



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:25 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

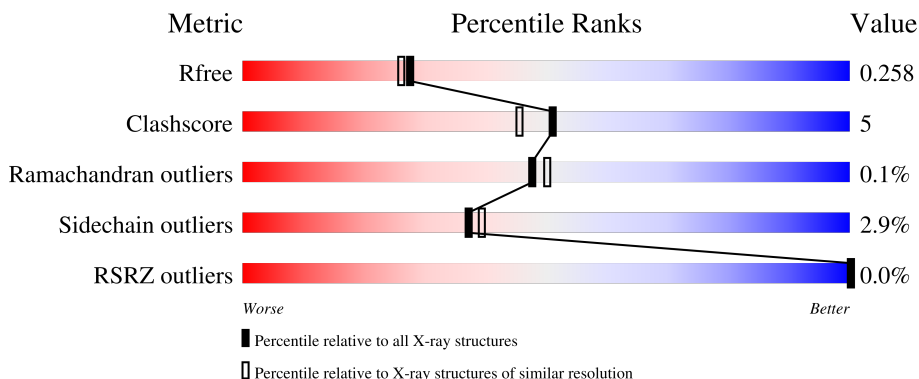
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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			

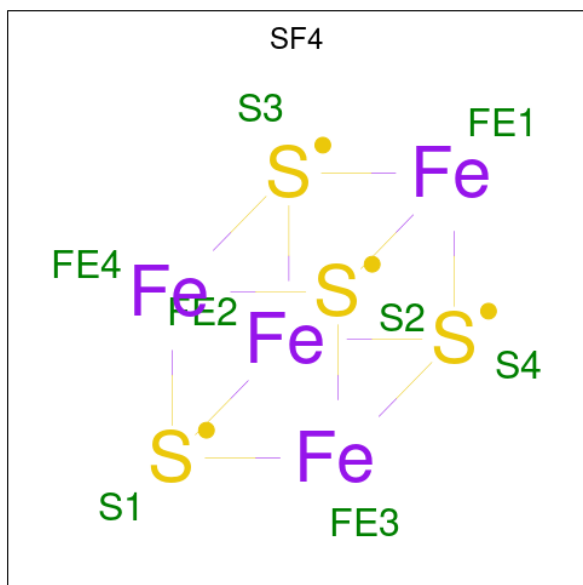
- Molecule 3 is a protein called 3-methylbenzoyl-CoA reductase delta subunit MbdP.

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_4S_4) (labeled as "Ligand of Interest" by depositor).



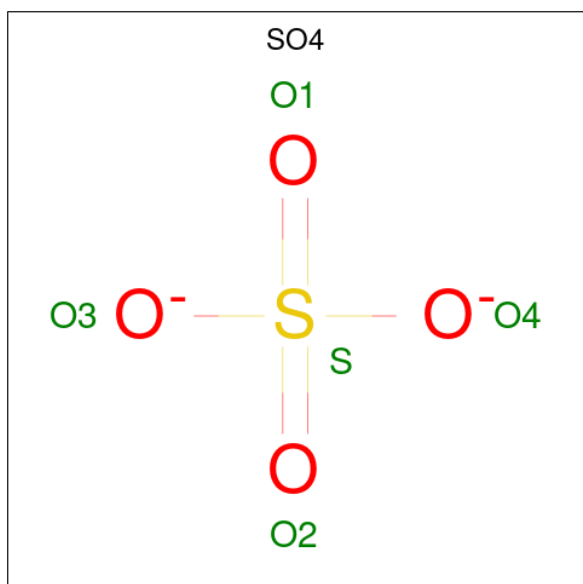
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	D	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		
5	F	1	Total	Fe	S	0	0
			8	4	4		
5	G	1	Total	Fe	S	0	0
			8	4	4		

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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: O₄S).



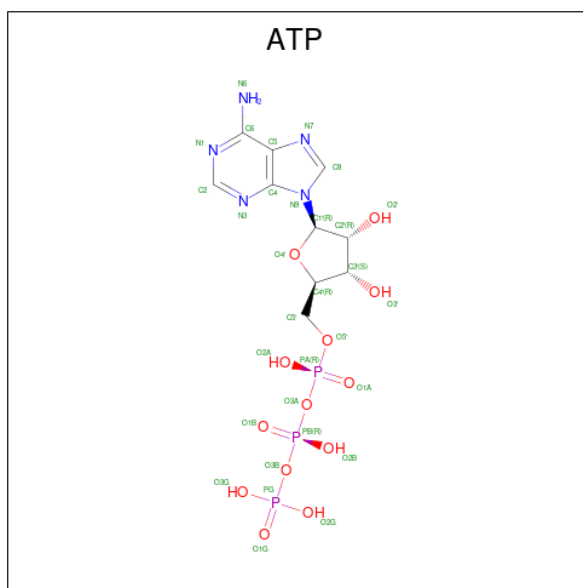
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		

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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).

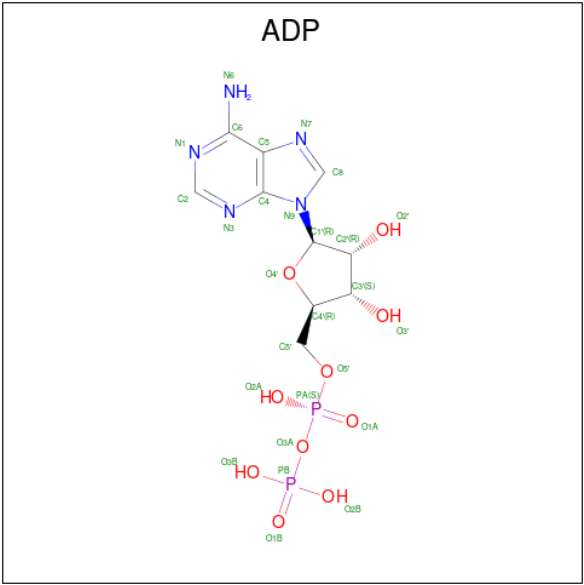


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- 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	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	G	1	Total	Mg	0	0
			1	1		
8	H	1	Total	Mg	0	0
			1	1		
8	K	1	Total	Mg	0	0
			1	1		
8	L	1	Total	Mg	0	0
			1	1		
8	O	1	Total	Mg	0	0
			1	1		
8	P	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

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

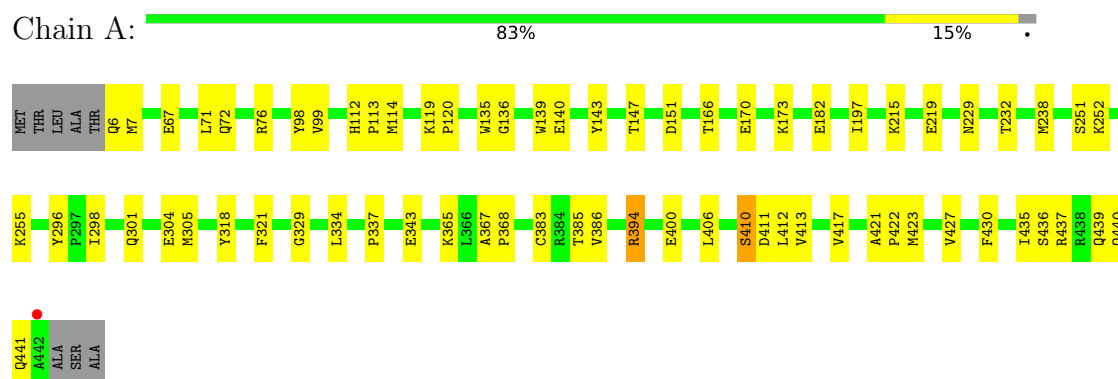
- Molecule 10 is water.

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

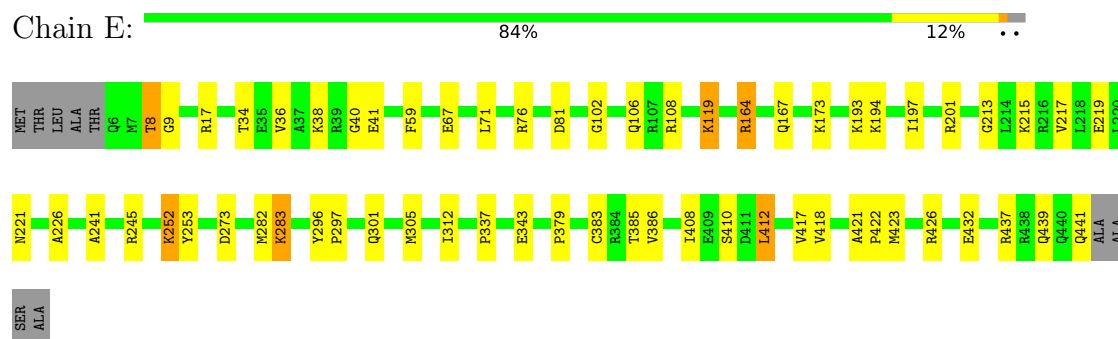
3 Residue-property plots

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.

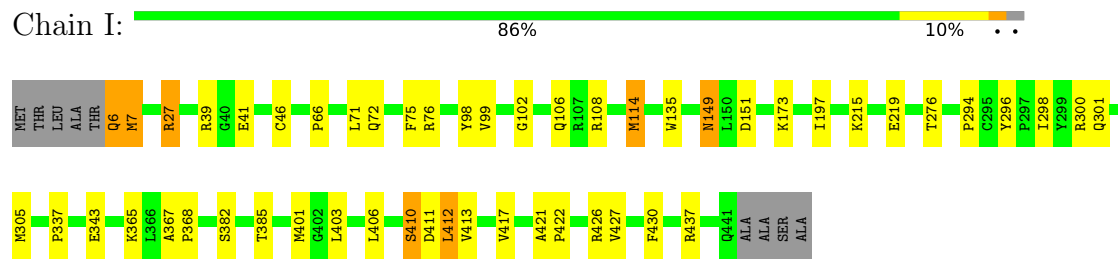
- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO



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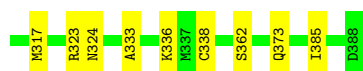
Met	THR	LEU	ALA	THR	Q6	R7	T8	I48	R57	L71	Q72	T73	R76	R77	V78	Y98	P113	W135	I138	V139	E140	T147	I148	N149	Y152	P153	M154	R164	Q167	K173	E188	G192	I197	N221	A226	V227	F228	A243	F248					
R438	Q439	Q440	A441	A442	ALA	SER	ALA	K252	L261	E262	V265	V266	D273	K274	E277	G278	T279	V280	K283	P284	C295	Y296	E304	Y332	P337	E343	M348	K364	A367	P368	T385	M401	L406	S410	D411	L412	V417	P422	R426	F430	L434	I435	S436	P437

R323	N324	A327	V330	A333	K336	Y359	F360	I361	S362	D372	Q373	D388																				
A2	L14	I17	E23	L61	G73	H74	E75	S78	D93	T97	L104	D112	K141	R152	I158	V161	R192	K193	P196	W197	A201	S204	M229	G247	V267	D270	L290	Y303	E315	H316	N317	V320

E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838
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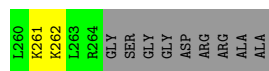
F219	A2	K12	E159	L104	D112	A118	N137	R152	L155	E159	S160	V161	R164	K165	I166	E170	R183	R192	A201	S204	A211
G247	K3	A29	E175	T97	A119	P119	N99	R152	L155	E159	S160	V161	R164	K165	I166	E170	R183	R192	A201	S204	A211
V267	K4	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166	E170
D282	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
Q310	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
E328	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
T329	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
A333	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
K336	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
P358	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
S362	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
Q373	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
M386	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
F387	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166
D388	K12	A29	K34	R42	A58	L61	N74	E75	R88	K89	T97	A98	N99	R152	L155	E159	S160	V161	R164	K165	I166

Item	MET	A2	A39	R183
MET	7			
A2		6		
A39			1	
R42			1	
V43			1	
I44			1	
Q48			1	
V49			1	
Y50			1	
F51			1	
P52			1	
L61			1	
R65			1	
T71			1	
D72			1	
G73			1	
N74			1	
E75			1	
D93			1	
T97			1	
K98			1	
L104			1	
D112			1	
A118			1	
P119			1	
N137			1	
V161			1	
R164			1	
K166			1	
E170			1	
R183				1
R192				1
K193				1
S204				1
Q238				1
G247				1
Y303				1
G316				1



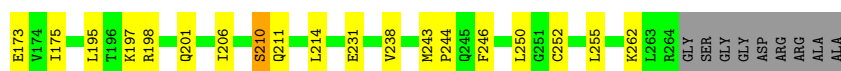
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain C: 84% 11% ..



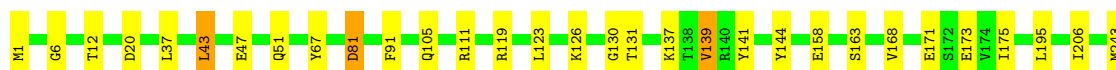
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain G: 78% 18% ..



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

Chain K: 84% 12% ..



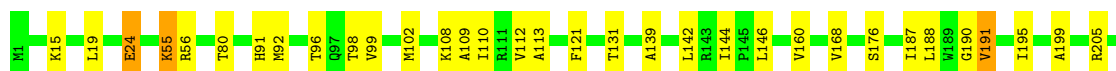
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

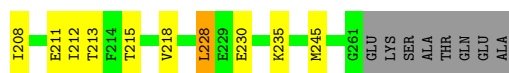
Chain O: 81% 15% ..



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

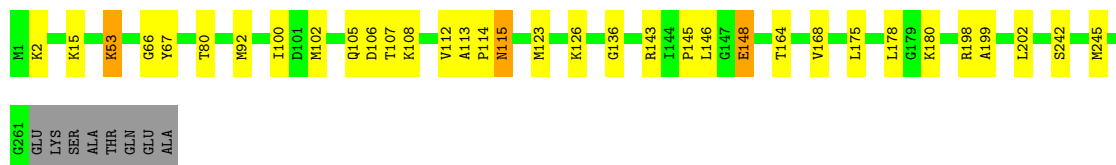
Chain D: 81% 14% ..





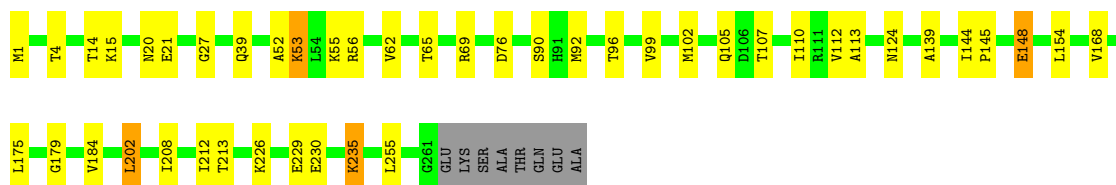
- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain H: 84% 12% ..



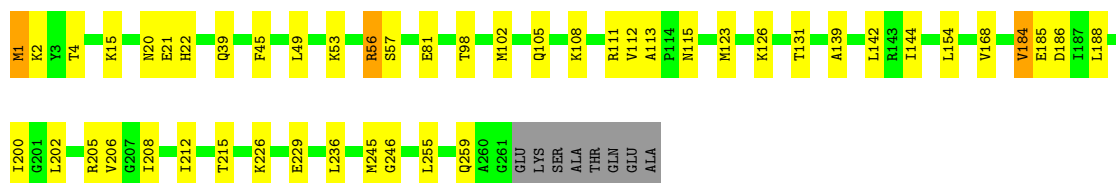
- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	45.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P	198/203 (98%)	189 (96%)	9 (4%)	24	22
All	All	4457/4500 (99%)	4328 (97%)	129 (3%)	37	39

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	116	HIS
3	O	261	LYS
2	F	165	LYS
2	F	61	LEU
4	P	21	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	193	GLN
1	M	202	GLN
1	M	267	HIS
1	E	223	ASN
1	E	202	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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%)
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

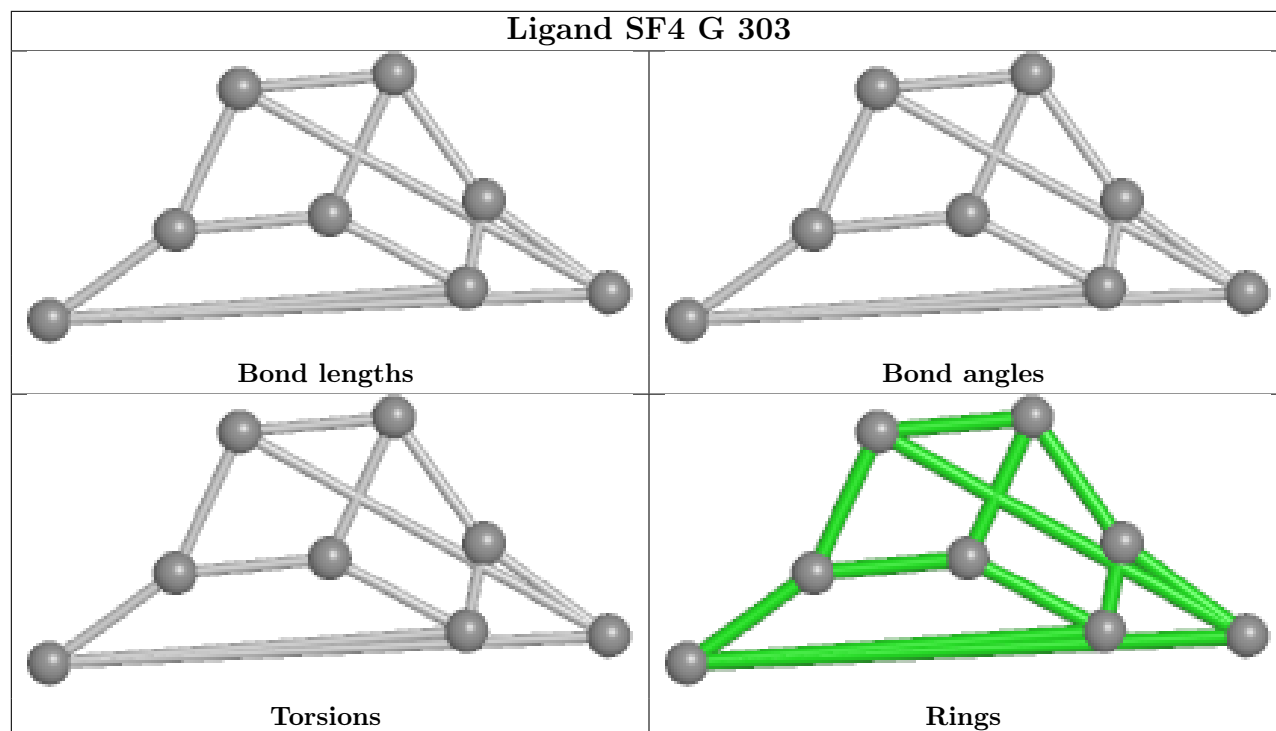
There are no ring outliers.

4 monomers are involved in 4 short contacts:

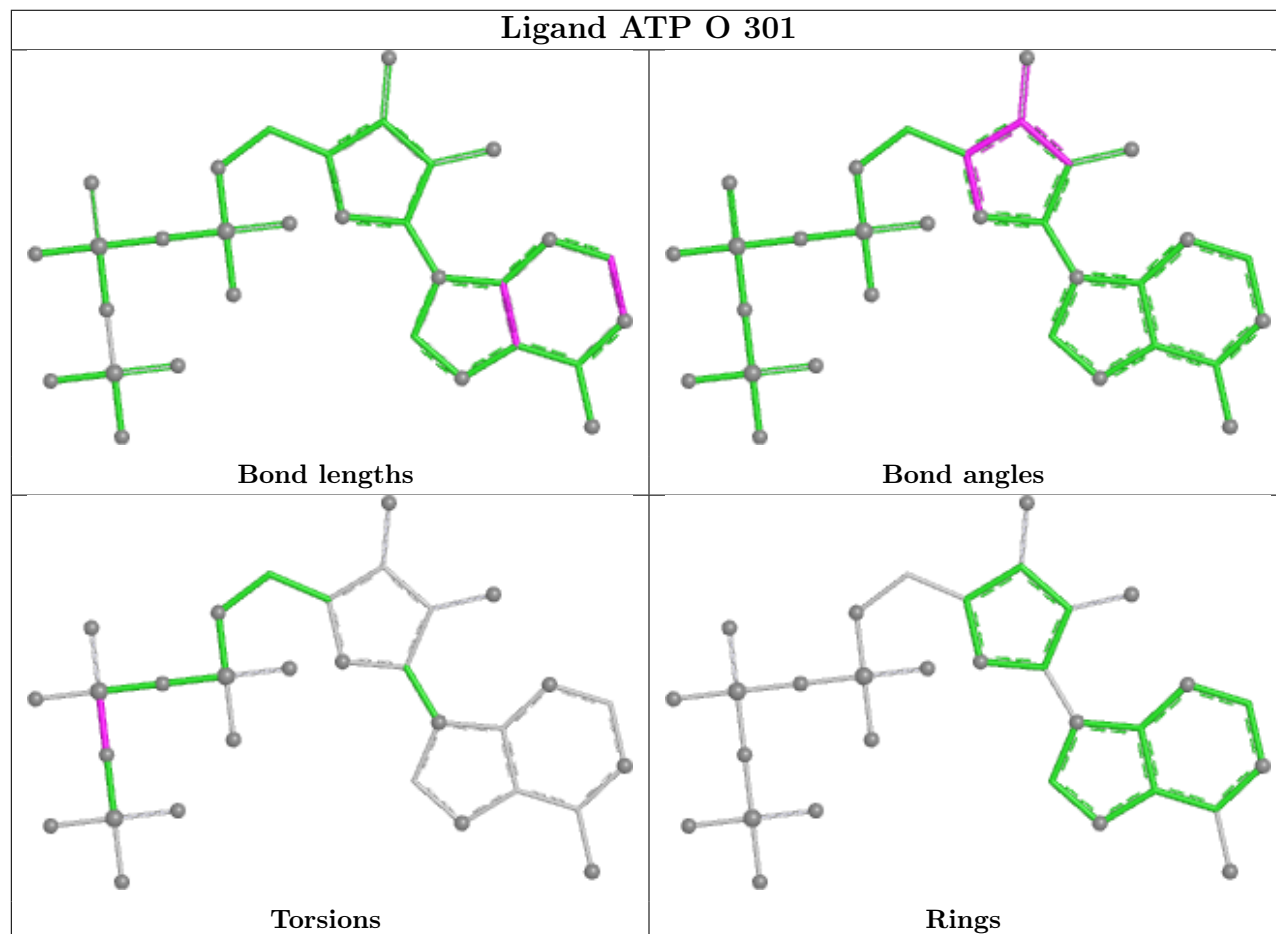
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	301	ADP	1	0
7	G	301	ATP	1	0
9	D	301	ADP	1	0
5	N	401	SF4	1	0

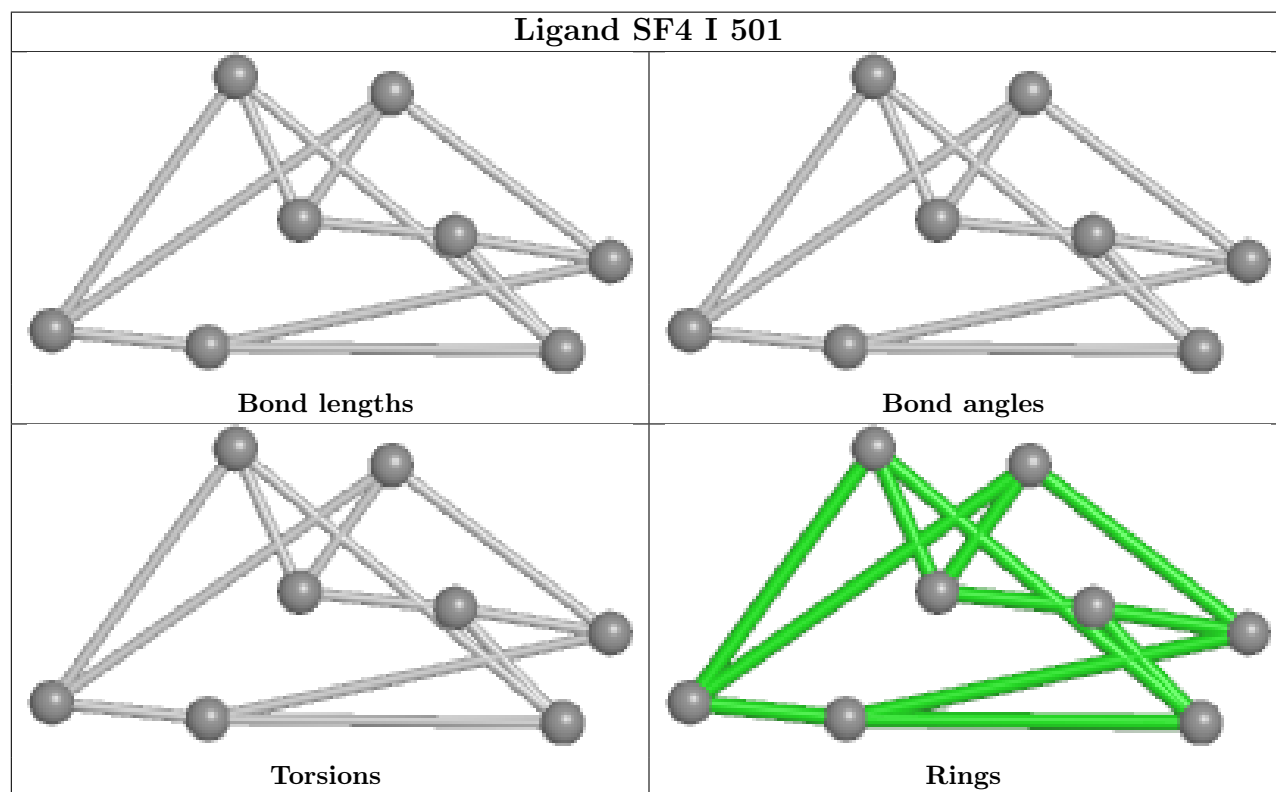
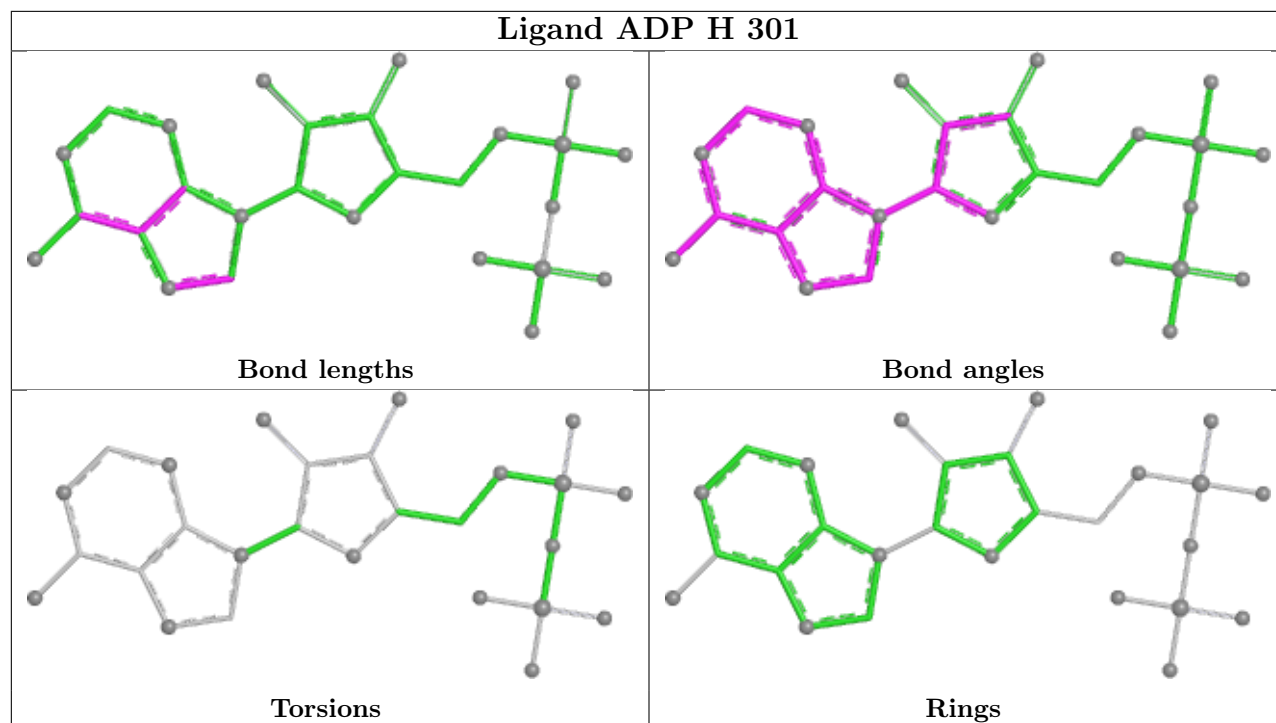
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 SF4 G 303

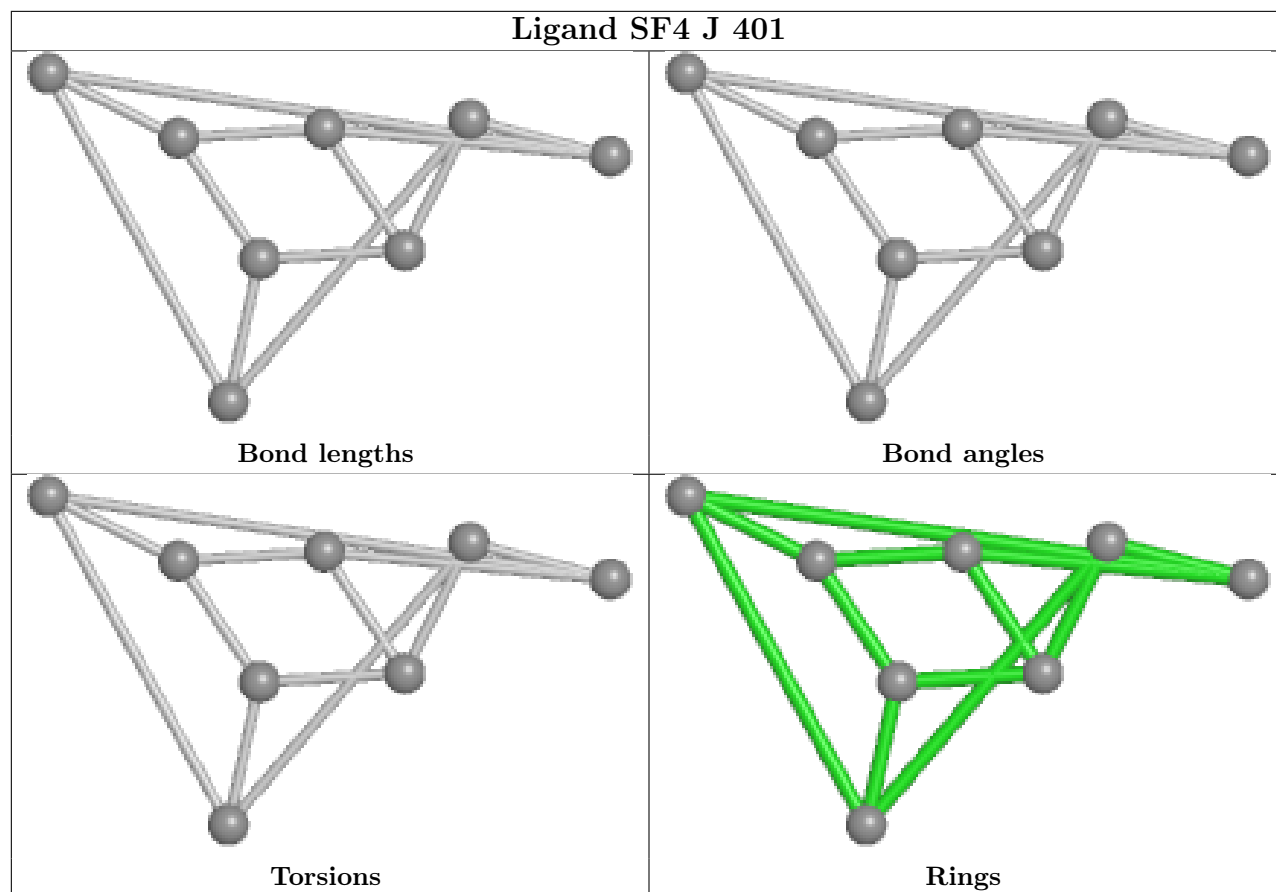


Ligand ATP O 301

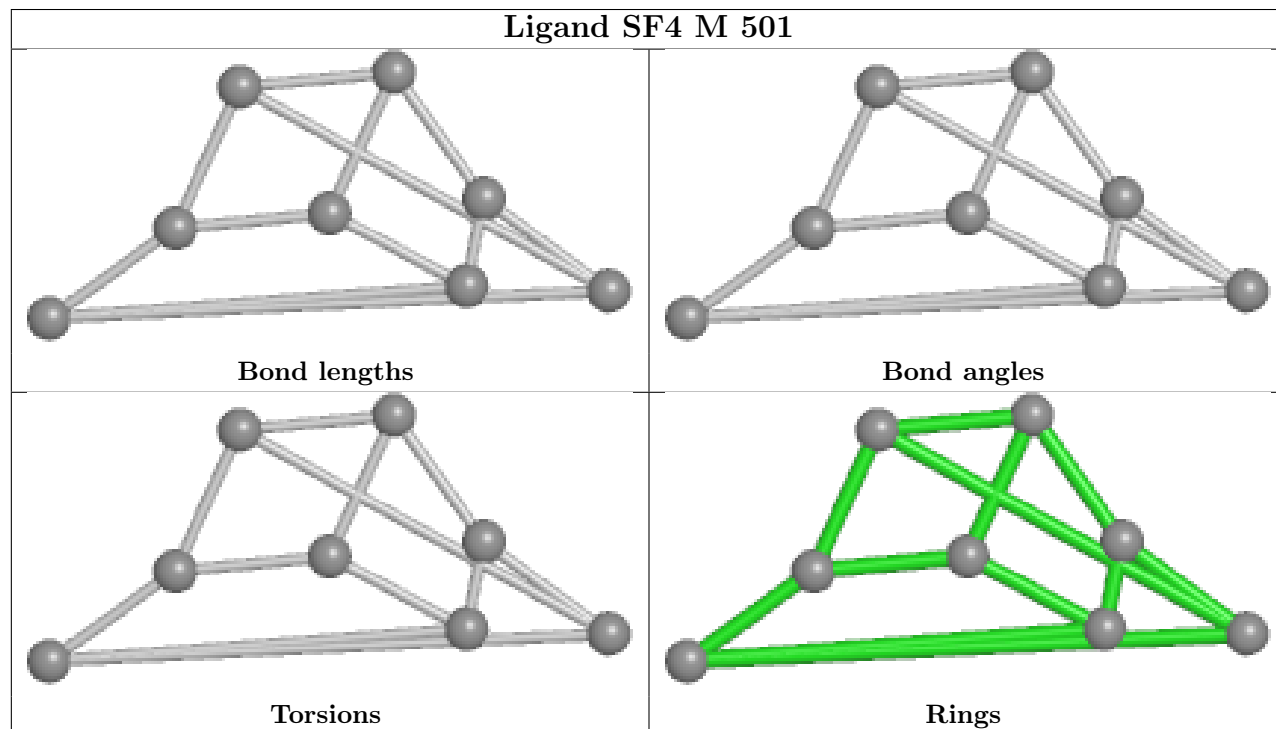




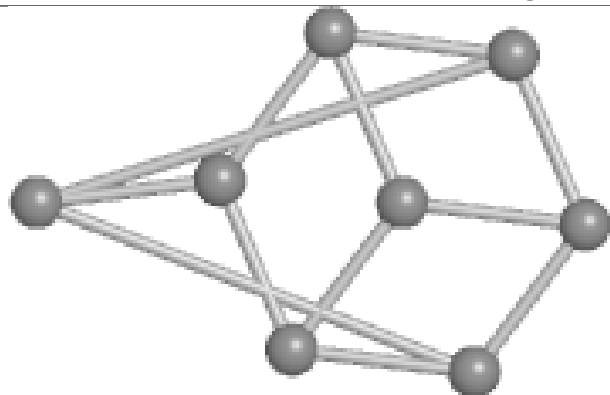
Ligand SF4 J 401



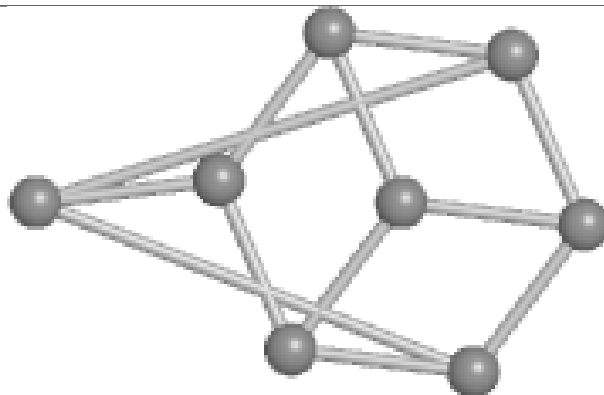
Ligand SF4 M 501



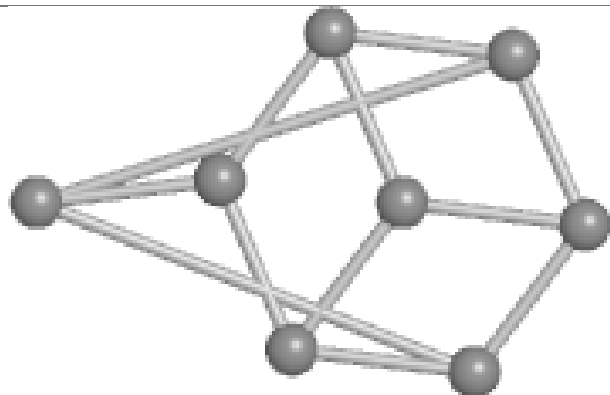
Ligand SF4 E 501



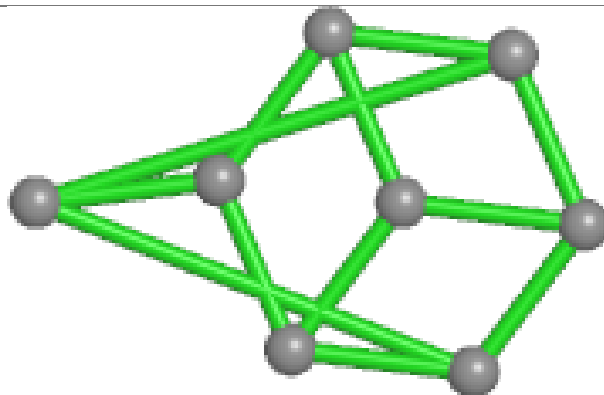
Bond lengths



Bond angles

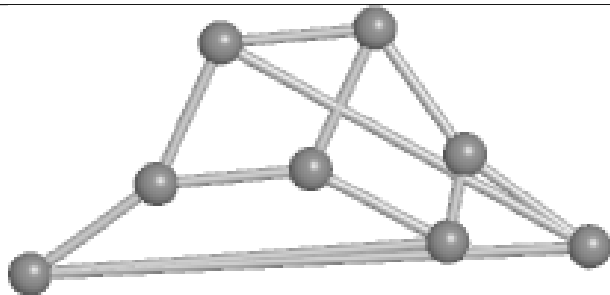


Torsions

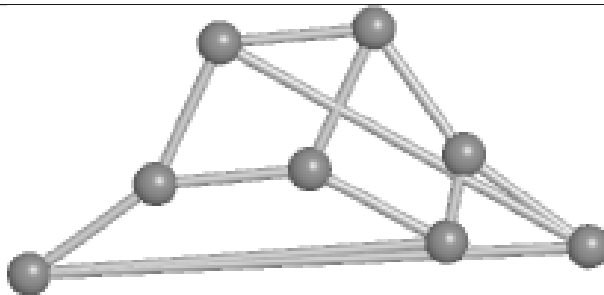


Rings

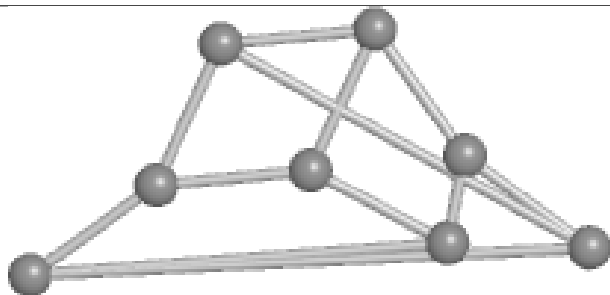
Ligand SF4 O 303



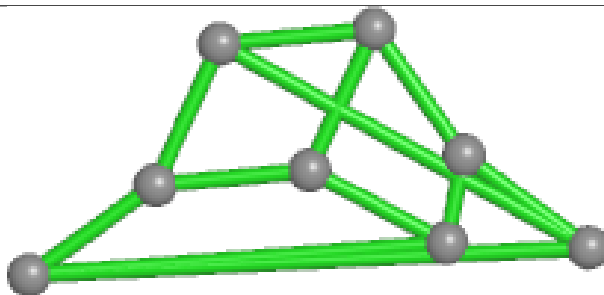
Bond lengths



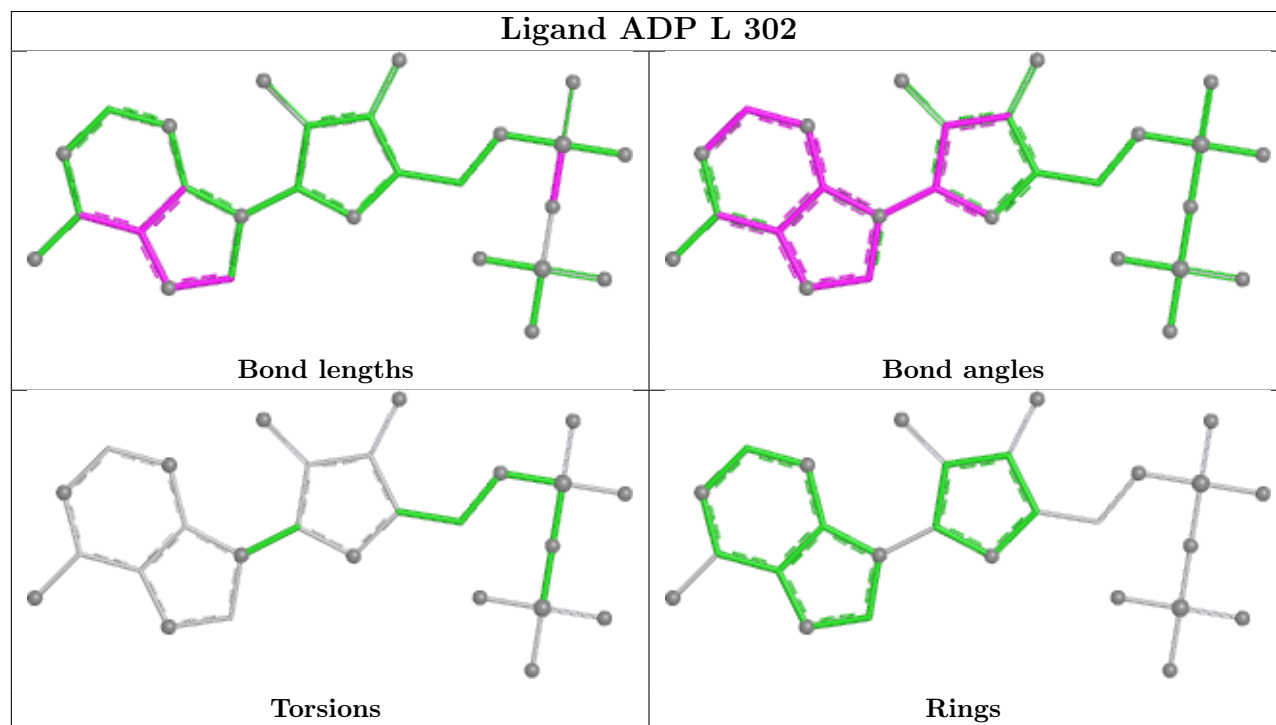
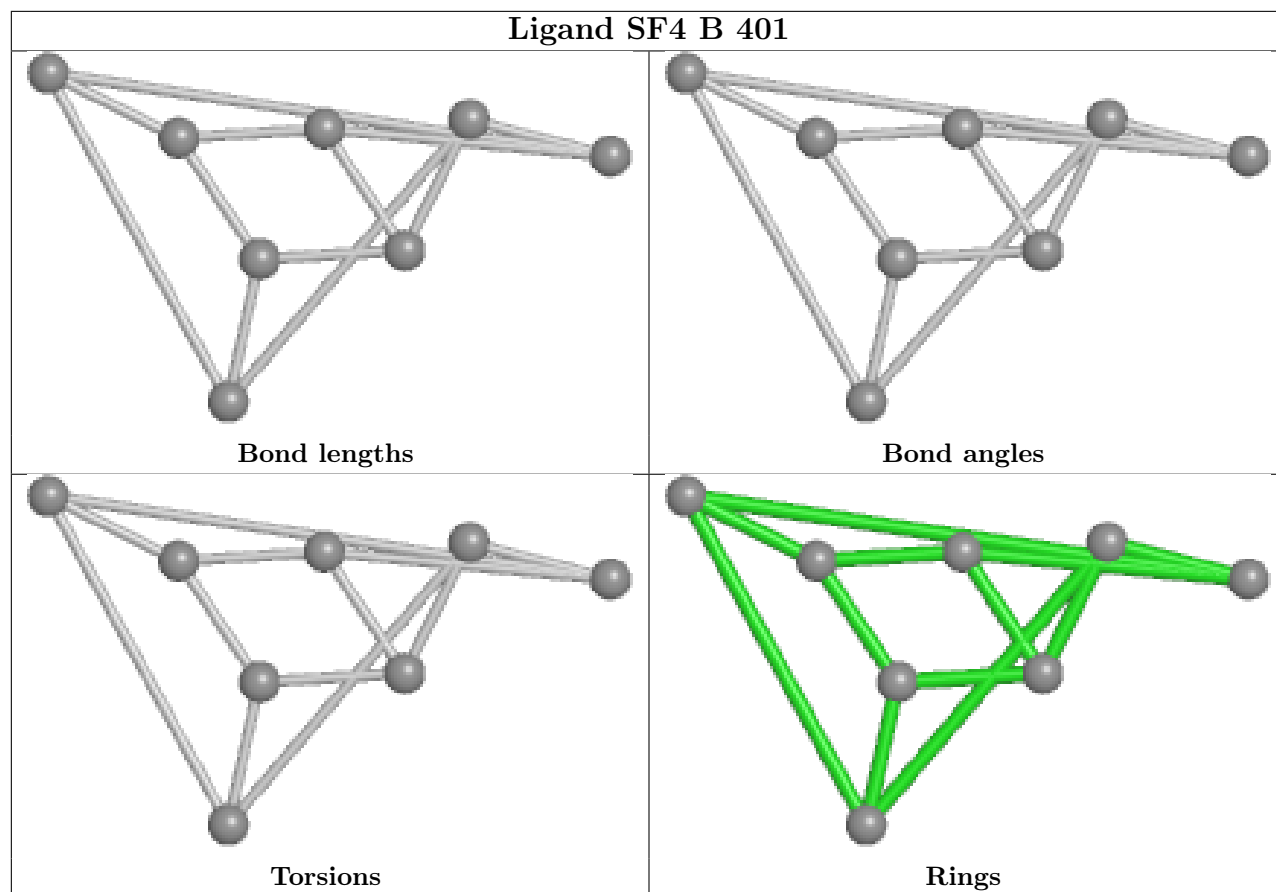
Bond angles

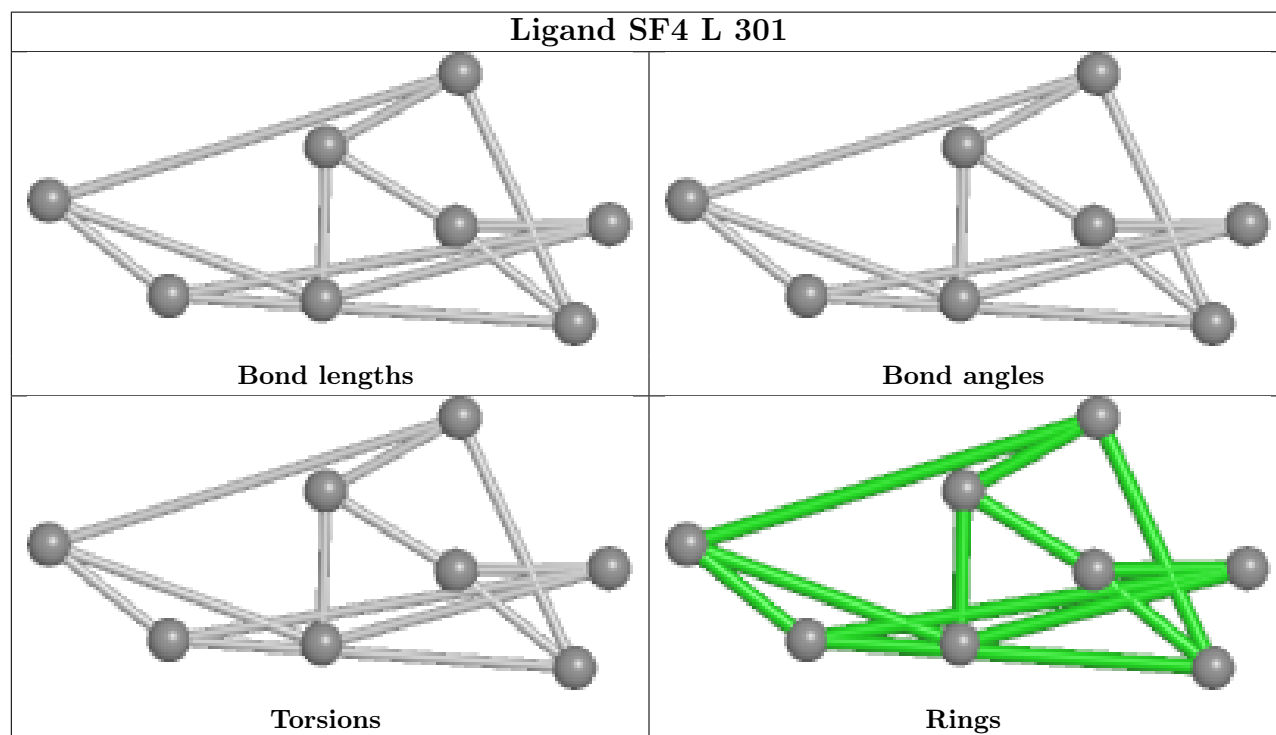
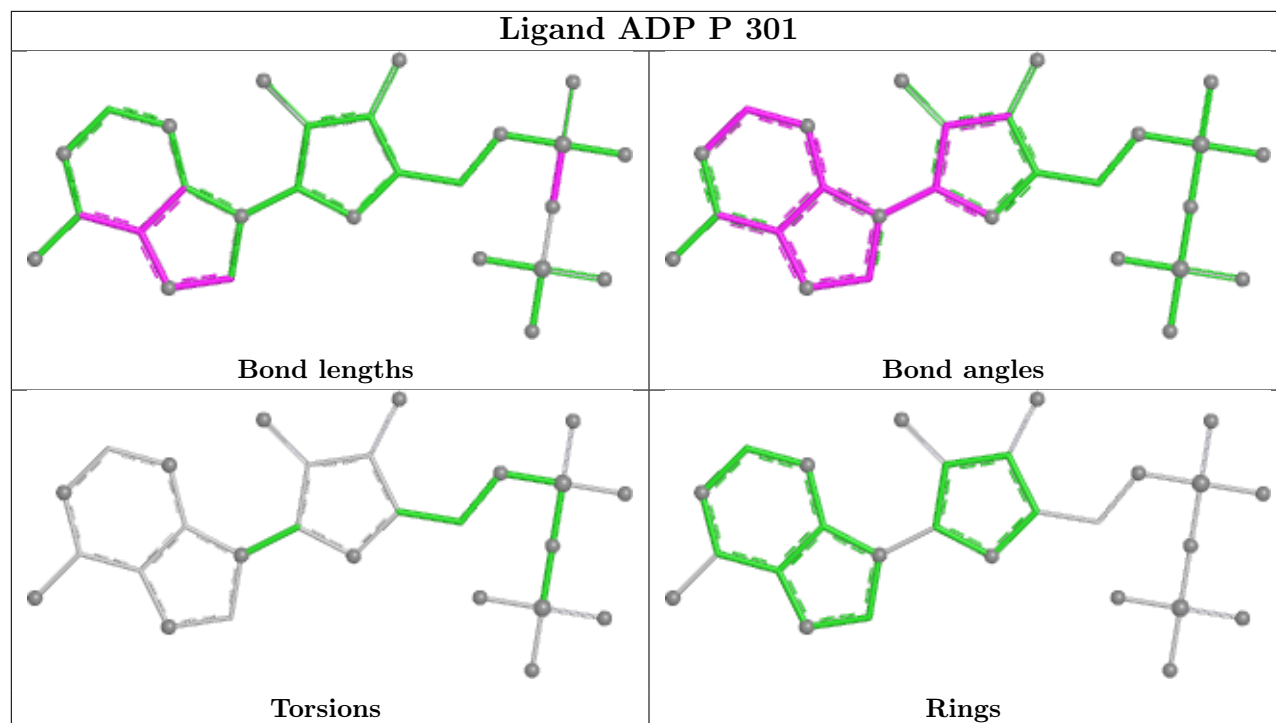


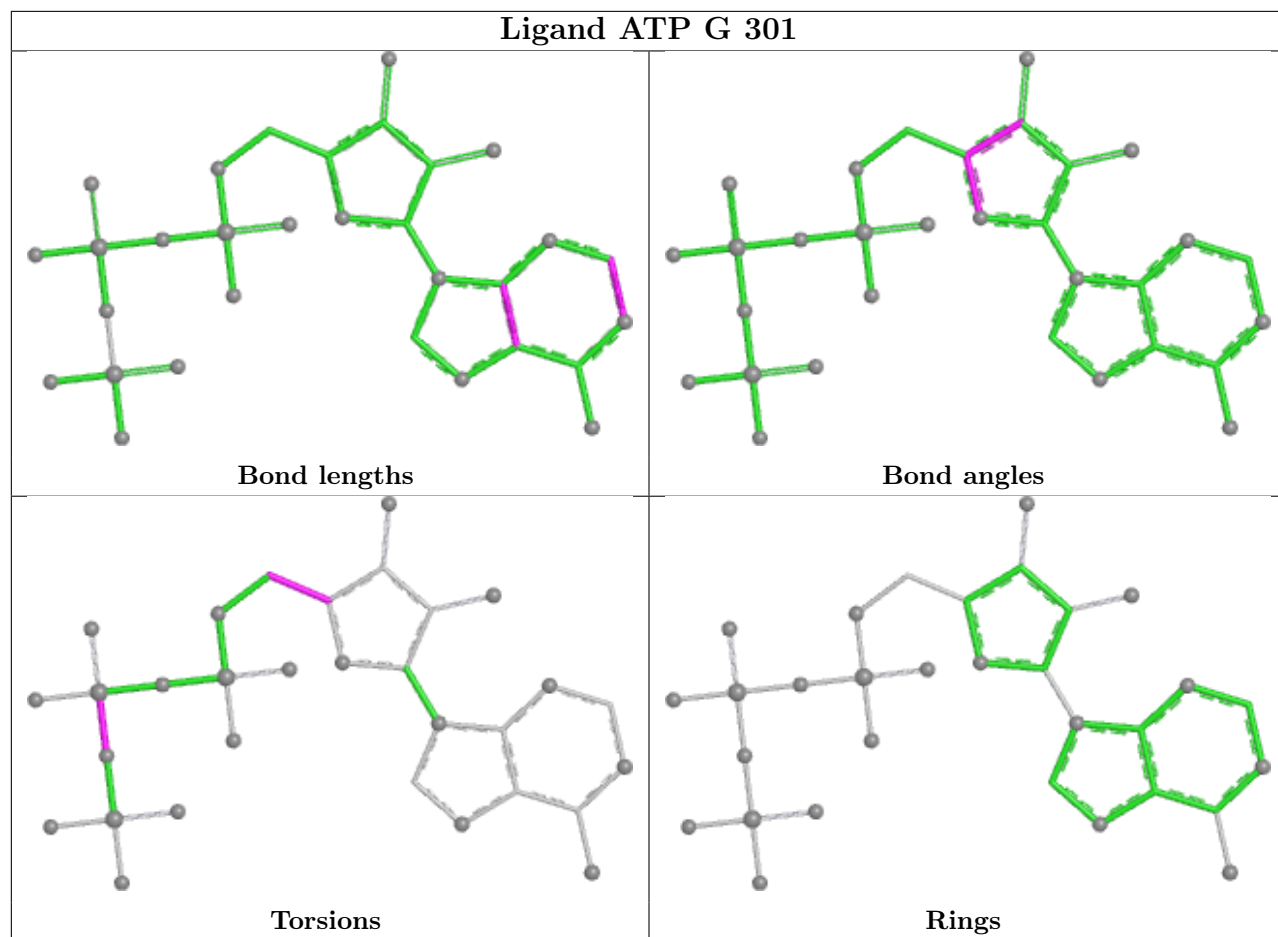
Torsions



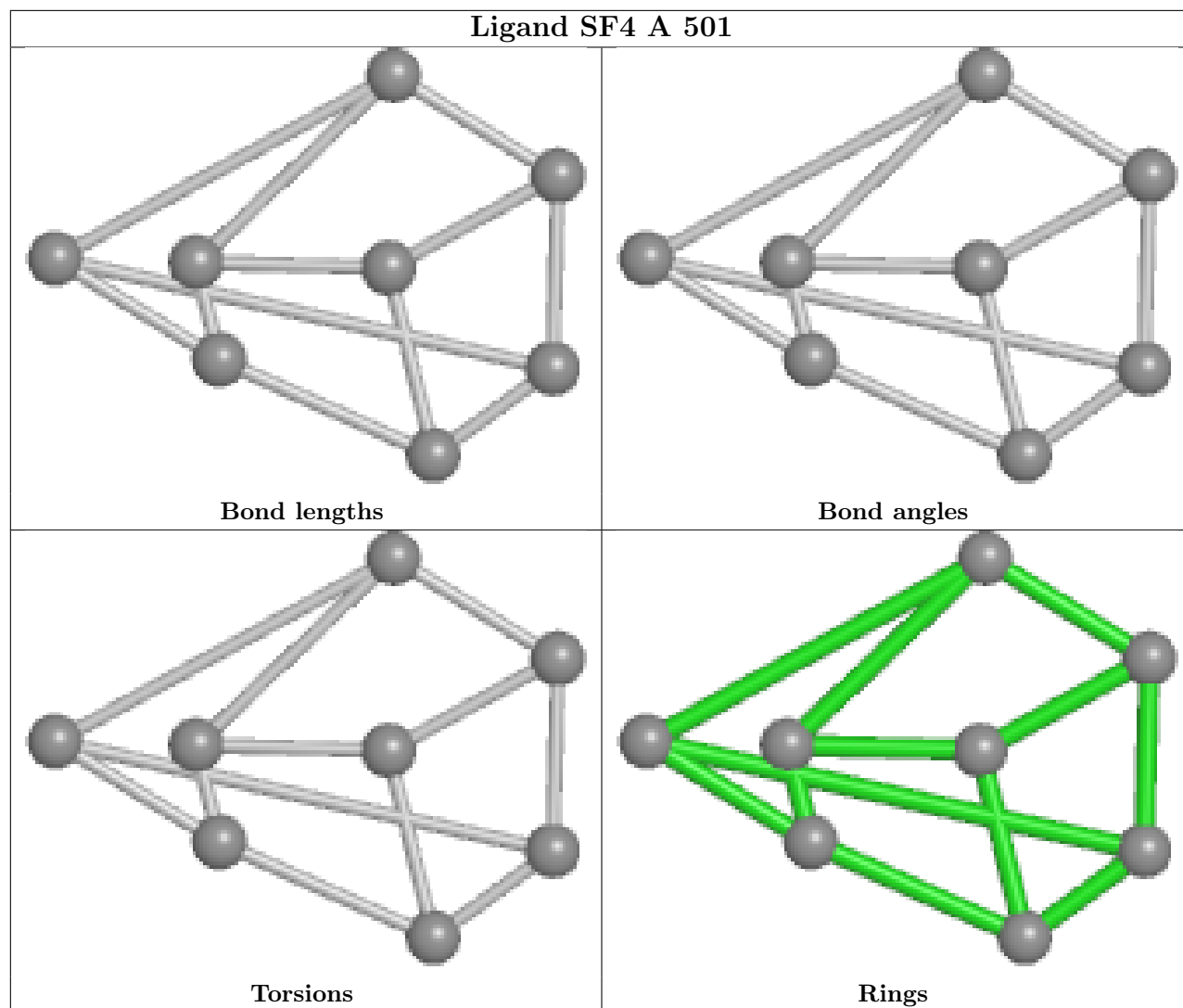
Rings

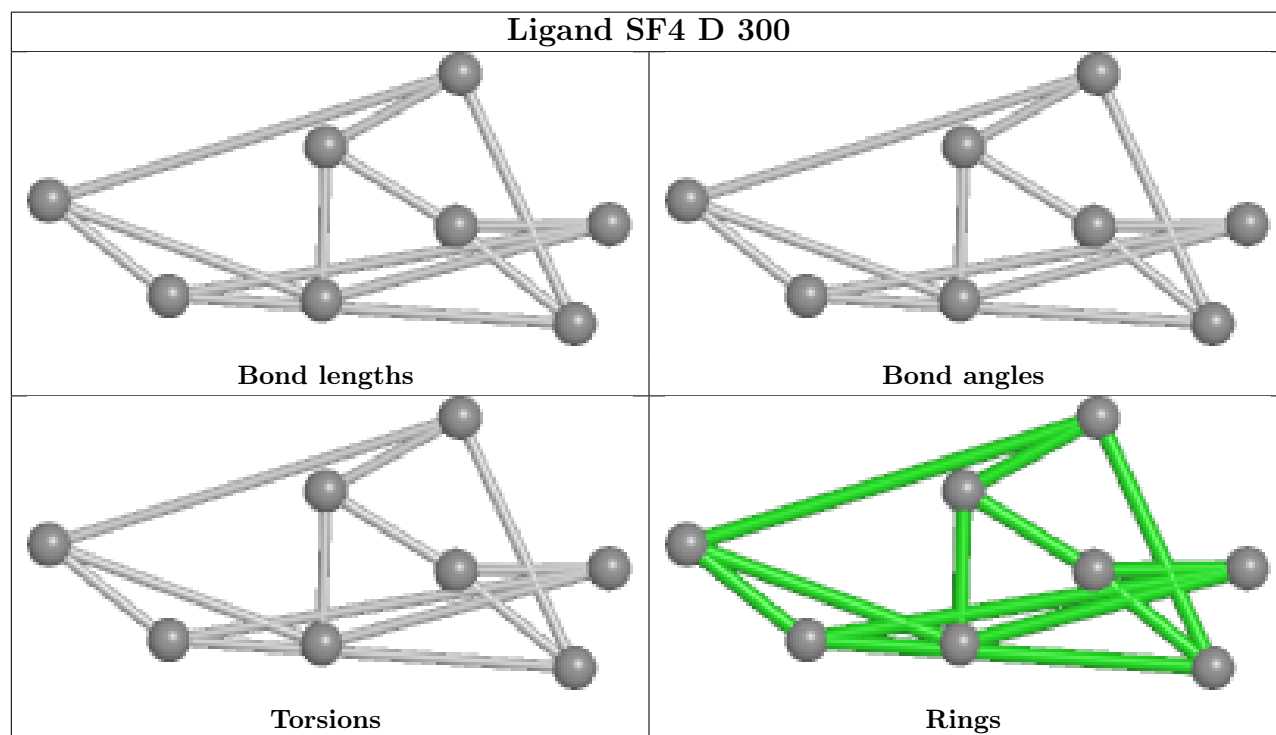
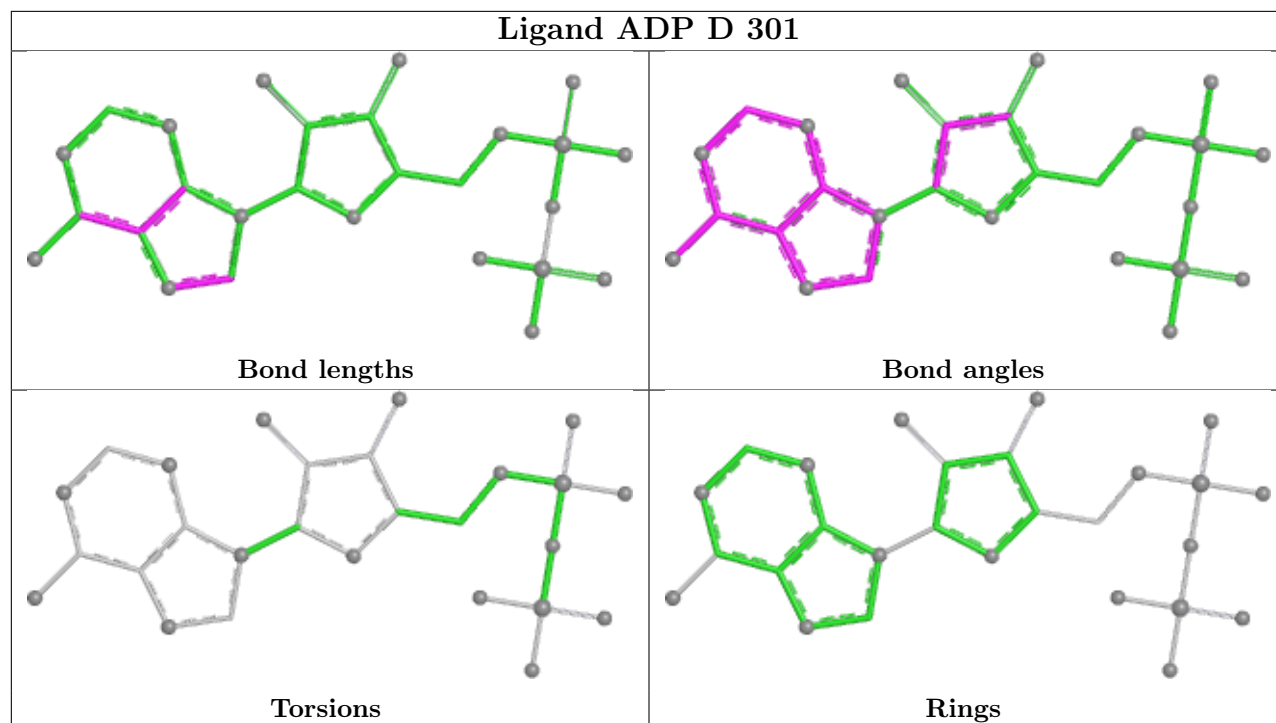


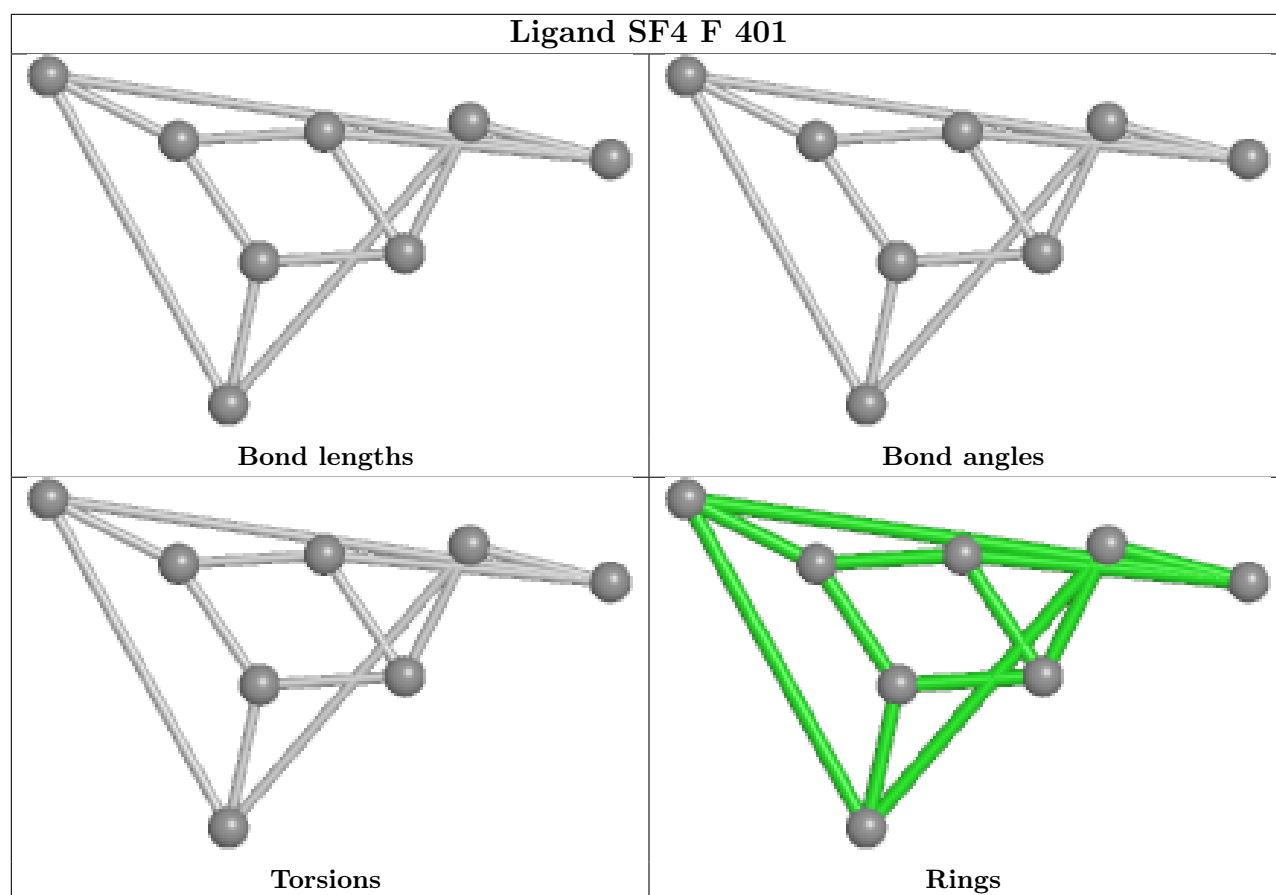


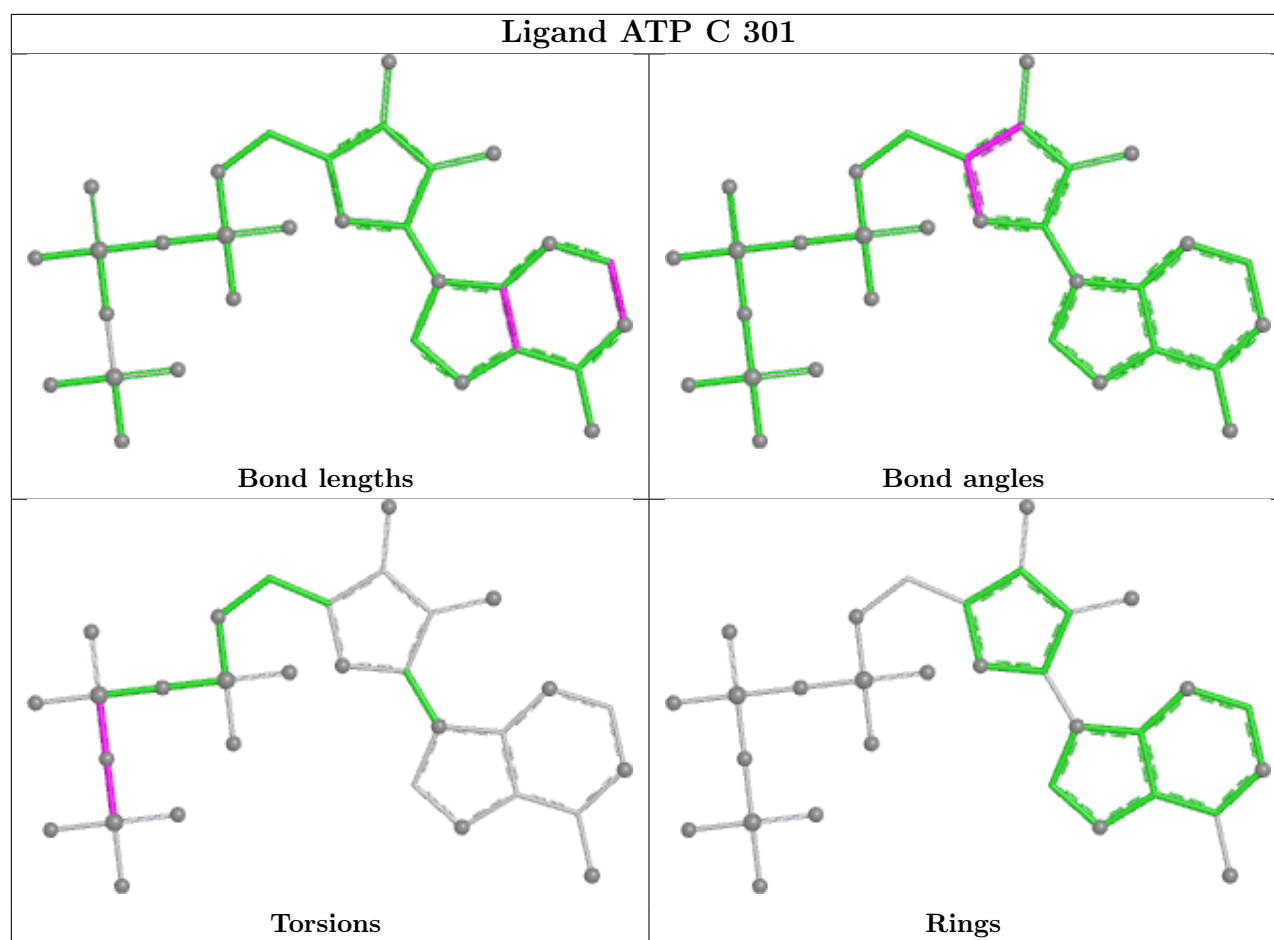


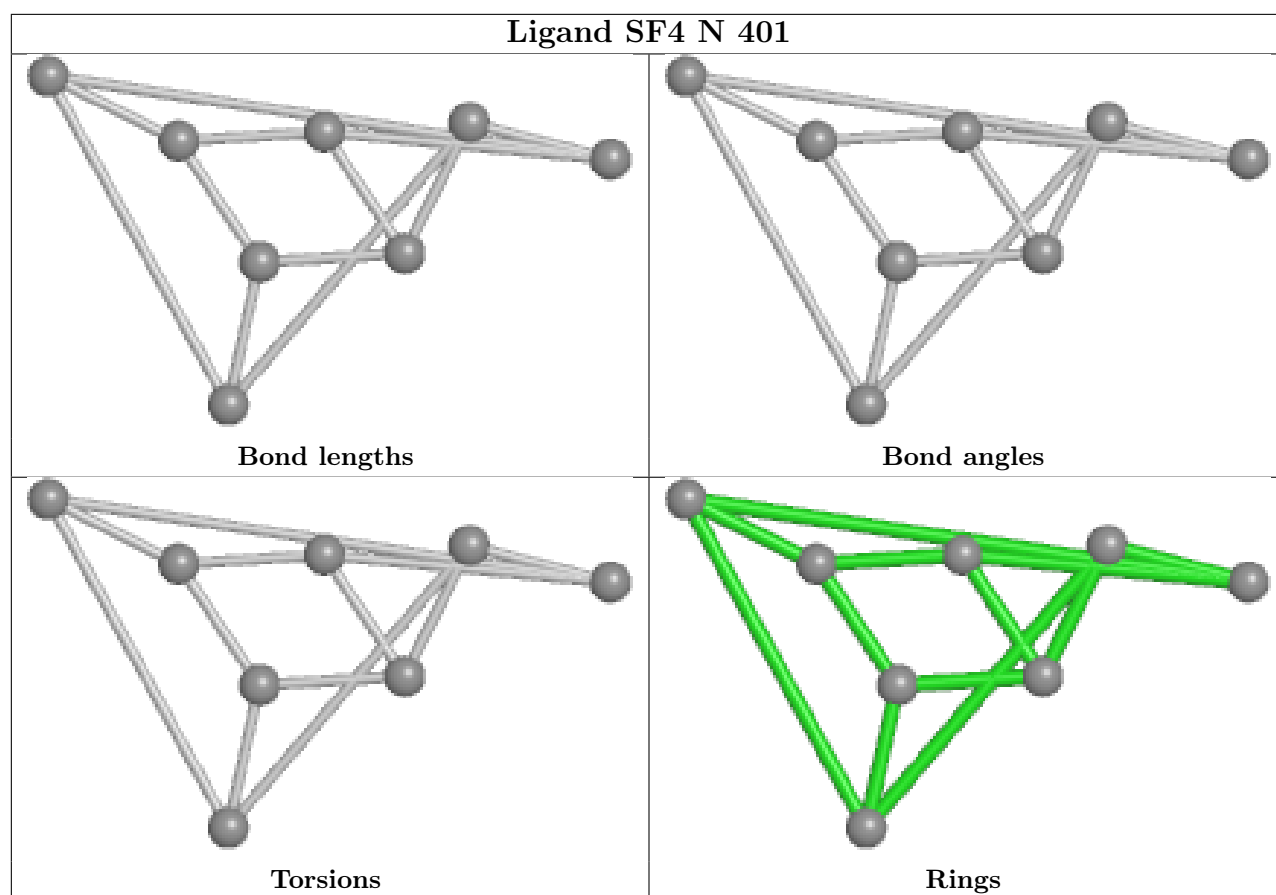
Ligand SF4 A 501

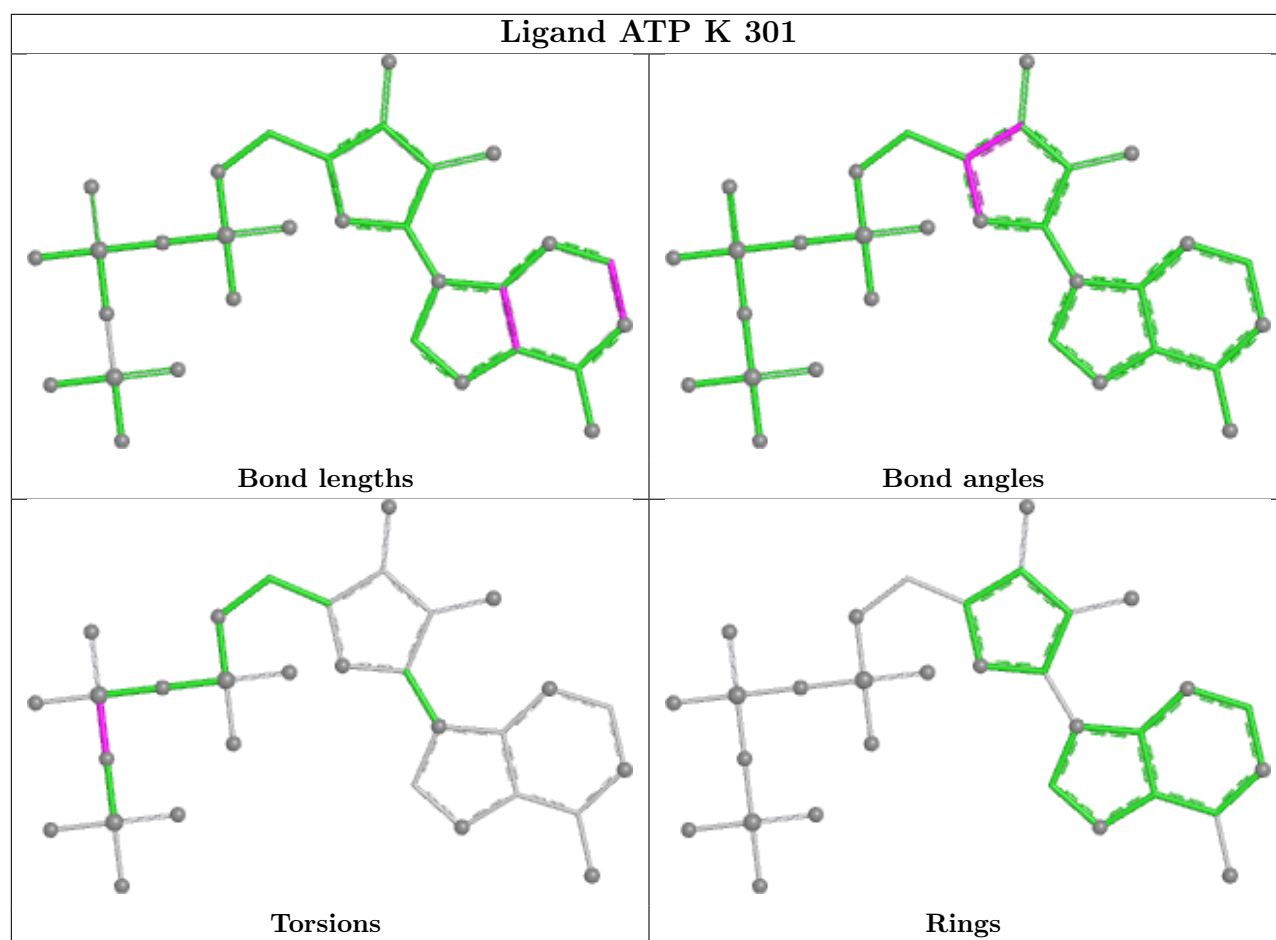












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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(\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.