



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 12:02 AM EDT

PDB ID : 2QC8
Title : Crystal structure of human glutamine synthetase in complex with ADP and methionine sulfoximine phosphate
Authors : Karlberg, T.; Lehtio, L.; Arrowsmith, C.H.; Berglund, H.; Busam, R.D.; Collins, R.; Dahlgren, L.G.; Edwards, A.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hogbom, M.; Johansson, I.; Kallas, A.; Kotenyova, T.; Moche, M.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Sundstrom, M.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Holmberg-Schiavone, L.; Structural Genomics Consortium (SGC)
Deposited on : 2007-06-19
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158

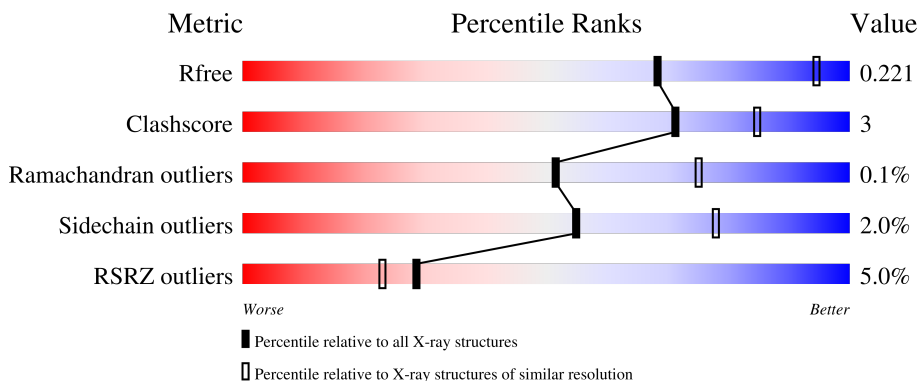
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	384	 3% 81% 11% 7%
1	B	384	 % 84% 8% 7%

Continued on next page...

CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	C	384	<p>% 82% 10% • 7%</p>
1	D	384	<p>% 83% 10% 7%</p>
1	E	384	<p>3% 82% 10% • 8%</p>
1	F	384	<p>6% 83% 9% • 7%</p>
1	G	384	<p>9% 83% 9% • 7%</p>
1	H	384	<p>7% 84% 8% • 7%</p>
1	I	384	<p>8% 83% 9% • 7%</p>
1	J	384	<p>10% 83% 9% • 7%</p>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28837 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2815	1768	503	522	22	0	0	0
1	B	356	2815	1768	503	522	22	0	0	0
1	C	356	2815	1768	503	522	22	0	0	0
1	D	356	2815	1768	503	522	22	0	0	0
1	E	355	2811	1766	502	521	22	0	0	0
1	F	356	2815	1768	503	522	22	0	0	0
1	G	356	2815	1768	503	522	22	0	0	0
1	H	356	2815	1768	503	522	22	0	0	0
1	I	356	2815	1768	503	522	22	0	0	0
1	J	356	2815	1768	503	522	22	0	0	0

There are 230 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P15104
A	-17	HIS	-	expression tag	UNP P15104
A	-16	HIS	-	expression tag	UNP P15104
A	-15	HIS	-	expression tag	UNP P15104
A	-14	HIS	-	expression tag	UNP P15104
A	-13	HIS	-	expression tag	UNP P15104
A	-12	HIS	-	expression tag	UNP P15104
A	-11	SER	-	expression tag	UNP P15104
A	-10	SER	-	expression tag	UNP P15104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP P15104
A	-8	VAL	-	expression tag	UNP P15104
A	-7	ASP	-	expression tag	UNP P15104
A	-6	LEU	-	expression tag	UNP P15104
A	-5	GLY	-	expression tag	UNP P15104
A	-4	THR	-	expression tag	UNP P15104
A	-3	GLU	-	expression tag	UNP P15104
A	-2	ASN	-	expression tag	UNP P15104
A	-1	LEU	-	expression tag	UNP P15104
A	0	TYR	-	expression tag	UNP P15104
A	1	PHE	-	expression tag	UNP P15104
A	2	GLN	-	expression tag	UNP P15104
A	3	SER	-	expression tag	UNP P15104
A	4	MET	-	expression tag	UNP P15104
B	-18	MET	-	expression tag	UNP P15104
B	-17	HIS	-	expression tag	UNP P15104
B	-16	HIS	-	expression tag	UNP P15104
B	-15	HIS	-	expression tag	UNP P15104
B	-14	HIS	-	expression tag	UNP P15104
B	-13	HIS	-	expression tag	UNP P15104
B	-12	HIS	-	expression tag	UNP P15104
B	-11	SER	-	expression tag	UNP P15104
B	-10	SER	-	expression tag	UNP P15104
B	-9	GLY	-	expression tag	UNP P15104
B	-8	VAL	-	expression tag	UNP P15104
B	-7	ASP	-	expression tag	UNP P15104
B	-6	LEU	-	expression tag	UNP P15104
B	-5	GLY	-	expression tag	UNP P15104
B	-4	THR	-	expression tag	UNP P15104
B	-3	GLU	-	expression tag	UNP P15104
B	-2	ASN	-	expression tag	UNP P15104
B	-1	LEU	-	expression tag	UNP P15104
B	0	TYR	-	expression tag	UNP P15104
B	1	PHE	-	expression tag	UNP P15104
B	2	GLN	-	expression tag	UNP P15104
B	3	SER	-	expression tag	UNP P15104
B	4	MET	-	expression tag	UNP P15104
C	-18	MET	-	expression tag	UNP P15104
C	-17	HIS	-	expression tag	UNP P15104
C	-16	HIS	-	expression tag	UNP P15104
C	-15	HIS	-	expression tag	UNP P15104
C	-14	HIS	-	expression tag	UNP P15104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP P15104
C	-12	HIS	-	expression tag	UNP P15104
C	-11	SER	-	expression tag	UNP P15104
C	-10	SER	-	expression tag	UNP P15104
C	-9	GLY	-	expression tag	UNP P15104
C	-8	VAL	-	expression tag	UNP P15104
C	-7	ASP	-	expression tag	UNP P15104
C	-6	LEU	-	expression tag	UNP P15104
C	-5	GLY	-	expression tag	UNP P15104
C	-4	THR	-	expression tag	UNP P15104
C	-3	GLU	-	expression tag	UNP P15104
C	-2	ASN	-	expression tag	UNP P15104
C	-1	LEU	-	expression tag	UNP P15104
C	0	TYR	-	expression tag	UNP P15104
C	1	PHE	-	expression tag	UNP P15104
C	2	GLN	-	expression tag	UNP P15104
C	3	SER	-	expression tag	UNP P15104
C	4	MET	-	expression tag	UNP P15104
D	-18	MET	-	expression tag	UNP P15104
D	-17	HIS	-	expression tag	UNP P15104
D	-16	HIS	-	expression tag	UNP P15104
D	-15	HIS	-	expression tag	UNP P15104
D	-14	HIS	-	expression tag	UNP P15104
D	-13	HIS	-	expression tag	UNP P15104
D	-12	HIS	-	expression tag	UNP P15104
D	-11	SER	-	expression tag	UNP P15104
D	-10	SER	-	expression tag	UNP P15104
D	-9	GLY	-	expression tag	UNP P15104
D	-8	VAL	-	expression tag	UNP P15104
D	-7	ASP	-	expression tag	UNP P15104
D	-6	LEU	-	expression tag	UNP P15104
D	-5	GLY	-	expression tag	UNP P15104
D	-4	THR	-	expression tag	UNP P15104
D	-3	GLU	-	expression tag	UNP P15104
D	-2	ASN	-	expression tag	UNP P15104
D	-1	LEU	-	expression tag	UNP P15104
D	0	TYR	-	expression tag	UNP P15104
D	1	PHE	-	expression tag	UNP P15104
D	2	GLN	-	expression tag	UNP P15104
D	3	SER	-	expression tag	UNP P15104
D	4	MET	-	expression tag	UNP P15104
E	-18	MET	-	expression tag	UNP P15104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	expression tag	UNP P15104
E	-16	HIS	-	expression tag	UNP P15104
E	-15	HIS	-	expression tag	UNP P15104
E	-14	HIS	-	expression tag	UNP P15104
E	-13	HIS	-	expression tag	UNP P15104
E	-12	HIS	-	expression tag	UNP P15104
E	-11	SER	-	expression tag	UNP P15104
E	-10	SER	-	expression tag	UNP P15104
E	-9	GLY	-	expression tag	UNP P15104
E	-8	VAL	-	expression tag	UNP P15104
E	-7	ASP	-	expression tag	UNP P15104
E	-6	LEU	-	expression tag	UNP P15104
E	-5	GLY	-	expression tag	UNP P15104
E	-4	THR	-	expression tag	UNP P15104
E	-3	GLU	-	expression tag	UNP P15104
E	-2	ASN	-	expression tag	UNP P15104
E	-1	LEU	-	expression tag	UNP P15104
E	0	TYR	-	expression tag	UNP P15104
E	1	PHE	-	expression tag	UNP P15104
E	2	GLN	-	expression tag	UNP P15104
E	3	SER	-	expression tag	UNP P15104
E	4	MET	-	expression tag	UNP P15104
F	-18	MET	-	expression tag	UNP P15104
F	-17	HIS	-	expression tag	UNP P15104
F	-16	HIS	-	expression tag	UNP P15104
F	-15	HIS	-	expression tag	UNP P15104
F	-14	HIS	-	expression tag	UNP P15104
F	-13	HIS	-	expression tag	UNP P15104
F	-12	HIS	-	expression tag	UNP P15104
F	-11	SER	-	expression tag	UNP P15104
F	-10	SER	-	expression tag	UNP P15104
F	-9	GLY	-	expression tag	UNP P15104
F	-8	VAL	-	expression tag	UNP P15104
F	-7	ASP	-	expression tag	UNP P15104
F	-6	LEU	-	expression tag	UNP P15104
F	-5	GLY	-	expression tag	UNP P15104
F	-4	THR	-	expression tag	UNP P15104
F	-3	GLU	-	expression tag	UNP P15104
F	-2	ASN	-	expression tag	UNP P15104
F	-1	LEU	-	expression tag	UNP P15104
F	0	TYR	-	expression tag	UNP P15104
F	1	PHE	-	expression tag	UNP P15104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	GLN	-	expression tag	UNP P15104
F	3	SER	-	expression tag	UNP P15104
F	4	MET	-	expression tag	UNP P15104
G	-18	MET	-	expression tag	UNP P15104
G	-17	HIS	-	expression tag	UNP P15104
G	-16	HIS	-	expression tag	UNP P15104
G	-15	HIS	-	expression tag	UNP P15104
G	-14	HIS	-	expression tag	UNP P15104
G	-13	HIS	-	expression tag	UNP P15104
G	-12	HIS	-	expression tag	UNP P15104
G	-11	SER	-	expression tag	UNP P15104
G	-10	SER	-	expression tag	UNP P15104
G	-9	GLY	-	expression tag	UNP P15104
G	-8	VAL	-	expression tag	UNP P15104
G	-7	ASP	-	expression tag	UNP P15104
G	-6	LEU	-	expression tag	UNP P15104
G	-5	GLY	-	expression tag	UNP P15104
G	-4	THR	-	expression tag	UNP P15104
G	-3	GLU	-	expression tag	UNP P15104
G	-2	ASN	-	expression tag	UNP P15104
G	-1	LEU	-	expression tag	UNP P15104
G	0	TYR	-	expression tag	UNP P15104
G	1	PHE	-	expression tag	UNP P15104
G	2	GLN	-	expression tag	UNP P15104
G	3	SER	-	expression tag	UNP P15104
G	4	MET	-	expression tag	UNP P15104
H	-18	MET	-	expression tag	UNP P15104
H	-17	HIS	-	expression tag	UNP P15104
H	-16	HIS	-	expression tag	UNP P15104
H	-15	HIS	-	expression tag	UNP P15104
H	-14	HIS	-	expression tag	UNP P15104
H	-13	HIS	-	expression tag	UNP P15104
H	-12	HIS	-	expression tag	UNP P15104
H	-11	SER	-	expression tag	UNP P15104
H	-10	SER	-	expression tag	UNP P15104
H	-9	GLY	-	expression tag	UNP P15104
H	-8	VAL	-	expression tag	UNP P15104
H	-7	ASP	-	expression tag	UNP P15104
H	-6	LEU	-	expression tag	UNP P15104
H	-5	GLY	-	expression tag	UNP P15104
H	-4	THR	-	expression tag	UNP P15104
H	-3	GLU	-	expression tag	UNP P15104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	ASN	-	expression tag	UNP P15104
H	-1	LEU	-	expression tag	UNP P15104
H	0	TYR	-	expression tag	UNP P15104
H	1	PHE	-	expression tag	UNP P15104
H	2	GLN	-	expression tag	UNP P15104
H	3	SER	-	expression tag	UNP P15104
H	4	MET	-	expression tag	UNP P15104
I	-18	MET	-	expression tag	UNP P15104
I	-17	HIS	-	expression tag	UNP P15104
I	-16	HIS	-	expression tag	UNP P15104
I	-15	HIS	-	expression tag	UNP P15104
I	-14	HIS	-	expression tag	UNP P15104
I	-13	HIS	-	expression tag	UNP P15104
I	-12	HIS	-	expression tag	UNP P15104
I	-11	SER	-	expression tag	UNP P15104
I	-10	SER	-	expression tag	UNP P15104
I	-9	GLY	-	expression tag	UNP P15104
I	-8	VAL	-	expression tag	UNP P15104
I	-7	ASP	-	expression tag	UNP P15104
I	-6	LEU	-	expression tag	UNP P15104
I	-5	GLY	-	expression tag	UNP P15104
I	-4	THR	-	expression tag	UNP P15104
I	-3	GLU	-	expression tag	UNP P15104
I	-2	ASN	-	expression tag	UNP P15104
I	-1	LEU	-	expression tag	UNP P15104
I	0	TYR	-	expression tag	UNP P15104
I	1	PHE	-	expression tag	UNP P15104
I	2	GLN	-	expression tag	UNP P15104
I	3	SER	-	expression tag	UNP P15104
I	4	MET	-	expression tag	UNP P15104
J	-18	MET	-	expression tag	UNP P15104
J	-17	HIS	-	expression tag	UNP P15104
J	-16	HIS	-	expression tag	UNP P15104
J	-15	HIS	-	expression tag	UNP P15104
J	-14	HIS	-	expression tag	UNP P15104
J	-13	HIS	-	expression tag	UNP P15104
J	-12	HIS	-	expression tag	UNP P15104
J	-11	SER	-	expression tag	UNP P15104
J	-10	SER	-	expression tag	UNP P15104
J	-9	GLY	-	expression tag	UNP P15104
J	-8	VAL	-	expression tag	UNP P15104
J	-7	ASP	-	expression tag	UNP P15104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-6	LEU	-	expression tag	UNP P15104
J	-5	GLY	-	expression tag	UNP P15104
J	-4	THR	-	expression tag	UNP P15104
J	-3	GLU	-	expression tag	UNP P15104
J	-2	ASN	-	expression tag	UNP P15104
J	-1	LEU	-	expression tag	UNP P15104
J	0	TYR	-	expression tag	UNP P15104
J	1	PHE	-	expression tag	UNP P15104
J	2	GLN	-	expression tag	UNP P15104
J	3	SER	-	expression tag	UNP P15104
J	4	MET	-	expression tag	UNP P15104

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Mn 3	0	0
2	B	3	Total 3	Mn 3	0	0
2	C	3	Total 3	Mn 3	0	0
2	D	3	Total 3	Mn 3	0	0
2	E	3	Total 3	Mn 3	0	0
2	F	3	Total 3	Mn 3	0	0
2	G	3	Total 3	Mn 3	0	0
2	H	3	Total 3	Mn 3	0	0
2	I	3	Total 3	Mn 3	0	0
2	J	3	Total 3	Mn 3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

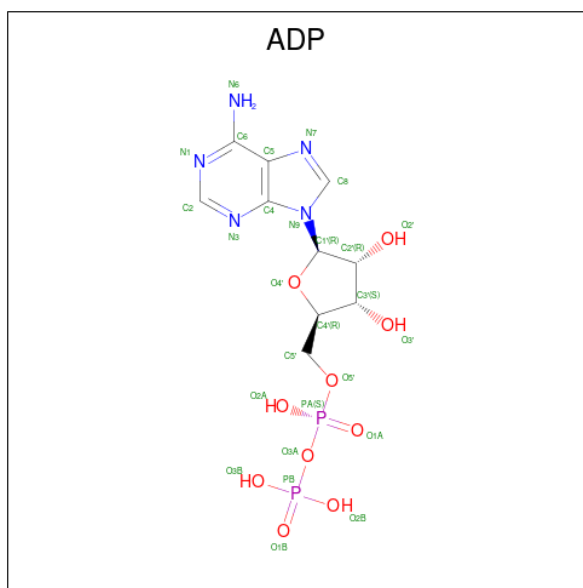
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	G	2	Total Cl 2 2	0	0
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



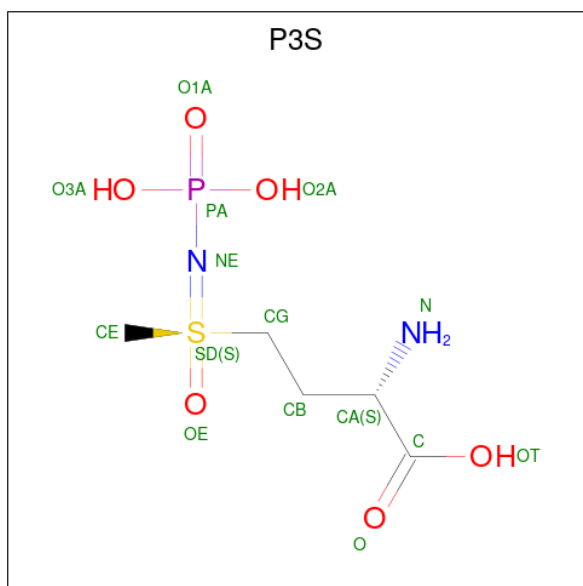
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 27 10 5 10 2	0	0
4	B	1	Total C N O P 27 10 5 10 2	0	0
4	C	1	Total C N O P 27 10 5 10 2	0	0
4	D	1	Total C N O P 27 10 5 10 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: C₅H₁₃N₂O₆PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	B	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	C	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	E	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	F	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	G	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	H	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	I	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
5	J	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		


- Molecule 6 is water.

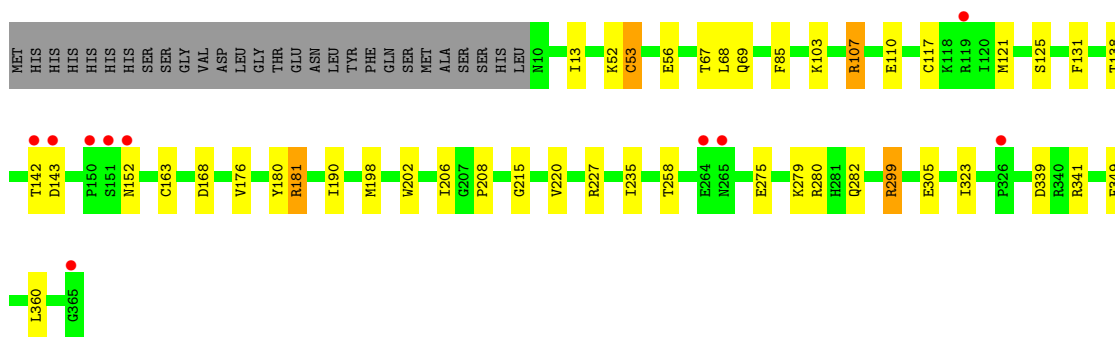
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	39	Total	O	0	0
			39	39		
6	C	39	Total	O	0	0
			39	39		
6	D	45	Total	O	0	0
			45	45		
6	E	32	Total	O	0	0
			32	32		
6	F	12	Total	O	0	0
			12	12		
6	G	5	Total	O	0	0
			5	5		
6	H	8	Total	O	0	0
			8	8		
6	I	10	Total	O	0	0
			10	10		
6	J	9	Total	O	0	0
			9	9		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

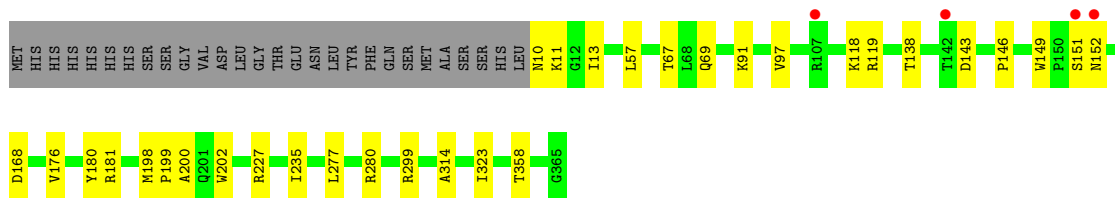
- Molecule 1: Glutamine synthetase

Chain A: 




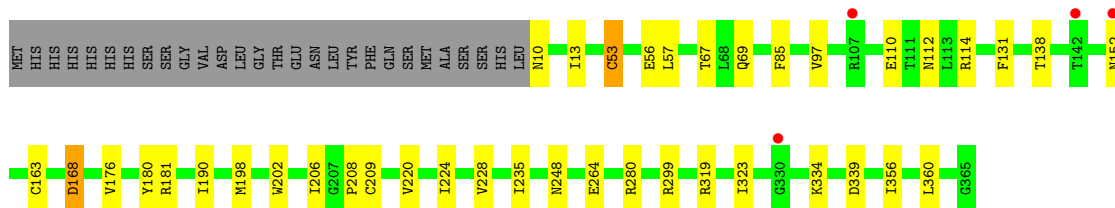
- Molecule 1: Glutamine synthetase

Chain B: 

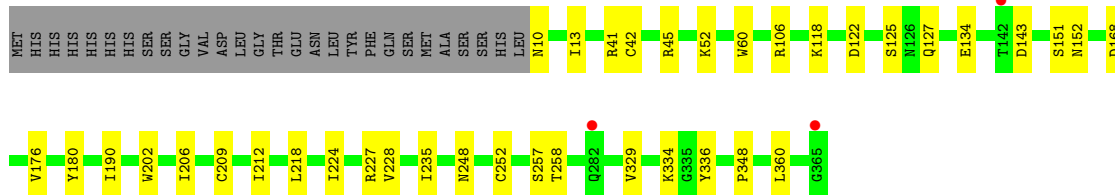
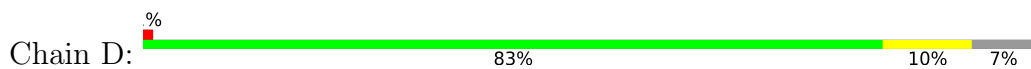


- Molecule 1: Glutamine synthetase

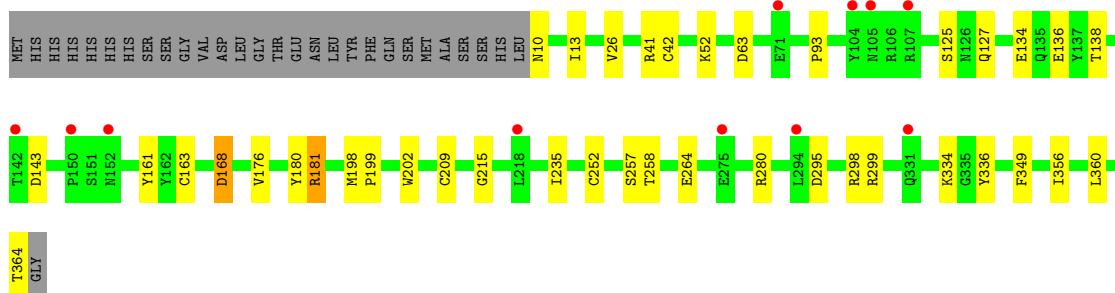
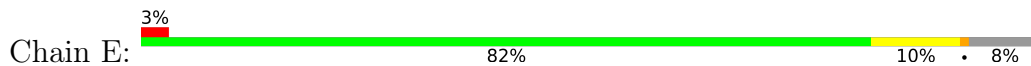
Chain C: 



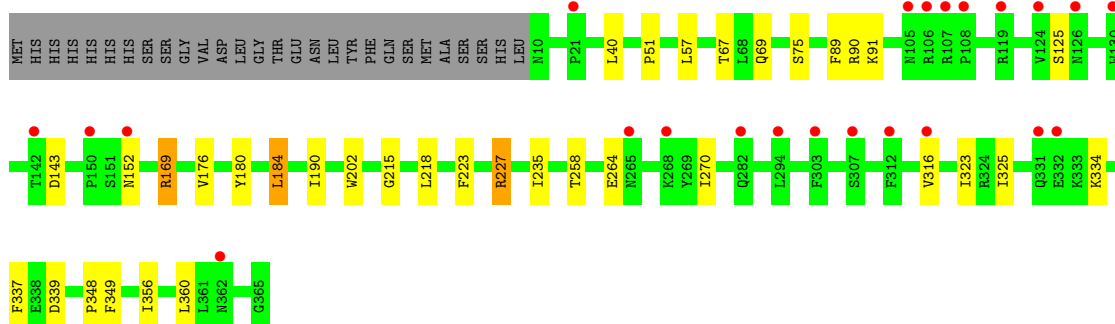
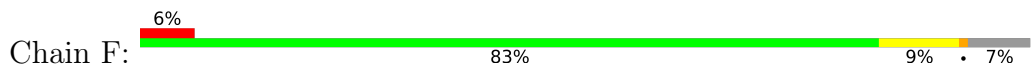
- Molecule 1: Glutamine synthetase



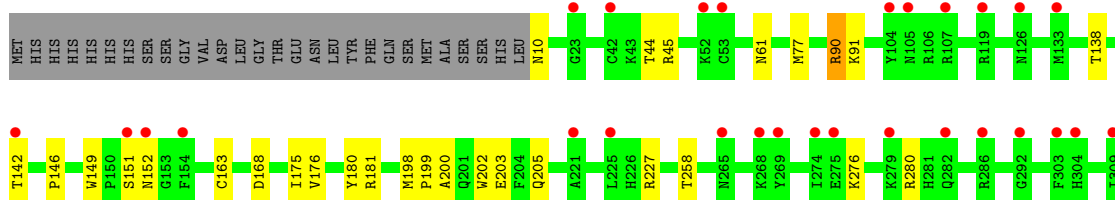
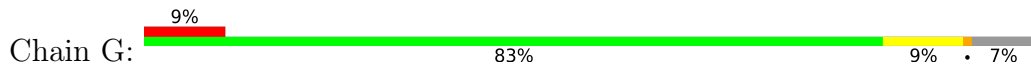
- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase

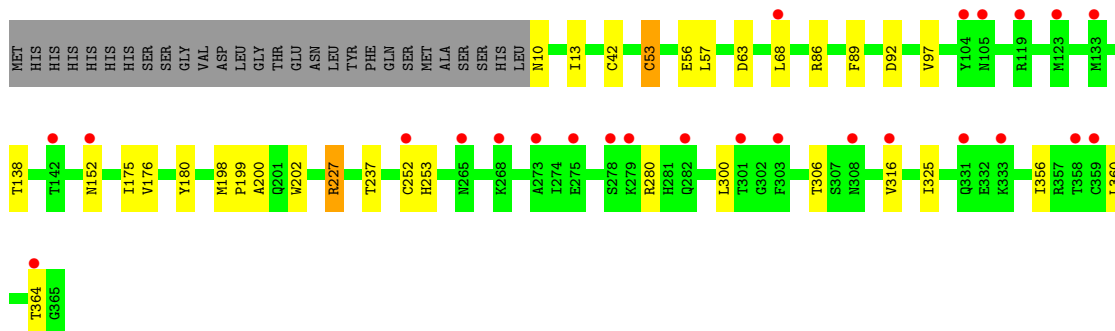
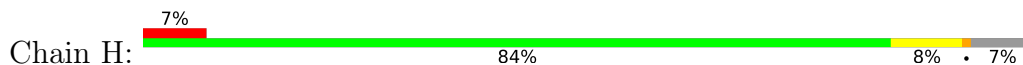


- Molecule 1: Glutamine synthetase

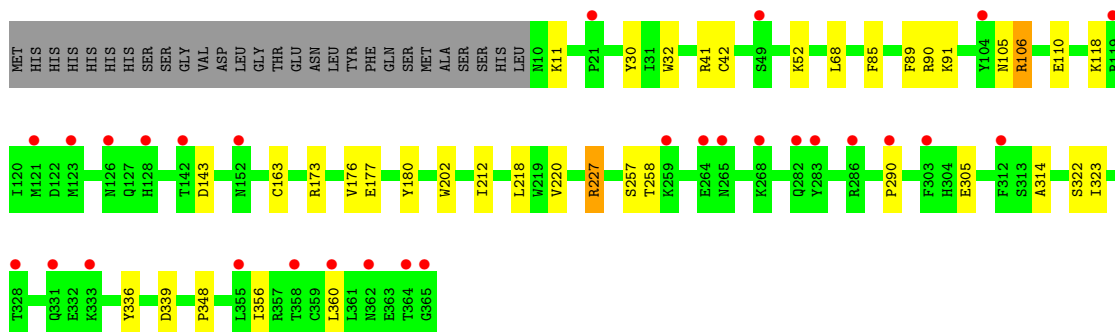
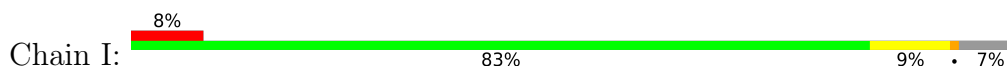




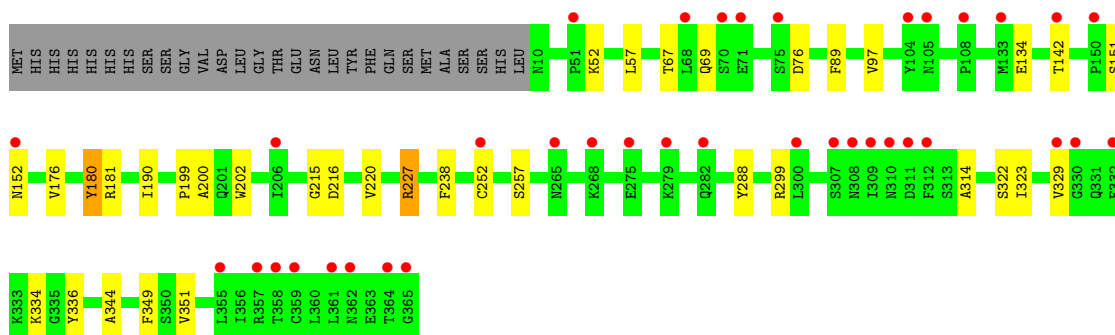
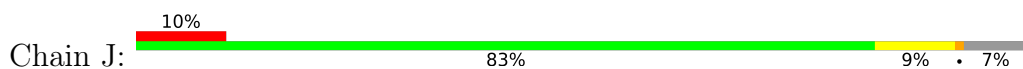
- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.21Å 126.08Å 188.17Å 90.00° 92.14° 90.00°	Depositor
Resolution (Å)	39.94 – 2.60 39.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.94-2.60) 100.0 (39.93-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.3.0032	Depositor
R, R_{free}	0.166 , 0.217 0.173 , 0.221	Depositor DCC
R_{free} test set	6497 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtrriage
Anisotropy	0.458	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28837	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: MN, ADP, CL, P3S

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	0.84	0/2890	0.79	2/3909 (0.1%)
1	B	0.86	0/2890	0.80	2/3909 (0.1%)
1	C	0.88	3/2890 (0.1%)	0.82	5/3909 (0.1%)
1	D	0.85	1/2890 (0.0%)	0.80	2/3909 (0.1%)
1	E	0.83	1/2886 (0.0%)	0.80	7/3904 (0.2%)
1	F	0.70	0/2890	0.69	0/3909
1	G	0.68	1/2890 (0.0%)	0.68	0/3909
1	H	0.70	1/2890 (0.0%)	0.70	0/3909
1	I	0.68	1/2890 (0.0%)	0.70	1/3909 (0.0%)
1	J	0.68	0/2890	0.72	1/3909 (0.0%)
All	All	0.77	8/28896 (0.0%)	0.75	20/39085 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	209	CYS	CB-SG	-6.88	1.70	1.82
1	D	209	CYS	CB-SG	-6.02	1.72	1.82
1	C	209	CYS	CB-SG	-6.01	1.72	1.82
1	G	163	CYS	CB-SG	-5.91	1.72	1.81
1	C	163	CYS	CB-SG	-5.56	1.72	1.81
1	H	252	CYS	CB-SG	-5.23	1.73	1.81
1	C	110	GLU	CG-CD	5.10	1.59	1.51
1	I	110	GLU	CG-CD	5.06	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	C	299	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	J	299	ARG	NE-CZ-NH1	7.77	124.19	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	D	122	ASP	CB-CG-OD1	6.63	124.27	118.30
1	E	41	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	B	299	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	E	295	ASP	CB-CG-OD1	6.30	123.97	118.30
1	D	41	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	E	41	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	299	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	114	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	299	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	107	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	E	168	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	298	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	299	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	319	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	I	106	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	168	ASP	CB-CG-OD1	5.02	122.82	118.30

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	2815	0	2700	26	1
1	B	2815	0	2700	18	0
1	C	2815	0	2699	19	1
1	D	2815	0	2700	18	0
1	E	2811	0	2697	24	0
1	F	2815	0	2700	22	0
1	G	2815	0	2700	22	0
1	H	2815	0	2700	25	0
1	I	2815	0	2700	22	0
1	J	2815	0	2700	17	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
4	G	27	0	12	0	0
4	H	27	0	12	0	0
4	I	27	0	12	0	0
4	J	27	0	12	0	0
5	A	15	0	10	0	0
5	B	15	0	10	0	0
5	C	15	0	10	0	0
5	D	15	0	10	0	0
5	E	15	0	10	0	0
5	F	15	0	10	0	0
5	G	15	0	10	0	0
5	H	15	0	10	1	0
5	I	15	0	10	0	0
5	J	15	0	10	0	0
6	A	32	0	0	0	0
6	B	39	0	0	1	0
6	C	39	0	0	0	0
6	D	45	0	0	0	0
6	E	32	0	0	1	0
6	F	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	5	0	0	0	0
6	H	8	0	0	1	0
6	I	10	0	0	0	0
6	J	9	0	0	0	0
All	All	28837	0	27216	193	1

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 3.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:CYS:SG	1:C:56:GLU:OE2	1.92	1.28
1:B:91:LYS:NZ	6:B:739:HOH:O	1.69	1.20
1:H:92:ASP:OD1	6:H:604:HOH:O	1.81	0.99
1:A:53:CYS:SG	1:A:56:GLU:OE2	2.26	0.94
1:D:258:THR:HG21	1:D:360:LEU:HD21	1.65	0.77
1:B:235:ILE:HD11	1:C:168:ASP:HB3	1.66	0.77
1:A:168:ASP:HB3	1:E:235:ILE:HD11	1.68	0.76
1:F:90:ARG:O	1:F:91:LYS:HB2	1.83	0.75
1:E:356:ILE:HD12	1:E:360:LEU:HD12	1.72	0.72
1:H:176:VAL:HG21	1:H:202:TRP:CE3	2.26	0.70
1:H:57:LEU:HD13	1:H:97:VAL:HG21	1.74	0.70
1:C:235:ILE:HD11	1:D:168:ASP:HB3	1.75	0.68
1:F:184:LEU:HD13	1:F:190:ILE:CG2	2.23	0.68
1:E:138:THR:HG21	1:E:198:MET:CE	2.24	0.67
1:E:258:THR:HG21	1:E:360:LEU:HD21	1.78	0.66
1:E:176:VAL:HG21	1:E:202:TRP:CE3	2.32	0.65
1:G:276:LYS:NZ	1:G:362:ASN:OD1	2.26	0.65
1:A:143:ASP:HA	1:F:152:ASN:HD21	1.64	0.62
1:E:138:THR:HG21	1:E:198:MET:HE1	1.80	0.62
1:I:356:ILE:HD12	1:I:360:LEU:HD12	1.82	0.61
1:J:176:VAL:HG21	1:J:202:TRP:CE3	2.35	0.61
1:G:175:ILE:H	1:G:175:ILE:HD12	1.66	0.61
1:C:176:VAL:HG21	1:C:202:TRP:CE3	2.36	0.60
1:B:10:ASN:HB3	1:B:13:ILE:HD12	1.82	0.60
1:B:176:VAL:HG21	1:B:202:TRP:CE3	2.37	0.60
1:I:176:VAL:HG21	1:I:202:TRP:CE3	2.37	0.59
1:F:176:VAL:HG21	1:F:202:TRP:CD2	2.38	0.59
1:I:323:ILE:HD12	1:I:339:ASP:HA	1.84	0.59
1:G:176:VAL:HG21	1:G:202:TRP:CE3	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:257:SER:HB3	1:J:336:TYR:HB3	1.84	0.58
1:A:235:ILE:HD11	1:B:168:ASP:HB3	1.85	0.58
1:D:176:VAL:HG21	1:D:202:TRP:CD2	2.40	0.57
1:A:138:THR:HG21	1:A:198:MET:HE1	1.88	0.56
1:F:258:THR:HG21	1:F:360:LEU:HD21	1.86	0.56
1:C:85:PHE:CE2	1:C:220:VAL:HG21	2.40	0.56
1:F:51:PRO:HG3	1:F:57:LEU:HD21	1.88	0.56
1:B:138:THR:HG21	1:B:198:MET:HE1	1.86	0.56
1:G:175:ILE:HD12	1:G:175:ILE:N	2.21	0.56
1:F:176:VAL:HG21	1:F:202:TRP:CE3	2.40	0.56
1:H:57:LEU:HD13	1:H:97:VAL:CG2	2.36	0.56
1:H:176:VAL:HG21	1:H:202:TRP:CD2	2.40	0.56
1:B:143:ASP:HA	1:J:152:ASN:HD21	1.71	0.55
1:G:329:VAL:HG21	1:G:336:TYR:O	2.07	0.55
1:H:138:THR:HG21	1:H:198:MET:CE	2.36	0.55
1:J:238:PHE:O	1:J:344:ALA:HB3	2.07	0.54
1:I:176:VAL:HG21	1:I:202:TRP:CD2	2.43	0.54
1:B:176:VAL:HG21	1:B:202:TRP:CD2	2.43	0.54
1:B:277:LEU:HD23	1:B:358:THR:HG21	1.89	0.54
1:J:288:TYR:CD1	1:J:351:VAL:HG22	2.43	0.54
1:C:138:THR:HG21	1:C:198:MET:HE1	1.88	0.54
1:G:138:THR:HG21	1:G:198:MET:HE1	1.89	0.53
1:D:127:GLN:OE1	1:D:360:LEU:HD22	2.09	0.53
1:C:176:VAL:HG21	1:C:202:TRP:CD2	2.43	0.53
1:E:280:ARG:HD2	1:E:364:THR:HA	1.91	0.53
1:H:138:THR:HG21	1:H:198:MET:HE1	1.91	0.52
1:H:280:ARG:HD2	1:H:364:THR:HA	1.92	0.52
1:J:57:LEU:HD13	1:J:97:VAL:HG21	1.91	0.52
1:I:258:THR:HG21	1:I:360:LEU:HD21	1.91	0.51
1:A:138:THR:HG21	1:A:198:MET:CE	2.40	0.51
1:C:152:ASN:HD21	1:I:143:ASP:HA	1.75	0.51
1:A:13:ILE:HG12	1:B:11:LYS:HG3	1.92	0.51
1:J:199:PRO:O	1:J:200:ALA:HB3	2.10	0.51
1:A:176:VAL:HG21	1:A:202:TRP:CE3	2.47	0.50
1:A:258:THR:HG21	1:A:360:LEU:HD21	1.93	0.50
1:H:356:ILE:HD12	1:H:360:LEU:HD12	1.92	0.50
1:D:176:VAL:HG21	1:D:202:TRP:CE3	2.47	0.50
1:J:216:ASP:O	1:J:220:VAL:HG23	2.11	0.50
1:A:142:THR:HA	1:A:235:ILE:HD12	1.93	0.50
1:D:190:ILE:HA	1:D:206:ILE:HD13	1.93	0.50
1:B:138:THR:HG21	1:B:198:MET:CE	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:CE2	1:A:220:VAL:HG21	2.47	0.49
1:G:356:ILE:HG23	1:G:360:LEU:HD12	1.92	0.49
1:C:356:ILE:HD12	1:C:360:LEU:HD12	1.94	0.49
1:B:138:THR:CG2	1:B:198:MET:CE	2.91	0.49
1:F:235:ILE:HD11	1:G:168:ASP:HB3	1.95	0.49
1:F:67:THR:OG1	1:F:69:GLN:NE2	2.32	0.48
1:J:67:THR:OG1	1:J:69:GLN:NE2	2.45	0.48
1:H:86:ARG:NH2	1:H:92:ASP:OD2	2.36	0.48
1:I:89:PHE:CZ	1:I:227:ARG:HB3	2.48	0.48
1:A:176:VAL:HG21	1:A:202:TRP:CD2	2.48	0.48
1:A:275:GLU:OE2	1:A:279:LYS:HE3	2.14	0.48
1:J:151:SER:O	1:J:152:ASN:HB2	2.14	0.48
1:A:103:LYS:NZ	1:A:110:GLU:OE2	2.40	0.48
1:F:270:ILE:HG23	1:F:337:PHE:CD2	2.49	0.48
1:G:151:SER:O	1:G:152:ASN:HB2	2.14	0.47
1:I:85:PHE:CE2	1:I:220:VAL:HG21	2.49	0.47
1:I:90:ARG:O	1:I:91:LYS:HB2	2.13	0.47
1:I:257:SER:HB3	1:I:336:TYR:HB3	1.96	0.47
1:F:184:LEU:HD13	1:F:190:ILE:HG22	1.97	0.47
1:C:67:THR:OG1	1:C:69:GLN:NE2	2.43	0.47
1:C:138:THR:HG21	1:C:198:MET:CE	2.45	0.47
1:G:90:ARG:O	1:G:91:LYS:HB2	2.13	0.47
1:A:67:THR:OG1	1:A:69:GLN:NE2	2.41	0.46
1:C:131:PHE:O	1:C:208:PRO:HA	2.15	0.46
1:E:26:VAL:HG22	1:E:93:PRO:HG2	1.97	0.46
1:G:258:THR:HG21	1:G:360:LEU:HD21	1.98	0.46
1:E:176:VAL:HG21	1:E:202:TRP:CD2	2.50	0.46
1:G:175:ILE:H	1:G:175:ILE:CD1	2.29	0.46
1:E:134:GLU:O	1:E:252:CYS:HA	2.15	0.46
1:J:215:GLY:HA3	1:J:349:PHE:CE1	2.50	0.46
1:C:224:ILE:O	1:C:228:VAL:HG23	2.15	0.46
1:G:314:ALA:HA	1:G:323:ILE:O	2.16	0.45
1:H:253:HIS:HE1	5:H:601:P3S:NE	2.15	0.45
1:J:329:VAL:HG13	1:J:334:LYS:O	2.16	0.45
1:E:264:GLU:OE2	1:E:334:LYS:NZ	2.40	0.45
1:G:176:VAL:HG21	1:G:202:TRP:CD2	2.51	0.45
1:J:322:SER:O	1:J:323:ILE:HD13	2.16	0.45
1:A:215:GLY:HA3	1:A:349:PHE:CE1	2.52	0.45
1:G:44:THR:HG22	1:G:45:ARG:N	2.31	0.45
1:I:173:ARG:HG2	1:I:177:GLU:HG2	1.98	0.45
1:J:180:TYR:HA	1:J:190:ILE:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:O	1:A:208:PRO:HA	2.16	0.45
1:D:10:ASN:HB3	1:D:13:ILE:HD12	1.99	0.45
1:D:235:ILE:HD11	1:E:168:ASP:HB3	1.99	0.45
1:H:89:PHE:CZ	1:H:227:ARG:HB3	2.52	0.45
1:H:237:THR:O	1:H:237:THR:HG23	2.18	0.44
1:A:163:CYS:HB3	1:E:42:CYS:O	2.18	0.44
1:I:30:TYR:O	1:I:42:CYS:HA	2.17	0.44
1:H:63:ASP:OD2	1:I:305:GLU:OE1	2.35	0.44
1:C:323:ILE:HD12	1:C:339:ASP:HA	1.98	0.44
1:I:322:SER:O	1:I:323:ILE:HD13	2.17	0.44
1:D:257:SER:HB3	1:D:336:TYR:HB3	2.00	0.44
1:F:264:GLU:OE2	1:F:334:LYS:NZ	2.39	0.43
1:I:218:LEU:HD23	1:I:348:PRO:HG3	1.99	0.43
1:A:190:ILE:HA	1:A:206:ILE:HD13	2.00	0.43
1:D:143:ASP:HA	1:H:152:ASN:HD21	1.80	0.43
1:E:215:GLY:HA3	1:E:349:PHE:CE1	2.53	0.43
1:C:264:GLU:OE2	1:C:334:LYS:NZ	2.37	0.43
1:D:151:SER:O	1:D:152:ASN:HB2	2.19	0.43
1:F:356:ILE:HD12	1:F:360:LEU:HD12	2.00	0.43
1:F:323:ILE:HD12	1:F:339:ASP:HA	2.00	0.43
1:G:199:PRO:O	1:G:200:ALA:HB3	2.18	0.43
1:D:329:VAL:HG13	1:D:334:LYS:O	2.17	0.43
1:F:40:LEU:HD13	1:F:223:PHE:HB2	2.01	0.43
1:B:181:ARG:HA	1:B:181:ARG:HD3	1.88	0.43
1:C:10:ASN:HB3	1:C:13:ILE:HD12	2.01	0.42
1:J:314:ALA:HA	1:J:323:ILE:O	2.19	0.42
1:A:299:ARG:NH2	1:A:341:ARG:O	2.52	0.42
1:H:42:CYS:O	1:I:163:CYS:HB3	2.19	0.42
1:F:169:ARG:HE	1:F:169:ARG:HB3	1.57	0.42
1:E:161:TYR:CD1	1:E:199:PRO:HB3	2.54	0.42
1:C:112:ASN:C	1:C:112:ASN:OD1	2.58	0.42
1:H:175:ILE:H	1:H:175:ILE:HD12	1.84	0.42
1:A:152:ASN:HD21	1:F:143:ASP:HA	1.84	0.42
1:E:257:SER:HB3	1:E:336:TYR:HB3	2.02	0.42
1:G:146:PRO:HB2	1:G:149:TRP:CD1	2.54	0.42
1:H:13:ILE:HG12	1:I:11:LYS:HG3	2.02	0.42
1:A:305:GLU:OE1	1:E:63:ASP:OD2	2.38	0.42
1:E:136:GLU:HG3	6:E:630:HOH:O	2.19	0.42
1:F:215:GLY:HA3	1:F:349:PHE:CE1	2.55	0.42
1:H:53:CYS:SG	1:H:56:GLU:HG3	2.60	0.42
1:H:199:PRO:O	1:H:200:ALA:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:134:GLU:O	1:J:252:CYS:HA	2.20	0.42
1:B:314:ALA:HA	1:B:323:ILE:O	2.19	0.42
1:C:190:ILE:HA	1:C:206:ILE:HD13	2.00	0.42
1:A:323:ILE:HD12	1:A:339:ASP:HA	2.02	0.42
1:B:67:THR:OG1	1:B:69:GLN:NE2	2.37	0.42
1:I:105:ASN:C	1:I:105:ASN:OD1	2.57	0.42
1:A:117:CYS:O	1:A:121:MET:HG2	2.20	0.41
1:B:146:PRO:HB2	1:B:149:TRP:CD1	2.54	0.41
1:F:316:VAL:HA	1:F:325:ILE:O	2.20	0.41
1:J:89:PHE:CZ	1:J:227:ARG:HB3	2.55	0.41
1:H:316:VAL:HA	1:H:325:ILE:O	2.20	0.41
1:E:181:ARG:HD3	1:E:181:ARG:HA	1.89	0.41
1:E:258:THR:CG2	1:E:360:LEU:HD21	2.49	0.41
1:H:68:LEU:HD23	1:H:68:LEU:HA	1.88	0.41
1:I:118:LYS:HA	1:I:212:ILE:HD13	2.02	0.41
1:D:42:CYS:O	1:E:163:CYS:HB3	2.21	0.41
1:E:127:GLN:OE1	1:E:360:LEU:HD22	2.21	0.41
1:H:300:LEU:HD23	1:H:306:THR:HB	2.03	0.41
1:I:32:TRP:CE2	1:I:41:ARG:HB2	2.56	0.41
1:A:138:THR:CG2	1:A:198:MET:CE	2.99	0.41
1:E:10:ASN:HB3	1:E:13:ILE:HD12	2.03	0.41
1:I:314:ALA:HA	1:I:323:ILE:O	2.21	0.41
1:D:212:ILE:HD12	1:D:212:ILE:HA	1.93	0.41
1:B:199:PRO:O	1:B:200:ALA:HB3	2.20	0.41
1:D:134:GLU:O	1:D:252:CYS:HA	2.20	0.41
1:F:89:PHE:CZ	1:F:227:ARG:HB3	2.56	0.41
1:G:61:ASN:HA	1:G:77:MET:O	2.21	0.41
1:G:138:THR:HG21	1:G:198:MET:CE	2.50	0.41
1:G:203:GLU:HG2	1:G:205:GLN:HE21	1.85	0.41
1:H:13:ILE:CG1	1:I:11:LYS:HG3	2.51	0.41
1:D:45:ARG:HB3	1:D:60:TRP:CH2	2.56	0.41
1:D:218:LEU:HD23	1:D:348:PRO:HB3	2.03	0.41
1:H:138:THR:CG2	1:H:198:MET:CE	2.98	0.41
1:C:57:LEU:HD13	1:C:97:VAL:CG2	2.51	0.40
1:B:57:LEU:HD13	1:B:97:VAL:HG21	2.03	0.40
1:F:218:LEU:HD23	1:F:348:PRO:HG3	2.04	0.40
1:F:270:ILE:HG23	1:F:337:PHE:HD2	1.86	0.40
1:G:280:ARG:HD2	1:G:364:THR:HA	2.02	0.40
1:A:181:ARG:HA	1:A:181:ARG:HD3	1.85	0.40
1:D:224:ILE:O	1:D:228:VAL:HG23	2.21	0.40
1:E:143:ASP:HA	1:G:152:ASN:HD21	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:CYS:SG	1:C:56:GLU:OE2[4_455]	2.05	0.15

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	354/384 (92%)	343 (97%)	11 (3%)	0	100	100
1	B	354/384 (92%)	341 (96%)	13 (4%)	0	100	100
1	C	354/384 (92%)	344 (97%)	10 (3%)	0	100	100
1	D	354/384 (92%)	344 (97%)	10 (3%)	0	100	100
1	E	353/384 (92%)	342 (97%)	11 (3%)	0	100	100
1	F	354/384 (92%)	342 (97%)	12 (3%)	0	100	100
1	G	354/384 (92%)	342 (97%)	11 (3%)	1 (0%)	41	64
1	H	354/384 (92%)	337 (95%)	17 (5%)	0	100	100
1	I	354/384 (92%)	343 (97%)	11 (3%)	0	100	100
1	J	354/384 (92%)	339 (96%)	14 (4%)	1 (0%)	41	64
All	All	3539/3840 (92%)	3417 (97%)	120 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	142	THR
1	J	142	THR

5.3.2 Protein sidechains [i](#)

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	297/323 (92%)	287 (97%)	10 (3%)	37	63
1	B	297/323 (92%)	290 (98%)	7 (2%)	49	74
1	C	297/323 (92%)	292 (98%)	5 (2%)	60	81
1	D	297/323 (92%)	290 (98%)	7 (2%)	49	74
1	E	297/323 (92%)	293 (99%)	4 (1%)	69	86
1	F	297/323 (92%)	291 (98%)	6 (2%)	55	78
1	G	297/323 (92%)	291 (98%)	6 (2%)	55	78
1	H	297/323 (92%)	293 (99%)	4 (1%)	69	86
1	I	297/323 (92%)	291 (98%)	6 (2%)	55	78
1	J	297/323 (92%)	292 (98%)	5 (2%)	60	81
All	All	2970/3230 (92%)	2910 (98%)	60 (2%)	55	78

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	CYS
1	A	68	LEU
1	A	107	ARG
1	A	125	SER
1	A	180	TYR
1	A	181	ARG
1	A	227	ARG
1	A	280	ARG
1	A	282	GLN
1	B	118	LYS
1	B	119	ARG
1	B	151	SER
1	B	152	ASN
1	B	180	TYR
1	B	227	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	ARG
1	C	53	CYS
1	C	180	TYR
1	C	181	ARG
1	C	248	ASN
1	C	280	ARG
1	D	52	LYS
1	D	106	ARG
1	D	118	LYS
1	D	125	SER
1	D	180	TYR
1	D	227	ARG
1	D	248	ASN
1	E	52	LYS
1	E	125	SER
1	E	180	TYR
1	E	181	ARG
1	F	75	SER
1	F	125	SER
1	F	169	ARG
1	F	180	TYR
1	F	184	LEU
1	F	227	ARG
1	G	10	ASN
1	G	90	ARG
1	G	180	TYR
1	G	181	ARG
1	G	227	ARG
1	G	364	THR
1	H	10	ASN
1	H	53	CYS
1	H	180	TYR
1	H	227	ARG
1	I	52	LYS
1	I	68	LEU
1	I	106	ARG
1	I	180	TYR
1	I	227	ARG
1	I	290	PRO
1	J	52	LYS
1	J	76	ASP
1	J	180	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	181	ARG
1	J	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	152	ASN
1	B	69	GLN
1	C	69	GLN
1	C	152	ASN
1	C	248	ASN
1	D	248	ASN
1	F	69	GLN
1	F	152	ASN
1	F	282	GLN
1	G	69	GLN
1	G	152	ASN
1	G	205	GLN
1	G	282	GLN
1	H	61	ASN
1	H	152	ASN
1	H	205	GLN
1	H	265	ASN
1	J	69	GLN
1	J	152	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 60 ligands modelled in this entry, 40 are monoatomic - leaving 20 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
4	ADP	G	501	2	24,29,29	0.89	1 (4%)	29,45,45	1.42	4 (13%)
4	ADP	I	501	2	24,29,29	0.92	1 (4%)	29,45,45	1.31	3 (10%)
4	ADP	B	501	2	24,29,29	1.04	1 (4%)	29,45,45	1.59	5 (17%)
5	P3S	D	601	2	11,14,14	2.91	4 (36%)	12,21,21	0.93	0
5	P3S	F	601	2	11,14,14	3.43	3 (27%)	12,21,21	0.88	0
5	P3S	H	601	2	11,14,14	2.55	3 (27%)	12,21,21	2.14	3 (25%)
4	ADP	H	501	2	24,29,29	0.83	0	29,45,45	1.68	3 (10%)
4	ADP	A	501	2	24,29,29	0.97	2 (8%)	29,45,45	1.43	5 (17%)
5	P3S	B	601	2	11,14,14	2.55	3 (27%)	12,21,21	1.36	2 (16%)
4	ADP	F	501	2	24,29,29	0.93	0	29,45,45	1.57	4 (13%)
5	P3S	A	601	2	11,14,14	2.39	1 (9%)	12,21,21	2.12	3 (25%)
4	ADP	C	501	2	24,29,29	0.98	1 (4%)	29,45,45	1.76	6 (20%)
5	P3S	I	601	2	11,14,14	3.02	3 (27%)	12,21,21	1.70	2 (16%)
5	P3S	E	601	2	11,14,14	2.21	3 (27%)	12,21,21	1.34	2 (16%)
4	ADP	D	501	2	24,29,29	1.00	2 (8%)	29,45,45	1.70	5 (17%)
4	ADP	J	501	2	24,29,29	1.02	1 (4%)	29,45,45	1.47	5 (17%)
5	P3S	G	601	2	11,14,14	3.72	3 (27%)	12,21,21	1.13	1 (8%)
5	P3S	C	601	2	11,14,14	2.06	2 (18%)	12,21,21	2.01	4 (33%)
5	P3S	J	601	2	11,14,14	3.53	2 (18%)	12,21,21	1.66	3 (25%)
4	ADP	E	501	2	24,29,29	1.04	2 (8%)	29,45,45	1.58	6 (20%)

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
4	ADP	G	501	2	-	4/12/32/32	0/3/3/3
4	ADP	I	501	2	-	6/12/32/32	0/3/3/3
4	ADP	B	501	2	-	5/12/32/32	0/3/3/3
5	P3S	D	601	2	-	4/9/16/16	-
5	P3S	F	601	2	-	4/9/16/16	-
5	P3S	H	601	2	-	4/9/16/16	-
4	ADP	H	501	2	-	4/12/32/32	0/3/3/3
4	ADP	A	501	2	-	6/12/32/32	0/3/3/3
5	P3S	B	601	2	-	5/9/16/16	-
4	ADP	F	501	2	-	4/12/32/32	0/3/3/3
5	P3S	A	601	2	-	4/9/16/16	-
4	ADP	C	501	2	-	3/12/32/32	0/3/3/3
5	P3S	I	601	2	-	4/9/16/16	-
5	P3S	E	601	2	-	4/9/16/16	-
4	ADP	D	501	2	-	4/12/32/32	0/3/3/3
4	ADP	J	501	2	-	5/12/32/32	0/3/3/3
5	P3S	G	601	2	-	5/9/16/16	-
5	P3S	C	601	2	-	4/9/16/16	-
5	P3S	J	601	2	-	6/9/16/16	-
4	ADP	E	501	2	-	4/12/32/32	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	601	P3S	PA-O1A	11.39	1.64	1.46
5	J	601	P3S	PA-O1A	11.05	1.63	1.46
5	F	601	P3S	PA-O1A	9.81	1.61	1.46
5	I	601	P3S	PA-O1A	8.64	1.59	1.46
5	D	601	P3S	PA-O1A	7.61	1.58	1.46
5	A	601	P3S	PA-O1A	7.07	1.57	1.46
5	B	601	P3S	PA-O1A	6.88	1.57	1.46
5	H	601	P3S	PA-O1A	6.87	1.57	1.46
5	C	601	P3S	PA-O1A	5.68	1.55	1.46
5	E	601	P3S	PA-O1A	5.49	1.55	1.46
5	F	601	P3S	PA-O3A	3.91	1.62	1.54
5	E	601	P3S	PA-O3A	3.73	1.62	1.54
5	D	601	P3S	PA-O3A	3.70	1.62	1.54
5	I	601	P3S	PA-O2A	-3.64	1.47	1.54
5	B	601	P3S	PA-O3A	3.64	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	601	P3S	PA-O3A	3.48	1.62	1.54
5	D	601	P3S	PA-O2A	-3.26	1.48	1.54
5	C	601	P3S	PA-O2A	-3.08	1.48	1.54
5	G	601	P3S	PA-O2A	-2.99	1.48	1.54
5	F	601	P3S	PA-O2A	-2.80	1.49	1.54
5	J	601	P3S	PA-O2A	-2.66	1.49	1.54
4	E	501	ADP	O4'-C1'	2.53	1.44	1.41
5	G	601	P3S	PA-O3A	2.48	1.60	1.54
4	E	501	ADP	C5-C4	2.35	1.47	1.40
4	D	501	ADP	C5-C4	2.34	1.47	1.40
4	D	501	ADP	O4'-C1'	2.33	1.44	1.41
5	D	601	P3S	CB-CG	-2.29	1.50	1.52
4	A	501	ADP	C5-C4	2.26	1.46	1.40
5	E	601	P3S	O-C	2.26	1.29	1.22
4	B	501	ADP	C5-C4	2.22	1.46	1.40
4	J	501	ADP	C5-C4	2.18	1.46	1.40
5	H	601	P3S	PA-O2A	-2.14	1.50	1.54
4	I	501	ADP	C2-N3	2.14	1.35	1.32
4	C	501	ADP	C5-C4	2.09	1.46	1.40
5	I	601	P3S	OT-C	-2.07	1.23	1.30
4	A	501	ADP	O4'-C1'	2.07	1.44	1.41
5	B	601	P3S	PA-O2A	-2.06	1.50	1.54
4	G	501	ADP	C5-C4	2.04	1.46	1.40

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	P3S	OE-SD-CG	5.61	112.76	108.37
5	H	601	P3S	OE-SD-CG	-5.40	104.14	108.37
4	H	501	ADP	C1'-N9-C4	-5.07	117.74	126.64
4	F	501	ADP	N3-C2-N1	-5.01	120.84	128.68
4	H	501	ADP	N3-C2-N1	-4.99	120.88	128.68
4	D	501	ADP	N3-C2-N1	-4.75	121.25	128.68
5	I	601	P3S	O3A-PA-O1A	-4.42	103.97	113.45
4	B	501	ADP	C1'-N9-C4	-4.18	119.29	126.64
4	E	501	ADP	N3-C2-N1	-4.14	122.21	128.68
4	G	501	ADP	N3-C2-N1	-4.12	122.23	128.68
4	J	501	ADP	N3-C2-N1	-4.05	122.35	128.68
5	C	601	P3S	OE-SD-CG	-4.03	105.21	108.37
4	J	501	ADP	C1'-N9-C4	-4.00	119.61	126.64
4	D	501	ADP	C2-N1-C6	3.97	125.55	118.75
4	C	501	ADP	O2B-PB-O1B	3.97	126.22	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	ADP	N3-C2-N1	-3.86	122.65	128.68
4	C	501	ADP	C1'-N9-C4	-3.73	120.09	126.64
4	A	501	ADP	N3-C2-N1	-3.72	122.87	128.68
4	B	501	ADP	N3-C2-N1	-3.63	123.01	128.68
4	I	501	ADP	N3-C2-N1	-3.62	123.02	128.68
5	H	601	P3S	O3A-PA-O1A	-3.57	105.80	113.45
5	C	601	P3S	O3A-PA-O1A	-3.51	105.92	113.45
5	A	601	P3S	OE-SD-CE	3.45	114.73	109.24
5	C	601	P3S	CE-SD-NE	3.38	119.31	107.48
5	J	601	P3S	O3A-PA-O1A	-3.26	106.47	113.45
4	E	501	ADP	C1'-N9-C4	-3.21	121.00	126.64
4	G	501	ADP	PA-O3A-PB	-3.15	122.02	132.83
4	D	501	ADP	O3B-PB-O1B	3.09	122.79	110.68
4	G	501	ADP	C4-C5-N7	-2.96	106.31	109.40
4	F	501	ADP	C1'-N9-C4	-2.93	121.49	126.64
4	I	501	ADP	C4-C5-N7	-2.93	106.34	109.40
5	E	601	P3S	O2A-PA-O1A	-2.92	107.20	113.45
5	I	601	P3S	OE-SD-CG	2.90	110.64	108.37
4	I	501	ADP	C1'-N9-C4	-2.85	121.64	126.64
4	D	501	ADP	C1'-N9-C4	-2.83	121.67	126.64
4	A	501	ADP	C4-C5-N7	-2.79	106.49	109.40
4	C	501	ADP	O3A-PB-O1B	-2.79	95.73	111.19
4	E	501	ADP	O2B-PB-O1B	2.72	121.34	110.68
4	A	501	ADP	C1'-N9-C4	-2.69	121.91	126.64
4	G	501	ADP	C1'-N9-C4	-2.58	122.11	126.64
4	B	501	ADP	C4-C5-N7	-2.45	106.85	109.40
5	J	601	P3S	OE-SD-CG	-2.42	106.47	108.37
4	E	501	ADP	N6-C6-N1	2.36	123.48	118.57
4	C	501	ADP	C3'-C2'-C1'	-2.36	97.43	100.98
4	F	501	ADP	PA-O3A-PB	-2.35	124.78	132.83
5	J	601	P3S	OE-SD-CE	-2.34	105.52	109.24
5	B	601	P3S	OE-SD-CE	-2.22	105.71	109.24
4	E	501	ADP	C2-N1-C6	2.20	122.53	118.75
4	B	501	ADP	O5'-PA-O1A	-2.20	100.48	109.07
4	F	501	ADP	C4-C5-N7	-2.20	107.11	109.40
4	C	501	ADP	O2A-PA-O1A	2.19	123.09	112.24
5	H	601	P3S	CE-SD-NE	2.19	115.14	107.48
4	A	501	ADP	C2-N1-C6	2.14	122.42	118.75
5	A	601	P3S	O3A-PA-O1A	-2.13	108.88	113.45
5	B	601	P3S	CE-SD-NE	2.11	114.85	107.48
4	A	501	ADP	PA-O3A-PB	-2.10	125.62	132.83
4	B	501	ADP	O2A-PA-O1A	2.09	122.58	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	501	ADP	C3'-C2'-C1'	-2.07	97.87	100.98
5	E	601	P3S	CE-SD-NE	2.06	114.69	107.48
4	H	501	ADP	O3B-PB-O2B	2.06	115.50	107.64
5	C	601	P3S	O2A-PA-O1A	2.05	117.85	113.45
4	J	501	ADP	C2-N1-C6	2.05	122.26	118.75
4	J	501	ADP	N6-C6-N1	2.05	122.82	118.57
4	D	501	ADP	O3A-PB-O1B	-2.04	99.86	111.19
4	E	501	ADP	O3A-PB-O1B	-2.02	100.01	111.19
5	G	601	P3S	OE-SD-CE	-2.02	106.03	109.24

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	ADP	C5'-O5'-PA-O1A
4	B	501	ADP	PA-O3A-PB-O3B
4	C	501	ADP	PA-O3A-PB-O3B
4	D	501	ADP	PA-O3A-PB-O3B
4	D	501	ADP	O4'-C4'-C5'-O5'
4	F	501	ADP	PA-O3A-PB-O3B
4	H	501	ADP	PA-O3A-PB-O3B
4	I	501	ADP	PA-O3A-PB-O3B
5	B	601	P3S	CB-CG-SD-OE
5	B	601	P3S	O-C-CA-N
5	C	601	P3S	O-C-CA-N
5	D	601	P3S	O-C-CA-N
5	E	601	P3S	O-C-CA-N
5	F	601	P3S	O-C-CA-N
5	G	601	P3S	O-C-CA-N
5	H	601	P3S	O-C-CA-N
5	J	601	P3S	CB-CG-SD-OE
5	J	601	P3S	O-C-CA-N
5	C	601	P3S	OT-C-CA-N
4	C	501	ADP	O4'-C4'-C5'-O5'
4	D	501	ADP	C3'-C4'-C5'-O5'
4	E	501	ADP	O4'-C4'-C5'-O5'
4	E	501	ADP	C3'-C4'-C5'-O5'
4	F	501	ADP	O4'-C4'-C5'-O5'
4	G	501	ADP	O4'-C4'-C5'-O5'
4	G	501	ADP	C3'-C4'-C5'-O5'
4	H	501	ADP	O4'-C4'-C5'-O5'
4	I	501	ADP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	501	ADP	C3'-C4'-C5'-O5'
4	J	501	ADP	O4'-C4'-C5'-O5'
4	J	501	ADP	C3'-C4'-C5'-O5'
5	G	601	P3S	OT-C-CA-N
5	B	601	P3S	OT-C-CA-N
5	D	601	P3S	OT-C-CA-N
5	E	601	P3S	OT-C-CA-N
5	F	601	P3S	OT-C-CA-N
4	C	501	ADP	C3'-C4'-C5'-O5'
5	J	601	P3S	OT-C-CA-N
4	F	501	ADP	C3'-C4'-C5'-O5'
4	H	501	ADP	C3'-C4'-C5'-O5'
5	A	601	P3S	OT-C-CA-N
5	H	601	P3S	OT-C-CA-N
5	I	601	P3S	OT-C-CA-N
4	G	501	ADP	PB-O3A-PA-O1A
5	A	601	P3S	O-C-CA-N
5	I	601	P3S	O-C-CA-N
4	A	501	ADP	PA-O3A-PB-O2B
4	J	501	ADP	PA-O3A-PB-O2B
4	A	501	ADP	C5'-O5'-PA-O3A
4	E	501	ADP	PB-O3A-PA-O2A
5	G	601	P3S	CB-CG-SD-OE
5	J	601	P3S	CB-CG-SD-CE
5	B	601	P3S	OT-C-CA-CB
4	B	501	ADP	O4'-C4'-C5'-O5'
5	A	601	P3S	O-C-CA-CB
5	B	601	P3S	O-C-CA-CB
5	H	601	P3S	O-C-CA-CB
5	I	601	P3S	O-C-CA-CB
4	G	501	ADP	PB-O3A-PA-O2A
4	I	501	ADP	PB-O3A-PA-O2A
4	J	501	ADP	PB-O3A-PA-O2A
5	C	601	P3S	O-C-CA-CB
5	D	601	P3S	O-C-CA-CB
5	E	601	P3S	O-C-CA-CB
4	I	501	ADP	PA-O3A-PB-O1B
5	A	601	P3S	OT-C-CA-CB
5	C	601	P3S	OT-C-CA-CB
5	G	601	P3S	O-C-CA-CB
5	D	601	P3S	OT-C-CA-CB
5	E	601	P3S	OT-C-CA-CB

Continued on next page...

Continued from previous page...

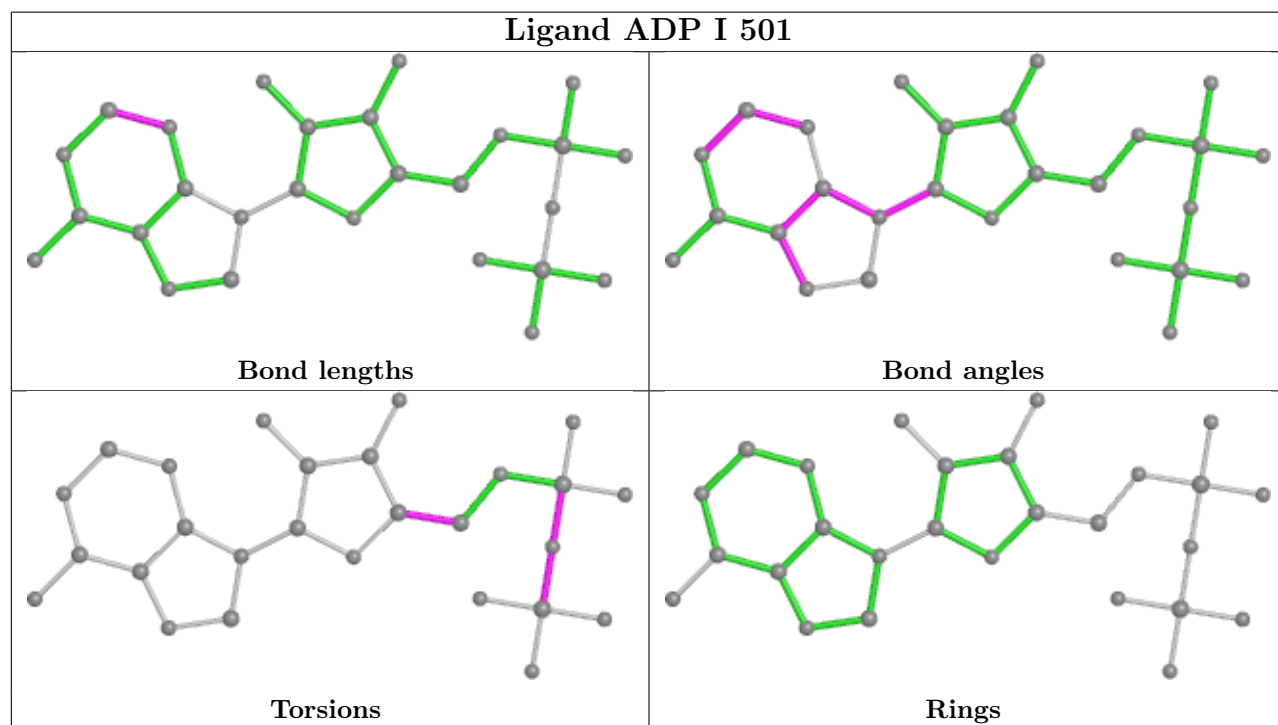
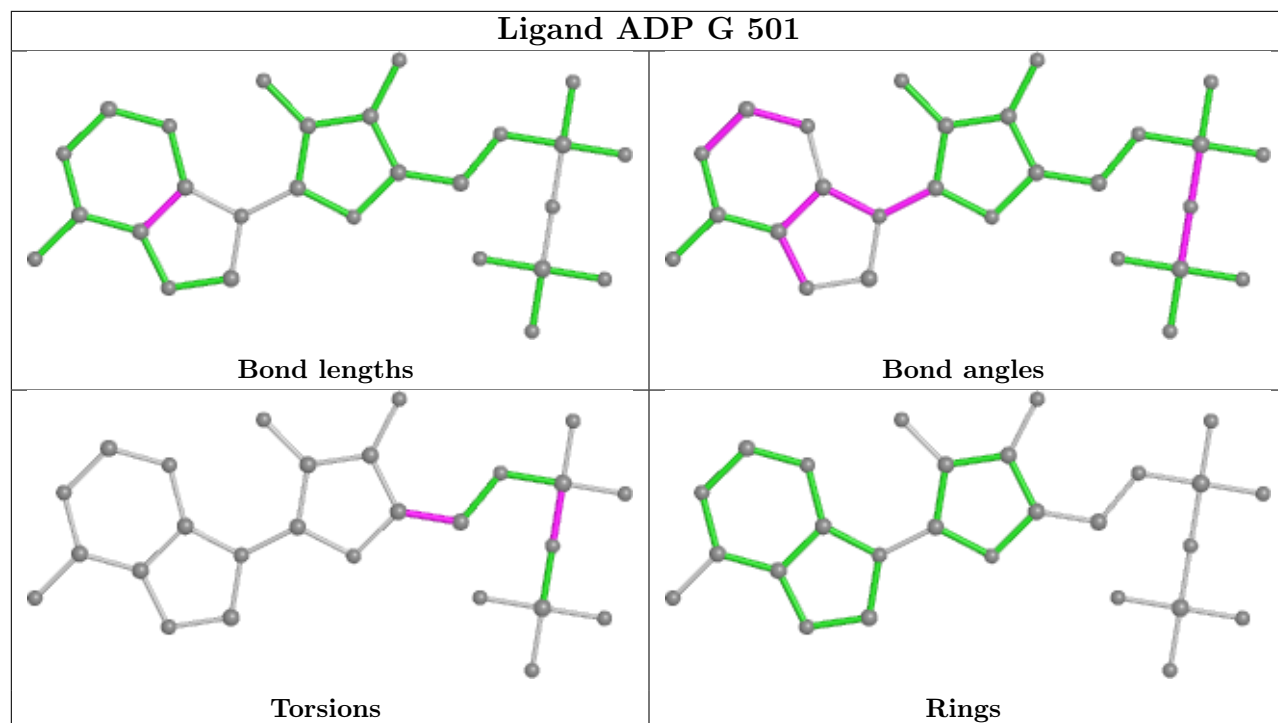
Mol	Chain	Res	Type	Atoms
5	F	601	P3S	O-C-CA-CB
5	H	601	P3S	OT-C-CA-CB
5	I	601	P3S	OT-C-CA-CB
4	E	501	ADP	PB-O3A-PA-O1A
4	I	501	ADP	PB-O3A-PA-O1A
4	B	501	ADP	PA-O3A-PB-O1B
5	J	601	P3S	O-C-CA-CB
4	D	501	ADP	PA-O3A-PB-O2B
4	H	501	ADP	PA-O3A-PB-O2B
5	F	601	P3S	OT-C-CA-CB
5	J	601	P3S	OT-C-CA-CB
4	A	501	ADP	O4'-C4'-C5'-O5'
4	A	501	ADP	PB-O3A-PA-O1A
4	B	501	ADP	PB-O3A-PA-O1A
4	F	501	ADP	PB-O3A-PA-O1A
4	J	501	ADP	PB-O3A-PA-O1A
5	G	601	P3S	OT-C-CA-CB
4	B	501	ADP	C3'-C4'-C5'-O5'
4	A	501	ADP	PA-O3A-PB-O1B

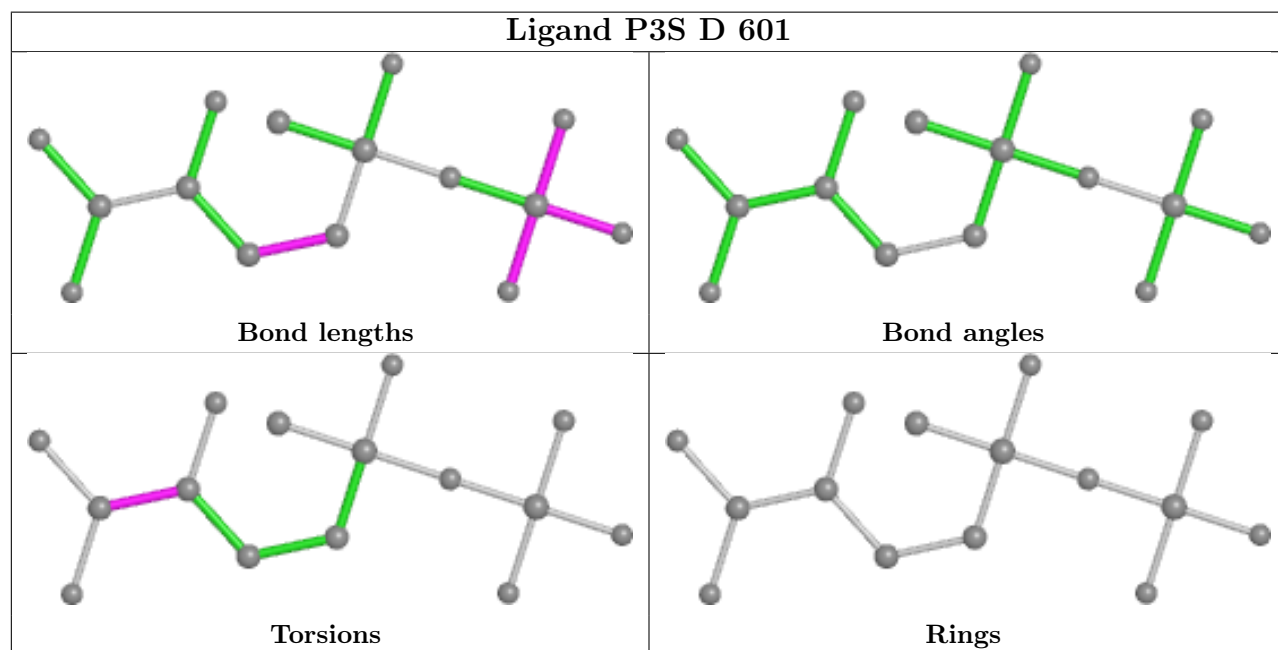
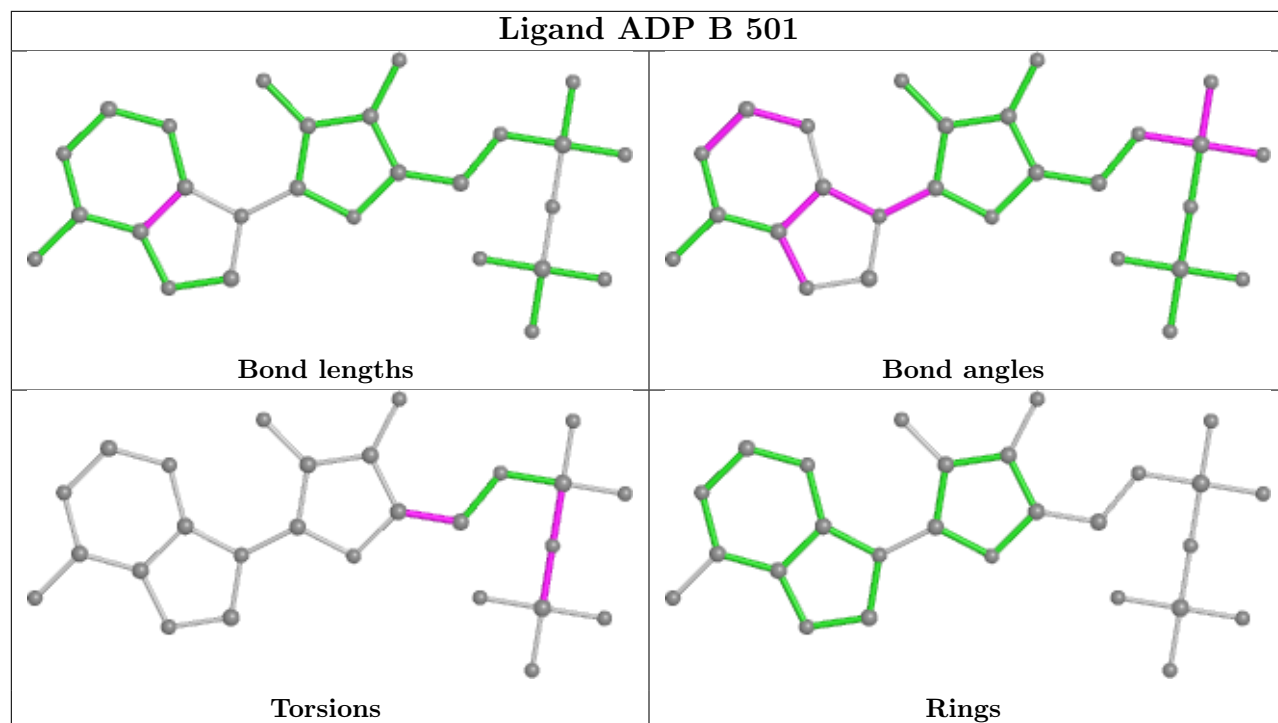
There are no ring outliers.

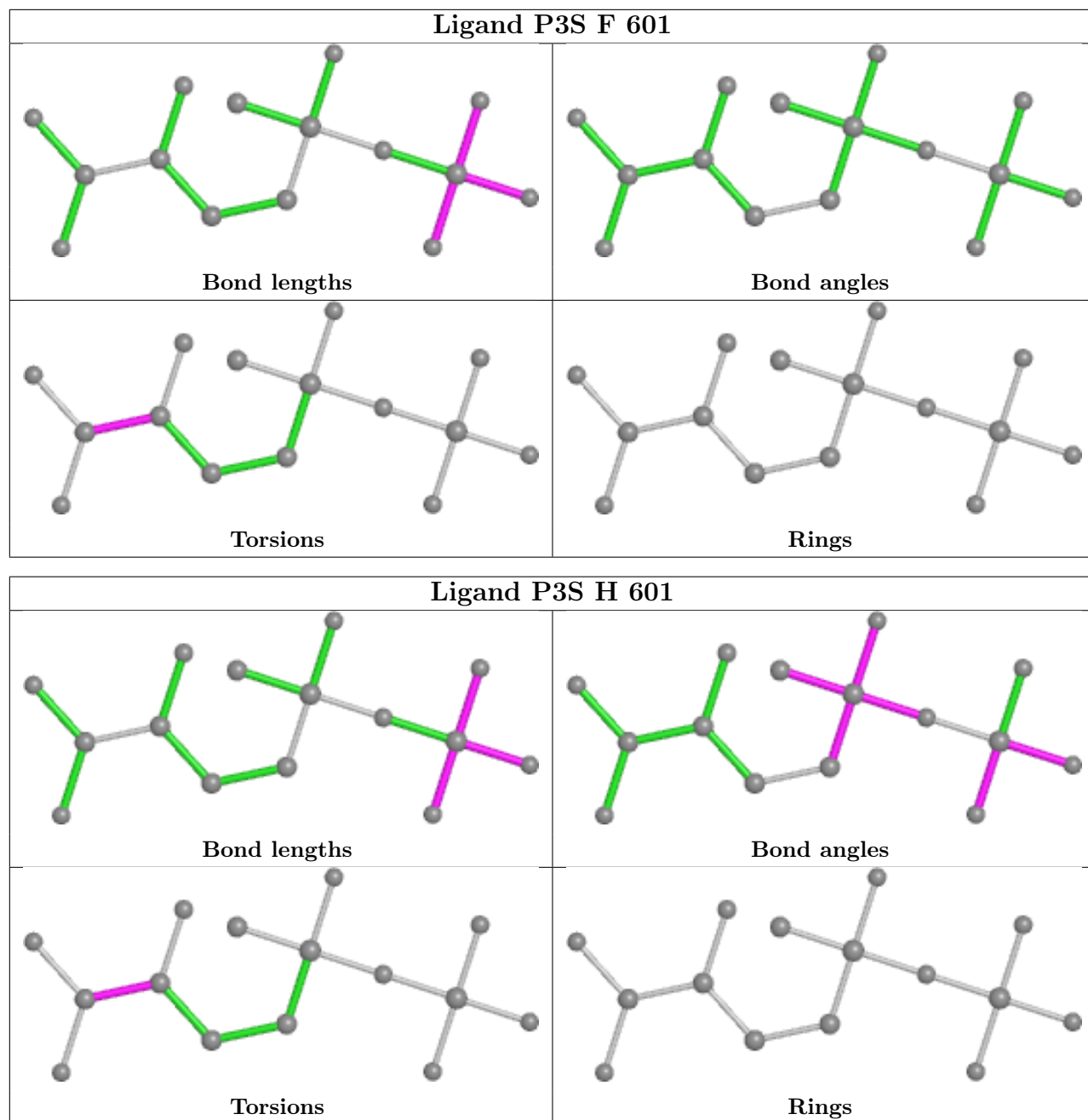
1 monomer is involved in 1 short contact:

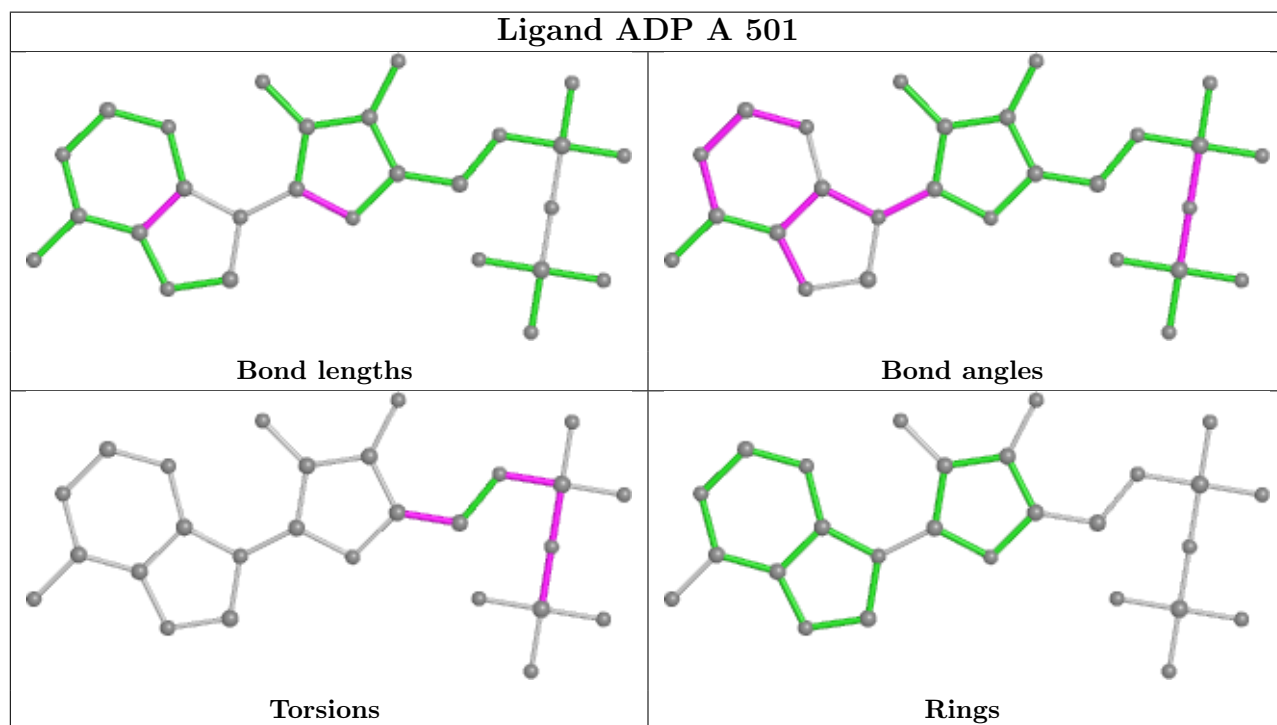
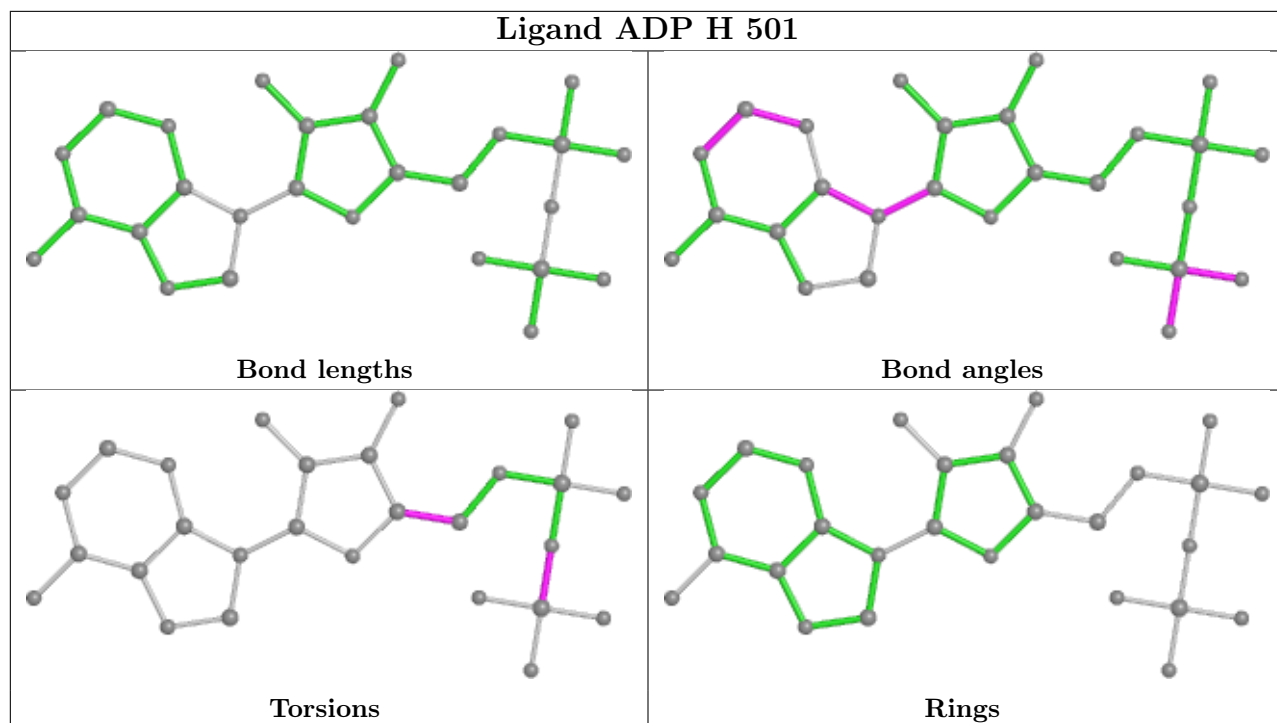
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	601	P3S	1	0

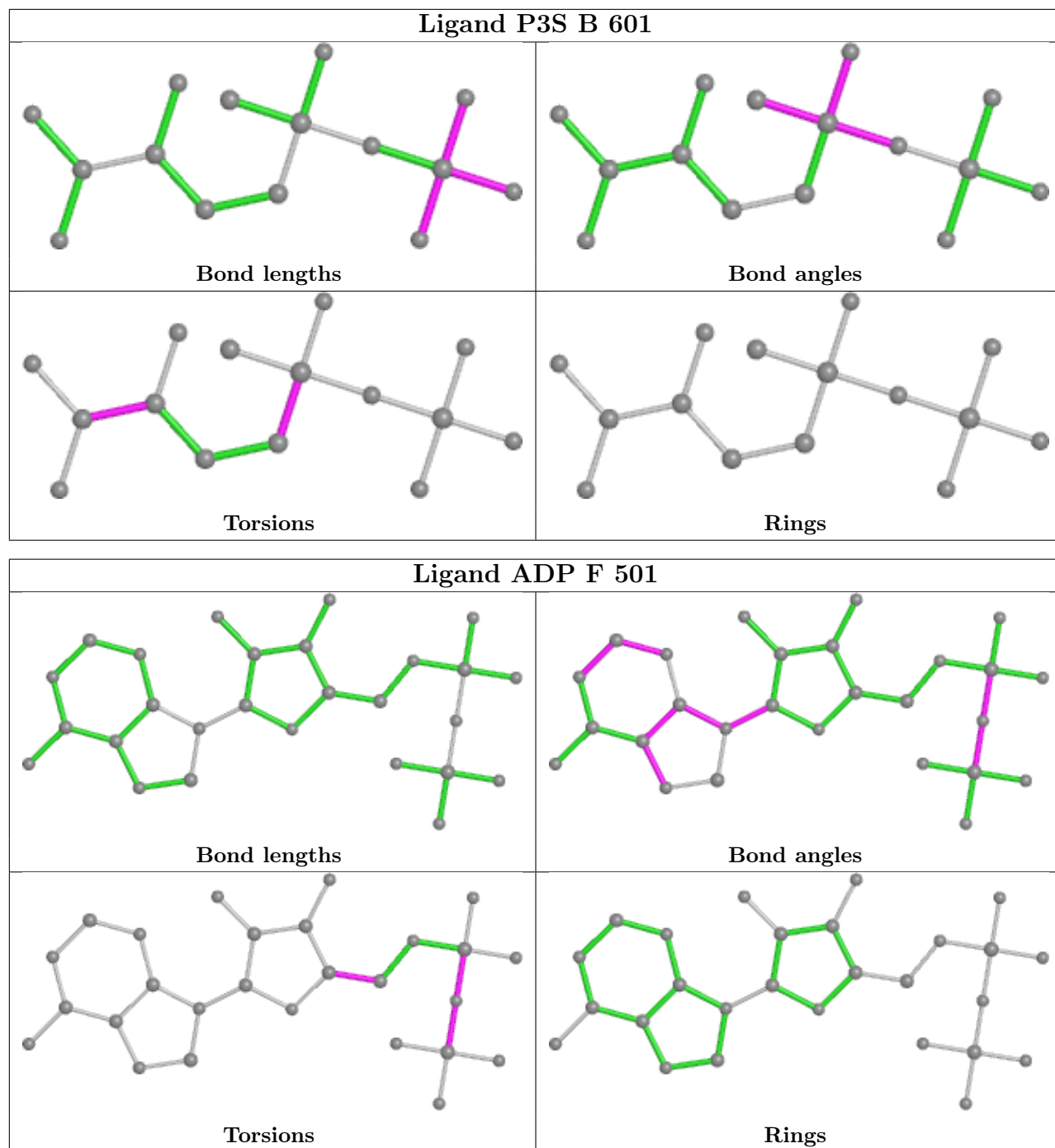
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

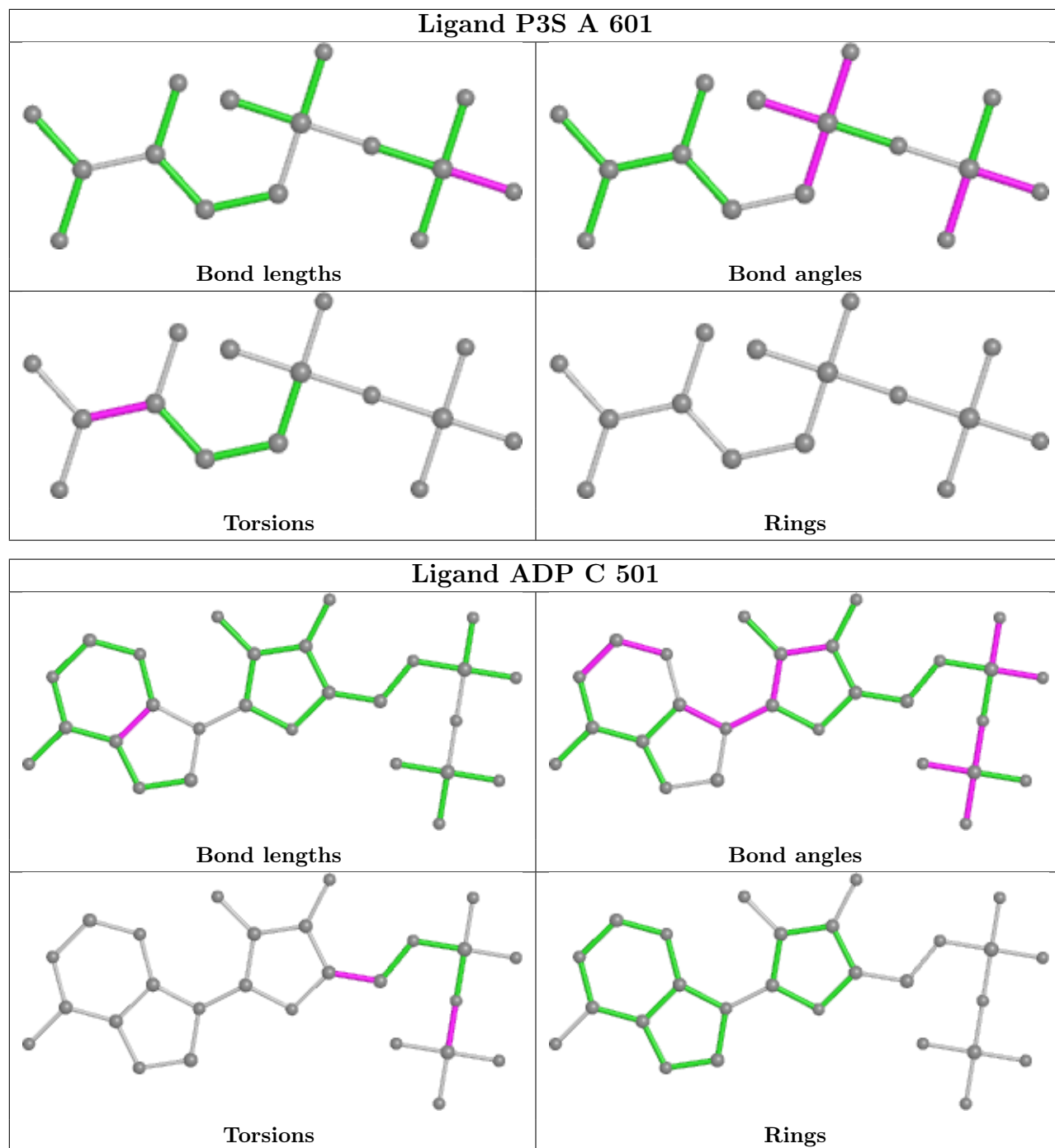


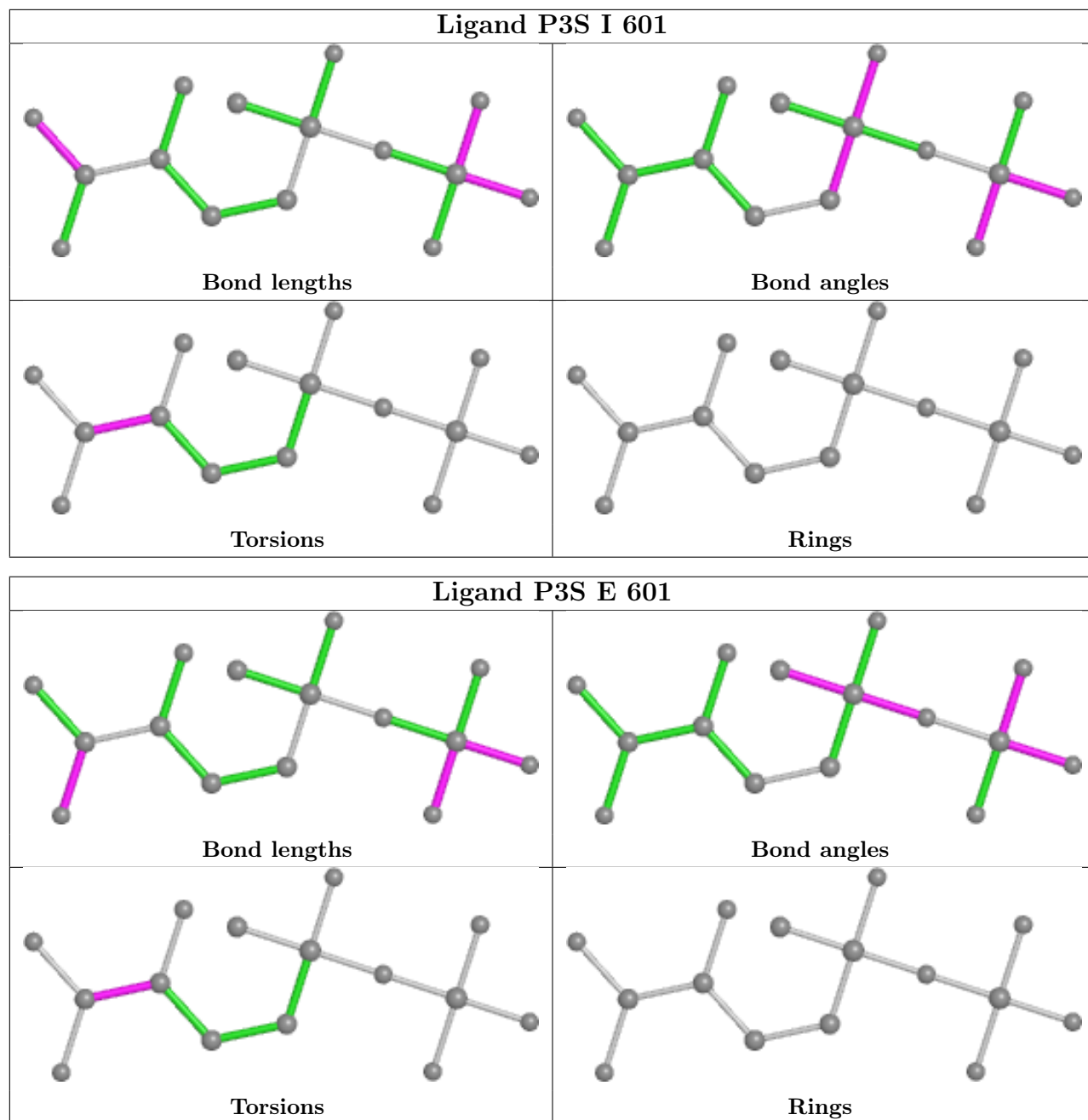


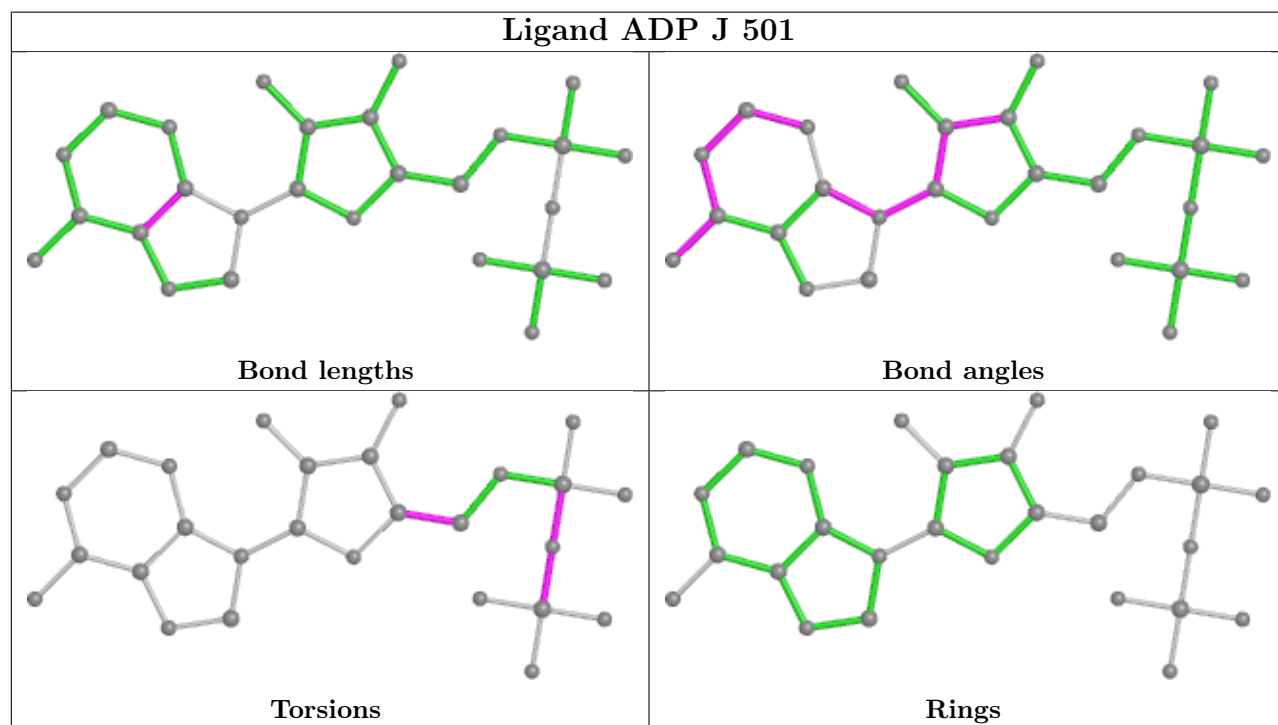
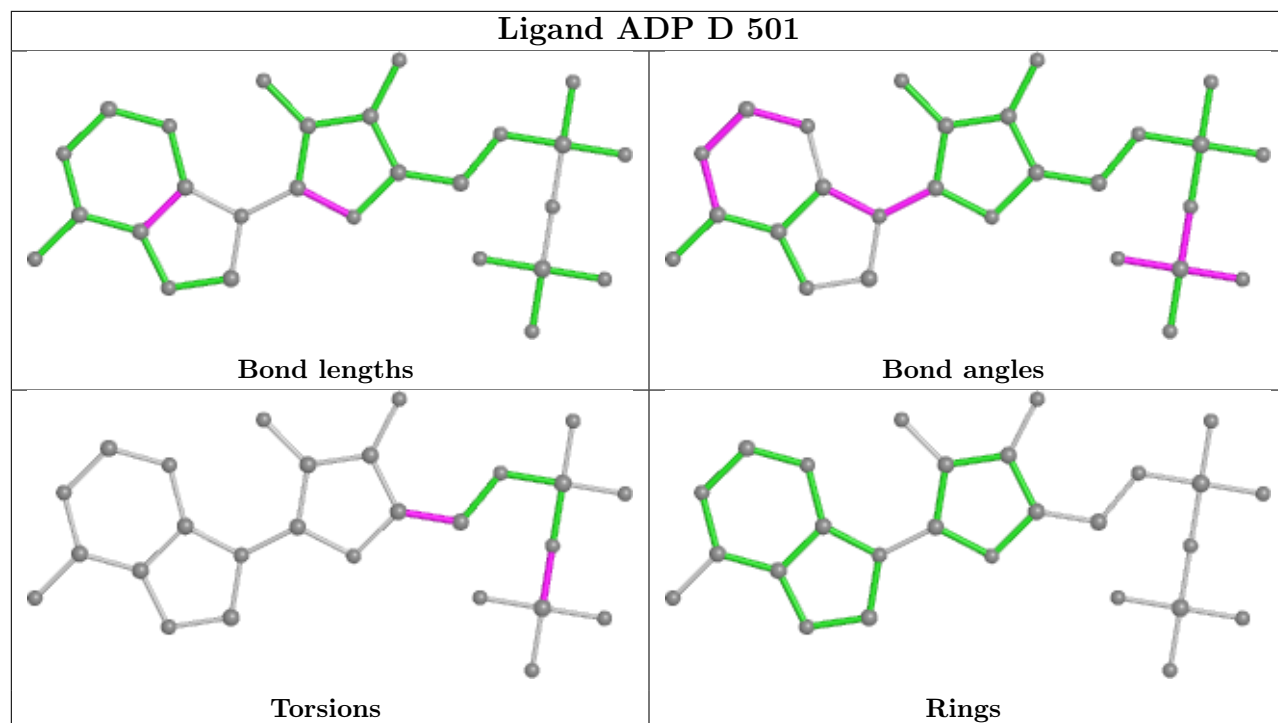


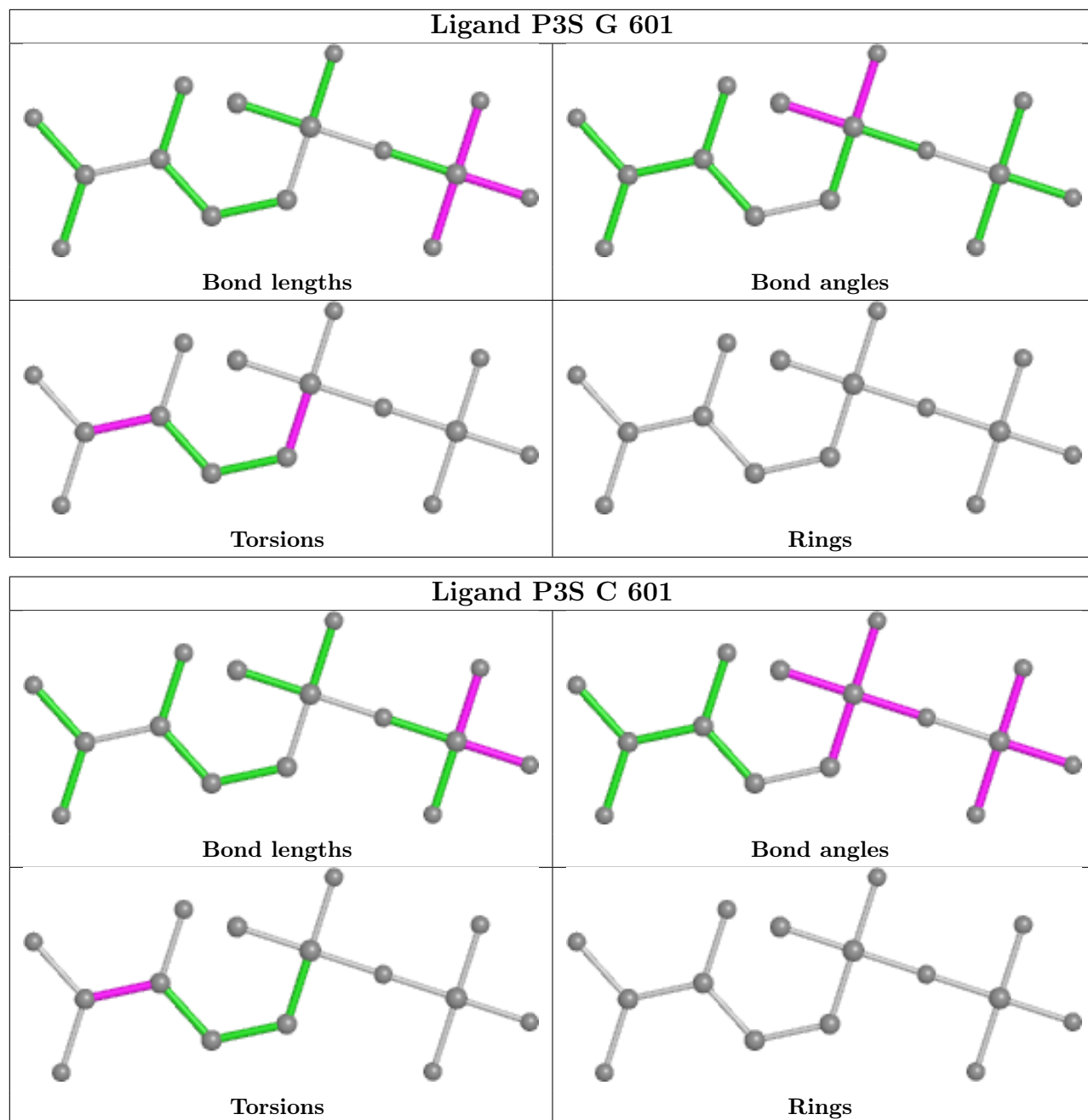


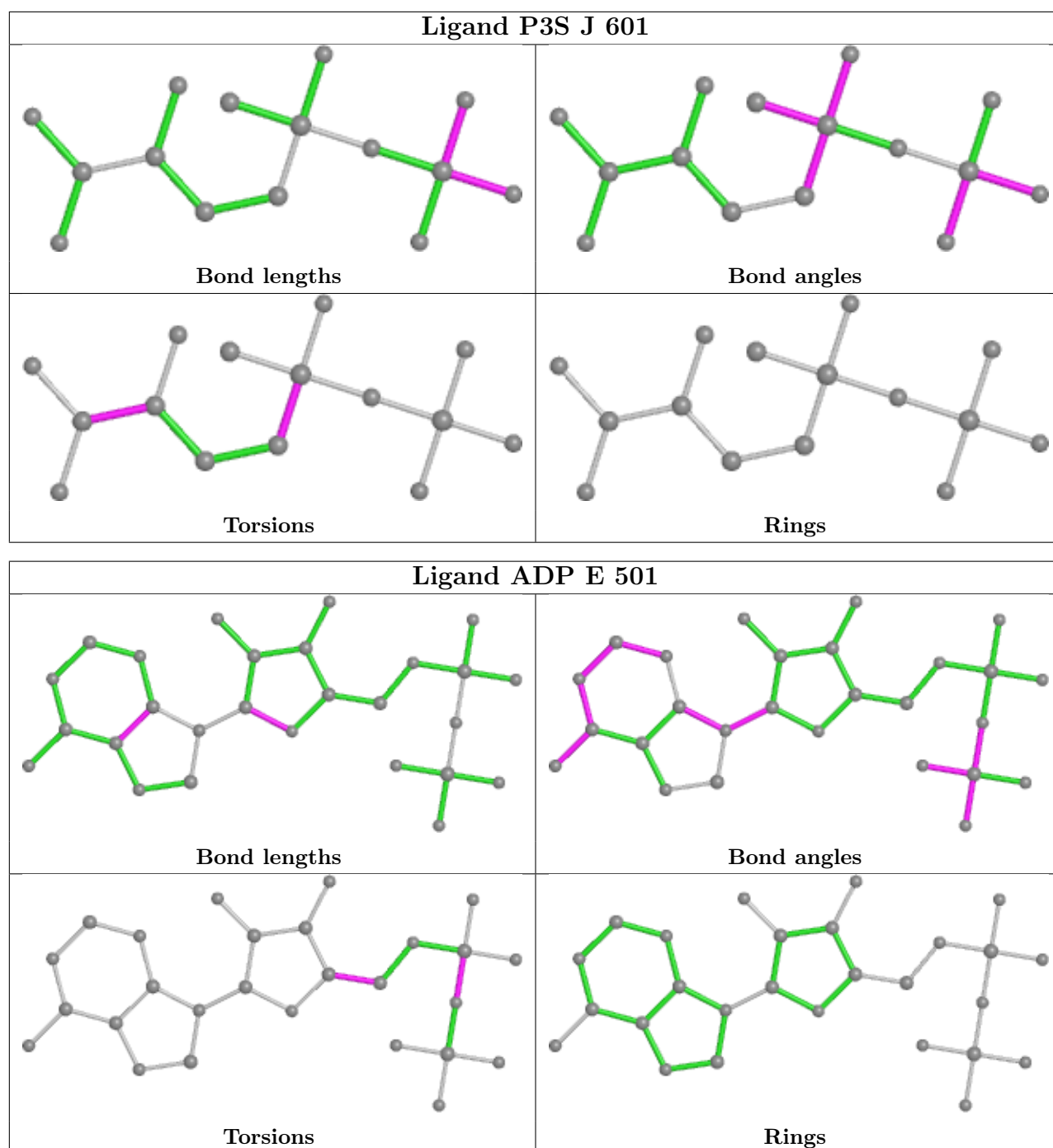












5.7 Other polymers [i](#)

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	356/384 (92%)	0.22	10 (2%) 53 46	35, 42, 54, 64	0
1	B	356/384 (92%)	0.14	4 (1%) 80 78	35, 42, 54, 62	0
1	C	356/384 (92%)	0.09	4 (1%) 80 78	35, 42, 54, 64	0
1	D	356/384 (92%)	0.19	3 (0%) 86 84	35, 42, 54, 63	0
1	E	355/384 (92%)	0.27	11 (3%) 49 42	35, 42, 54, 63	0
1	F	356/384 (92%)	0.42	23 (6%) 18 14	35, 42, 53, 63	0
1	G	356/384 (92%)	0.56	33 (9%) 8 6	35, 42, 53, 63	0
1	H	356/384 (92%)	0.47	25 (7%) 16 12	35, 42, 54, 62	0
1	I	356/384 (92%)	0.53	29 (8%) 12 8	35, 42, 53, 63	0
1	J	356/384 (92%)	0.71	37 (10%) 6 4	35, 42, 53, 63	0
All	All	3559/3840 (92%)	0.36	179 (5%) 28 23	35, 42, 54, 64	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	GLY	5.8
1	F	265	ASN	4.7
1	J	268	LYS	4.6
1	F	119	ARG	4.4
1	H	142	THR	4.4
1	I	104	TYR	4.3
1	D	365	GLY	4.2
1	J	142	THR	4.2
1	J	104	TYR	4.1
1	G	286	ARG	4.1
1	F	331	GLN	4.1
1	H	265	ASN	4.0
1	J	362	ASN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	303	PHE	4.0
1	I	362	ASN	3.9
1	G	52	LYS	3.8
1	J	307	SER	3.8
1	A	142	THR	3.7
1	J	279	LYS	3.7
1	H	119	ARG	3.5
1	G	265	ASN	3.5
1	F	268	LYS	3.5
1	G	105	ASN	3.5
1	E	104	TYR	3.4
1	I	126	ASN	3.4
1	E	107	ARG	3.4
1	H	308	ASN	3.3
1	B	107	ARG	3.3
1	I	142	THR	3.2
1	G	107	ARG	3.2
1	I	333	LYS	3.2
1	I	358	THR	3.2
1	A	264	GLU	3.2
1	J	71	GLU	3.2
1	J	361	LEU	3.2
1	F	303	PHE	3.2
1	F	142	THR	3.1
1	J	308	ASN	3.1
1	J	282	GLN	3.1
1	G	151	SER	3.1
1	E	275	GLU	3.1
1	G	279	LYS	3.1
1	J	133	MET	3.0
1	H	152	ASN	3.0
1	I	265	ASN	3.0
1	I	259	LYS	3.0
1	J	152	ASN	3.0
1	G	309	ILE	3.0
1	J	330	GLY	3.0
1	A	119	ARG	3.0
1	J	105	ASN	3.0
1	G	53	CYS	3.0
1	G	119	ARG	3.0
1	H	359	CYS	2.9
1	J	265	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	365	GLY	2.9
1	A	143	ASP	2.9
1	C	152	ASN	2.9
1	J	309	ILE	2.9
1	I	282	GLN	2.8
1	J	51	PRO	2.8
1	G	269	TYR	2.8
1	I	355	LEU	2.8
1	I	303	PHE	2.8
1	F	126	ASN	2.8
1	G	152	ASN	2.8
1	A	151	SER	2.7
1	G	333	LYS	2.7
1	J	312	PHE	2.7
1	J	364	THR	2.7
1	H	104	TYR	2.7
1	G	303	PHE	2.7
1	J	68	LEU	2.7
1	H	316	VAL	2.6
1	H	105	ASN	2.6
1	F	294	LEU	2.6
1	H	252	CYS	2.6
1	G	310	ASN	2.6
1	G	331	GLN	2.6
1	F	362	ASN	2.6
1	J	358	THR	2.6
1	A	265	ASN	2.6
1	B	152	ASN	2.5
1	E	331	GLN	2.5
1	F	108	PRO	2.5
1	I	312	PHE	2.5
1	D	142	THR	2.5
1	G	275	GLU	2.5
1	G	268	LYS	2.5
1	C	142	THR	2.5
1	F	130	TRP	2.5
1	J	252	CYS	2.5
1	I	268	LYS	2.5
1	J	70	SER	2.5
1	J	150	PRO	2.5
1	I	123	MET	2.5
1	D	282	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	282	GLN	2.4
1	H	273	ALA	2.4
1	F	312	PHE	2.4
1	J	332	GLU	2.4
1	B	142	THR	2.4
1	H	278	SER	2.4
1	F	316	VAL	2.4
1	I	119	ARG	2.4
1	H	68	LEU	2.4
1	J	206	ILE	2.4
1	J	275	GLU	2.4
1	E	294	LEU	2.4
1	F	282	GLN	2.4
1	G	154	PHE	2.4
1	G	332	GLU	2.4
1	G	282	GLN	2.4
1	J	310	ASN	2.4
1	F	107	ARG	2.4
1	E	150	PRO	2.3
1	G	104	TYR	2.3
1	I	364	THR	2.3
1	A	152	ASN	2.3
1	H	279	LYS	2.3
1	H	358	THR	2.3
1	F	332	GLU	2.3
1	F	124	VAL	2.3
1	J	359	CYS	2.3
1	G	337	PHE	2.3
1	J	365	GLY	2.2
1	I	21	PRO	2.2
1	E	152	ASN	2.2
1	I	152	ASN	2.2
1	F	21	PRO	2.2
1	G	274	ILE	2.2
1	I	286	ARG	2.2
1	G	225	LEU	2.2
1	I	121	MET	2.2
1	G	23	GLY	2.2
1	H	275	GLU	2.2
1	B	151	SER	2.2
1	F	150	PRO	2.2
1	H	301	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	364	THR	2.2
1	E	218	LEU	2.2
1	I	290	PRO	2.2
1	I	331	GLN	2.2
1	I	328	THR	2.2
1	I	128	HIS	2.1
1	G	221	ALA	2.1
1	I	283	TYR	2.1
1	C	107	ARG	2.1
1	J	357	ARG	2.1
1	F	152	ASN	2.1
1	J	355	LEU	2.1
1	E	71	GLU	2.1
1	H	133	MET	2.1
1	G	42	CYS	2.1
1	H	333	LYS	2.1
1	G	142	THR	2.1
1	H	331	GLN	2.1
1	E	105	ASN	2.1
1	J	329	VAL	2.1
1	A	150	PRO	2.1
1	I	49	SER	2.1
1	G	304	HIS	2.1
1	J	300	LEU	2.1
1	I	264	GLU	2.1
1	I	360	LEU	2.1
1	G	126	ASN	2.1
1	E	142	THR	2.1
1	F	307	SER	2.1
1	A	326	PRO	2.0
1	G	133	MET	2.0
1	J	75	SER	2.0
1	F	105	ASN	2.0
1	C	330	GLY	2.0
1	J	311	ASP	2.0
1	H	123	MET	2.0
1	F	106	ARG	2.0
1	H	268	LYS	2.0
1	G	292	GLY	2.0
1	J	108	PRO	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 monosaccharides 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
3	CL	G	707	1/1	0.93	0.12	44,44,44,44	0
2	MN	J	401	1/1	0.94	0.05	54,54,54,54	0
3	CL	J	710	1/1	0.94	0.12	45,45,45,45	0
2	MN	G	403	1/1	0.95	0.07	49,49,49,49	0
4	ADP	H	501	27/27	0.95	0.14	47,59,61,62	0
5	P3S	I	601	15/15	0.95	0.12	48,50,54,55	0
2	MN	I	401	1/1	0.96	0.06	52,52,52,52	0
4	ADP	E	501	27/27	0.96	0.11	30,38,40,41	0
4	ADP	F	501	27/27	0.96	0.15	43,61,62,63	0
4	ADP	G	501	27/27	0.96	0.18	44,59,63,63	0
3	CL	G	708	1/1	0.96	0.12	45,45,45,45	0
4	ADP	J	501	27/27	0.96	0.12	44,62,64,65	0
5	P3S	F	601	15/15	0.96	0.13	44,51,53,54	0
5	P3S	G	601	15/15	0.96	0.14	46,51,57,57	0
3	CL	I	709	1/1	0.96	0.07	40,40,40,40	0
4	ADP	D	501	27/27	0.97	0.10	26,35,37,38	0
3	CL	F	706	1/1	0.97	0.11	45,45,45,45	0
2	MN	G	401	1/1	0.97	0.05	51,51,51,51	0
2	MN	H	401	1/1	0.97	0.05	47,47,47,47	0
3	CL	B	701	1/1	0.97	0.11	31,31,31,31	0
4	ADP	I	501	27/27	0.97	0.18	45,60,61,61	0
3	CL	B	705	1/1	0.97	0.08	32,32,32,32	0
5	P3S	E	601	15/15	0.97	0.12	29,30,34,38	0
4	ADP	A	501	27/27	0.97	0.11	31,40,43,44	0
4	ADP	B	501	27/27	0.97	0.10	29,33,35,37	0
5	P3S	H	601	15/15	0.97	0.14	42,45,47,48	0
4	ADP	C	501	27/27	0.97	0.10	23,28,33,35	0

Continued on next page...

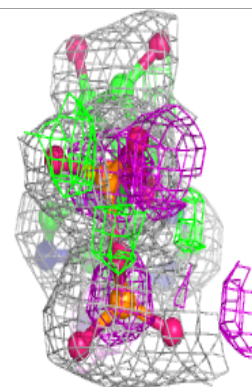
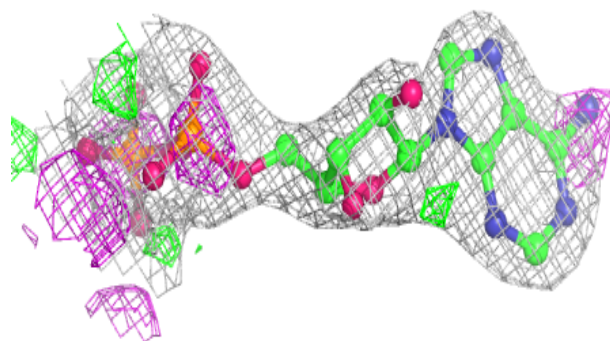
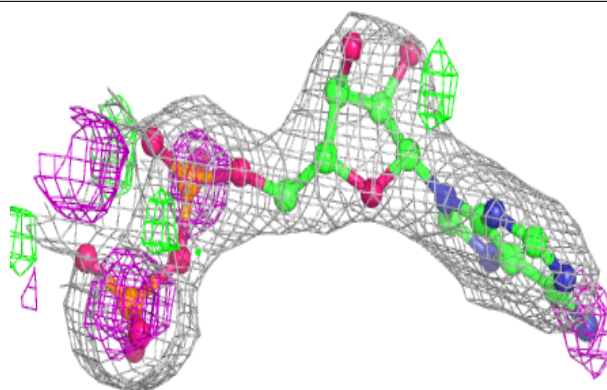
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	P3S	J	601	15/15	0.97	0.12	50,51,53,54	0
2	MN	I	403	1/1	0.98	0.11	47,47,47,47	0
2	MN	D	402	1/1	0.98	0.02	35,35,35,35	0
2	MN	J	402	1/1	0.98	0.09	52,52,52,52	0
2	MN	J	403	1/1	0.98	0.04	52,52,52,52	0
3	CL	A	703	1/1	0.98	0.08	33,33,33,33	0
2	MN	F	401	1/1	0.98	0.04	50,50,50,50	0
2	MN	F	402	1/1	0.98	0.04	55,55,55,55	0
3	CL	C	702	1/1	0.98	0.06	29,29,29,29	0
3	CL	D	704	1/1	0.98	0.06	31,31,31,31	0
5	P3S	A	601	15/15	0.98	0.12	31,34,35,36	0
5	P3S	B	601	15/15	0.98	0.12	26,27,30,32	0
5	P3S	C	601	15/15	0.98	0.10	23,24,31,34	0
5	P3S	D	601	15/15	0.98	0.12	27,29,30,33	0
2	MN	A	403	1/1	0.98	0.03	40,40,40,40	0
2	MN	B	402	1/1	0.98	0.05	34,34,34,34	0
2	MN	C	402	1/1	0.98	0.04	33,33,33,33	0
2	MN	H	402	1/1	0.98	0.05	55,55,55,55	0
2	MN	H	403	1/1	0.98	0.07	47,47,47,47	0
2	MN	D	401	1/1	0.98	0.03	31,31,31,31	0
2	MN	B	403	1/1	0.99	0.03	31,31,31,31	0
2	MN	D	403	1/1	0.99	0.03	30,30,30,30	0
2	MN	E	401	1/1	0.99	0.03	34,34,34,34	0
2	MN	E	402	1/1	0.99	0.03	36,36,36,36	0
2	MN	C	401	1/1	0.99	0.02	31,31,31,31	0
2	MN	I	402	1/1	0.99	0.04	52,52,52,52	0
2	MN	A	401	1/1	0.99	0.03	37,37,37,37	0
2	MN	F	403	1/1	0.99	0.05	51,51,51,51	0
2	MN	A	402	1/1	0.99	0.04	37,37,37,37	0
2	MN	G	402	1/1	0.99	0.05	54,54,54,54	0
2	MN	C	403	1/1	1.00	0.02	31,31,31,31	0
2	MN	B	401	1/1	1.00	0.04	32,32,32,32	0
2	MN	E	403	1/1	1.00	0.03	31,31,31,31	0

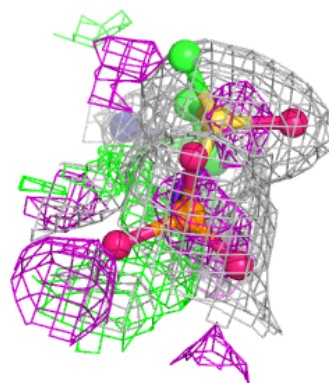
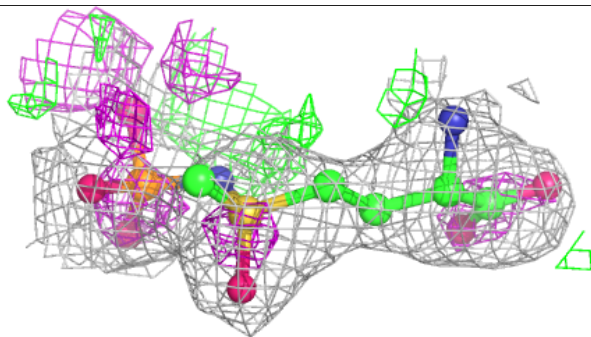
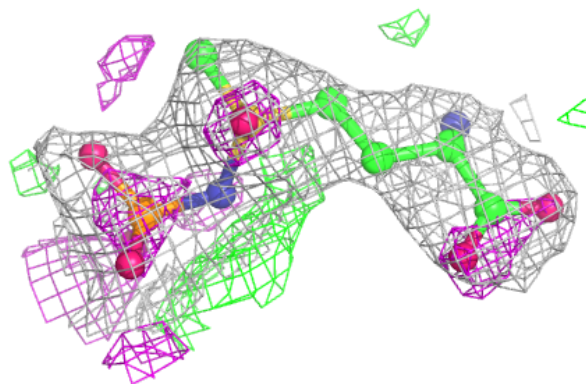
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP H 501:

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

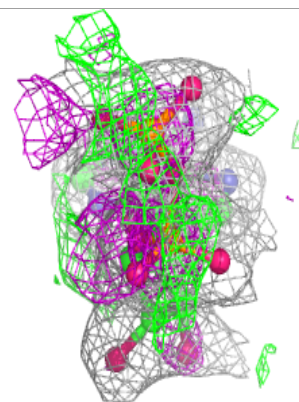
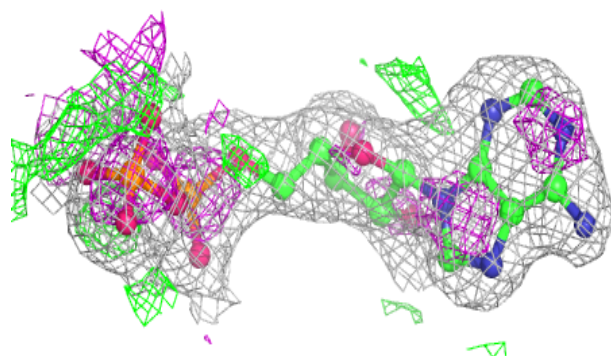
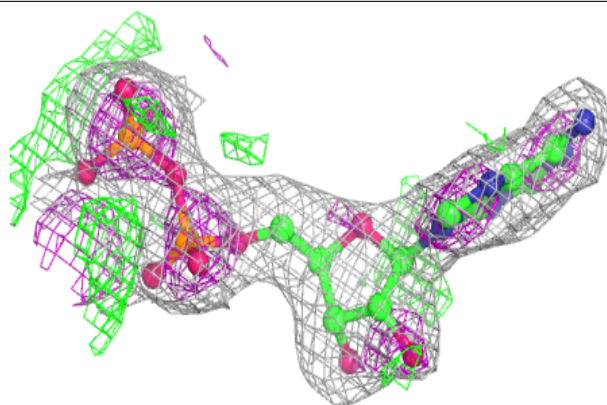
**Electron density around P3S I 601:**

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

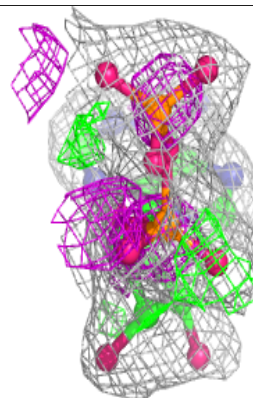
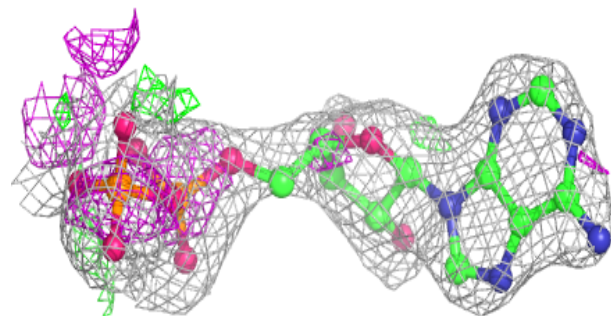
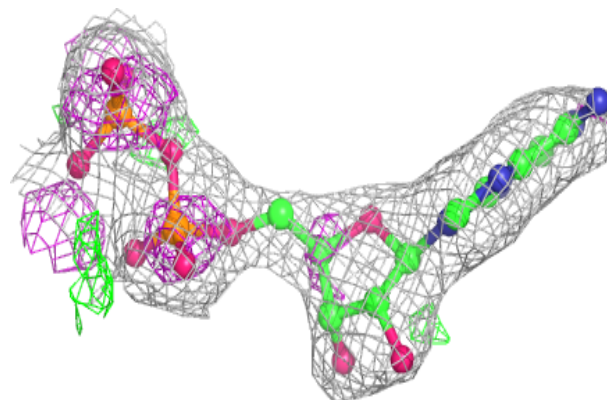


Electron density around ADP E 501:

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

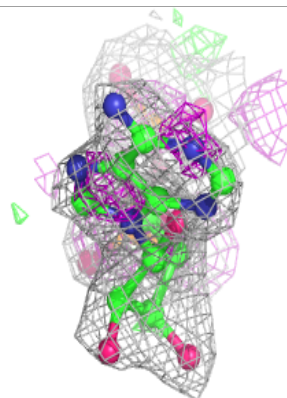
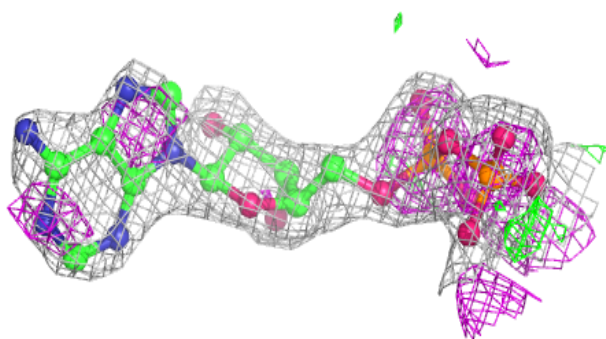
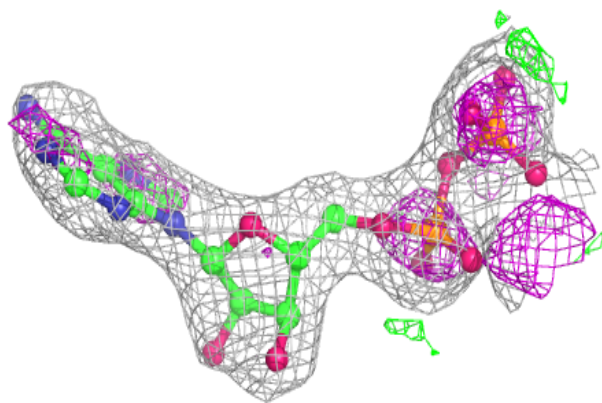
**Electron density around ADP F 501:**

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

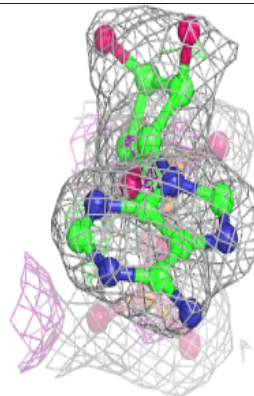
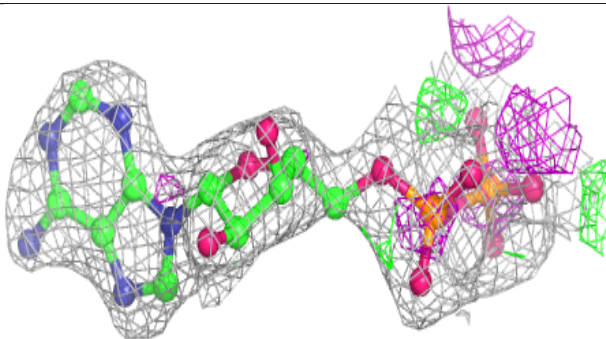
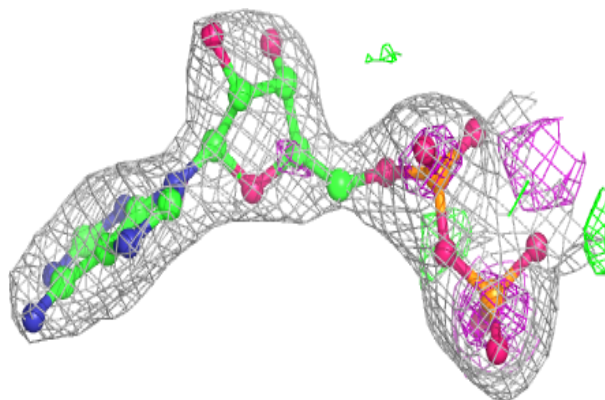


Electron density around ADP G 501:

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

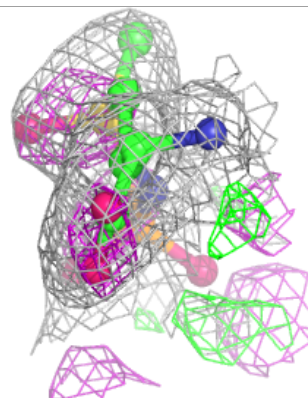
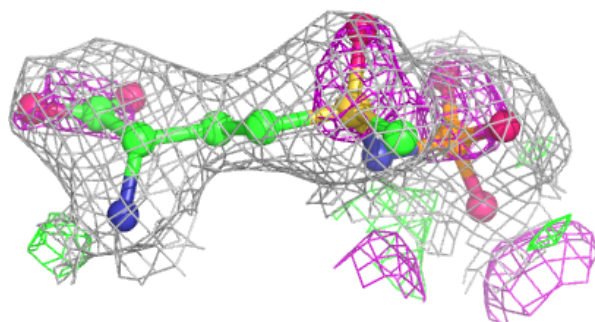
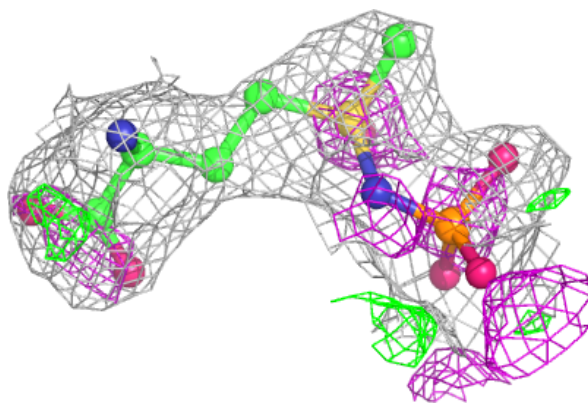
**Electron density around ADP J 501:**

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

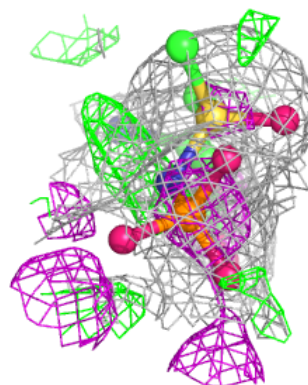
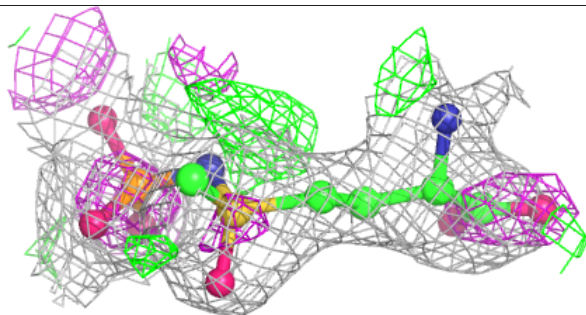
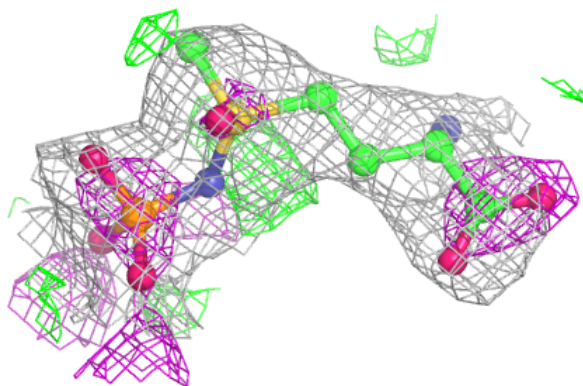


Electron density around P3S F 601:

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

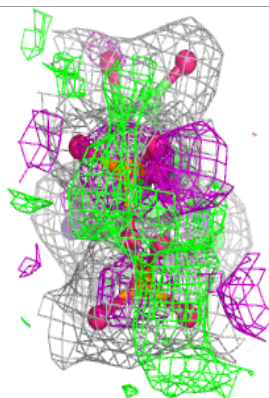
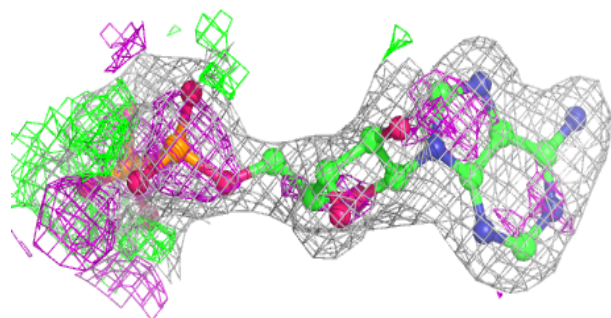
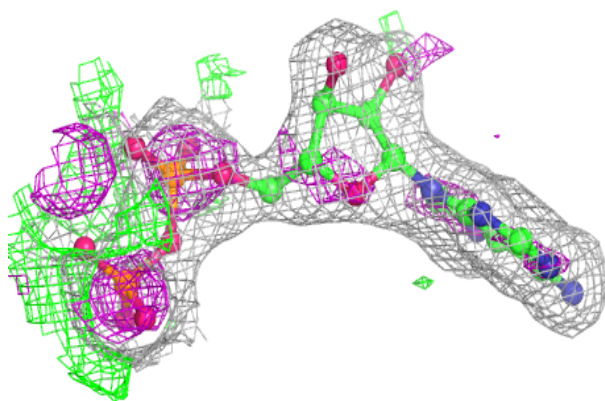
**Electron density around P3S G 601:**

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

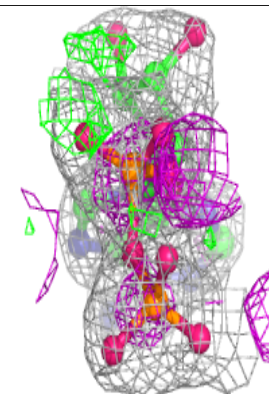
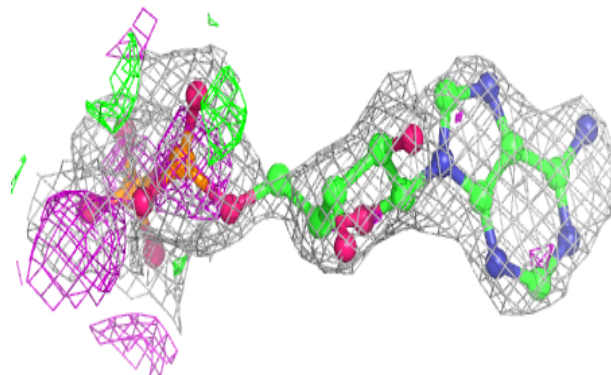
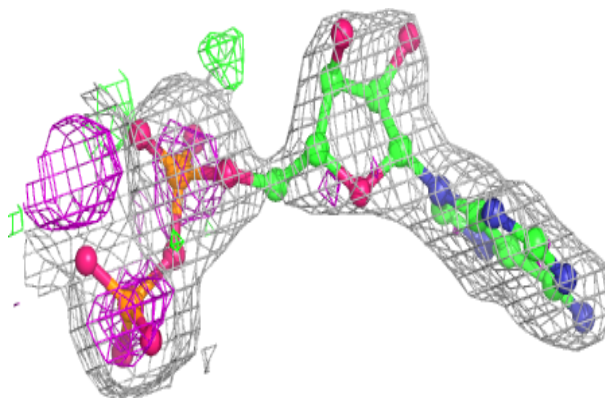


Electron density around ADP D 501:

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

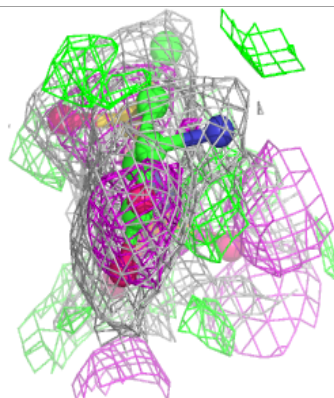
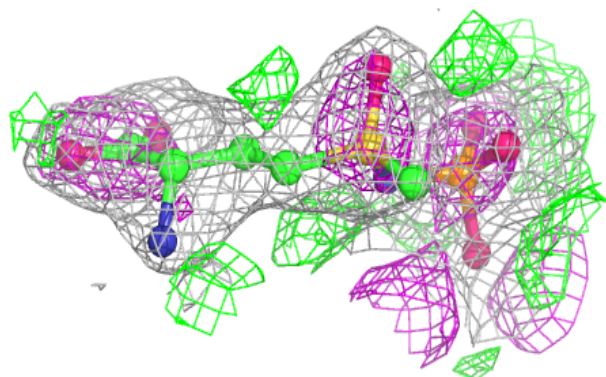
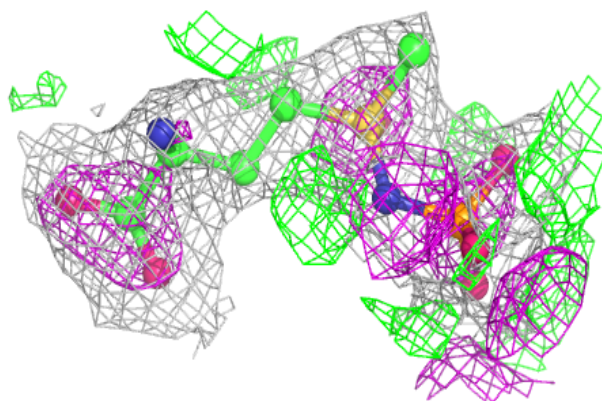
**Electron density around ADP I 501:**

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

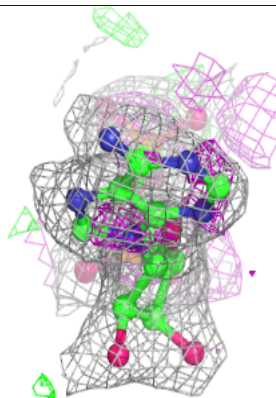
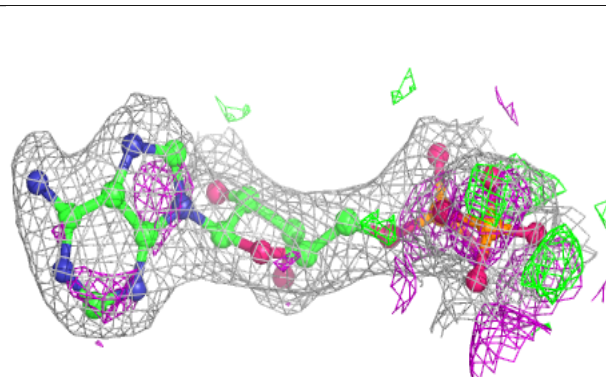
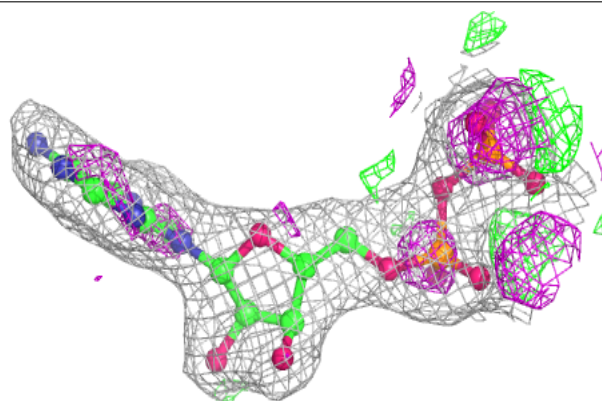


Electron density around P3S E 601:

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

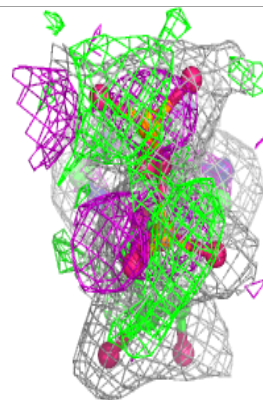
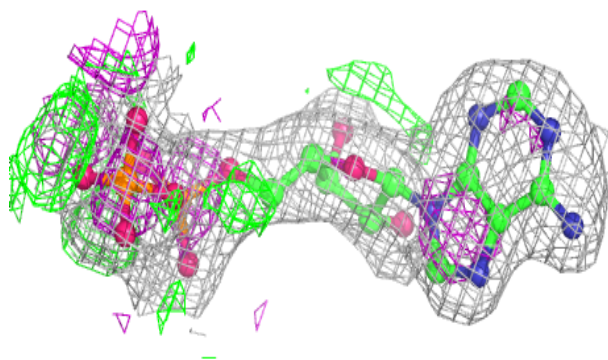
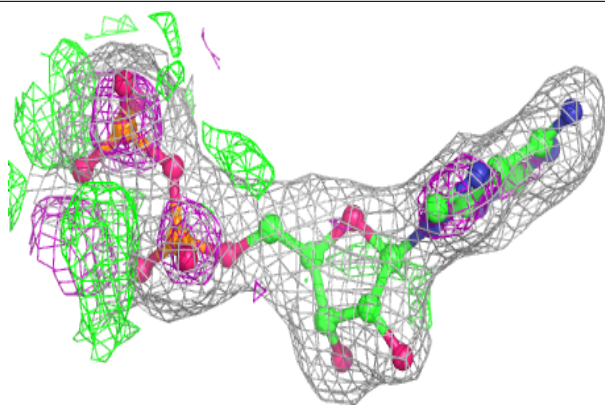
**Electron density around ADP A 501:**

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

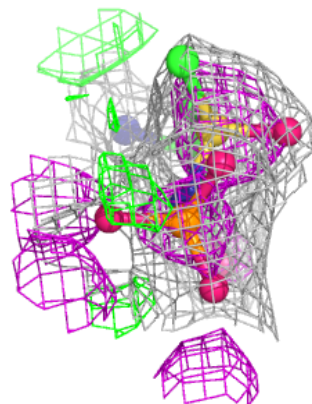
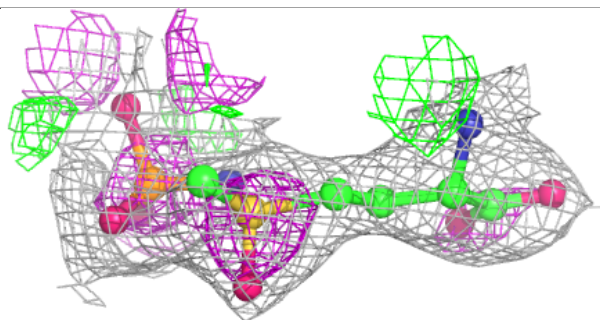
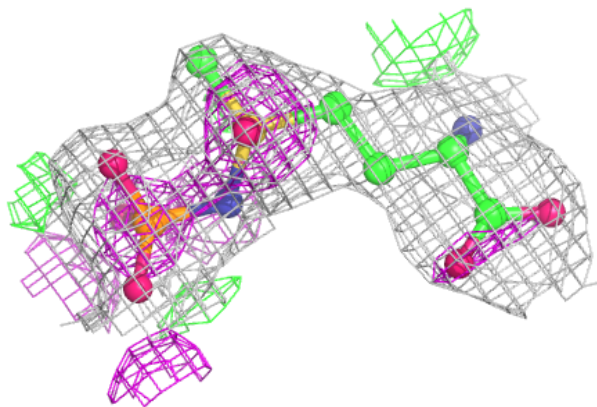


Electron density around ADP B 501:

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

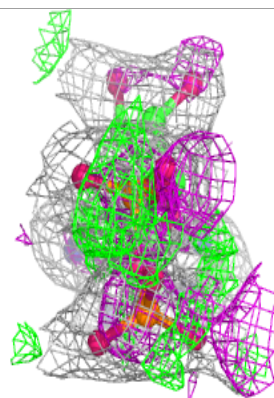
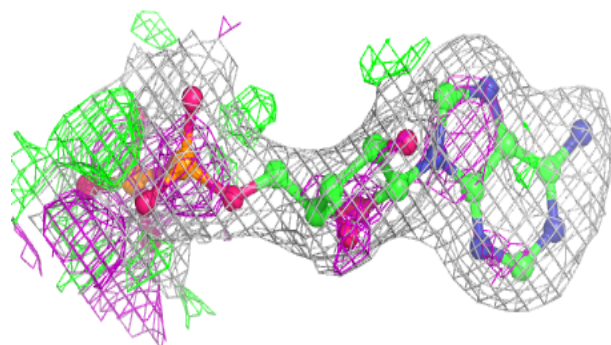
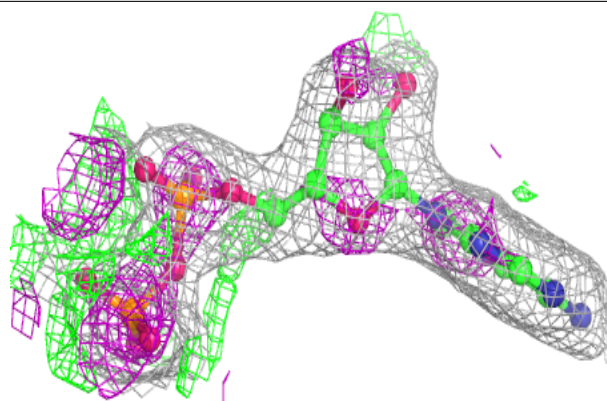
**Electron density around P3S H 601:**

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

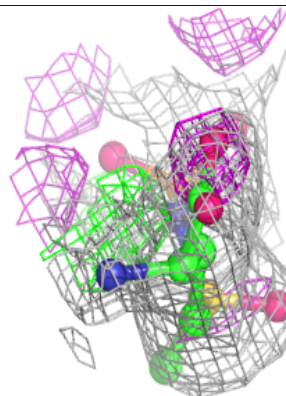
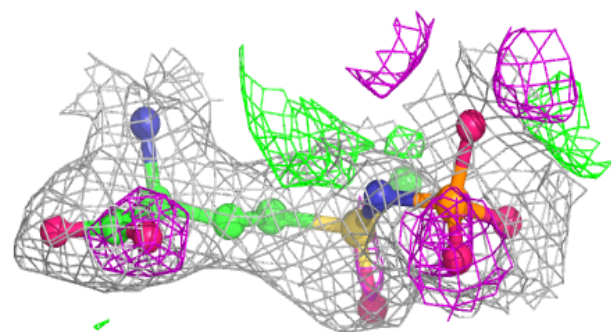
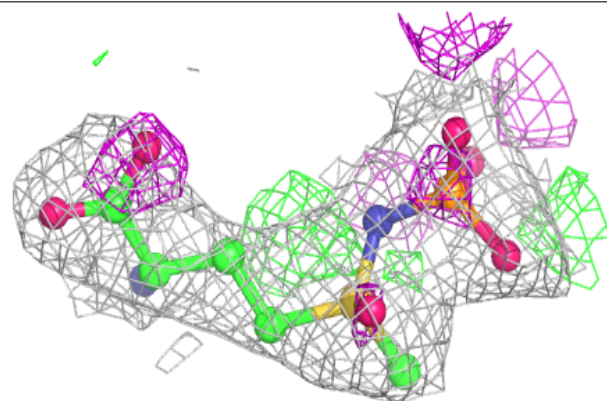


Electron density around ADP C 501:

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

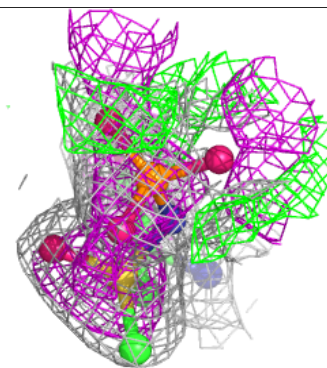
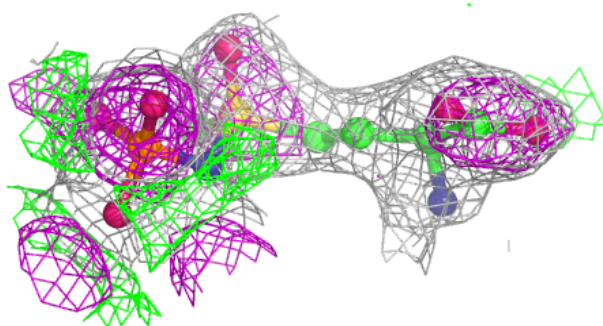
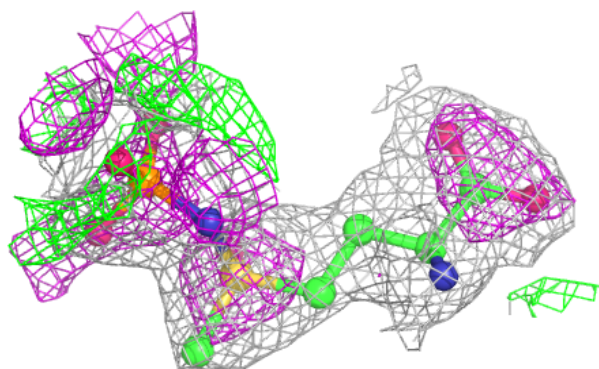
**Electron density around P3S J 601:**

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

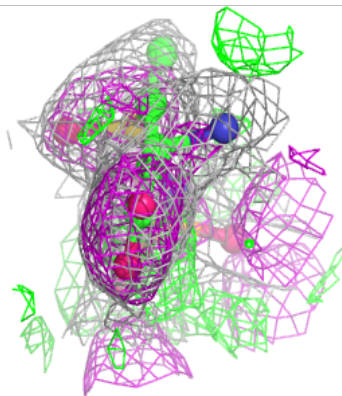
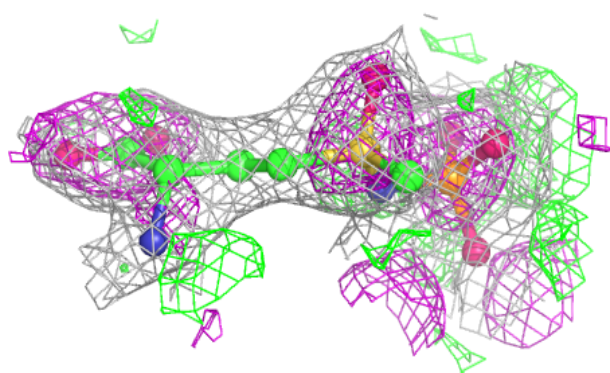
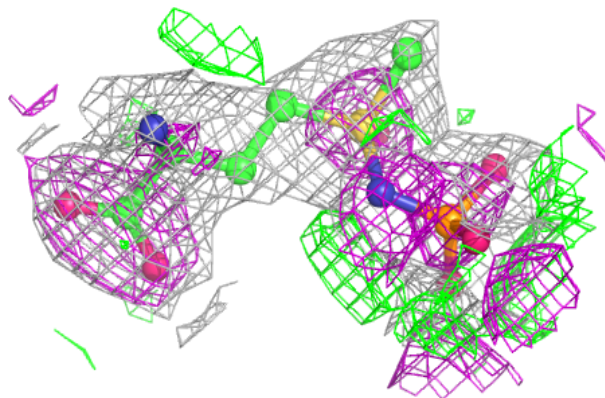


Electron density around P3S A 601:

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

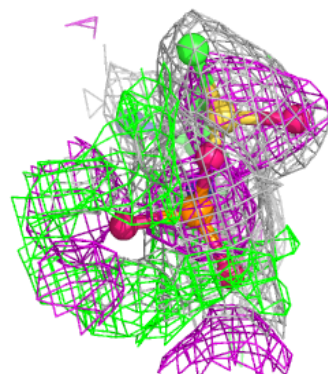
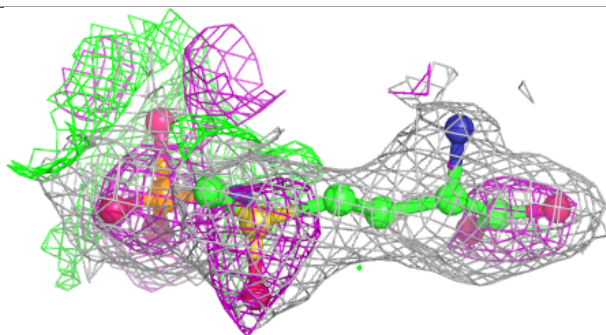
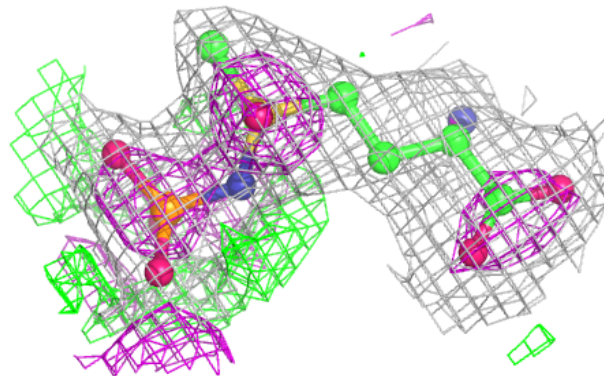
**Electron density around P3S B 601:**

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

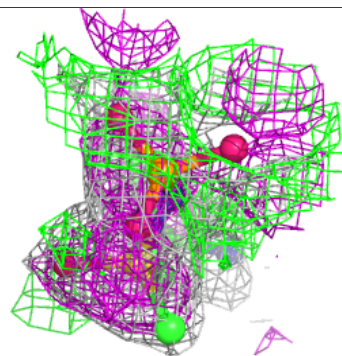
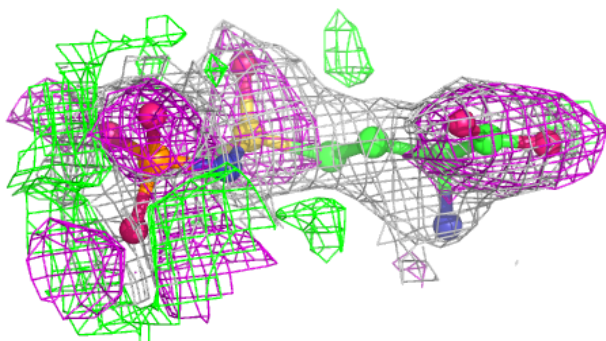
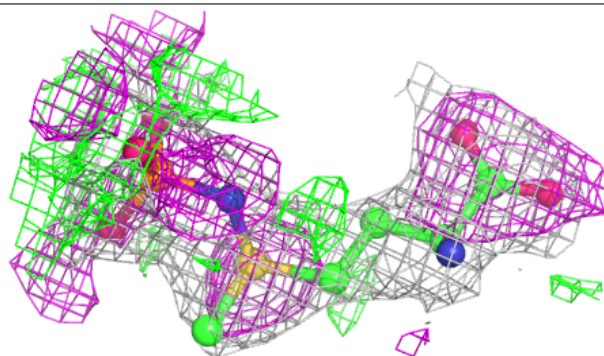


Electron density around P3S C 601:

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

**Electron density around P3S D 601:**

$2mF_o-DF_c$ (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.