



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:33 AM UTC

PDB ID : 9GBA / pdb_00009gba
Title : 3-methylbenzoyl-CoA reductase from *Thauera chlorobenzoica* (MbdONPQ) + AMPPNP
Authors : Ermler, U.; Boll, M.; Demmer, U.; Fuchs, J.
Deposited on : 2024-07-30
Resolution : 3.00 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

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

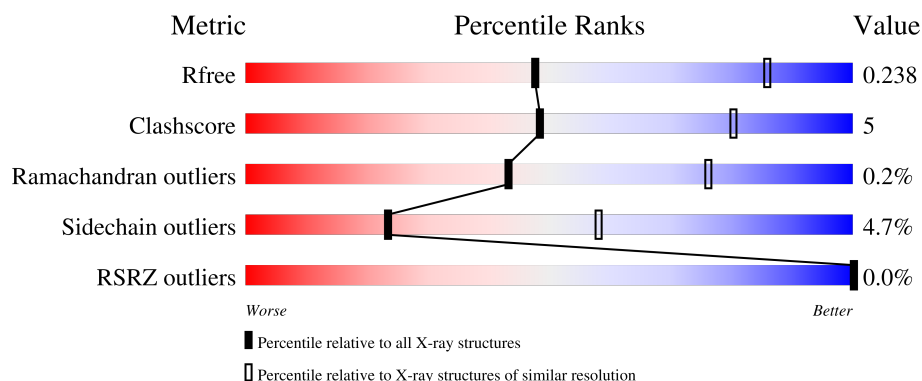
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	 86% 11% ..
1	E	445	 87% 10% ..
2	B	388	 83% 15% .
2	F	388	 87% 12% .
3	C	273	 81% 14% ..

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Mol	Chain	Length	Quality of chain
3	G	273	<div><div></div><div>84%</div><div>10%</div><div></div><div></div></div>
4	D	269	<div><div></div><div>71%</div><div>22%</div><div></div><div></div></div>
4	H	269	<div><div></div><div>69%</div><div>23%</div><div>5%</div><div></div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21237 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	436	Total	C	N	O	S	0	2	0
			3464	2196	598	652	18			
1	E	436	Total	C	N	O	S	0	2	0
			3464	2196	597	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	2	0
			3114	1977	532	590	15			
2	F	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	1	0
			2004	1254	355	381	14			
3	G	264	Total	C	N	O	S	0	3	0
			2026	1266	363	383	14			

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

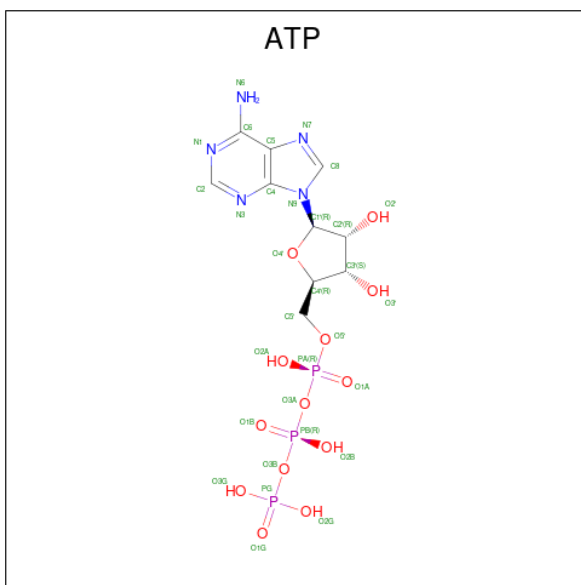
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	260	Total	C	N	O	S	0	1	0
			1933	1215	344	363	11			
4	H	261	Total	C	N	O	S	0	1	0
			1939	1218	348	362	11			

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (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	C	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		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

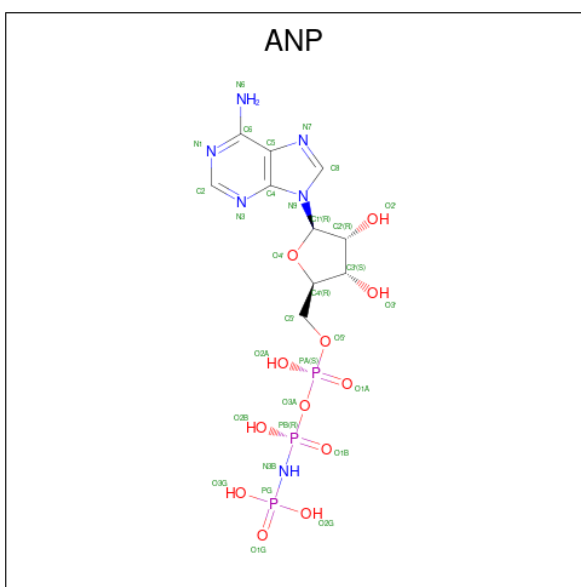


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
6	G	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

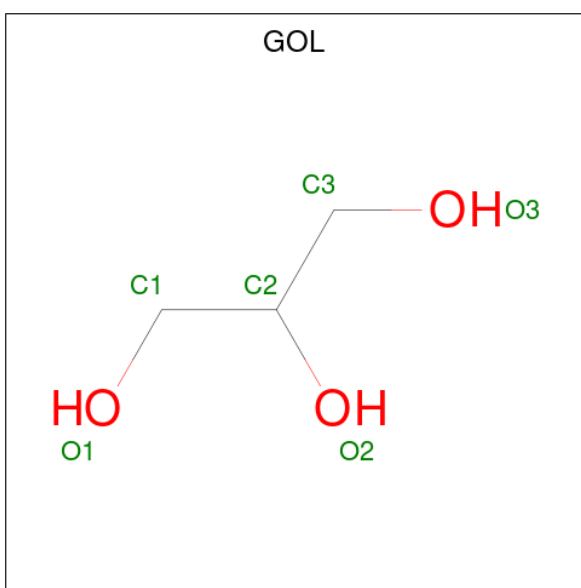
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	G	1	Total Mg 1 1	0	0
7	H	1	Total Mg 1 1	0	0

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total 31	C 10	N 6	O 12	P 3	0	0
8	H	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	4	Total 4	O 4	0	0
10	D	4	Total 4	O 4	0	0
10	E	1	Total 1	O 1	0	0
10	F	1	Total 1	O 1	0	0
10	G	4	Total 4	O 4	0	0
10	H	4	Total 4	O 4	0	0

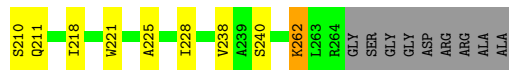
- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO





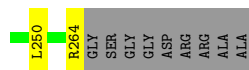
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain C: 81% 14% ..



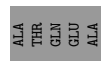
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain G: 84% 10% ..



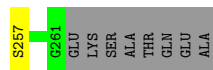
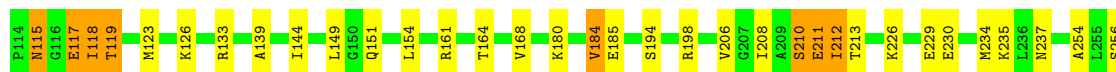
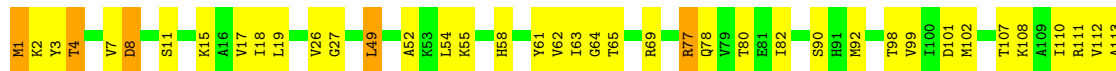
- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain D: 71% 22% . .



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

Chain H: 69% 23% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	148.41Å 243.18Å 164.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.22 – 3.00 46.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.22-3.00) 97.0 (46.22-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.204 , 0.238 0.204 , 0.238	Depositor DCC
R_{free} test set	2848 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	91.2	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.001 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21237	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GOL, MG, ANP, SF4

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	0.11	0/3539	0.30	0/4783
1	E	0.11	0/3539	0.31	0/4783
2	B	0.16	1/3181 (0.0%)	0.31	0/4310
2	F	0.11	0/3159	0.30	0/4281
3	C	0.14	0/2031	0.35	0/2740
3	G	0.14	0/2053	0.35	0/2768
4	D	0.15	0/1961	0.35	0/2641
4	H	0.17	0/1967	0.39	0/2648
All	All	0.13	1/21430 (0.0%)	0.33	0/28954

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	227	ILE	CA-CB	6.26	1.57	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3464	0	3392	24	0
1	E	3464	0	3390	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3114	0	3054	38	0
2	F	3093	0	3036	28	0
3	C	2004	0	2032	23	0
3	G	2026	0	2056	16	0
4	D	1933	0	1964	45	0
4	H	1939	0	1974	49	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
5	C	8	0	0	0	0
5	E	8	0	0	0	0
5	F	8	0	0	1	0
5	G	8	0	0	0	0
6	C	31	0	12	0	0
6	G	31	0	12	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	D	31	0	12	1	0
8	H	31	0	12	0	0
9	E	6	0	8	0	0
10	C	4	0	0	0	0
10	D	4	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	4	0	0	0	0
10	H	4	0	0	0	0
All	All	21237	0	20954	230	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 (230) 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)
4:D:4:THR:HG22	4:D:19:LEU:HB3	1.62	0.81
4:H:98:THR:HB	4:H:212:ILE:HG13	1.67	0.76
4:H:101:ASP:HB3	4:H:108:LYS:HB2	1.69	0.74
4:H:115:ASN:OD1	4:H:115:ASN:N	2.19	0.74
4:H:144:ILE:HD11	4:H:184:VAL:HG11	1.78	0.66
4:H:99:VAL:HB	4:H:110:ILE:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LYS:NZ	2:B:221:GLU:OE1	2.26	0.65
2:F:42:ARG:HB2	2:F:61:LEU:HD22	1.77	0.65
4:H:52:ALA:HB1	4:H:54:LEU:HD12	1.77	0.65
4:D:86:GLY:HA3	4:D:118:ILE:HD11	1.79	0.65
3:C:139:VAL:HG22	3:C:144:TYR:HB2	1.78	0.65
4:H:108:LYS:HG2	4:H:123:MET:HG2	1.78	0.65
4:D:115:ASN:OD1	4:D:115:ASN:N	2.27	0.64
4:D:100:ILE:HD11	4:D:199:ALA:HB1	1.80	0.63
2:B:323:ARG:NH2	2:B:324:ASN:OD1	2.32	0.63
3:G:81:ASP:OD1	3:G:81:ASP:N	2.32	0.62
3:G:164:GLY:O	3:G:198:ARG:NH1	2.25	0.62
4:H:164:THR:O	4:H:198[B]:ARG:NE	2.33	0.62
1:A:227:VAL:HB	1:A:261:LEU:HD22	1.82	0.62
4:H:1:MET:HG2	4:H:3:TYR:HE1	1.65	0.61
1:E:298:ILE:HB	1:E:301:GLN:HB2	1.82	0.60
4:D:42:HIS:NE2	4:D:73:THR:OG1	2.33	0.60
1:E:134:LYS:NZ	2:F:344:GLU:OE1	2.33	0.60
1:E:426:ARG:HE	4:H:123:MET:HE2	1.67	0.60
3:C:175:ILE:HD11	4:D:133:ARG:HH21	1.67	0.60
2:B:152[A]:ARG:HD3	2:B:290:LEU:HD12	1.83	0.59
4:D:102:MET:HG2	4:D:107:THR:HG23	1.82	0.59
2:B:14:LEU:HD23	2:B:233:ARG:HG3	1.84	0.59
1:E:285:SER:O	1:E:438:ARG:NH2	2.35	0.59
3:C:8:ASP:HB3	3:C:15:LYS:HB2	1.85	0.59
4:H:111:ARG:NH1	4:H:206:VAL:O	2.30	0.59
4:H:1:MET:HG2	4:H:3:TYR:CE1	2.38	0.58
4:D:18:ILE:HD11	4:D:48:ALA:C	2.28	0.58
4:D:23:GLN:OE1	4:D:91:HIS:NE2	2.29	0.58
4:D:69:ARG:HH11	4:D:69:ARG:HB2	1.68	0.57
1:A:197:ILE:HD11	1:A:337:PRO:HG2	1.86	0.57
2:B:322:VAL:HG13	2:B:327:ALA:HB3	1.86	0.57
4:D:65:THR:HA	4:D:69:ARG:HG2	1.86	0.56
2:B:135:PRO:HD3	2:B:147:LEU:HD13	1.86	0.56
3:G:168:VAL:HG23	4:H:168:VAL:HG23	1.85	0.56
4:H:213:THR:HA	4:H:237:ASN:HB2	1.88	0.56
1:E:294:PRO:HG2	1:E:296:TYR:CZ	2.40	0.56
2:B:383:GLU:HG2	2:B:386:MET:HE2	1.88	0.55
4:H:77:ARG:HG2	4:H:78:GLN:N	2.21	0.55
1:E:197:ILE:HD11	1:E:337:PRO:HG2	1.88	0.55
4:H:18:ILE:HD13	4:H:49:LEU:HD13	1.88	0.55
1:A:211:ASN:OD1	1:A:245:ARG:NH2	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:HD13	1:A:430:PHE:HB2	1.89	0.54
4:D:208:ILE:HG23	4:D:212:ILE:HD11	1.88	0.54
2:B:104:LEU:HG	2:B:161:VAL:HG21	1.89	0.54
3:C:81:ASP:OD1	3:C:81:ASP:N	2.39	0.54
3:C:7:VAL:HB	3:C:64:THR:HG22	1.90	0.54
2:F:104:LEU:HG	2:F:161:VAL:HG21	1.90	0.54
2:F:322:VAL:HG13	2:F:327:ALA:HB3	1.89	0.54
2:B:307:GLN:O	2:B:314:LYS:NZ	2.40	0.54
4:D:1:MET:HE3	4:D:20:ASN:HB2	1.90	0.53
1:E:222:ARG:HD3	1:E:369:GLU:HB3	1.90	0.53
4:D:5:GLY:HA3	4:D:62:VAL:HG22	1.91	0.53
2:F:192:ARG:NH1	2:F:270:ASP:OD2	2.37	0.53
4:H:27:GLY:HA3	4:H:52:ALA:HB2	1.91	0.53
1:A:294:PRO:HG2	1:A:296:TYR:CZ	2.43	0.53
4:H:90:SER:HB2	4:H:112:VAL:HG11	1.88	0.53
2:B:90:THR:OG1	2:B:366:GLU:OE2	2.18	0.53
4:D:63:ILE:HD12	4:D:254:ALA:HA	1.91	0.53
2:B:138:PRO:HB2	2:B:298:ILE:HG23	1.91	0.52
1:A:195:PHE:CE2	1:A:338:ILE:HD11	2.45	0.52
4:D:19:LEU:HD21	4:D:23:GLN:HA	1.91	0.52
4:D:101:ASP:CG	4:D:108:LYS:HE3	2.35	0.52
4:D:5:GLY:N	4:D:61:TYR:O	2.42	0.52
3:G:137:LYS:O	3:G:141:TYR:HD1	1.92	0.52
4:H:151:GLN:N	4:H:151:GLN:OE1	2.42	0.52
2:F:179:ASN:OD1	2:F:182:ARG:NH2	2.43	0.51
4:H:164:THR:HG22	4:H:194:SER:HB2	1.92	0.51
4:D:15:LYS:HD3	4:D:243:HIS:O	2.11	0.51
4:H:55:LYS:HG2	4:H:58:HIS:HE1	1.76	0.51
4:D:125:ASP:OD1	4:D:205:ARG:NH2	2.44	0.51
4:D:214:PHE:HB3	4:D:238:VAL:HG22	1.93	0.51
2:F:138:PRO:HB2	2:F:298:ILE:HG23	1.92	0.50
3:C:72:TYR:O	3:C:75:ARG:NH1	2.41	0.50
4:D:113:ALA:HB1	4:D:114:PRO:HD2	1.93	0.50
4:H:8:ASP:OD2	4:H:15:LYS:HE2	2.11	0.50
3:C:175:ILE:HD13	4:D:11:SER:HB2	1.94	0.50
2:F:77:GLU:CD	4:H:198[B]:ARG:HH12	2.19	0.50
4:D:66:GLY:O	4:D:69:ARG:HG3	2.11	0.50
1:E:378:HIS:NE2	1:E:410:SER:OG	2.43	0.50
3:G:91:PHE:CD1	3:G:250:LEU:HD21	2.47	0.49
1:A:151:ASP:OD2	2:B:137:ASN:N	2.46	0.49
4:D:151:GLN:N	4:D:151:GLN:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ALA:HB3	2:B:119:PRO:HD3	1.94	0.49
1:E:241:ALA:O	1:E:245:ARG:HB2	2.13	0.49
2:F:323:ARG:NH2	2:F:324:ASN:OD1	2.46	0.49
4:H:111:ARG:HG2	4:H:206:VAL:HB	1.95	0.48
2:B:197:TRP:CE3	2:B:237:ARG:HB2	2.48	0.48
3:C:31:ARG:NH2	3:C:47:GLU:OE2	2.46	0.48
3:C:105:GLN:HA	3:C:130:GLY:HA2	1.95	0.48
4:H:63:ILE:HG12	4:H:254:ALA:HB2	1.95	0.48
1:A:207:SER:OG	1:A:245:ARG:NH1	2.45	0.48
1:A:168:LYS:HA	1:A:171:TYR:CE2	2.48	0.48
3:C:262:LYS:HD3	3:C:262:LYS:HA	1.68	0.48
2:F:247:GLY:HA3	2:F:333:ALA:O	2.13	0.48
3:C:196:THR:HG23	3:C:228:ILE:HG13	1.96	0.48
4:H:49:LEU:HD12	4:H:54:LEU:HB2	1.96	0.48
3:G:229:ARG:O	3:G:233:ASN:N	2.46	0.48
1:A:7:MET:O	1:A:24:ARG:NH2	2.47	0.48
4:H:65:THR:HA	4:H:69:ARG:HB3	1.96	0.48
2:B:251:GLU:HG3	2:B:366:GLU:HB3	1.95	0.47
4:D:220:LYS:HE3	4:D:243:HIS:HB2	1.96	0.47
1:E:436:SER:O	1:E:440:GLN:HG2	2.14	0.47
3:C:150:ASP:HB2	3:C:221:TRP:CD1	2.48	0.47
4:D:4:THR:CG2	4:D:19:LEU:HB3	2.39	0.47
4:D:13:GLN:HB2	4:D:15:LYS:NZ	2.28	0.47
1:E:410:SER:OG	1:E:411:ASP:N	2.48	0.47
2:F:329:THR:HG23	2:F:358:PRO:HB2	1.95	0.47
2:F:244:VAL:HG21	2:F:322:VAL:HA	1.96	0.47
1:A:410:SER:OG	1:A:411:ASP:N	2.48	0.47
2:B:201:ALA:HB2	2:B:267:VAL:HB	1.97	0.47
4:D:61:TYR:CD2	4:D:254:ALA:HB1	2.50	0.47
1:A:156:ARG:NH1	1:A:172:GLU:OE2	2.47	0.47
1:A:437:ARG:O	1:A:440:GLN:HG2	2.15	0.47
4:D:242:SER:HA	4:D:245:MET:HG2	1.96	0.47
2:B:323:ARG:HH21	2:B:324:ASN:HA	1.79	0.47
4:H:82:ILE:HG22	4:H:118:ILE:HG12	1.96	0.46
2:B:373:GLN:O	2:B:377:GLN:HG3	2.15	0.46
4:H:113:ALA:HB2	4:H:119:THR:HG23	1.97	0.46
1:A:378:HIS:NE2	1:A:410:SER:OG	2.45	0.46
4:H:11:SER:O	4:H:133:ARG:NH2	2.46	0.46
2:F:201:ALA:HB2	2:F:267:VAL:HB	1.97	0.46
3:C:12:THR:OG1	3:C:104:GLY:HA3	2.15	0.46
4:D:15:LYS:HE2	4:D:243:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ARG:NH1	1:E:414:ASP:OD2	2.48	0.46
3:G:20:ASP:OD2	3:G:24:ASN:HB2	2.15	0.46
1:A:140:GLU:HG3	1:A:147:THR:HG21	1.97	0.46
1:A:134:LYS:NZ	2:B:344:GLU:OE1	2.31	0.45
3:C:13:TYR:O	3:C:15:LYS:NZ	2.42	0.45
2:F:280:VAL:HG23	2:F:281:GLU:HG3	1.99	0.45
1:A:321:PHE:CE1	1:A:386:VAL:HG11	2.52	0.45
4:H:210:SER:HA	4:H:211:GLU:HA	1.66	0.45
1:A:396:ILE:HG13	2:B:123:ARG:HD2	1.98	0.45
4:D:196:ALA:O	4:D:200:ILE:HG22	2.17	0.45
3:G:8:ASP:HB3	3:G:15:LYS:HB2	1.99	0.45
2:B:192:ARG:NH1	2:B:270:ASP:OD2	2.47	0.45
1:E:383:CYS:SG	1:E:386:VAL:HG22	2.57	0.45
2:B:368:GLN:HE22	2:B:373:GLN:HE22	1.62	0.44
3:C:225:ALA:HB1	3:C:238:VAL:HG21	1.99	0.44
4:H:49:LEU:HD12	4:H:54:LEU:CB	2.47	0.44
3:C:1:MET:HE3	3:C:3:TYR:HE1	1.82	0.44
2:F:70:GLN:HB3	4:H:161:ARG:HH12	1.81	0.44
2:F:152:ARG:HD3	2:F:290:LEU:HD12	2.00	0.44
2:F:338:CYS:HA	5:F:401:SF4:S1	2.57	0.44
3:G:210:SER:HA	3:G:211:GLN:HA	1.64	0.44
4:H:102:MET:HG2	4:H:107:THR:HG23	2.00	0.44
3:C:168:VAL:HG23	4:D:168:VAL:HG23	1.98	0.44
1:E:149:ASN:HB3	2:F:137:ASN:CG	2.42	0.44
1:E:429:ALA:HA	4:H:80:THR:HG21	1.98	0.44
2:F:385:ILE:H	2:F:385:ILE:HG13	1.59	0.44
2:B:314:LYS:HG3	2:B:344:GLU:CD	2.43	0.43
2:B:88:ILE:HD13	2:B:113:ALA:HB1	1.99	0.43
1:E:94:ASP:O	1:E:384:ARG:NH2	2.32	0.43
1:E:293:THR:HG21	1:E:412:LEU:HD23	2.00	0.43
2:B:373:GLN:CD	2:B:373:GLN:H	2.26	0.43
2:B:333:ALA:HA	2:B:362:SER:O	2.18	0.43
2:F:52:PRO:HG3	2:F:151:TYR:CE1	2.53	0.43
4:H:229:GLU:OE2	4:H:235:LYS:HD3	2.17	0.43
2:B:271:ASP:HB3	2:B:321:ARG:HH12	1.84	0.43
1:E:128:TYR:O	2:F:115:ARG:NH2	2.44	0.43
2:B:192:ARG:HD2	2:B:204:SER:HB2	2.00	0.43
3:C:169:PHE:CE1	4:D:126:LYS:HG2	2.53	0.43
4:D:200:ILE:O	4:D:204:ARG:HG3	2.18	0.43
3:G:119[A]:ARG:HA	3:G:119[A]:ARG:HD3	1.47	0.43
4:H:102:MET:HE2	4:H:102:MET:HB3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:154:LEU:HD22	4:H:226:LYS:HD2	2.00	0.43
1:A:323:SER:HB2	1:A:326:ALA:HB3	2.01	0.43
3:G:185:GLU:H	3:G:185:GLU:CD	2.27	0.43
3:G:208:VAL:HG21	3:G:234:LEU:HD12	2.01	0.43
4:H:208:ILE:HG23	4:H:212:ILE:HD11	2.01	0.43
4:D:146:LEU:HD21	8:D:301:ANP:H2'	2.01	0.43
4:D:79:VAL:HG12	4:D:80:THR:H	1.83	0.42
4:H:4:THR:OG1	4:H:61:TYR:O	2.26	0.42
4:H:139:ALA:HB2	4:H:149:LEU:HD13	2.01	0.42
3:C:189:TYR:CE1	3:C:193:MET:HE3	2.54	0.42
3:G:105:GLN:NE2	3:G:133:MET:SD	2.81	0.42
4:H:7:VAL:O	4:H:64:GLY:HA2	2.19	0.42
2:F:243:VAL:HG12	2:F:329:THR:HB	2.02	0.42
3:C:3:TYR:CE2	3:C:54:ILE:HG21	2.54	0.42
4:D:61:TYR:HD2	4:D:254:ALA:HB1	1.85	0.42
1:E:97:GLY:H	1:E:382:SER:CB	2.32	0.42
4:H:55:LYS:HG2	4:H:58:HIS:CE1	2.54	0.42
3:C:210:SER:HA	3:C:211:GLN:HA	1.73	0.42
3:G:169:PHE:CE1	4:H:126:LYS:HG2	2.54	0.42
4:D:6:GLY:HA2	4:D:63:ILE:O	2.19	0.42
4:D:84:CYS:O	4:D:249:GLY:HA3	2.19	0.42
1:E:417:VAL:O	4:H:126:LYS:HE2	2.19	0.42
2:F:84:LEU:O	2:F:89:LYS:NZ	2.53	0.42
2:B:243:VAL:HG12	2:B:329:THR:HB	2.01	0.42
4:H:117:GLU:H	4:H:117:GLU:HG2	1.68	0.42
2:F:192:ARG:HD2	2:F:204:SER:HB2	2.02	0.42
3:G:139:VAL:HG22	3:G:144:TYR:HB2	2.02	0.42
2:B:42:ARG:HB2	2:B:61:LEU:HD22	2.02	0.41
1:E:318:TYR:HA	1:E:321:PHE:CZ	2.55	0.41
4:D:108:LYS:CG	4:D:123:MET:HG2	2.50	0.41
1:E:222:ARG:HG2	1:E:369:GLU:O	2.19	0.41
2:B:164:ARG:NH1	2:B:170:GLU:OE2	2.53	0.41
2:B:196:PRO:HD2	2:B:197:TRP:CZ3	2.55	0.41
3:C:200:VAL:HG22	3:C:228:ILE:HG23	2.01	0.41
1:E:301:GLN:O	1:E:305:MET:HG3	2.21	0.41
2:F:271:ASP:HB3	2:F:321:ARG:HH12	1.86	0.41
1:A:293:THR:HG21	1:A:412:LEU:HD23	2.03	0.41
1:E:168:LYS:NZ	1:E:172:GLU:OE2	2.51	0.41
1:E:357:PHE:HB3	2:F:119:PRO:HG2	2.02	0.41
1:A:123:GLY:HA3	1:A:147:THR:HG22	2.03	0.41
2:B:34:LYS:HE3	2:B:99:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:TYR:CD1	2:B:317:MET:HB3	2.56	0.41
4:D:15:LYS:H	4:D:15:LYS:HG2	1.66	0.41
4:D:156:SER:HB2	4:D:185:GLU:O	2.21	0.41
1:E:426:ARG:HE	4:H:123:MET:CE	2.30	0.41
2:F:54:GLU:HG2	2:F:175:VAL:HA	2.02	0.41
2:B:363:GLU:OE1	3:C:125:ASP:HB2	2.21	0.41
4:D:108:LYS:HG2	4:D:123:MET:HG2	2.03	0.41
1:E:8:THR:HG23	1:E:24:ARG:HH21	1.86	0.41
1:A:389:GLY:HA2	2:B:120:ILE:HD11	2.03	0.40
2:B:247:GLY:HA3	2:B:333:ALA:O	2.21	0.40
1:E:227:VAL:HB	1:E:261:LEU:HD22	2.03	0.40
4:H:8:ASP:HB2	4:H:65:THR:HG23	2.02	0.40
1:A:18:GLY:HA3	1:A:257:LEU:HD13	2.03	0.40
2:B:29:ALA:HB1	2:B:34:LYS:NZ	2.36	0.40
4:H:82:ILE:HD12	4:H:82:ILE:H	1.86	0.40
1:A:36:VAL:HG13	1:A:41:GLU:HB2	2.03	0.40
3:G:224:MET:HE2	3:G:224:MET:HB3	1.84	0.40
4:D:189:TRP:CH2	4:D:226:LYS:HD3	2.57	0.40
2:F:383:GLU:HA	2:F:386:MET:HB2	2.03	0.40

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	436/445 (98%)	423 (97%)	11 (2%)	2 (0%)	24	60
1	E	436/445 (98%)	424 (97%)	10 (2%)	2 (0%)	24	60
2	B	387/388 (100%)	379 (98%)	8 (2%)	0	100	100
2	F	385/388 (99%)	378 (98%)	7 (2%)	0	100	100
3	C	263/273 (96%)	258 (98%)	4 (2%)	1 (0%)	30	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	265/273 (97%)	258 (97%)	6 (2%)	1 (0%)	30	65
4	D	259/269 (96%)	256 (99%)	3 (1%)	0	100	100
4	H	260/269 (97%)	256 (98%)	4 (2%)	0	100	100
All	All	2691/2750 (98%)	2632 (98%)	53 (2%)	6 (0%)	43	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	207	ASN
1	E	410	SER
1	A	410	SER
1	A	413	VAL
3	G	207	ASN
1	E	413	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%)	354 (96%)	14 (4%)	29	63
1	E	368/371 (99%)	361 (98%)	7 (2%)	50	76
2	B	337/336 (100%)	328 (97%)	9 (3%)	39	71
2	F	335/336 (100%)	329 (98%)	6 (2%)	51	77
3	C	212/215 (99%)	202 (95%)	10 (5%)	23	58
3	G	214/215 (100%)	200 (94%)	14 (6%)	15	47
4	D	198/203 (98%)	176 (89%)	22 (11%)	6	25
4	H	198/203 (98%)	173 (87%)	25 (13%)	4	20
All	All	2230/2250 (99%)	2123 (95%)	107 (5%)	23	57

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	MET
1	A	77	ASN
1	A	114	MET
1	A	119	LYS
1	A	164	ARG
1	A	227	VAL
1	A	238	MET
1	A	249	VAL
1	A	272	LEU
1	A	300	ARG
1	A	426	ARG
1	A	436	SER
1	A	441	GLN
2	B	152[A]	ARG
2	B	152[B]	ARG
2	B	169	GLN
2	B	203	GLU
2	B	232	ASP
2	B	237	ARG
2	B	323	ARG
2	B	373	GLN
2	B	387	PHE
3	C	1	MET
3	C	37	LEU
3	C	55	ASN
3	C	81	ASP
3	C	122[A]	ARG
3	C	122[B]	ARG
3	C	126	LYS
3	C	218	ILE
3	C	240	SER
3	C	262	LYS
4	D	1	MET
4	D	4	THR
4	D	15	LYS
4	D	17	VAL
4	D	18	ILE
4	D	25	ILE
4	D	26	VAL
4	D	54	LEU
4	D	69	ARG
4	D	77	ARG

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Mol	Chain	Res	Type
4	D	79	VAL
4	D	80	THR
4	D	108	LYS
4	D	112	VAL
4	D	115	ASN
4	D	117	GLU
4	D	118	ILE
4	D	119	THR
4	D	185	GLU
4	D	205	ARG
4	D	211	GLU
4	D	213	THR
1	E	194	LYS
1	E	227	VAL
1	E	249	VAL
1	E	412	LEU
1	E	437	ARG
1	E	438	ARG
1	E	439	GLN
2	F	74	ASN
2	F	169	GLN
2	F	237	ARG
2	F	336	LYS
2	F	385	ILE
2	F	386	MET
3	G	20	ASP
3	G	43	LEU
3	G	81	ASP
3	G	119[A]	ARG
3	G	119[B]	ARG
3	G	125	ASP
3	G	139	VAL
3	G	173	GLU
3	G	178	LEU
3	G	197	LYS
3	G	218	ILE
3	G	224	MET
3	G	234	LEU
3	G	264	ARG
4	H	1	MET
4	H	2	LYS
4	H	4	THR

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Mol	Chain	Res	Type
4	H	8	ASP
4	H	17	VAL
4	H	19	LEU
4	H	26	VAL
4	H	49	LEU
4	H	62	VAL
4	H	77	ARG
4	H	92	MET
4	H	115	ASN
4	H	117	GLU
4	H	118	ILE
4	H	119	THR
4	H	180	LYS
4	H	184	VAL
4	H	185	GLU
4	H	210	SER
4	H	211	GLU
4	H	212	ILE
4	H	230	GLU
4	H	234	MET
4	H	256	SER
4	H	257	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	202	GLN
1	A	267	HIS
1	A	358	HIS
2	B	149	ASN
2	B	300	HIS
2	B	373	GLN
3	C	24	ASN
3	C	180	ASN
4	D	39	GLN
1	E	6	GLN
1	E	235	ASN
1	E	267	HIS
1	E	440	GLN
2	F	300	HIS
2	F	373	GLN

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Mol	Chain	Res	Type
3	G	29	HIS
3	G	71	GLN
4	H	39	GLN
4	H	58	HIS
4	H	192	HIS
4	H	193	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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z > 2$
5	SF4	E	501	1	0,12,12	-	-	-		
6	ATP	G	301	7	32,33,33	0.29	0	48,52,52	0.41	0
5	SF4	G	303	4,3	0,12,12	-	-	-		
8	ANP	D	301	7	33,33,33	3.06	14 (42%)	45,52,52	1.93	7 (15%)
9	GOL	E	502	-	5,5,5	0.98	0	5,5,5	1.01	0
8	ANP	H	301	7	33,33,33	3.07	14 (42%)	45,52,52	1.94	7 (15%)
5	SF4	B	401	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	C	303	4,3	0,12,12	-	-	-		
5	SF4	F	401	2	0,12,12	-	-	-		
6	ATP	C	301	7	32,33,33	0.27	0	48,52,52	0.37	0
5	SF4	A	501	1	0,12,12	-	-	-		

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	E	501	1	-	-	0/6/5/5
6	ATP	G	301	7	-	3/22/38/38	0/3/3/3
5	SF4	G	303	4,3	-	-	0/6/5/5
8	ANP	D	301	7	-	1/18/38/38	0/3/3/3
9	GOL	E	502	-	-	1/4/4/4	-
8	ANP	H	301	7	-	1/18/38/38	0/3/3/3
5	SF4	B	401	2	-	-	0/6/5/5
5	SF4	C	303	4,3	-	-	0/6/5/5
5	SF4	F	401	2	-	-	0/6/5/5
6	ATP	C	301	7	-	2/22/38/38	0/3/3/3
5	SF4	A	501	1	-	-	0/6/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	301	ANP	O3'-C3'	-9.67	1.19	1.43
8	D	301	ANP	O3'-C3'	-9.65	1.19	1.43
8	H	301	ANP	PA-O3A	5.45	1.65	1.59
8	D	301	ANP	PA-O3A	5.23	1.65	1.59
8	H	301	ANP	PB-O3A	5.05	1.65	1.59
8	D	301	ANP	C5-N7	4.99	1.48	1.39
8	H	301	ANP	C5-N7	4.99	1.48	1.39
8	D	301	ANP	PB-O3A	4.89	1.65	1.59
8	D	301	ANP	C6-N6	4.50	1.45	1.34
8	H	301	ANP	C6-N6	4.48	1.45	1.34
8	H	301	ANP	PG-O2G	-3.96	1.46	1.56
8	D	301	ANP	PB-O2B	-3.95	1.46	1.56
8	H	301	ANP	PB-O2B	-3.90	1.46	1.56
8	D	301	ANP	PG-O3G	-3.85	1.46	1.56
8	D	301	ANP	PG-O2G	-3.84	1.46	1.56
8	H	301	ANP	PG-O3G	-3.83	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	301	ANP	C8-N9	-3.17	1.32	1.37
8	D	301	ANP	C8-N9	-3.05	1.32	1.37
8	D	301	ANP	PG-N3B	2.88	1.70	1.63
8	D	301	ANP	PB-N3B	2.88	1.70	1.63
8	H	301	ANP	PG-N3B	2.73	1.70	1.63
8	H	301	ANP	C2'-C3'	-2.72	1.46	1.53
8	H	301	ANP	PB-N3B	2.69	1.70	1.63
8	D	301	ANP	C2'-C3'	-2.67	1.46	1.53
8	H	301	ANP	C4-N9	-2.44	1.32	1.37
8	D	301	ANP	C4-N9	-2.38	1.32	1.37
8	D	301	ANP	C8-N7	2.03	1.35	1.31
8	H	301	ANP	C8-N7	2.01	1.35	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	301	ANP	C4-N9-C8	7.94	114.08	105.74
8	D	301	ANP	C4-N9-C8	7.89	114.02	105.74
8	H	301	ANP	O2B-PB-O1B	-4.06	101.16	109.87
8	D	301	ANP	O2B-PB-O1B	-3.82	101.66	109.87
8	D	301	ANP	O3G-PG-O1G	-3.66	104.28	113.45
8	H	301	ANP	O3G-PG-O1G	-3.62	104.38	113.45
8	D	301	ANP	O2G-PG-O1G	-3.43	104.84	113.45
8	H	301	ANP	O2G-PG-O1G	-3.34	105.09	113.45
8	D	301	ANP	C3'-C2'-C1'	3.09	107.30	101.46
8	H	301	ANP	C3'-C2'-C1'	3.08	107.29	101.46
8	H	301	ANP	O2A-PA-O1A	-2.51	100.75	112.44
8	D	301	ANP	O2A-PA-O1A	-2.38	101.35	112.44
8	D	301	ANP	C5-C4-N9	-2.19	103.43	105.81
8	H	301	ANP	C5-C4-N9	-2.13	103.49	105.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	301	ATP	C5'-O5'-PA-O3A
8	D	301	ANP	PB-N3B-PG-O1G
9	E	502	GOL	O2-C2-C3-O3
6	C	301	ATP	PG-O3B-PB-O1B
6	G	301	ATP	PG-O3B-PB-O1B
8	H	301	ANP	C3'-C4'-C5'-O5'
6	C	301	ATP	PG-O3B-PB-O2B

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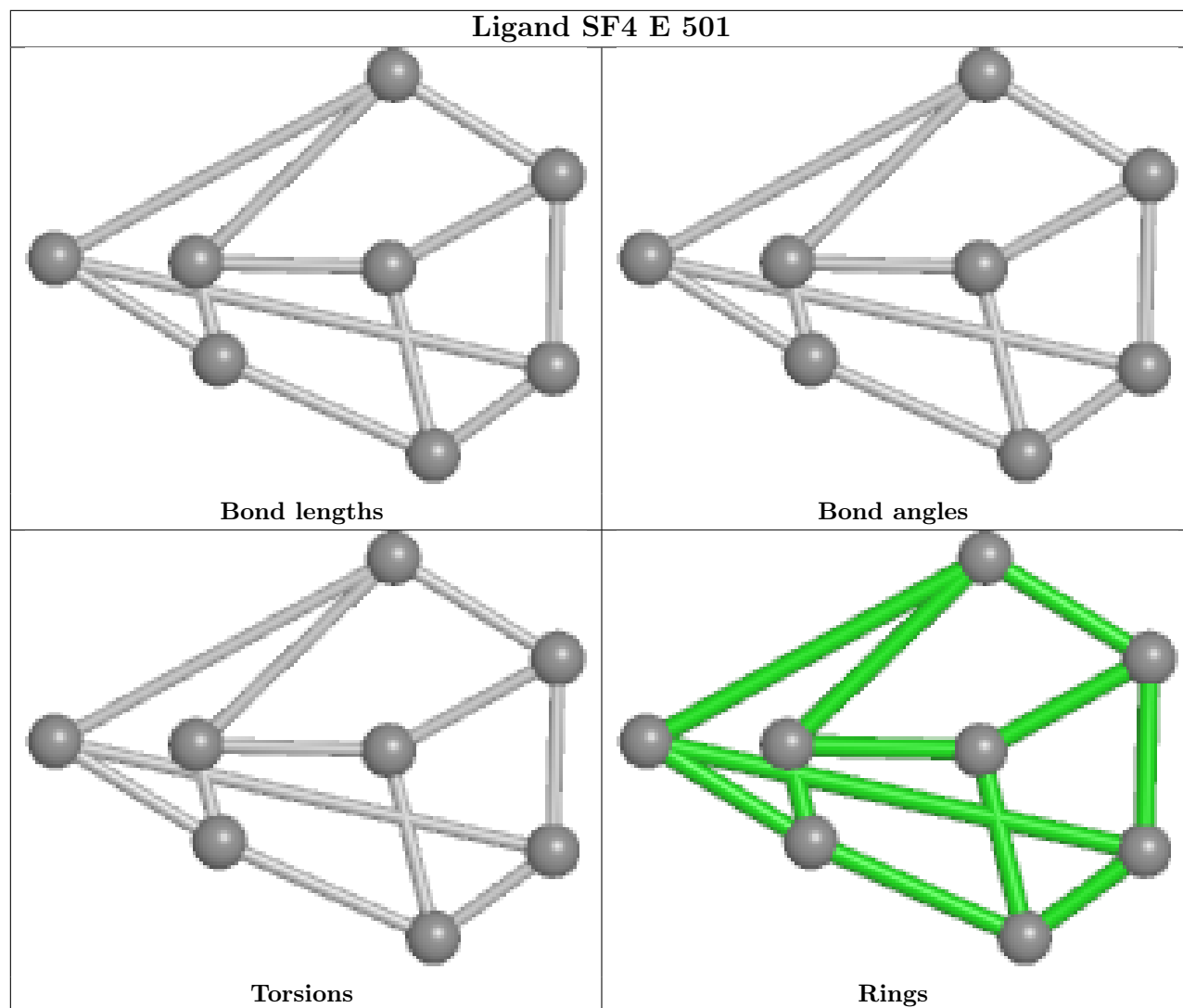
Mol	Chain	Res	Type	Atoms
6	G	301	ATP	PG-O3B-PB-O2B

There are no ring outliers.

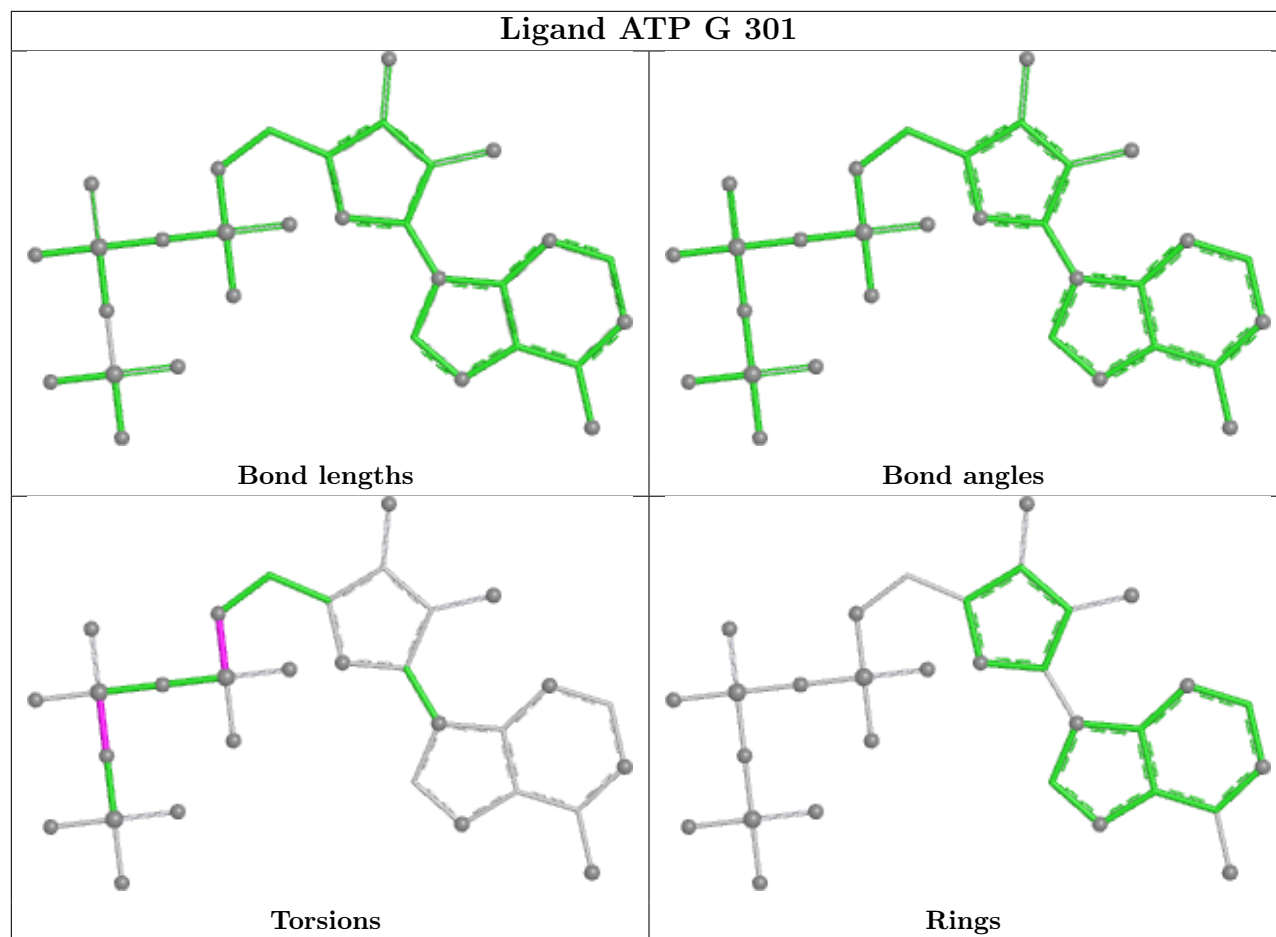
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	301	ANP	1	0
5	F	401	SF4	1	0

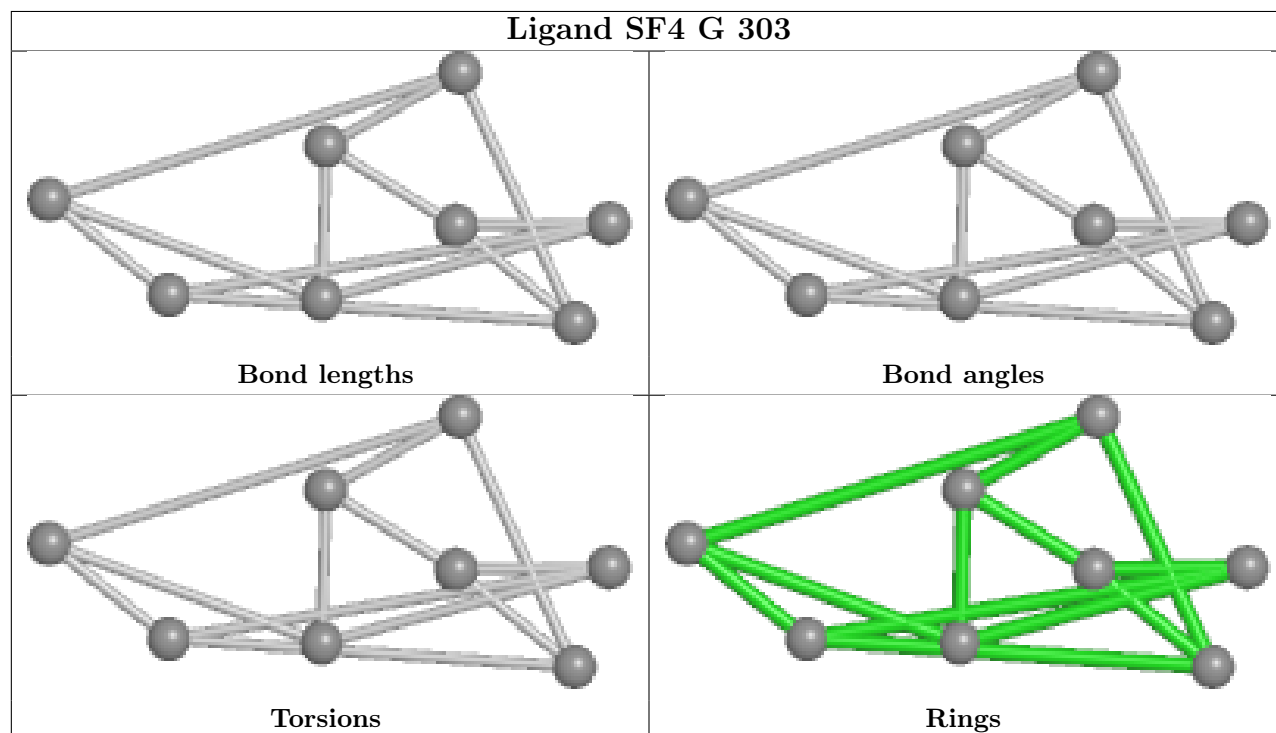
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

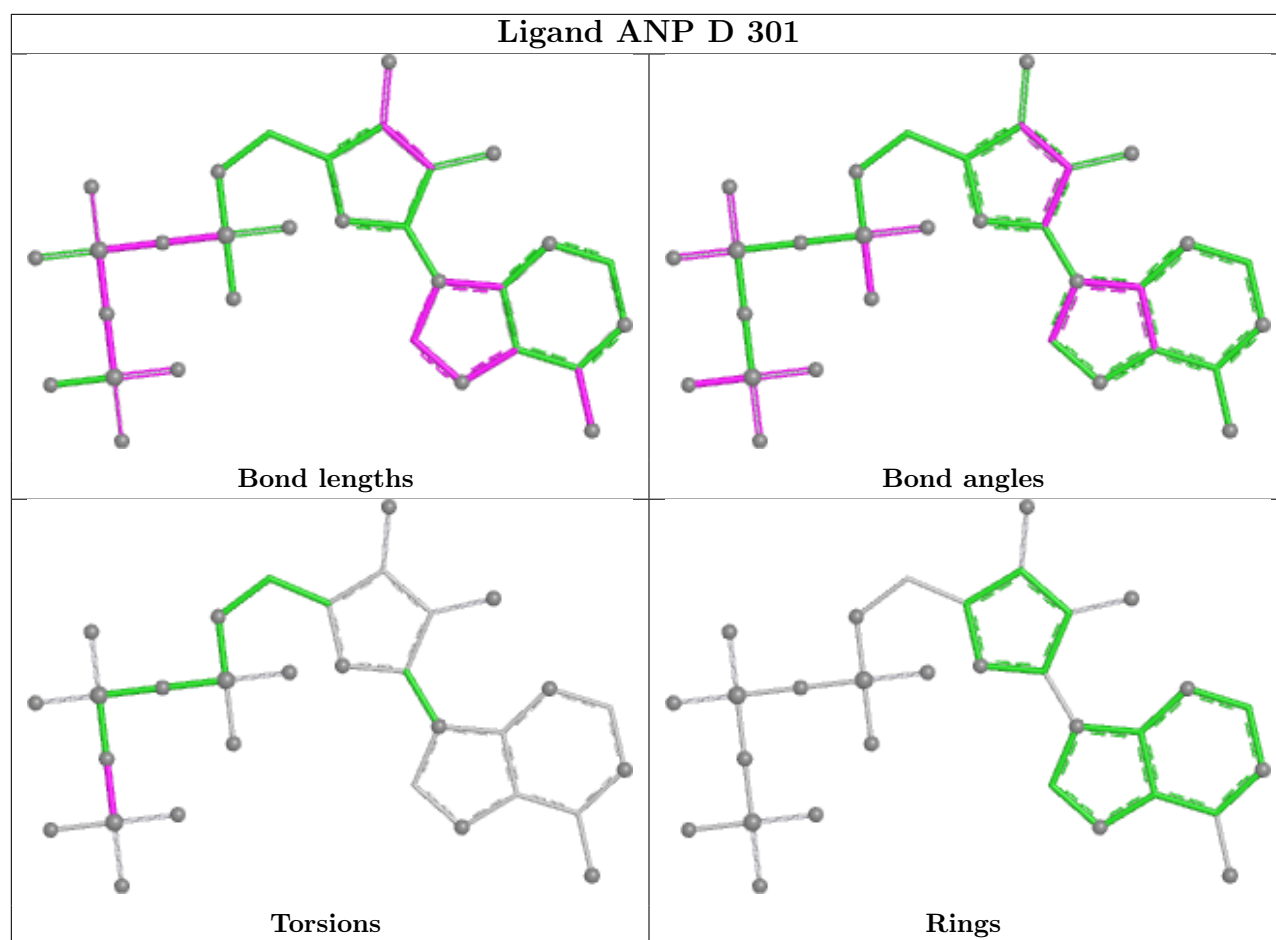


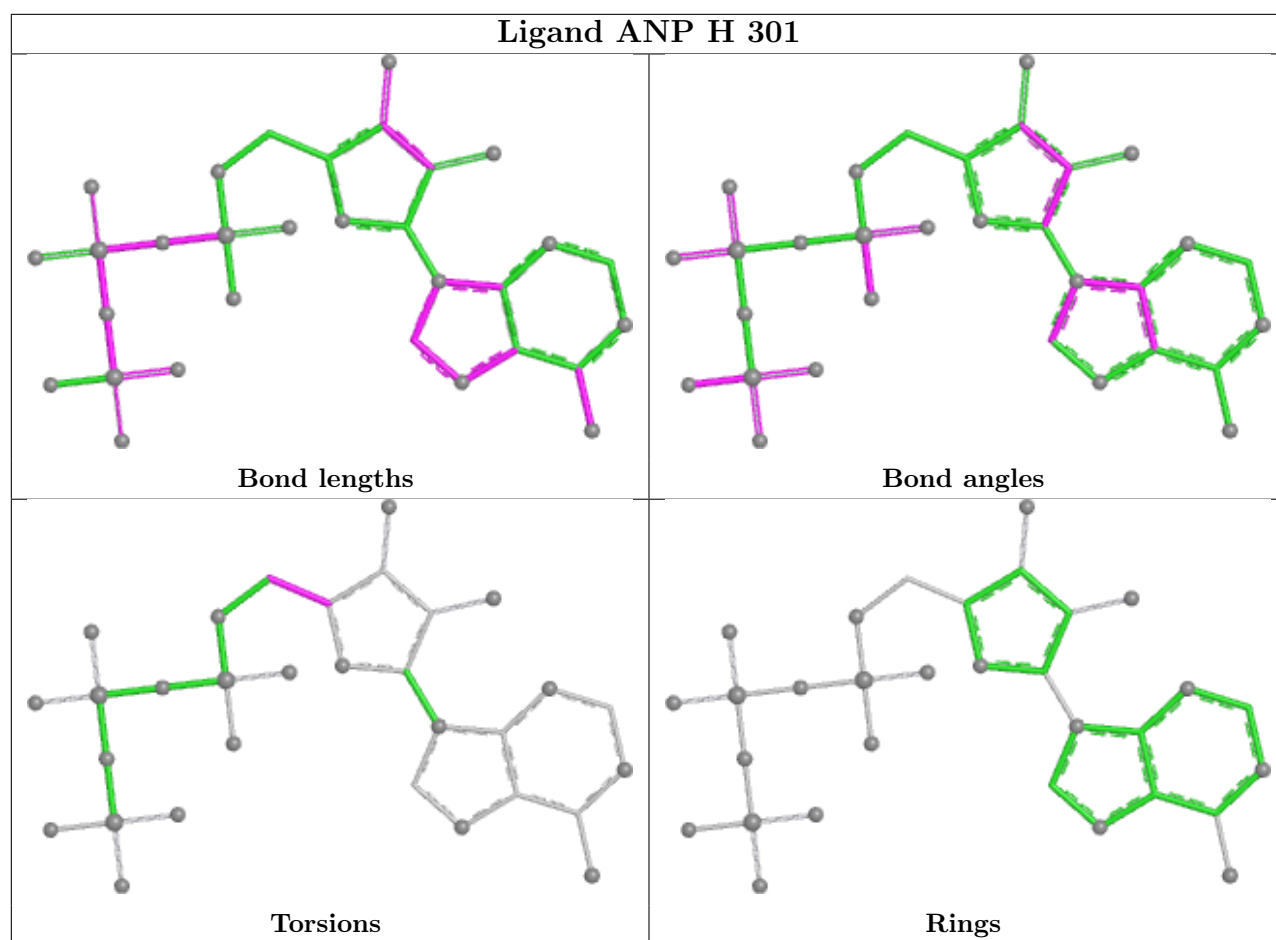
Ligand ATP G 301



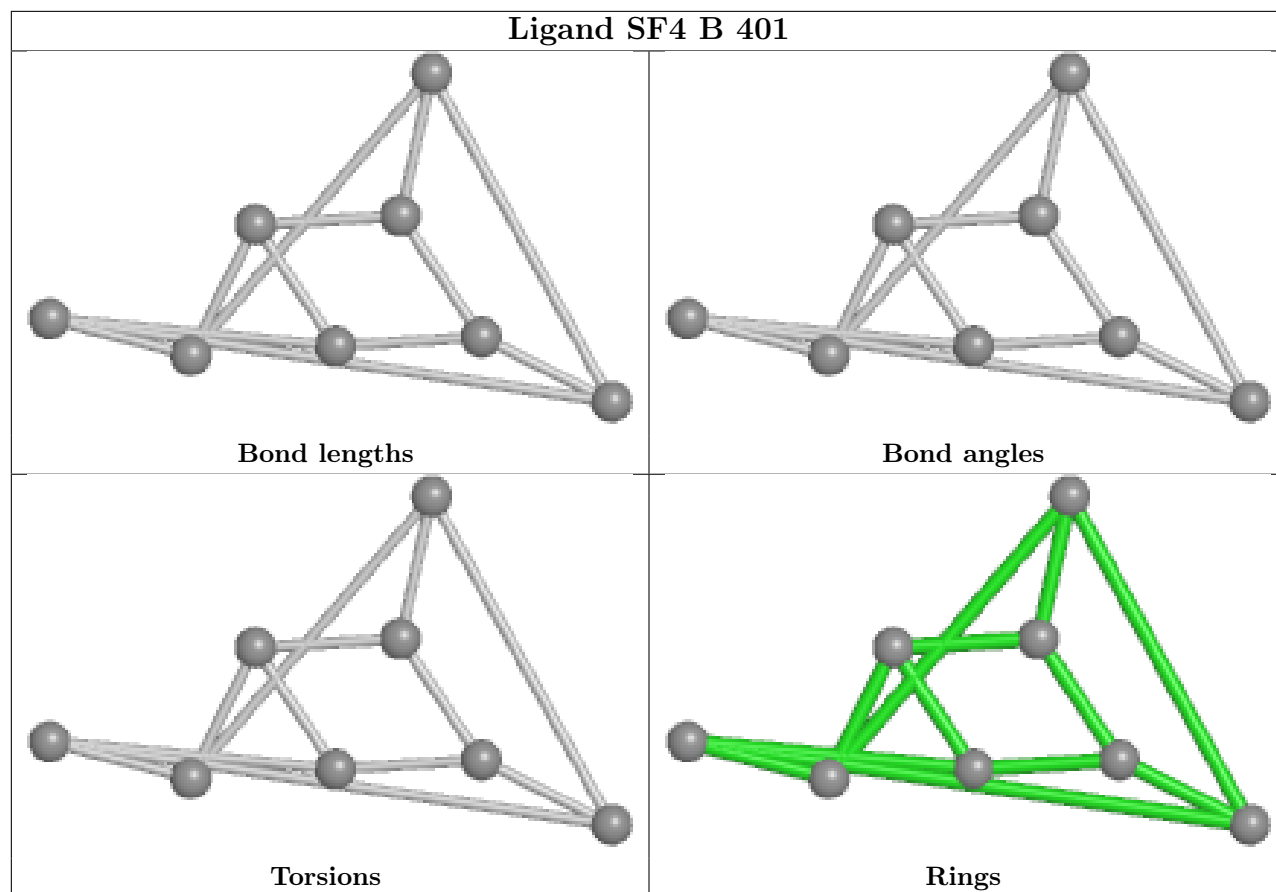
Ligand SF4 G 303



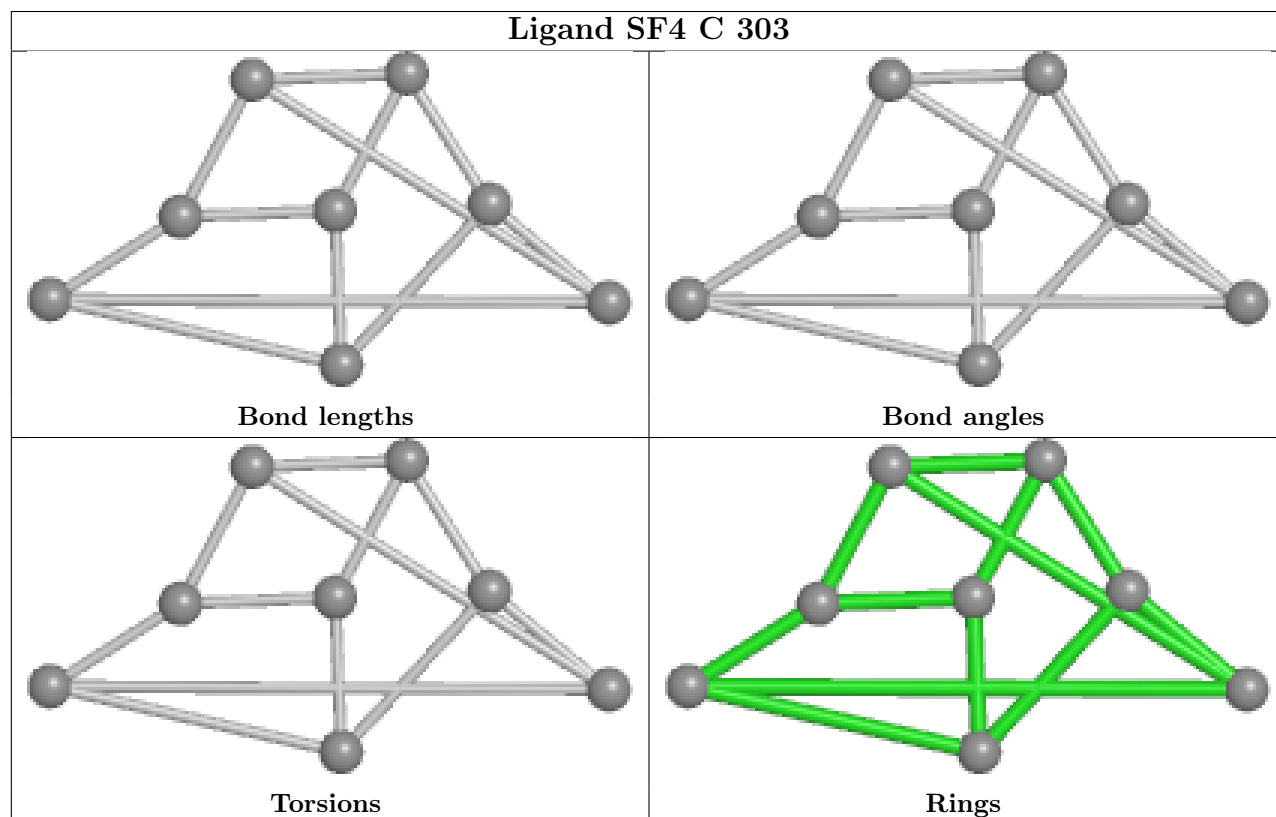


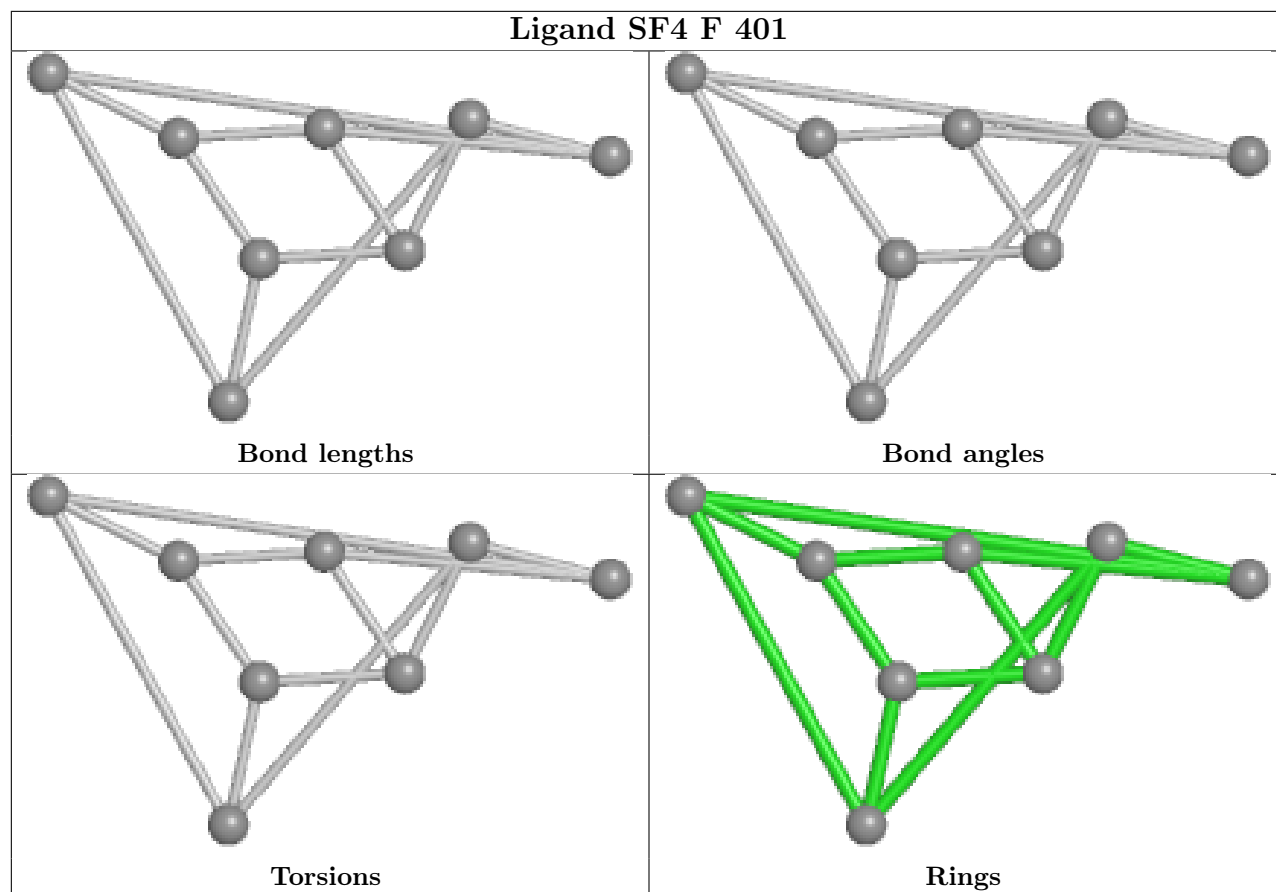


Ligand SF4 B 401

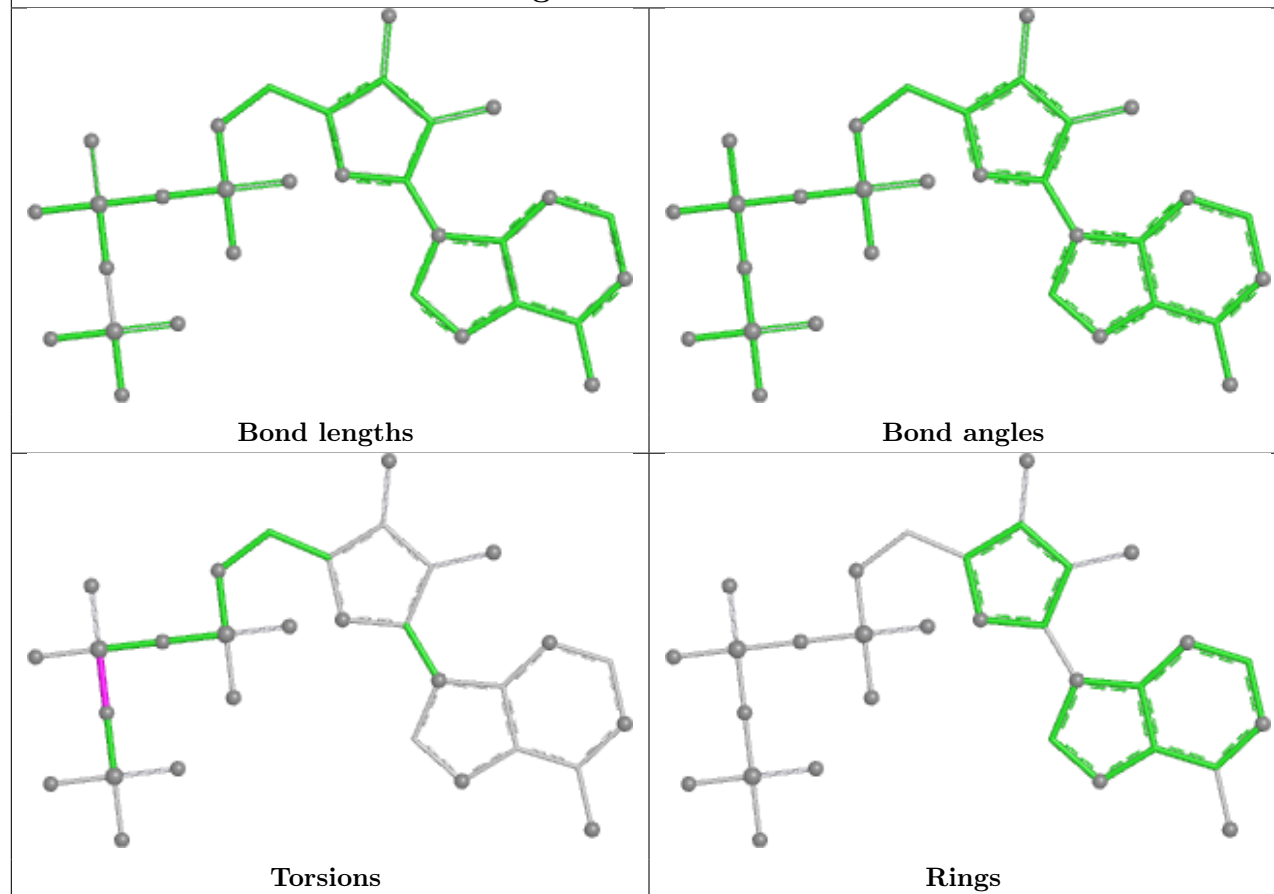


Ligand SF4 C 303

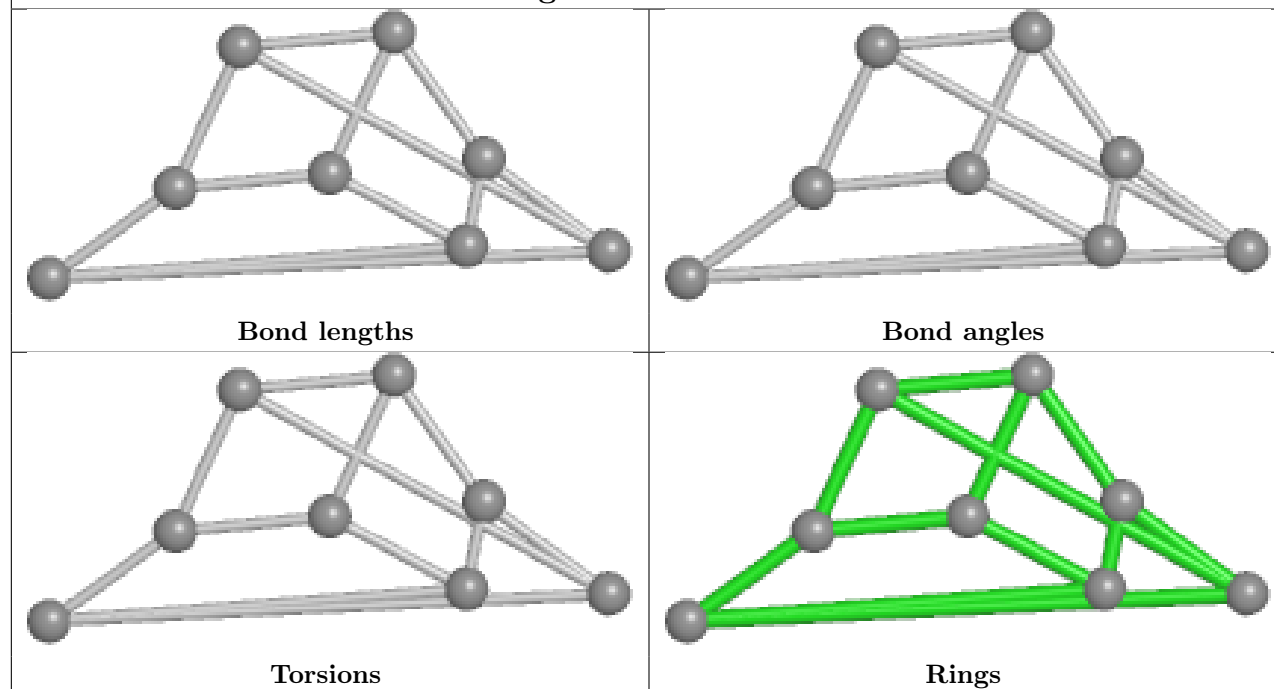




Ligand ATP C 301



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/445 (97%)	-0.57	0 100 100	39, 91, 110, 133	2 (0%)
1	E	436/445 (97%)	-0.60	0 100 100	37, 85, 107, 137	2 (0%)
2	B	387/388 (99%)	-0.60	1 (0%) 90 79	39, 90, 109, 129	2 (0%)
2	F	387/388 (99%)	-0.66	0 100 100	67, 81, 100, 130	0
3	C	264/273 (96%)	-0.57	0 100 100	41, 93, 115, 126	1 (0%)
3	G	264/273 (96%)	-0.48	0 100 100	39, 95, 122, 138	3 (1%)
4	D	260/269 (96%)	-0.41	0 100 100	53, 108, 136, 155	1 (0%)
4	H	261/269 (97%)	-0.41	0 100 100	46, 106, 137, 154	1 (0%)
All	All	2695/2750 (98%)	-0.55	1 (0%) 100 100	37, 92, 121, 155	12 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	316[A]	HIS	5.6

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.

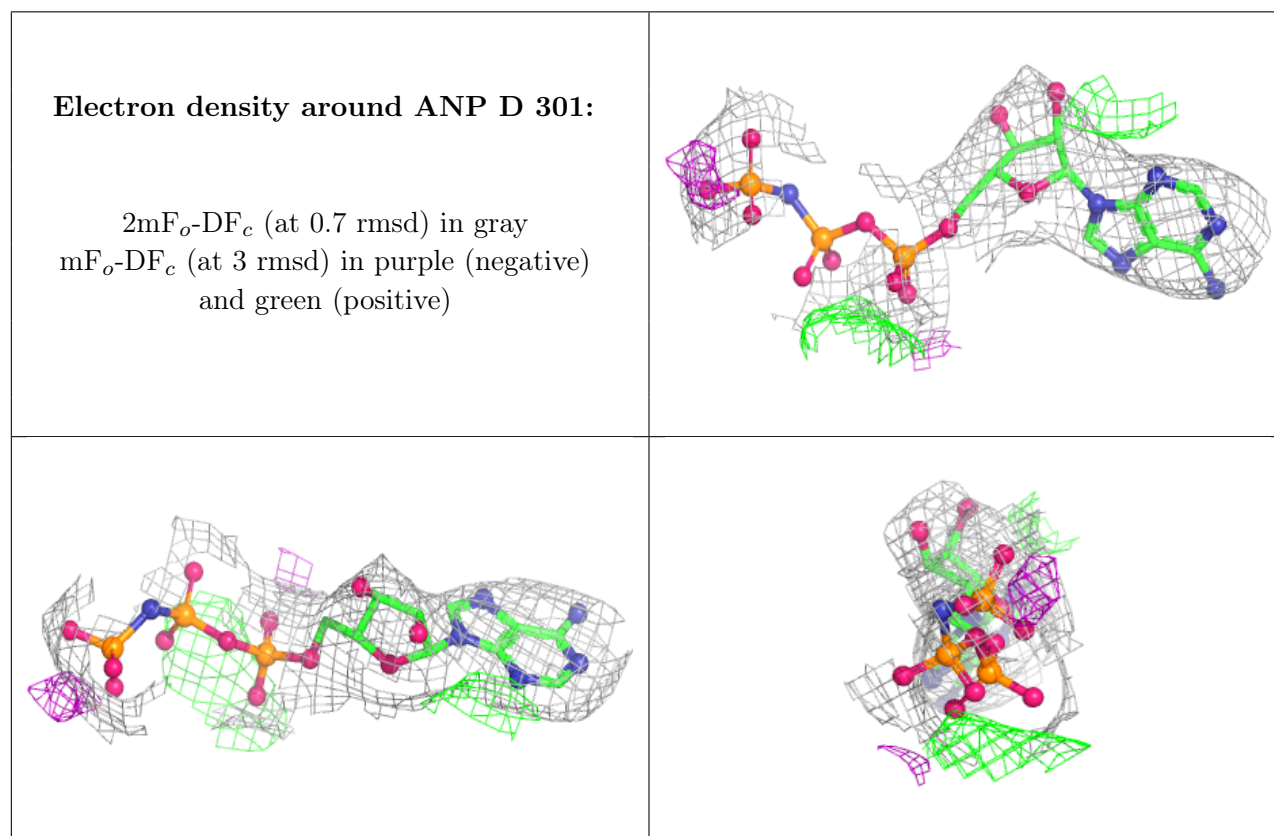
6.4 Ligands [i](#)

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.

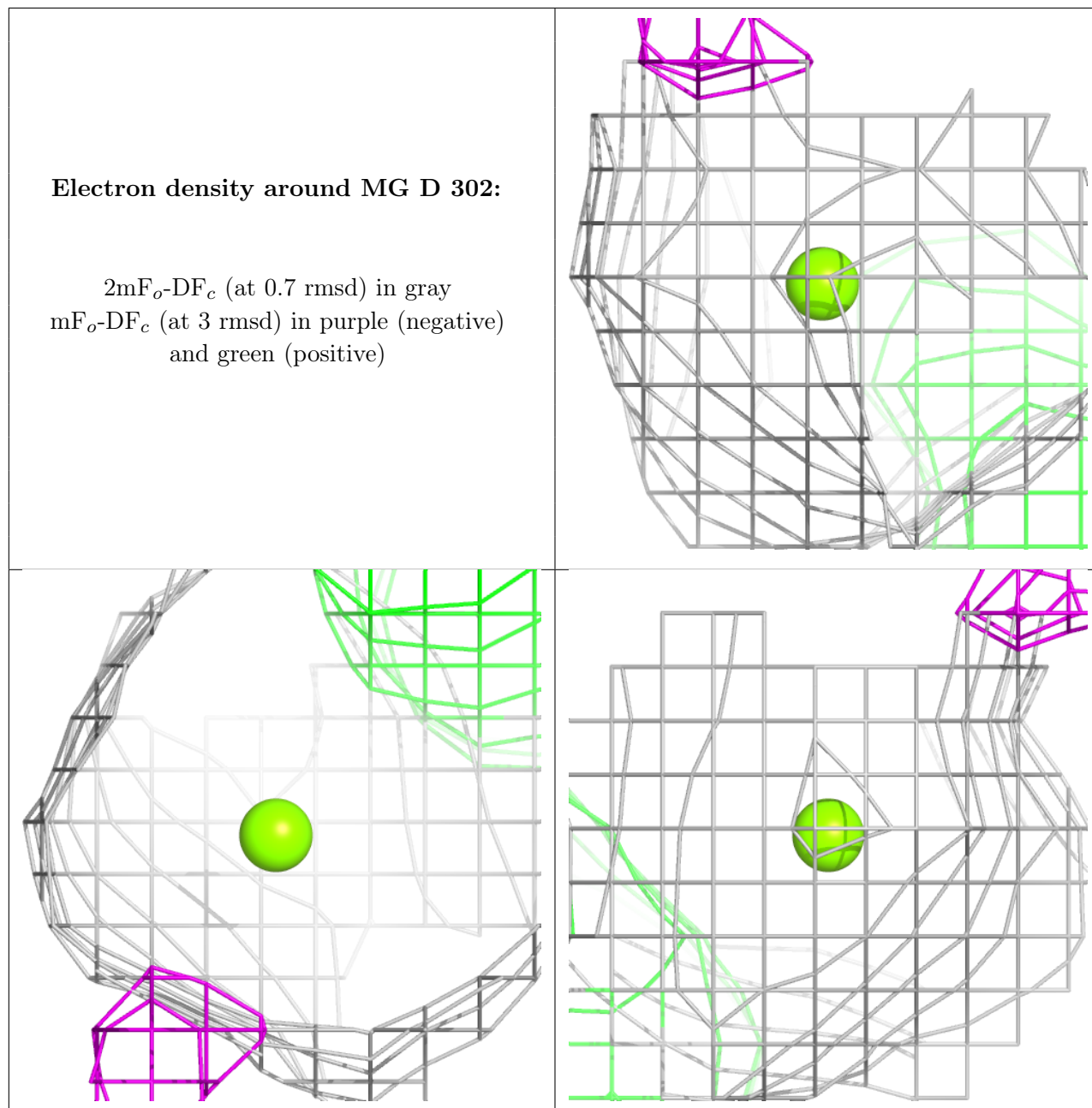
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GOL	E	502	6/6	0.84	0.17	70,77,78,88	0
8	ANP	D	301	31/31	0.89	0.07	94,101,106,110	0
7	MG	D	302	1/1	0.91	0.07	126,126,126,126	0
8	ANP	H	301	31/31	0.95	0.06	84,94,106,109	0
6	ATP	G	301	31/31	0.95	0.06	81,89,96,97	0
6	ATP	C	301	31/31	0.96	0.06	89,93,98,98	0
7	MG	H	302	1/1	0.97	0.05	105,105,105,105	0
5	SF4	B	401	8/8	0.99	0.03	72,75,81,90	0
7	MG	C	302	1/1	0.99	0.04	84,84,84,84	0
5	SF4	C	303	8/8	0.99	0.04	78,81,91,96	0
7	MG	G	302	1/1	0.99	0.05	86,86,86,86	0
5	SF4	E	501	8/8	0.99	0.04	61,69,72,82	0
5	SF4	F	401	8/8	0.99	0.03	58,68,71,84	0
5	SF4	G	303	8/8	0.99	0.04	76,79,85,92	0
5	SF4	A	501	8/8	0.99	0.04	69,74,80,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



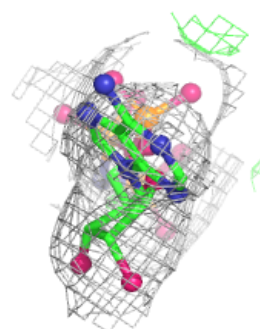
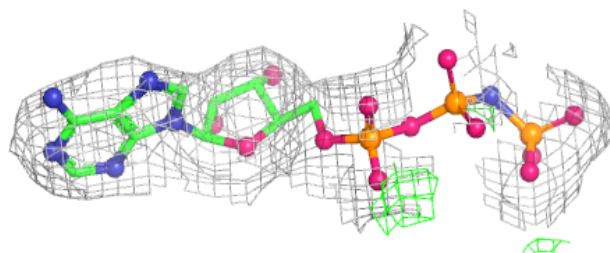
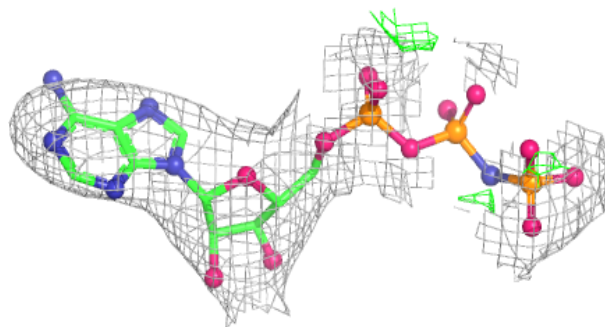
Electron density around MG D 302:

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

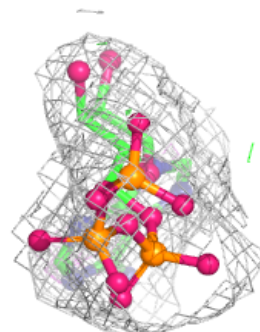
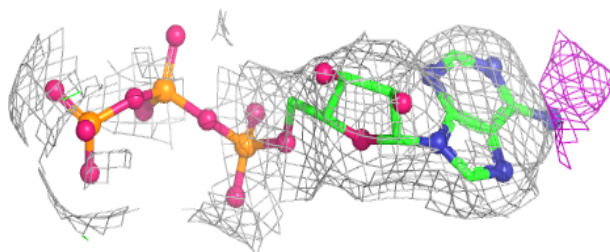
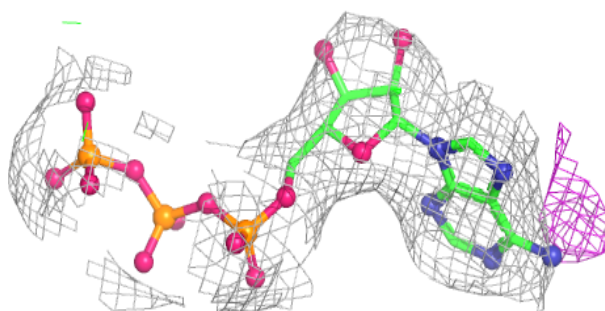


Electron density around ANP H 301:

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

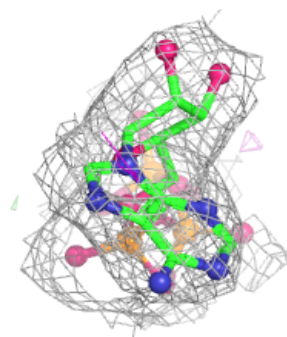
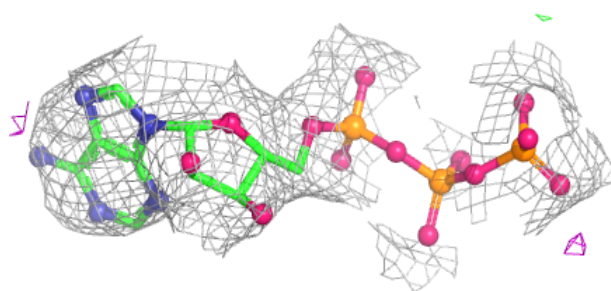
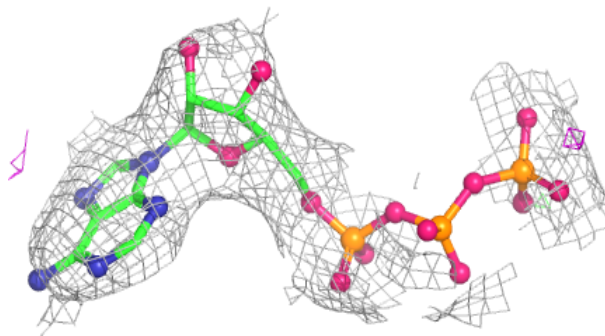
**Electron density around ATP G 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



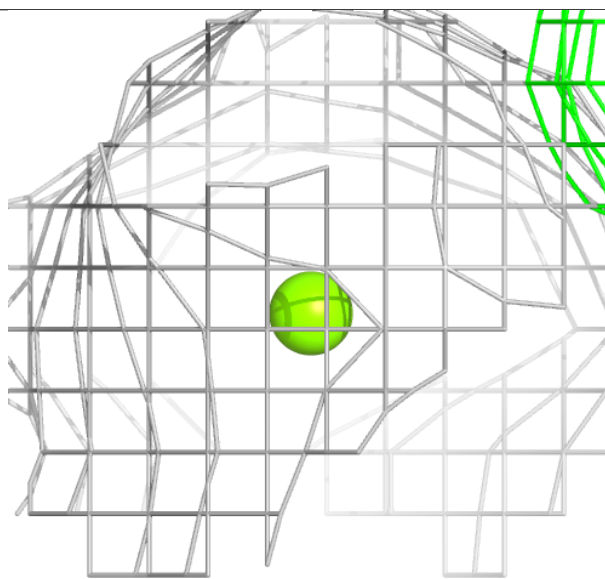
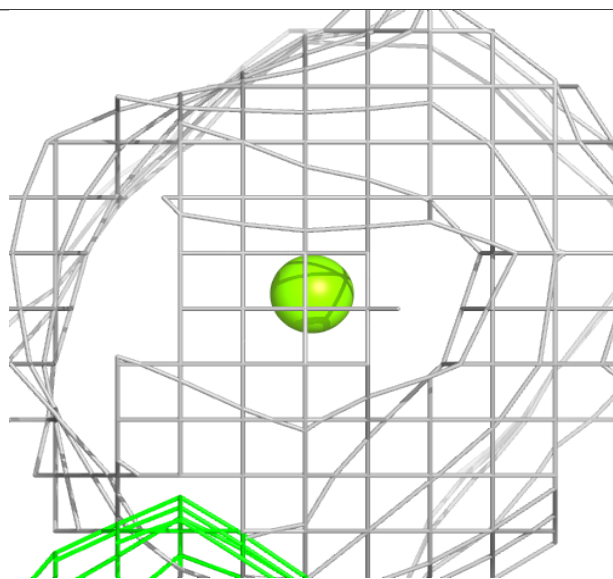
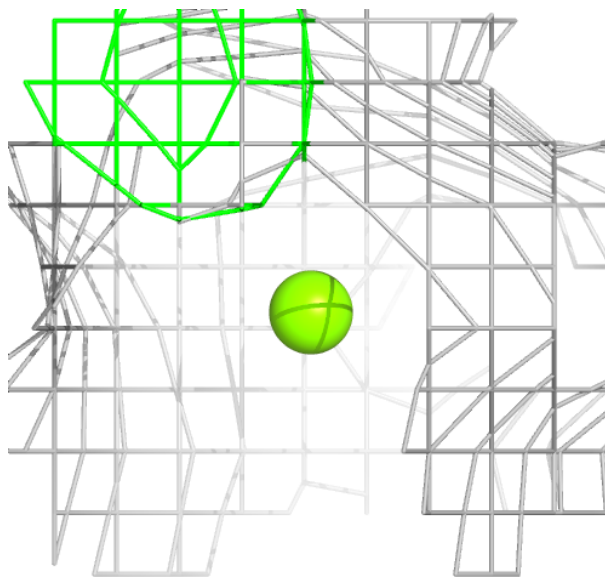
Electron density around ATP C 301:

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



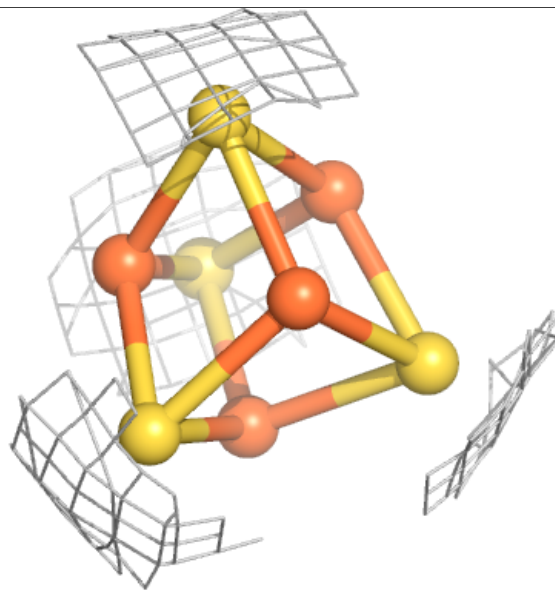
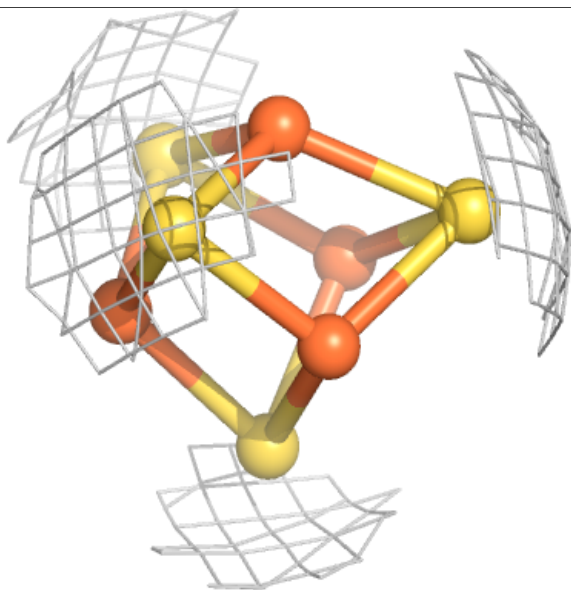
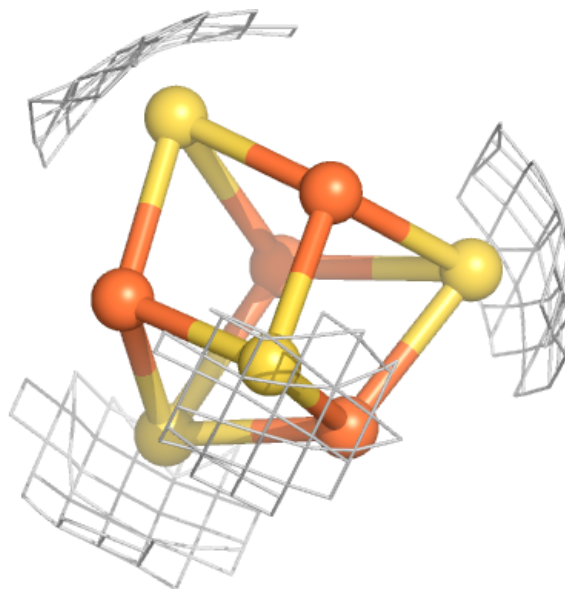
Electron density around MG H 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



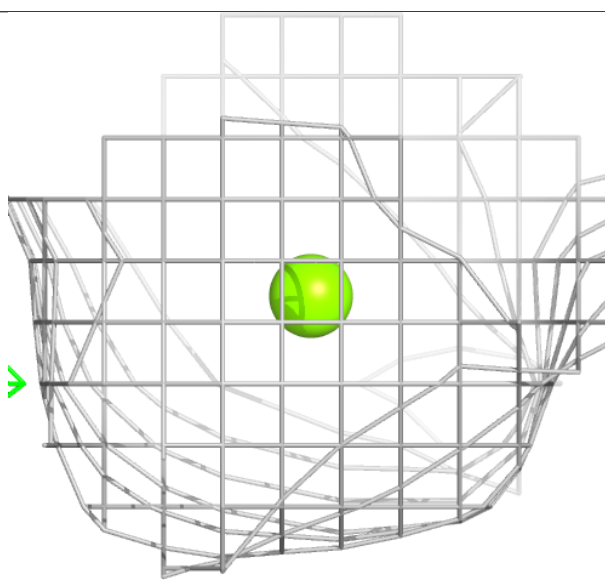
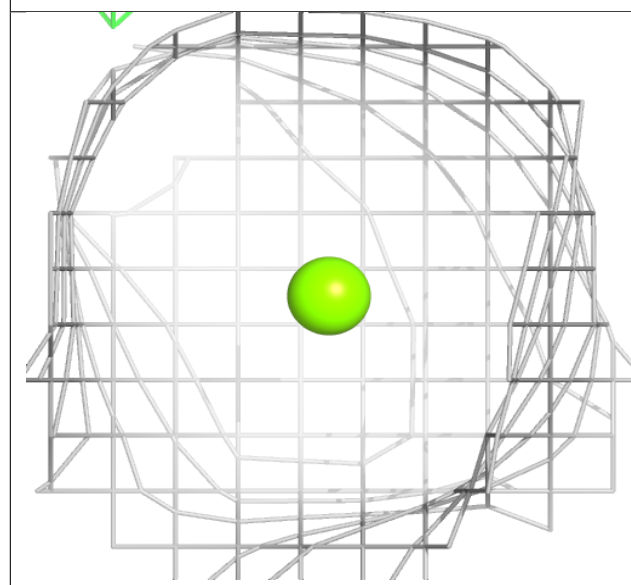
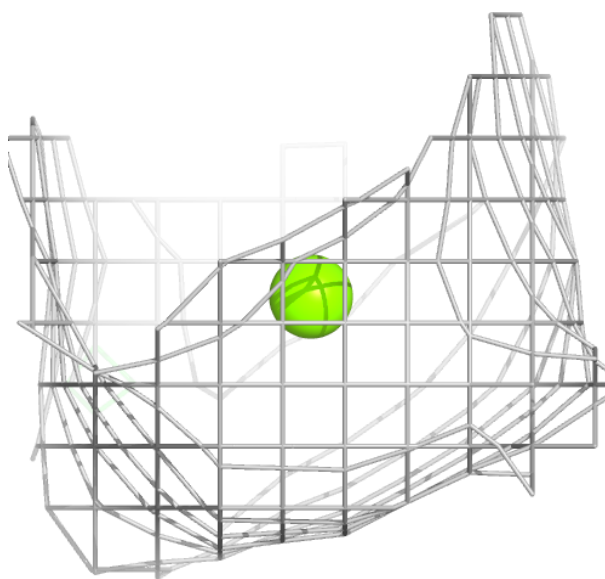
Electron density around SF4 B 401:

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



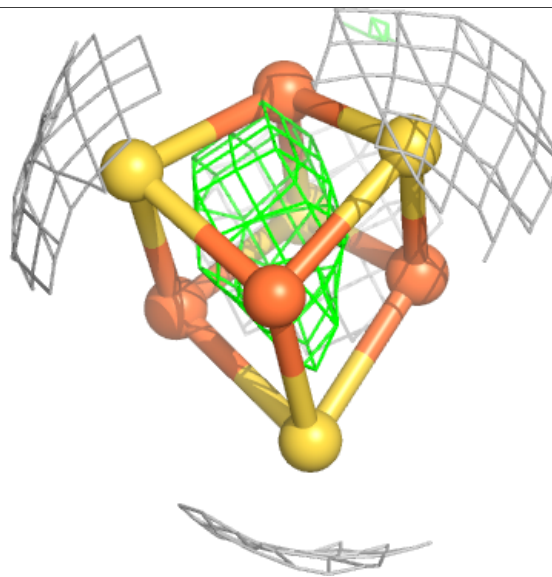
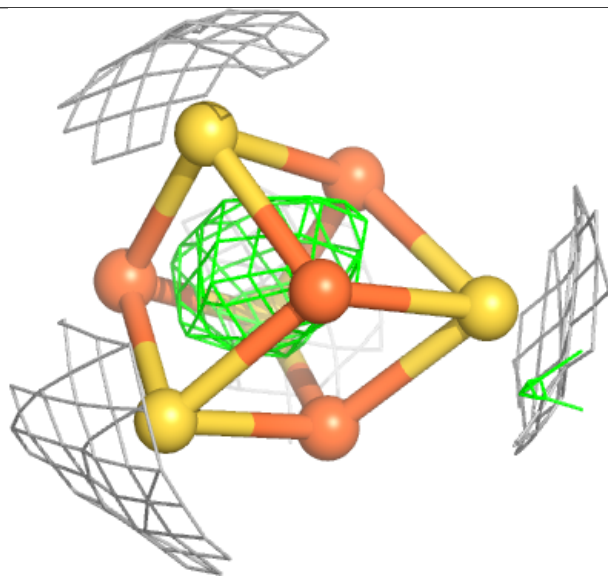
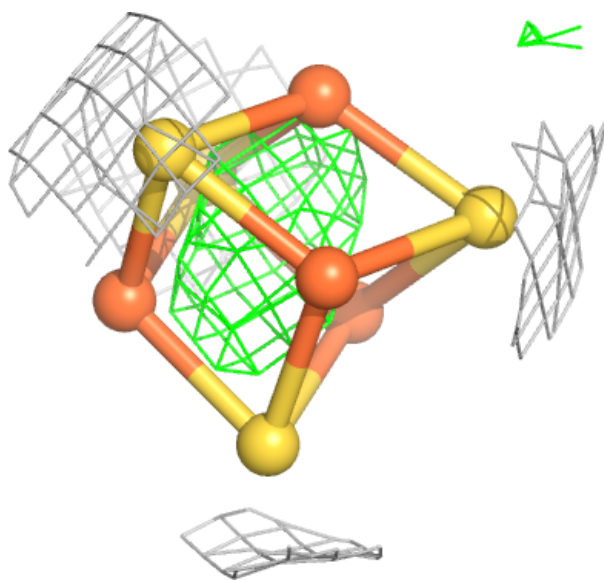
Electron density around MG C 302:

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



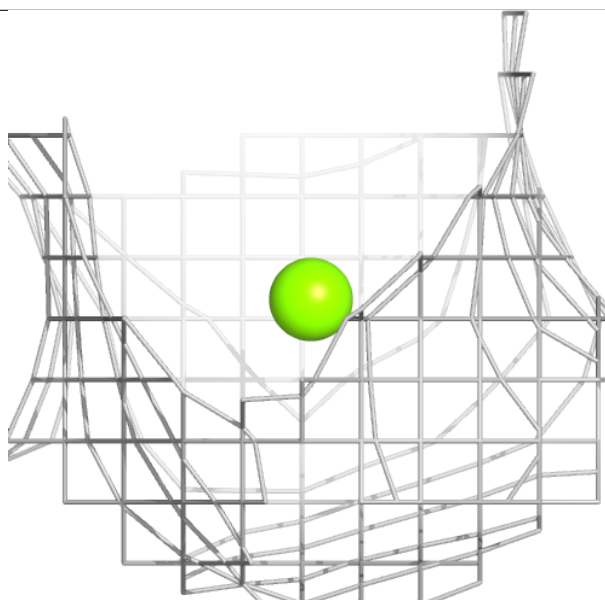
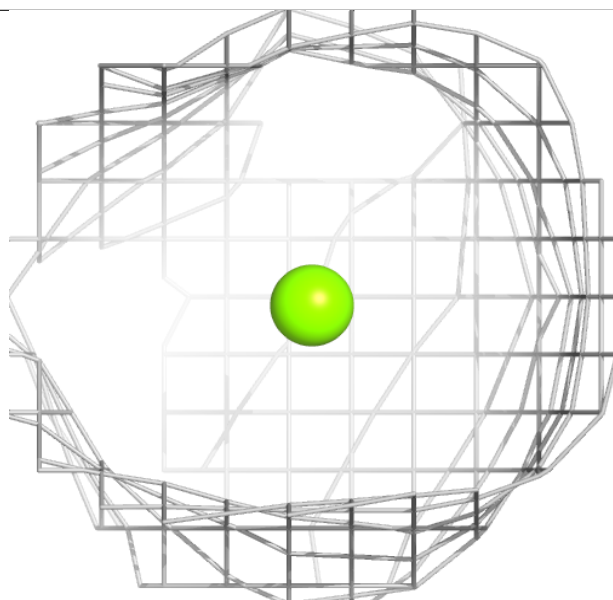
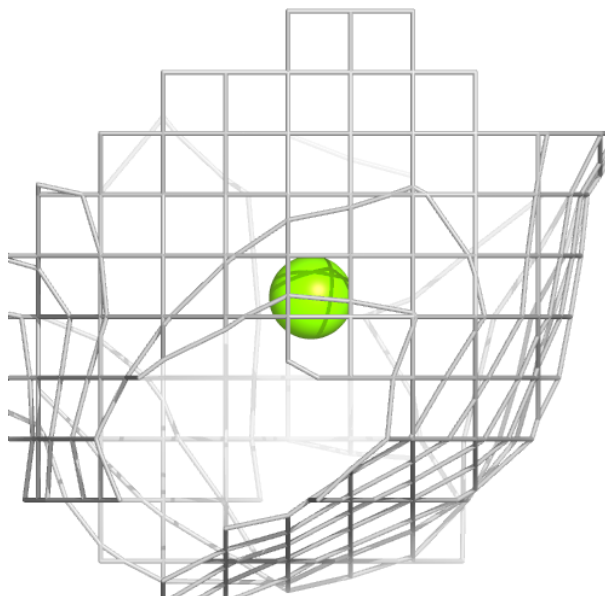
Electron density around SF4 C 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



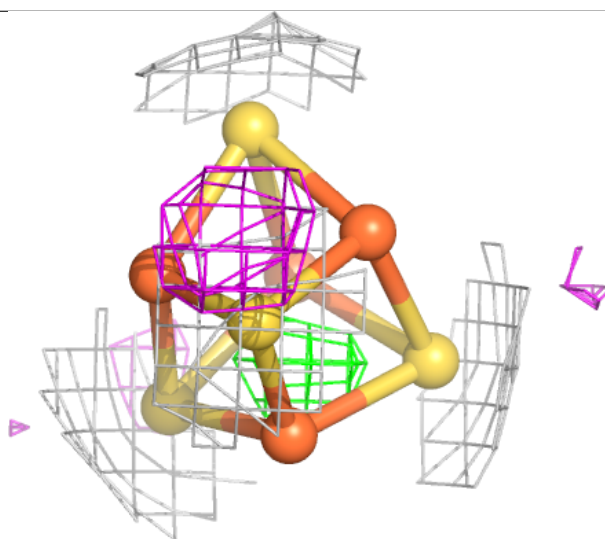
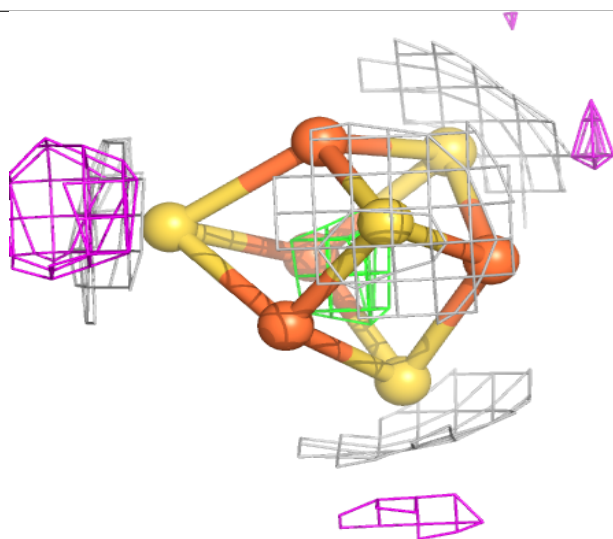
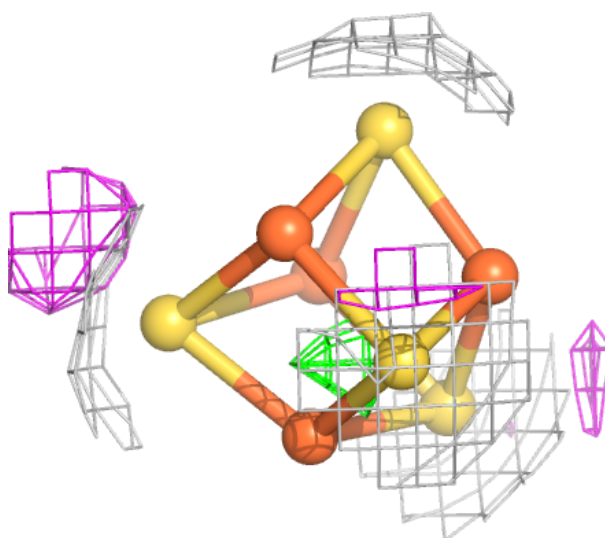
Electron density around MG G 302:

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and green (positive)



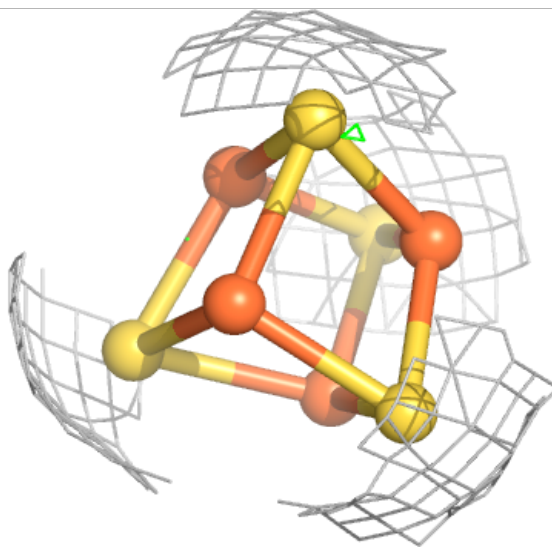
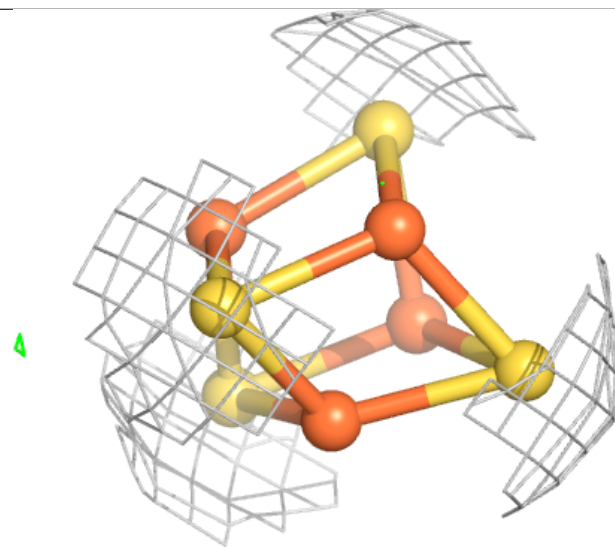
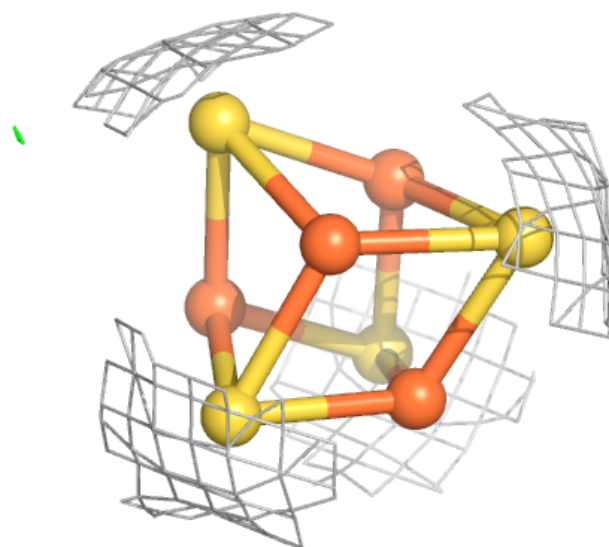
Electron density around SF4 E 501:

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and green (positive)



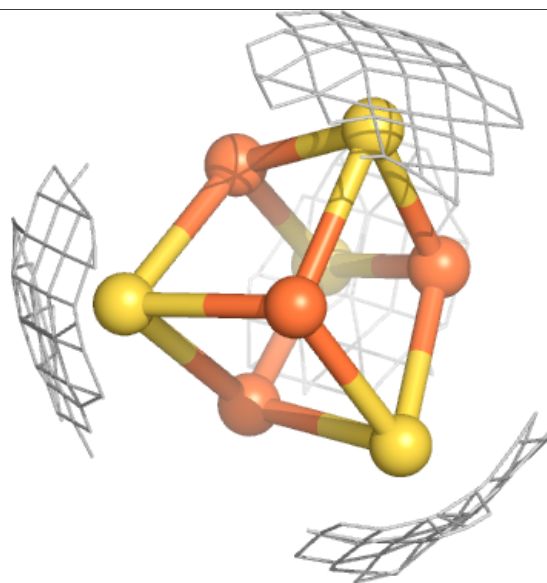
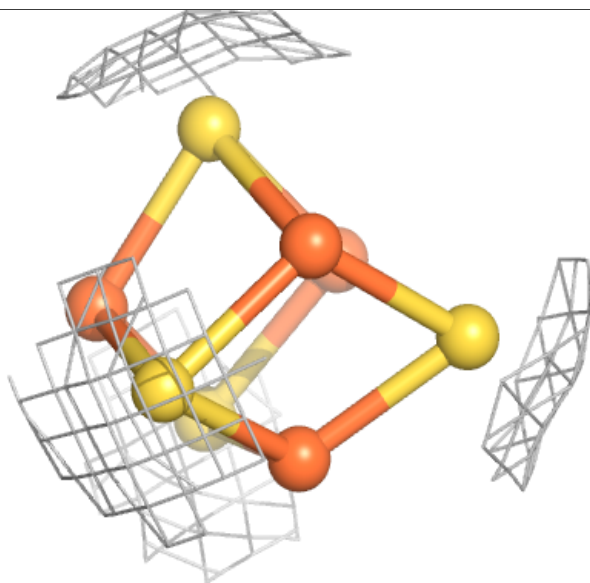
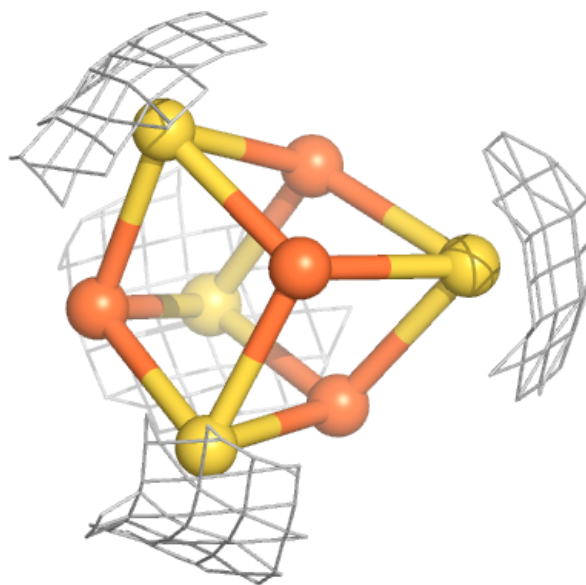
Electron density around SF4 F 401:

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and green (positive)



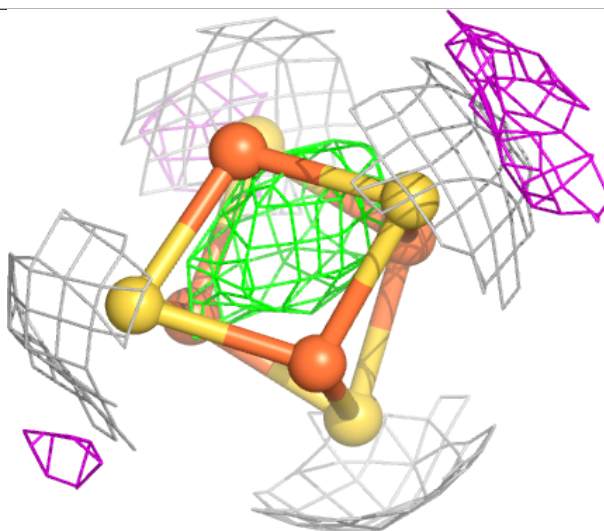
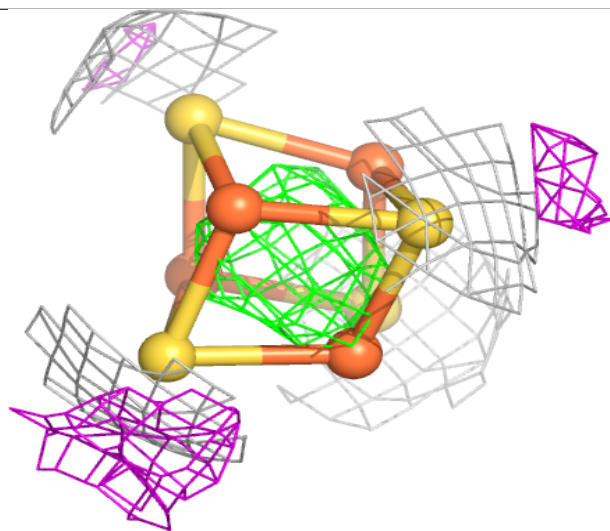
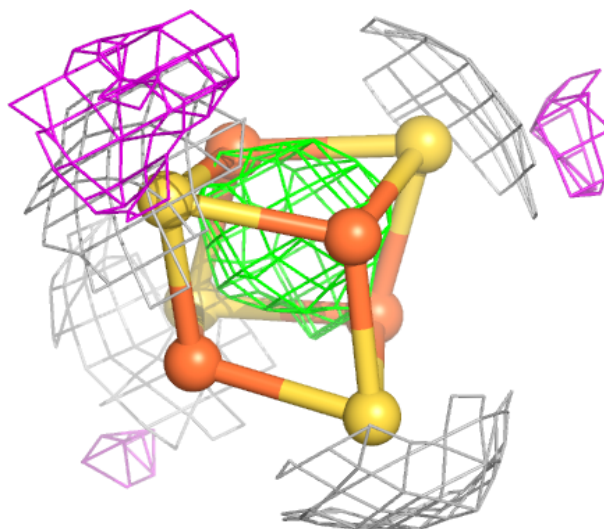
Electron density around SF4 G 303:

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



Electron density around SF4 A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.