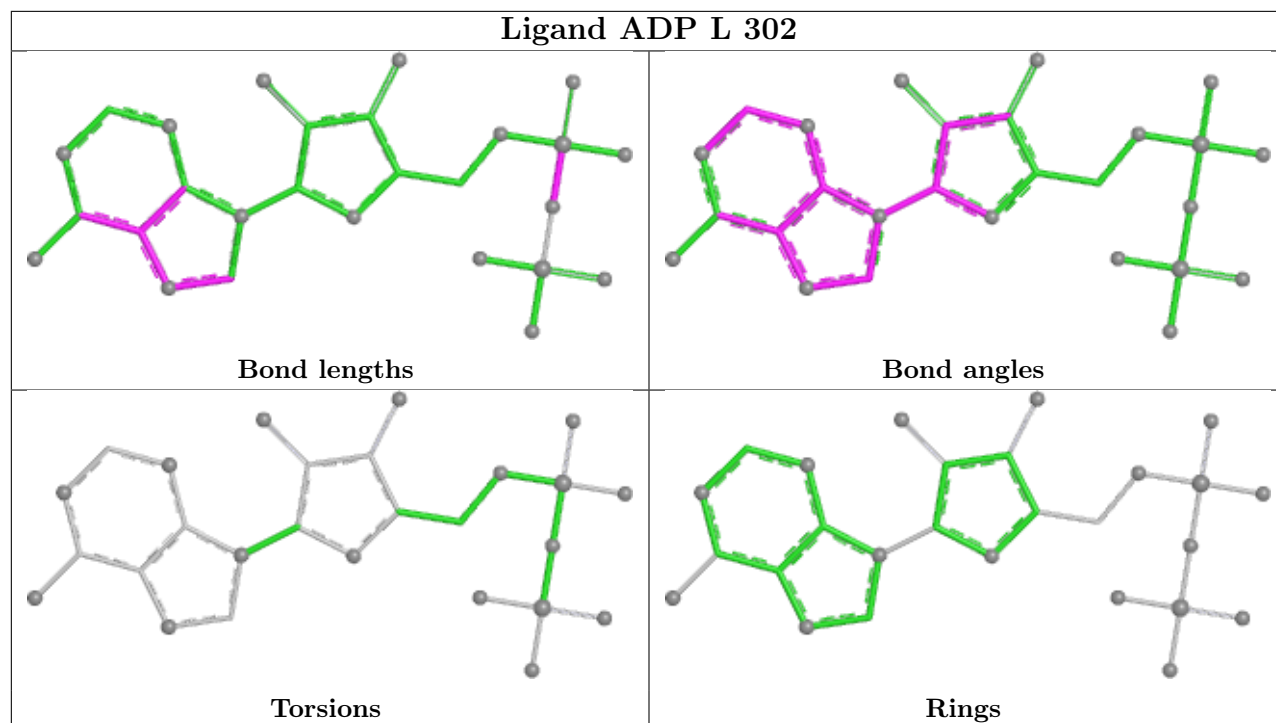


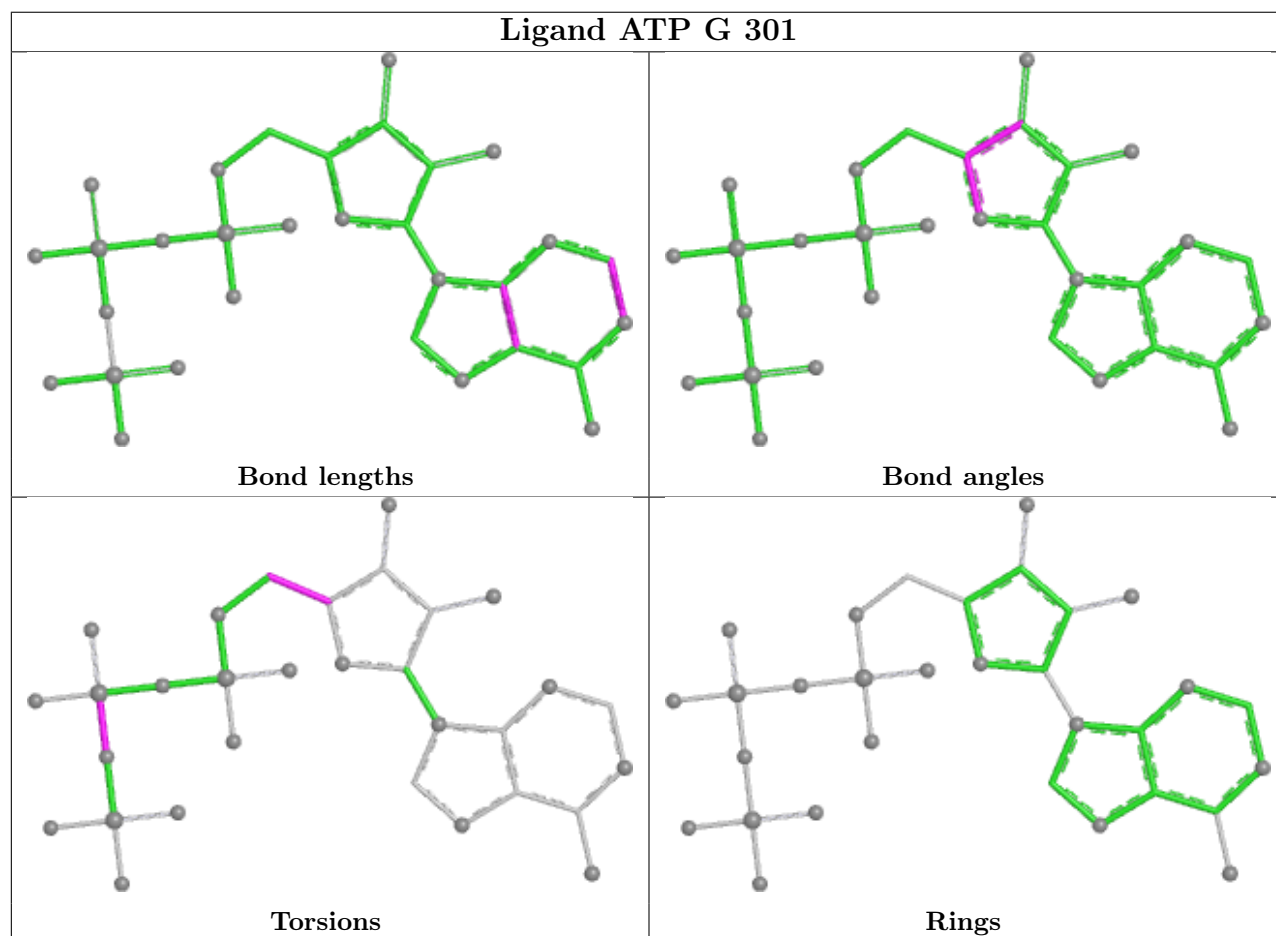
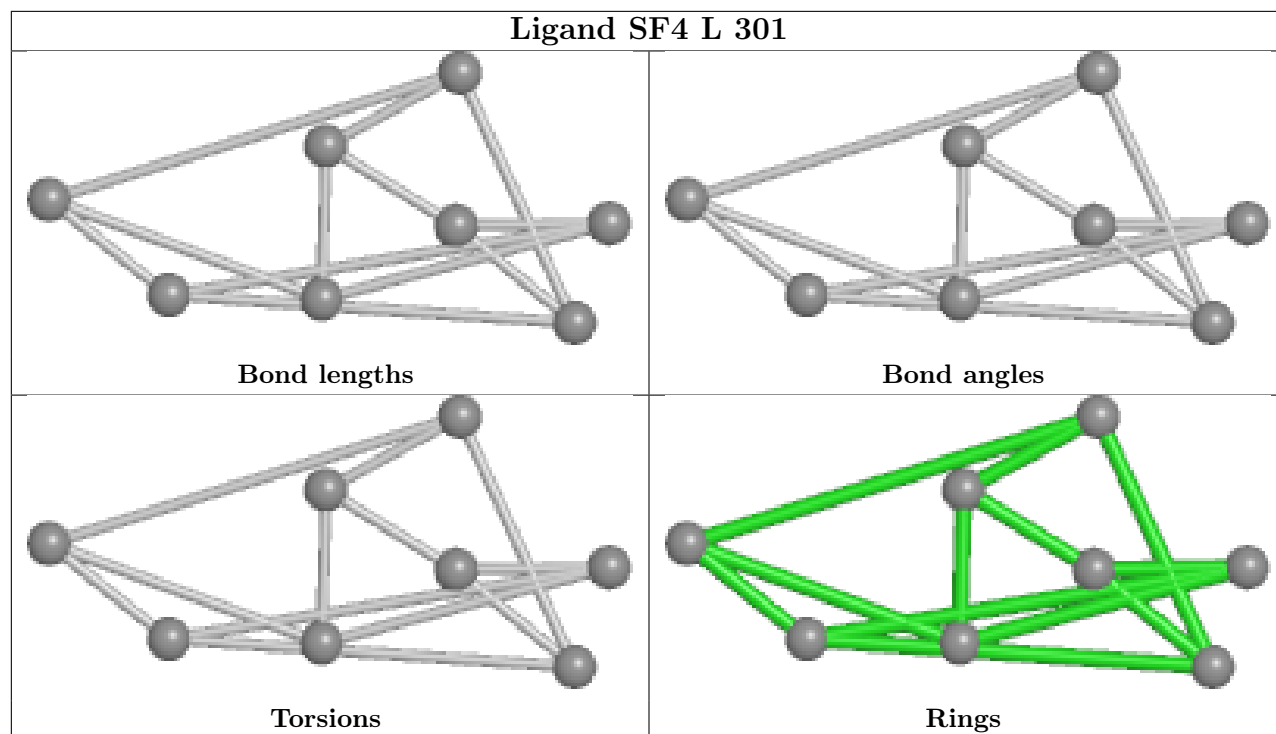
## Ligand SF4 O 303

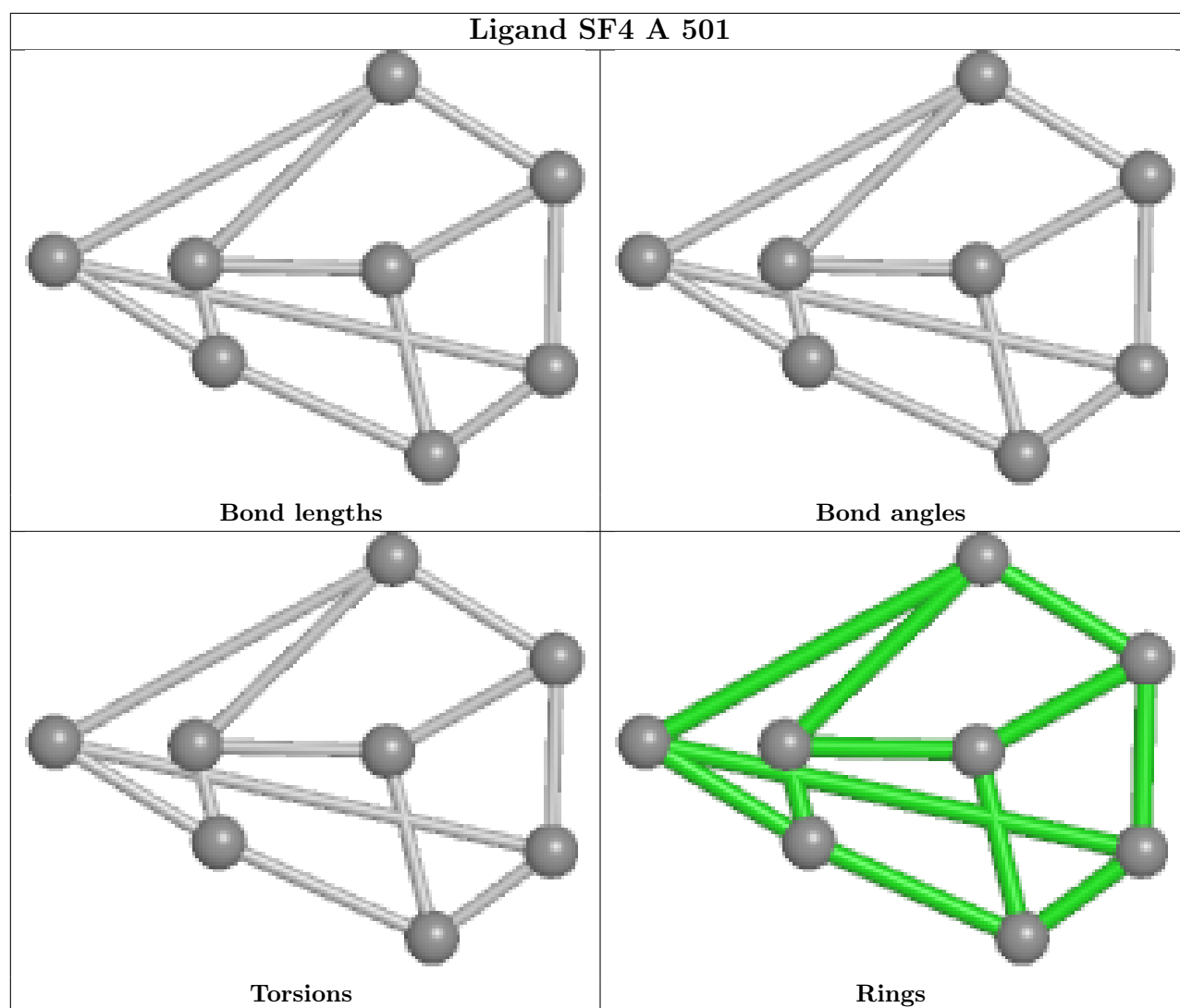


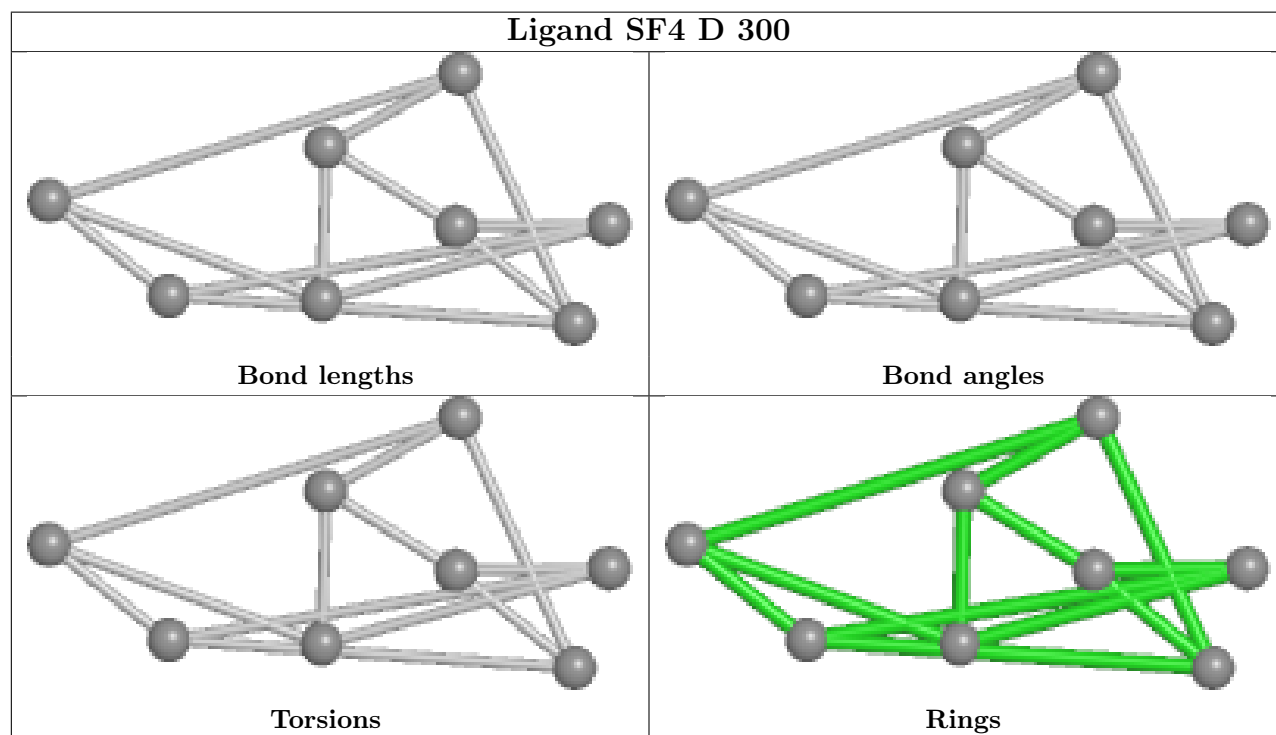
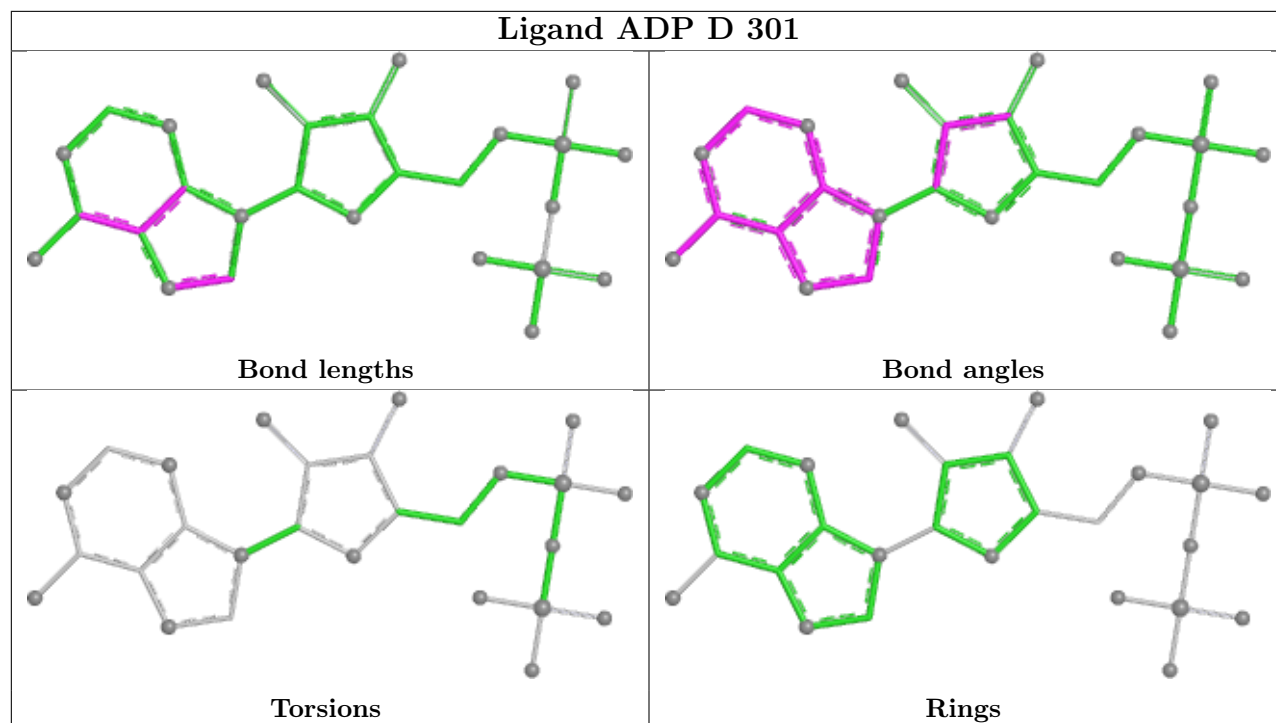
## Ligand SF4 B 401

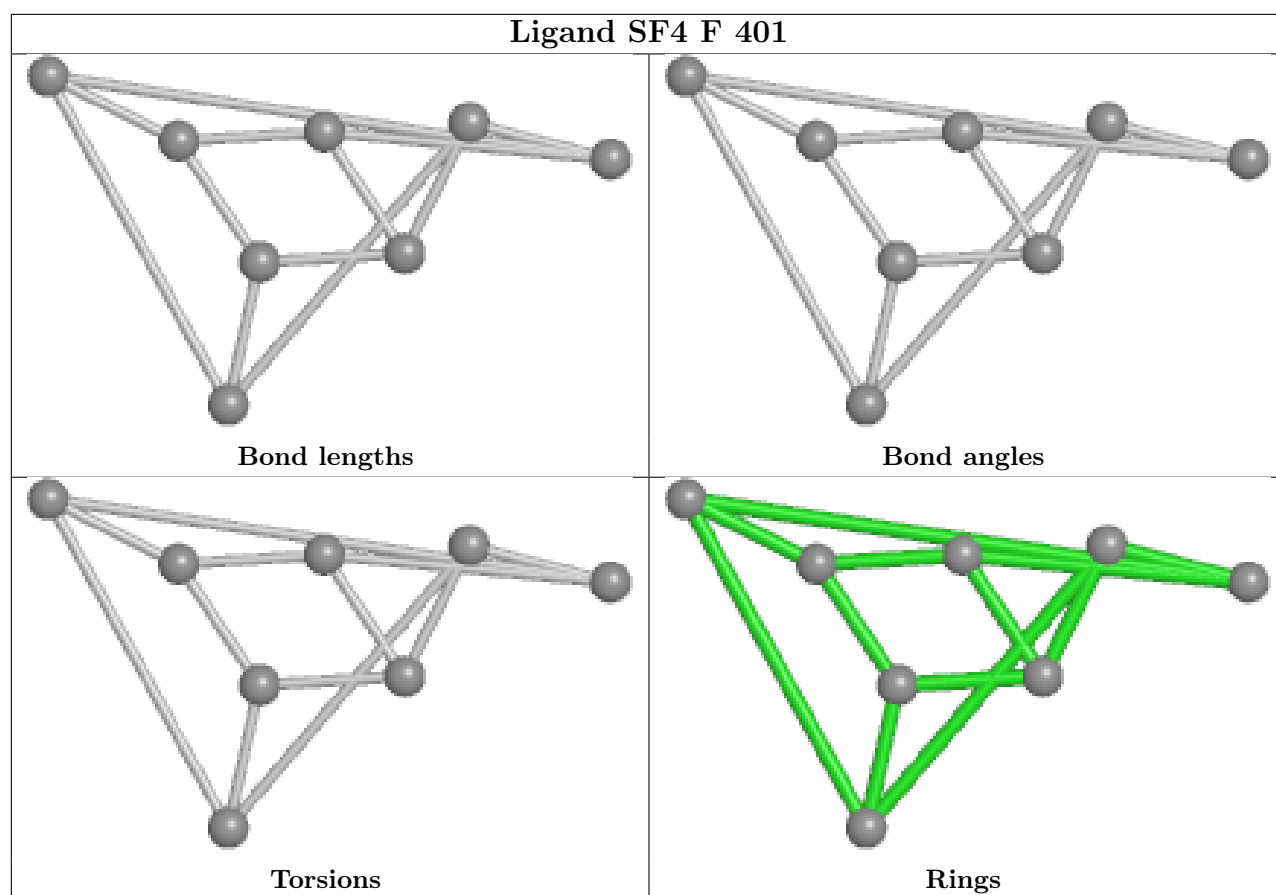




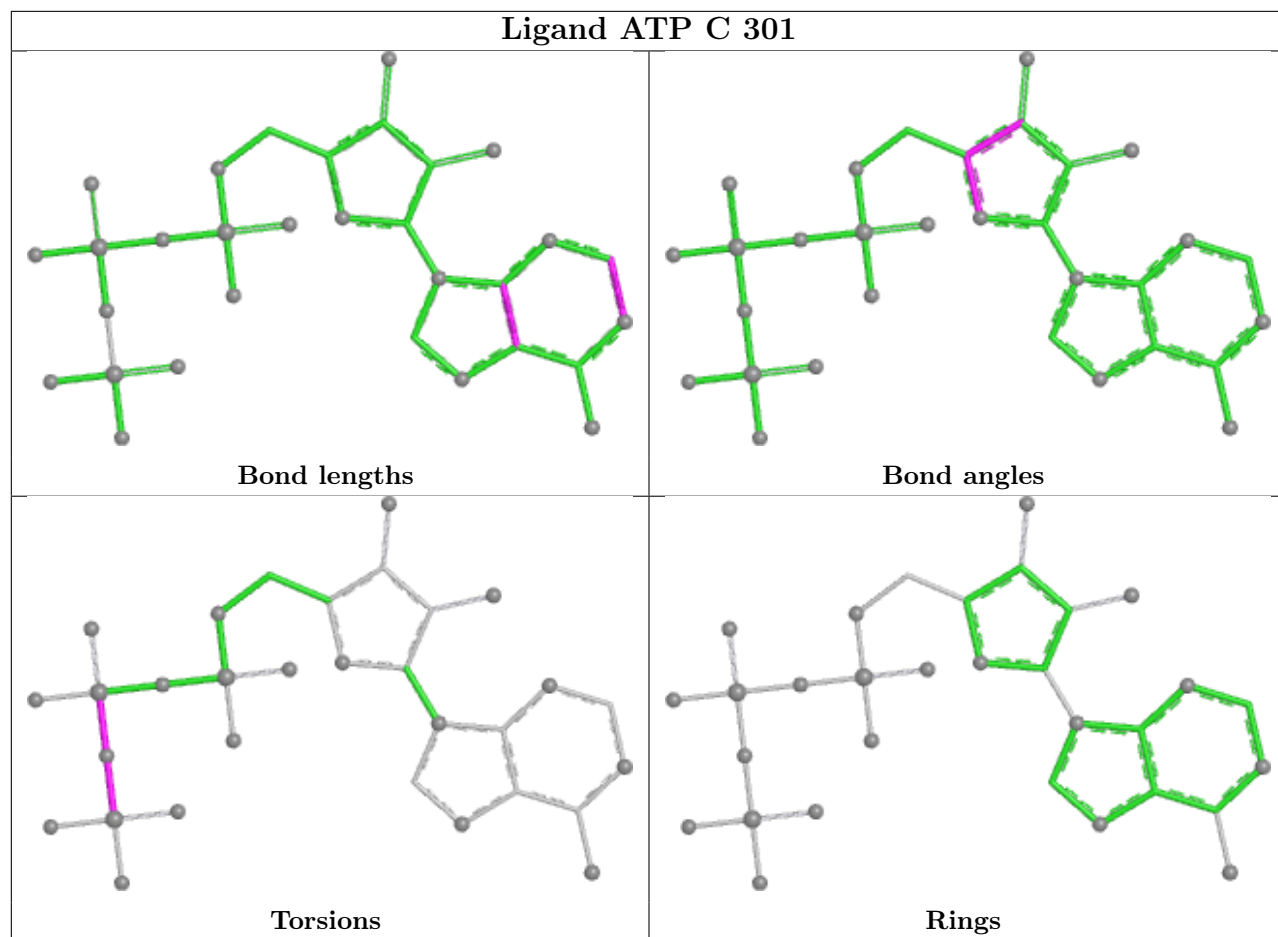


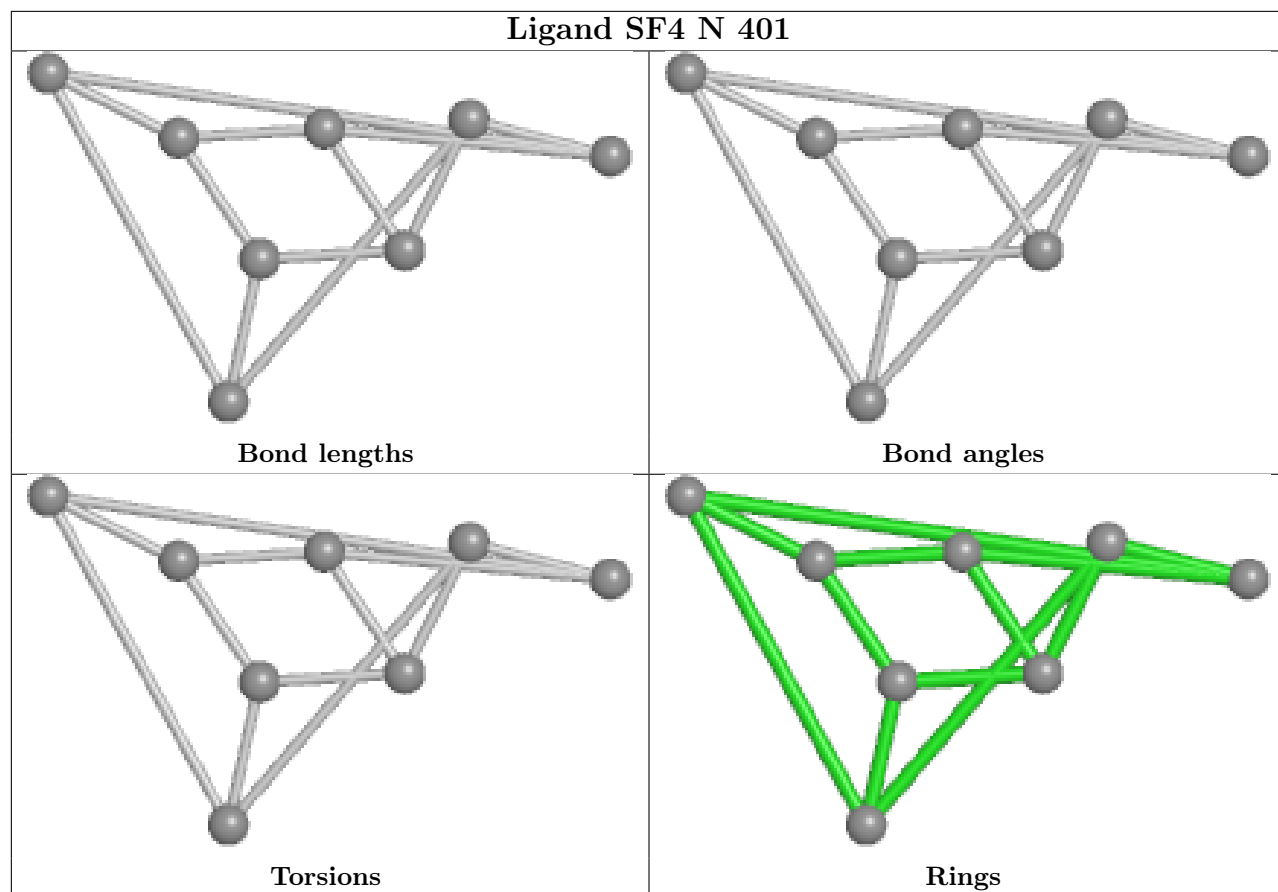


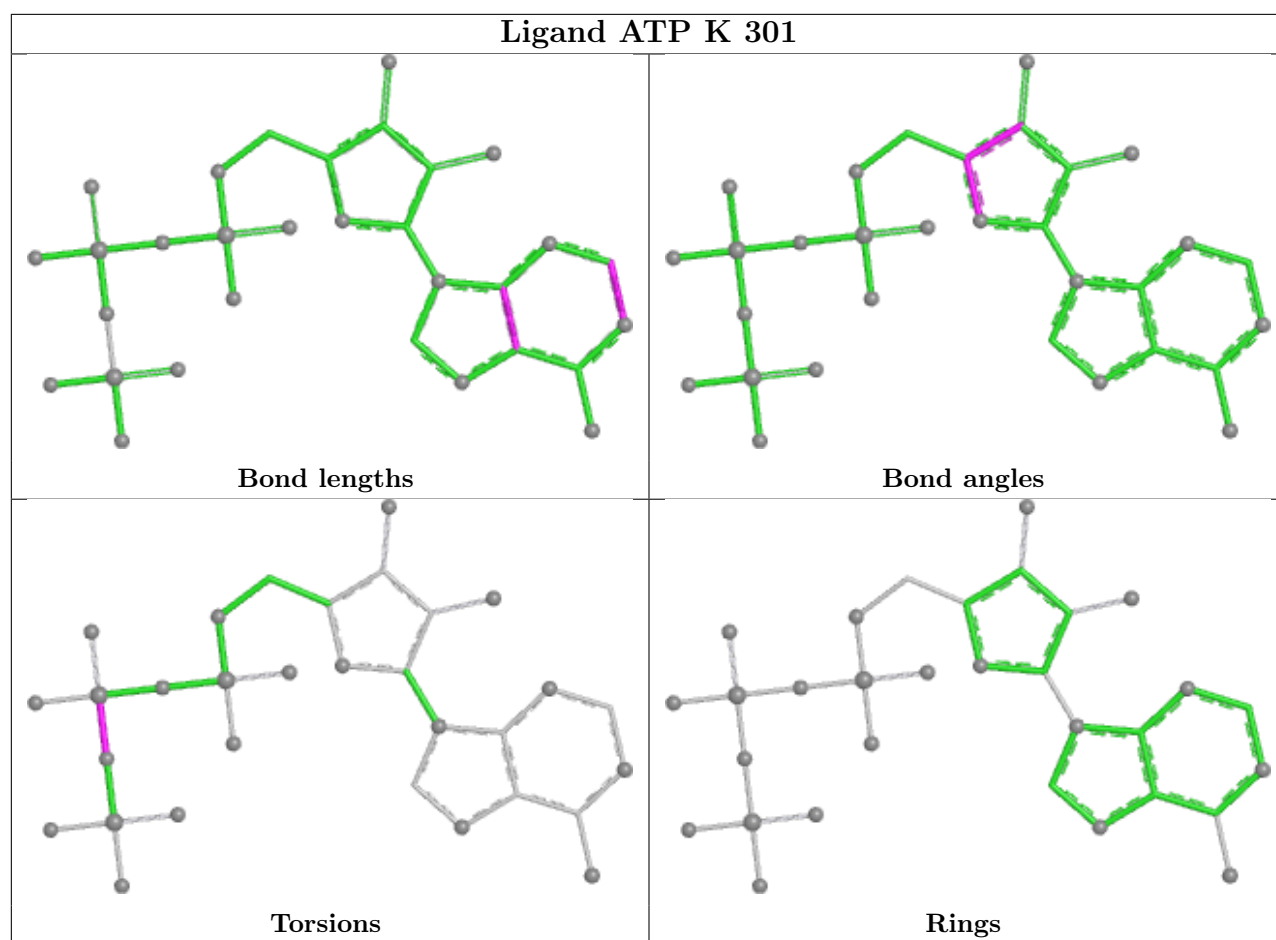












## 5.7 Other polymers [i](#)

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	437/445 (98%)	-1.00	1 (0%) 91 92	21, 47, 62, 103	2 (0%)
1	E	436/445 (97%)	-1.05	0 100 100	19, 46, 59, 84	2 (0%)
1	I	436/445 (97%)	-1.02	0 100 100	20, 48, 64, 91	3 (0%)
1	M	437/445 (98%)	-0.90	0 100 100	23, 53, 70, 97	2 (0%)
2	B	387/388 (99%)	-1.07	0 100 100	38, 47, 58, 83	0
2	F	387/388 (99%)	-1.06	0 100 100	35, 45, 59, 76	0
2	J	387/388 (99%)	-1.07	0 100 100	36, 46, 60, 73	0
2	N	387/388 (99%)	-0.84	1 (0%) 90 91	39, 55, 73, 88	0
3	C	264/273 (96%)	-0.95	0 100 100	22, 52, 71, 82	3 (1%)
3	G	264/273 (96%)	-1.02	0 100 100	21, 46, 65, 74	3 (1%)
3	K	264/273 (96%)	-1.04	0 100 100	21, 46, 60, 72	1 (0%)
3	O	264/273 (96%)	-1.01	0 100 100	21, 48, 66, 81	2 (0%)
4	D	261/269 (97%)	-0.85	0 100 100	25, 60, 75, 85	1 (0%)
4	H	261/269 (97%)	-0.92	0 100 100	40, 53, 69, 92	0
4	L	261/269 (97%)	-0.96	0 100 100	26, 52, 66, 75	1 (0%)
4	P	261/269 (97%)	-0.91	0 100 100	26, 54, 66, 80	1 (0%)
All	All	5394/5500 (98%)	-0.98	2 (0%) 100 100	19, 49, 68, 103	21 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	38	ALA	2.6
1	A	442	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
6	SO4	E	502	5/5	0.96	0.09	50,52,55,75	0
6	SO4	P	303	5/5	0.96	0.04	55,56,60,85	0
6	SO4	K	303	5/5	0.97	0.09	53,56,58,59	0
6	SO4	L	304	5/5	0.97	0.14	53,54,56,77	0
6	SO4	M	502	5/5	0.97	0.10	50,51,58,76	0
6	SO4	O	304	5/5	0.97	0.03	55,56,58,81	0
6	SO4	C	303	5/5	0.97	0.09	50,54,59,74	0
6	SO4	J	402	5/5	0.98	0.05	48,49,51,56	0
6	SO4	G	304	5/5	0.98	0.04	50,52,60,62	1
6	SO4	N	402	5/5	0.99	0.04	54,55,62,62	0
6	SO4	F	402	5/5	0.99	0.06	46,49,52,54	0
6	SO4	B	402	5/5	0.99	0.04	45,49,50,51	0
7	ATP	C	301	31/31	0.99	0.03	46,51,56,58	0
7	ATP	K	301	31/31	0.99	0.03	35,42,48,49	0
7	ATP	O	301	31/31	0.99	0.03	39,44,47,49	0
9	ADP	D	301	27/27	0.99	0.04	46,52,58,60	0
9	ADP	H	301	27/27	0.99	0.03	40,46,48,49	0
9	ADP	P	301	27/27	0.99	0.03	42,47,50,52	0
5	SF4	I	501	8/8	1.00	0.02	35,43,46,47	0
5	SF4	J	401	8/8	1.00	0.02	31,34,39,42	0
5	SF4	L	301	8/8	1.00	0.02	35,37,38,41	0
5	SF4	M	501	8/8	1.00	0.01	39,42,44,45	0
5	SF4	N	401	8/8	1.00	0.01	38,42,43,47	0
5	SF4	O	303	8/8	1.00	0.02	36,40,43,46	0
5	SF4	A	501	8/8	1.00	0.02	36,40,43,47	0
7	ATP	G	301	31/31	1.00	0.03	37,42,46,48	0
5	SF4	B	401	8/8	1.00	0.02	34,39,40,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SF4	D	300	8/8	1.00	0.02	37,39,42,43	0
8	MG	C	302	1/1	1.00	0.02	48,48,48,48	0
8	MG	D	302	1/1	1.00	0.02	51,51,51,51	0
8	MG	G	302	1/1	1.00	0.01	39,39,39,39	0
8	MG	H	302	1/1	1.00	0.01	47,47,47,47	0
8	MG	K	302	1/1	1.00	0.01	39,39,39,39	0
8	MG	L	303	1/1	1.00	0.02	42,42,42,42	0
8	MG	O	302	1/1	1.00	0.01	51,51,51,51	0
8	MG	P	302	1/1	1.00	0.01	46,46,46,46	0
5	SF4	E	501	8/8	1.00	0.02	37,38,41,42	0
5	SF4	F	401	8/8	1.00	0.02	31,34,39,40	0
9	ADP	L	302	27/27	1.00	0.03	39,43,48,49	0
5	SF4	G	303	8/8	1.00	0.02	32,36,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.