



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2025 – 12:38 pm GMT

PDB ID : 9RAS / pdb\_00009ras  
Title : Streptococcus pyogenes GapN in complex with imidazoline-2,4-dione  
Authors : Wirsing, R.; Schindelin, H.  
Deposited on : 2025-05-21  
Resolution : 1.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

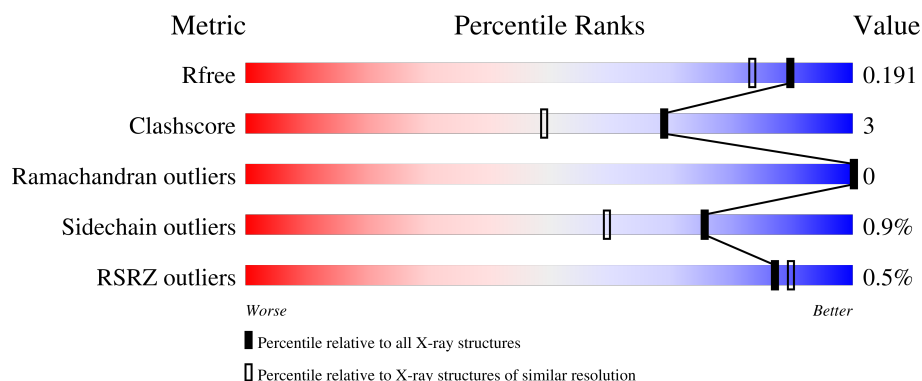
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 1.57 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))
$R_{free}$	164625	7165 (1.60-1.56)
Clashscore	180529	1026 (1.58-1.58)
Ramachandran outliers	177936	1005 (1.58-1.58)
Sidechain outliers	177891	1004 (1.58-1.58)
RSRZ outliers	164620	7163 (1.60-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	
1	B	496	
1	C	496	
1	D	496	
1	E	496	

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Mol	Chain	Length	Quality of chain
1	F	496	 88% 7% •
1	G	496	 90% 5% •
1	H	496	 90% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	E	503	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65210 atoms, of which 30754 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 NADP-dependent glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	474	Total	C	H	N	O	S	0	29	0
			7461	2352	3784	599	716	10			
1	B	474	Total	C	H	N	O	S	0	38	0
			7565	2391	3839	605	721	9			
1	C	474	Total	C	H	N	O	S	0	34	0
			7574	2384	3857	606	718	9			
1	D	475	Total	C	H	N	O	S	0	29	0
			7463	2352	3787	600	715	9			
1	E	474	Total	C	H	N	O	S	0	28	0
			7462	2353	3789	597	715	8			
1	F	474	Total	C	H	N	O	S	0	41	0
			7585	2387	3853	609	726	10			
1	G	474	Total	C	H	N	O	S	8	36	0
			7591	2388	3871	605	717	10			
1	H	480	Total	C	H	N	O	S	0	29	0
			7556	2378	3839	611	718	10			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	ALA	-	expression tag	UNP A0A4U9C786
A	-19	SER	-	expression tag	UNP A0A4U9C786
A	-18	TRP	-	expression tag	UNP A0A4U9C786
A	-17	SER	-	expression tag	UNP A0A4U9C786
A	-16	HIS	-	expression tag	UNP A0A4U9C786
A	-15	PRO	-	expression tag	UNP A0A4U9C786
A	-14	GLN	-	expression tag	UNP A0A4U9C786
A	-13	PHE	-	expression tag	UNP A0A4U9C786
A	-12	GLU	-	expression tag	UNP A0A4U9C786
A	-11	LYS	-	expression tag	UNP A0A4U9C786
A	-10	ILE	-	expression tag	UNP A0A4U9C786
A	-9	GLU	-	expression tag	UNP A0A4U9C786
A	-8	GLY	-	expression tag	UNP A0A4U9C786

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ARG	-	expression tag	UNP A0A4U9C786
A	-6	ARG	-	expression tag	UNP A0A4U9C786
A	-5	ASP	-	expression tag	UNP A0A4U9C786
A	-4	ARG	-	expression tag	UNP A0A4U9C786
A	-3	GLY	-	expression tag	UNP A0A4U9C786
A	-2	PRO	-	expression tag	UNP A0A4U9C786
A	-1	GLU	-	expression tag	UNP A0A4U9C786
A	0	PHE	-	expression tag	UNP A0A4U9C786
A	1	LEU	MET	conflict	UNP A0A4U9C786
A	58	THR	ALA	conflict	UNP A0A4U9C786
A	284	SER	CYS	conflict	UNP A0A4U9C786
B	-20	ALA	-	expression tag	UNP A0A4U9C786
B	-19	SER	-	expression tag	UNP A0A4U9C786
B	-18	TRP	-	expression tag	UNP A0A4U9C786
B	-17	SER	-	expression tag	UNP A0A4U9C786
B	-16	HIS	-	expression tag	UNP A0A4U9C786
B	-15	PRO	-	expression tag	UNP A0A4U9C786
B	-14	GLN	-	expression tag	UNP A0A4U9C786
B	-13	PHE	-	expression tag	UNP A0A4U9C786
B	-12	GLU	-	expression tag	UNP A0A4U9C786
B	-11	LYS	-	expression tag	UNP A0A4U9C786
B	-10	ILE	-	expression tag	UNP A0A4U9C786
B	-9	GLU	-	expression tag	UNP A0A4U9C786
B	-8	GLY	-	expression tag	UNP A0A4U9C786
B	-7	ARG	-	expression tag	UNP A0A4U9C786
B	-6	ARG	-	expression tag	UNP A0A4U9C786
B	-5	ASP	-	expression tag	UNP A0A4U9C786
B	-4	ARG	-	expression tag	UNP A0A4U9C786
B	-3	GLY	-	expression tag	UNP A0A4U9C786
B	-2	PRO	-	expression tag	UNP A0A4U9C786
B	-1	GLU	-	expression tag	UNP A0A4U9C786
B	0	PHE	-	expression tag	UNP A0A4U9C786
B	1	LEU	MET	conflict	UNP A0A4U9C786
B	58	THR	ALA	conflict	UNP A0A4U9C786
B	284	SER	CYS	conflict	UNP A0A4U9C786
C	-20	ALA	-	expression tag	UNP A0A4U9C786
C	-19	SER	-	expression tag	UNP A0A4U9C786
C	-18	TRP	-	expression tag	UNP A0A4U9C786
C	-17	SER	-	expression tag	UNP A0A4U9C786
C	-16	HIS	-	expression tag	UNP A0A4U9C786
C	-15	PRO	-	expression tag	UNP A0A4U9C786
C	-14	GLN	-	expression tag	UNP A0A4U9C786

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	PHE	-	expression tag	UNP A0A4U9C786
C	-12	GLU	-	expression tag	UNP A0A4U9C786
C	-11	LYS	-	expression tag	UNP A0A4U9C786
C	-10	ILE	-	expression tag	UNP A0A4U9C786
C	-9	GLU	-	expression tag	UNP A0A4U9C786
C	-8	GLY	-	expression tag	UNP A0A4U9C786
C	-7	ARG	-	expression tag	UNP A0A4U9C786
C	-6	ARG	-	expression tag	UNP A0A4U9C786
C	-5	ASP	-	expression tag	UNP A0A4U9C786
C	-4	ARG	-	expression tag	UNP A0A4U9C786
C	-3	GLY	-	expression tag	UNP A0A4U9C786
C	-2	PRO	-	expression tag	UNP A0A4U9C786
C	-1	GLU	-	expression tag	UNP A0A4U9C786
C	0	PHE	-	expression tag	UNP A0A4U9C786
C	1	LEU	MET	conflict	UNP A0A4U9C786
C	58	THR	ALA	conflict	UNP A0A4U9C786
C	284	SER	CYS	conflict	UNP A0A4U9C786
D	-20	ALA	-	expression tag	UNP A0A4U9C786
D	-19	SER	-	expression tag	UNP A0A4U9C786
D	-18	TRP	-	expression tag	UNP A0A4U9C786
D	-17	SER	-	expression tag	UNP A0A4U9C786
D	-16	HIS	-	expression tag	UNP A0A4U9C786
D	-15	PRO	-	expression tag	UNP A0A4U9C786
D	-14	GLN	-	expression tag	UNP A0A4U9C786
D	-13	PHE	-	expression tag	UNP A0A4U9C786
D	-12	GLU	-	expression tag	UNP A0A4U9C786
D	-11	LYS	-	expression tag	UNP A0A4U9C786
D	-10	ILE	-	expression tag	UNP A0A4U9C786
D	-9	GLU	-	expression tag	UNP A0A4U9C786
D	-8	GLY	-	expression tag	UNP A0A4U9C786
D	-7	ARG	-	expression tag	UNP A0A4U9C786
D	-6	ARG	-	expression tag	UNP A0A4U9C786
D	-5	ASP	-	expression tag	UNP A0A4U9C786
D	-4	ARG	-	expression tag	UNP A0A4U9C786
D	-3	GLY	-	expression tag	UNP A0A4U9C786
D	-2	PRO	-	expression tag	UNP A0A4U9C786
D	-1	GLU	-	expression tag	UNP A0A4U9C786
D	0	PHE	-	expression tag	UNP A0A4U9C786
D	1	LEU	MET	conflict	UNP A0A4U9C786
D	58	THR	ALA	conflict	UNP A0A4U9C786
D	284	SER	CYS	conflict	UNP A0A4U9C786
E	-20	ALA	-	expression tag	UNP A0A4U9C786

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	SER	-	expression tag	UNP A0A4U9C786
E	-18	TRP	-	expression tag	UNP A0A4U9C786
E	-17	SER	-	expression tag	UNP A0A4U9C786
E	-16	HIS	-	expression tag	UNP A0A4U9C786
E	-15	PRO	-	expression tag	UNP A0A4U9C786
E	-14	GLN	-	expression tag	UNP A0A4U9C786
E	-13	PHE	-	expression tag	UNP A0A4U9C786
E	-12	GLU	-	expression tag	UNP A0A4U9C786
E	-11	LYS	-	expression tag	UNP A0A4U9C786
E	-10	ILE	-	expression tag	UNP A0A4U9C786
E	-9	GLU	-	expression tag	UNP A0A4U9C786
E	-8	GLY	-	expression tag	UNP A0A4U9C786
E	-7	ARG	-	expression tag	UNP A0A4U9C786
E	-6	ARG	-	expression tag	UNP A0A4U9C786
E	-5	ASP	-	expression tag	UNP A0A4U9C786
E	-4	ARG	-	expression tag	UNP A0A4U9C786
E	-3	GLY	-	expression tag	UNP A0A4U9C786
E	-2	PRO	-	expression tag	UNP A0A4U9C786
E	-1	GLU	-	expression tag	UNP A0A4U9C786
E	0	PHE	-	expression tag	UNP A0A4U9C786
E	1	LEU	MET	conflict	UNP A0A4U9C786
E	58	THR	ALA	conflict	UNP A0A4U9C786
E	284	SER	CYS	conflict	UNP A0A4U9C786
F	-20	ALA	-	expression tag	UNP A0A4U9C786
F	-19	SER	-	expression tag	UNP A0A4U9C786
F	-18	TRP	-	expression tag	UNP A0A4U9C786
F	-17	SER	-	expression tag	UNP A0A4U9C786
F	-16	HIS	-	expression tag	UNP A0A4U9C786
F	-15	PRO	-	expression tag	UNP A0A4U9C786
F	-14	GLN	-	expression tag	UNP A0A4U9C786
F	-13	PHE	-	expression tag	UNP A0A4U9C786
F	-12	GLU	-	expression tag	UNP A0A4U9C786
F	-11	LYS	-	expression tag	UNP A0A4U9C786
F	-10	ILE	-	expression tag	UNP A0A4U9C786
F	-9	GLU	-	expression tag	UNP A0A4U9C786
F	-8	GLY	-	expression tag	UNP A0A4U9C786
F	-7	ARG	-	expression tag	UNP A0A4U9C786
F	-6	ARG	-	expression tag	UNP A0A4U9C786
F	-5	ASP	-	expression tag	UNP A0A4U9C786
F	-4	ARG	-	expression tag	UNP A0A4U9C786
F	-3	GLY	-	expression tag	UNP A0A4U9C786
F	-2	PRO	-	expression tag	UNP A0A4U9C786

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLU	-	expression tag	UNP A0A4U9C786
F	0	PHE	-	expression tag	UNP A0A4U9C786
F	1	LEU	MET	conflict	UNP A0A4U9C786
F	58	THR	ALA	conflict	UNP A0A4U9C786
F	284	SER	CYS	conflict	UNP A0A4U9C786
G	-20	ALA	-	expression tag	UNP A0A4U9C786
G	-19	SER	-	expression tag	UNP A0A4U9C786
G	-18	TRP	-	expression tag	UNP A0A4U9C786
G	-17	SER	-	expression tag	UNP A0A4U9C786
G	-16	HIS	-	expression tag	UNP A0A4U9C786
G	-15	PRO	-	expression tag	UNP A0A4U9C786
G	-14	GLN	-	expression tag	UNP A0A4U9C786
G	-13	PHE	-	expression tag	UNP A0A4U9C786
G	-12	GLU	-	expression tag	UNP A0A4U9C786
G	-11	LYS	-	expression tag	UNP A0A4U9C786
G	-10	ILE	-	expression tag	UNP A0A4U9C786
G	-9	GLU	-	expression tag	UNP A0A4U9C786
G	-8	GLY	-	expression tag	UNP A0A4U9C786
G	-7	ARG	-	expression tag	UNP A0A4U9C786
G	-6	ARG	-	expression tag	UNP A0A4U9C786
G	-5	ASP	-	expression tag	UNP A0A4U9C786
G	-4	ARG	-	expression tag	UNP A0A4U9C786
G	-3	GLY	-	expression tag	UNP A0A4U9C786
G	-2	PRO	-	expression tag	UNP A0A4U9C786
G	-1	GLU	-	expression tag	UNP A0A4U9C786
G	0	PHE	-	expression tag	UNP A0A4U9C786
G	1	LEU	MET	conflict	UNP A0A4U9C786
G	58	THR	ALA	conflict	UNP A0A4U9C786
G	284	SER	CYS	conflict	UNP A0A4U9C786
H	-22	ALA	-	expression tag	UNP A0A4U9C786
H	-21	SER	-	expression tag	UNP A0A4U9C786
H	-20	TRP	-	expression tag	UNP A0A4U9C786
H	-19	SER	-	expression tag	UNP A0A4U9C786
H	-18	HIS	-	expression tag	UNP A0A4U9C786
H	-17	PRO	-	expression tag	UNP A0A4U9C786
H	-16	GLN	-	expression tag	UNP A0A4U9C786
H	-15	PHE	-	expression tag	UNP A0A4U9C786
H	-14	GLU	-	expression tag	UNP A0A4U9C786
H	-13	LYS	-	expression tag	UNP A0A4U9C786
H	-12	ILE	-	expression tag	UNP A0A4U9C786
H	-11	GLU	-	expression tag	UNP A0A4U9C786
H	-10	GLY	-	expression tag	UNP A0A4U9C786

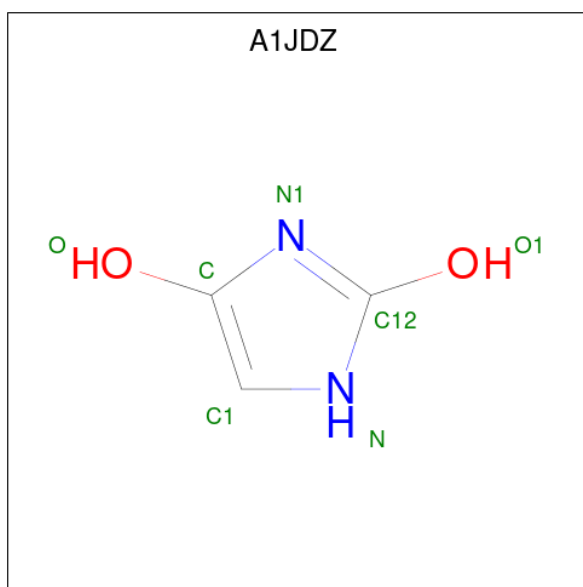
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	ARG	-	expression tag	UNP A0A4U9C786
H	-8	ARG	-	expression tag	UNP A0A4U9C786
H	-7	ASP	-	expression tag	UNP A0A4U9C786
H	-4	ARG	-	expression tag	UNP A0A4U9C786
H	-3	GLY	-	expression tag	UNP A0A4U9C786
H	-2	PRO	-	expression tag	UNP A0A4U9C786
H	-1	GLU	-	expression tag	UNP A0A4U9C786
H	0	PHE	-	expression tag	UNP A0A4U9C786
H	1	LEU	MET	conflict	UNP A0A4U9C786
H	58	THR	ALA	conflict	UNP A0A4U9C786
H	284	SER	CYS	conflict	UNP A0A4U9C786

- Molecule 2 is 1 {H}-imidazole-2,4-diol (CCD ID: A1JDZ) (formula: C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



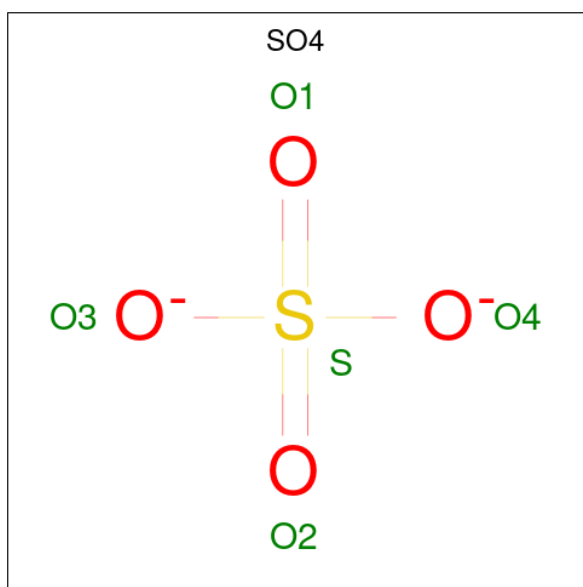
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 10	C 3	H 3	N 2	O 2	0	0
2	A	1	Total 10	C 3	H 3	N 2	O 2	0	0
2	B	1	Total 10	C 3	H 3	N 2	O 2	0	0
2	B	1	Total 10	C 3	H 3	N 2	O 2	0	0
2	B	1	Total 10	C 3	H 3	N 2	O 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	C	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	C	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	D	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	D	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	D	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	E	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	E	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	F	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	F	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	G	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	G	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	G	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	H	1	Total	C	H	N	O	0	0
			10	3	3	2	2		
2	H	1	Total	C	H	N	O	0	0
			10	3	3	2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	578	Total	O	0	0
			578	578		
5	B	523	Total	O	0	0
			523	523		
5	C	676	Total	O	0	1
			677	677		

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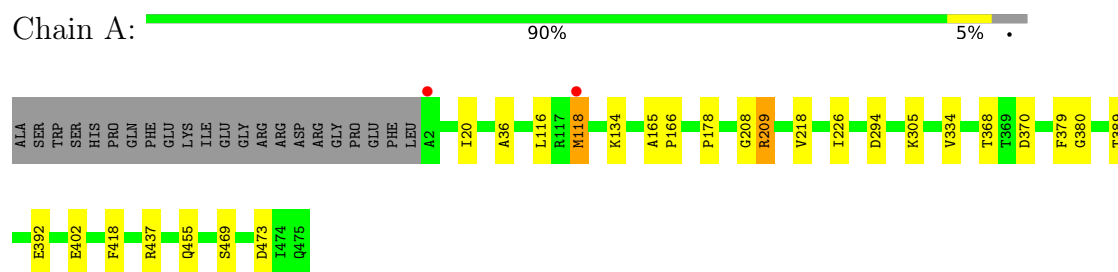
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	571	Total 571	O 571	0	0
5	E	473	Total 473	O 473	0	0
5	F	587	Total 587	O 587	0	0
5	G	652	Total 652	O 652	0	0
5	H	496	Total 496	O 496	0	0

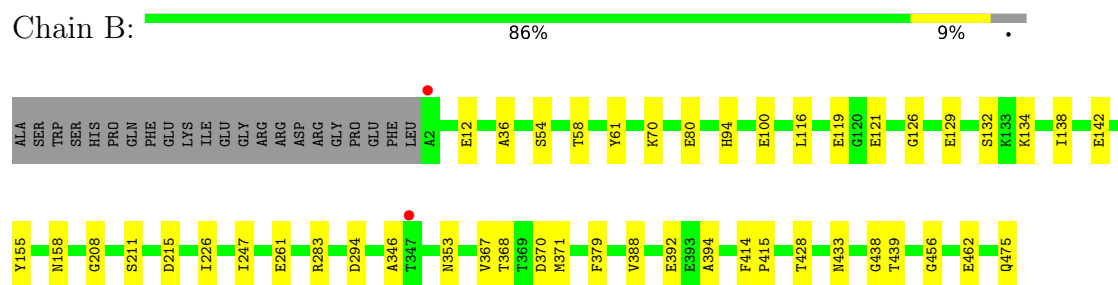
### 3 Residue-property plots

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

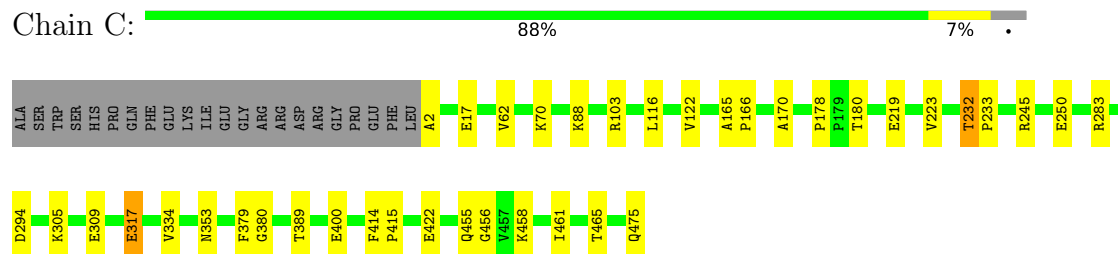
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



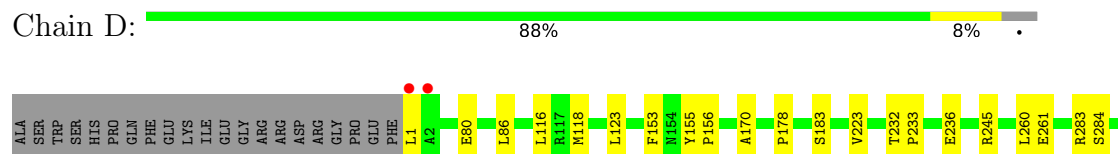
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

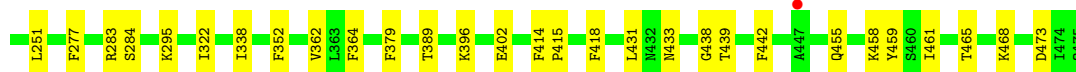
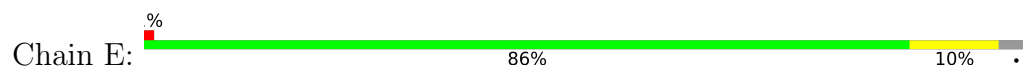


- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

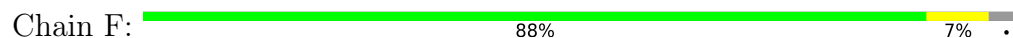




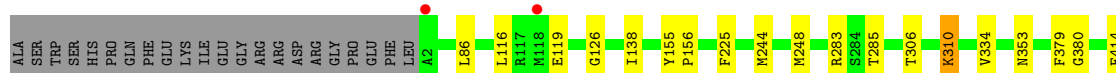
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



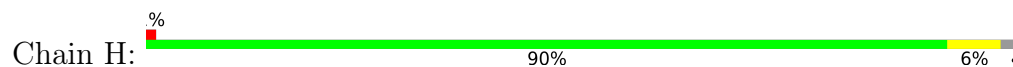
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.15Å 97.15Å 100.70Å 76.94° 77.99° 68.28°	Depositor
Resolution (Å)	46.58 – 1.57 46.58 – 1.57	Depositor EDS
% Data completeness (in resolution range)	81.6 (46.58-1.57) 82.2 (46.58-1.57)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 1.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.155 , 0.191 0.155 , 0.191	Depositor DCC
$R_{free}$ test set	19206 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	65210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, A1JDZ, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.19	0/3822	0.42	0/5179
1	B	0.18	0/3913	0.41	1/5304 (0.0%)
1	C	0.21	0/3889	0.47	1/5272 (0.0%)
1	D	0.19	0/3830	0.42	0/5194
1	E	0.19	0/3817	0.40	0/5174
1	F	0.19	0/3933	0.43	0/5327
1	G	0.20	0/3889	0.44	1/5271 (0.0%)
1	H	0.18	0/3874	0.39	0/5247
All	All	0.19	0/30967	0.42	3/41968 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	456	GLY	N-CA-C	-6.95	104.07	112.48
1	G	456	GLY	N-CA-C	-6.57	104.53	112.48
1	B	456	GLY	N-CA-C	-5.00	106.15	112.65

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	455	GLN	Peptide
1	D	455	GLN	Peptide
1	E	455	GLN	Peptide
1	H	455	GLN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3677	3784	3754	22	0
1	B	3726	3839	3770	35	0
1	C	3717	3857	3815	29	0
1	D	3676	3787	3744	26	0
1	E	3673	3789	3764	38	0
1	F	3732	3853	3756	31	0
1	G	3720	3871	3841	20	0
1	H	3717	3839	3791	32	0
2	A	14	6	0	1	0
2	B	21	9	0	0	0
2	C	21	9	0	0	0
2	D	21	9	0	1	0
2	E	14	6	0	2	0
2	F	14	6	0	1	0
2	G	21	9	0	1	0
2	H	21	9	0	1	0
3	A	10	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	10	0	0	1	0
3	E	5	0	0	2	0
3	F	10	0	0	0	0
3	G	5	0	0	0	0
3	H	10	0	0	0	0
4	A	6	8	8	1	0
4	B	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	8	8	1	0
4	E	6	8	8	1	0
4	F	6	8	8	1	0
4	G	12	16	16	0	0
4	H	6	8	8	0	0
5	A	578	0	0	5	0
5	B	523	0	0	11	3
5	C	677	0	0	12	5
5	D	571	0	0	6	3
5	E	473	0	0	11	2
5	F	587	0	0	10	1
5	G	652	0	0	2	7
5	H	496	0	0	6	1
All	All	34456	30754	30307	208	11

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 (208) 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:F:455:GLN:OE1	5:F:601:HOH:O	1.79	0.99
1:C:2:ALA:N	5:C:601:HOH:O	1.95	0.98
1:C:88[A]:LYS:NZ	5:C:602:HOH:O	2.00	0.88
1:A:118[A]:MET:SD	5:A:901:HOH:O	2.34	0.85
1:B:121:GLU:OE1	5:B:602:HOH:O	1.94	0.84
1:E:122[B]:VAL:HG11	1:H:138[B]:ILE:HG23	1.57	0.84
1:B:462:GLU:OE1	5:B:601:HOH:O	1.94	0.84
1:A:473:ASP:OD2	1:B:433[B]:ASN:ND2	2.12	0.83
1:C:294[B]:ASP:OD2	1:C:389:THR:HG22	1.78	0.82
1:G:433[B]:ASN:ND2	1:H:473:ASP:OD2	2.13	0.81
1:F:240:LYS:O	5:F:602:HOH:O	1.96	0.81
3:E:503:SO4:S	5:E:605:HOH:O	2.38	0.81
1:D:80[A]:GLU:OE1	5:D:601:HOH:O	1.99	0.79
1:H:305[A]:LYS:NZ	5:H:603:HOH:O	2.18	0.77
1:H:475:GLN:OXT	5:H:601:HOH:O	2.02	0.77
1:C:17:GLU:OE2	5:C:603:HOH:O	2.03	0.75
1:E:473:ASP:OD2	1:F:433[B]:ASN:ND2	2.20	0.75
1:D:283:ARG:NH1	3:D:503:SO4:O4	2.20	0.75
1:B:475:GLN:OE1	5:B:603:HOH:O	2.05	0.74
1:C:219:GLU:OE1	5:C:604:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ARG:NH1	5:C:606:HOH:O	2.21	0.73
1:F:462:GLU:OE1	5:F:603:HOH:O	2.05	0.73
1:B:392:GLU:OE1	5:B:604:HOH:O	2.07	0.72
1:C:475:GLN:NE2	5:C:607:HOH:O	2.22	0.71
1:B:119:GLU:OE2	5:B:606:HOH:O	2.09	0.70
1:B:61[B]:TYR:OH	5:B:605:HOH:O	2.08	0.69
1:F:2:ALA:N	5:F:607:HOH:O	2.26	0.68
2:F:501:A1JDZ:O1	5:F:604:HOH:O	2.12	0.68
1:F:129[A]:GLU:OE2	1:F:132:SER:OG	2.10	0.67
3:E:503:SO4:O1	5:E:601:HOH:O	2.11	0.67
1:H:191:GLU:OE2	5:H:602:HOH:O	2.12	0.66
1:G:306[B]:THR:HG23	5:G:704:HOH:O	1.95	0.66
1:D:284[C]:SER:OG	2:D:501:A1JDZ:O	2.13	0.66
1:C:305:LYS:NZ	1:C:309:GLU:OE2	2.26	0.65
2:E:501:A1JDZ:O1	5:E:602:HOH:O	2.13	0.65
1:F:309[B]:GLU:OE2	5:F:605:HOH:O	2.13	0.64
1:D:260:LEU:HD22	1:D:391:VAL:HG12	1.80	0.64
1:F:458:LYS:NZ	1:H:119:GLU:OE1	2.24	0.61
1:A:118[A]:MET:HE2	1:A:118[A]:MET:HA	1.81	0.61
1:F:248[B]:MET:HE2	1:F:455:GLN:HG2	1.83	0.61
1:E:122[A]:VAL:HG21	1:H:138[A]:ILE:HG23	1.85	0.59
1:E:458[A]:LYS:NZ	1:G:119:GLU:OE1	2.29	0.59
1:C:414[B]:PHE:HB3	1:C:415:PRO:HD3	1.86	0.58
1:D:80[B]:GLU:OE2	5:D:602:HOH:O	2.17	0.58
1:G:353:ASN:OD1	5:G:602:HOH:O	2.17	0.58
1:F:462:GLU:OE2	5:F:606:HOH:O	2.16	0.58
1:C:475:GLN:OE1	5:C:605:HOH:O	2.18	0.57
1:E:121:GLU:N	1:H:122[B]:VAL:HG12	2.21	0.56
1:A:118[A]:MET:HE3	5:A:676:HOH:O	2.05	0.55
1:E:433[B]:ASN:OD1	5:E:603:HOH:O	2.18	0.55
1:C:170:ALA:HB1	1:C:465:THR:HG22	1.88	0.55
1:D:309:GLU:OE1	5:D:603:HOH:O	2.18	0.55
1:E:74:ILE:HD13	1:E:195:GLU:HB3	1.89	0.55
1:E:170:ALA:HB1	1:E:465:THR:HG22	1.88	0.54
1:B:226:ILE:HB	1:B:247:ILE:HG22	1.89	0.54
1:F:218:VAL:HG13	1:F:226:ILE:HD13	1.90	0.53
1:B:142:GLU:OE2	5:B:608:HOH:O	2.19	0.53
1:C:116:LEU:C	1:C:116:LEU:HD12	2.32	0.53
1:E:389[A]:THR:OG1	5:E:604:HOH:O	2.19	0.53
1:H:334:VAL:HG21	1:H:380:GLY:HA3	1.89	0.53
1:E:116:LEU:HD12	1:E:116:LEU:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22[A]:ILE:HD12	1:E:184:ILE:HG13	1.92	0.52
1:H:141:ARG:HD2	1:H:467:VAL:HG12	1.92	0.52
1:G:334:VAL:HG21	1:G:380:GLY:HA3	1.92	0.51
1:A:294:ASP:OD2	1:A:389[A]:THR:HG22	2.11	0.51
1:B:283:ARG:NH1	5:B:620:HOH:O	2.34	0.51
1:H:3:LYS:NZ	5:H:602:HOH:O	2.43	0.51
1:D:236:GLU:OE2	1:D:449:LYS:NZ	2.33	0.51
1:B:368:THR:OG1	1:B:370:ASP:OD1	2.26	0.51
1:C:317[A]:GLU:CD	5:C:619:HOH:O	2.54	0.51
1:A:334:VAL:HG21	1:A:380:GLY:HA3	1.93	0.50
1:D:412:THR:HG22	5:D:1050:HOH:O	2.10	0.50
1:E:461:ILE:O	1:E:465:THR:HG23	2.12	0.50
1:D:223:VAL:O	1:D:245:ARG:HD2	2.11	0.50
1:F:248[B]:MET:HE1	1:F:460[B]:SER:HA	1.94	0.49
1:F:405[B]:LEU:HG	1:F:450:SER:HB3	1.95	0.49
1:E:414[B]:PHE:CE2	1:E:431:LEU:HD12	2.48	0.49
1:E:118:MET:HE2	5:E:766:HOH:O	2.12	0.49
1:G:244[B]:MET:HE1	1:H:251:LEU:CD1	2.42	0.49
1:B:138[A]:ILE:HG23	1:C:122:VAL:HG21	1.94	0.48
1:E:120:GLY:C	1:H:122[B]:VAL:HG12	2.38	0.48
1:G:285[B]:THR:O	1:G:285[B]:THR:OG1	2.31	0.48
1:B:261:GLU:O	5:B:609:HOH:O	2.20	0.48
1:E:418[A]:PHE:HZ	1:F:138[A]:ILE:HD12	1.79	0.48
1:A:178:PRO:HB3	5:A:677:HOH:O	2.13	0.48
1:F:122:VAL:HG21	1:G:138[B]:ILE:HG23	1.94	0.48
1:F:317[B]:GLU:H	1:F:317[B]:GLU:CD	2.21	0.48
1:G:116:LEU:C	1:G:116:LEU:HD12	2.38	0.48
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.96	0.48
1:F:62[A]:VAL:HG23	1:G:126:GLY:O	2.14	0.48
1:C:317[A]:GLU:CD	5:C:864:HOH:O	2.56	0.47
1:H:368:THR:OG1	1:H:370:ASP:OD1	2.22	0.47
1:A:418[A]:PHE:HZ	1:B:138[A]:ILE:HD12	1.80	0.47
1:E:414[B]:PHE:HB3	1:E:415:PRO:HD3	1.97	0.47
1:E:126:GLY:O	1:H:62[A]:VAL:HG23	2.15	0.47
1:E:219[A]:GLU:HG3	5:E:906:HOH:O	2.14	0.47
1:E:338:ILE:HD13	1:E:362:VAL:HG21	1.97	0.47
1:B:215:ASP:OD1	5:B:610:HOH:O	2.20	0.47
1:F:287:VAL:HG22	5:F:965:HOH:O	2.14	0.46
1:A:134:LYS:NZ	1:C:422:GLU:OE1	2.46	0.46
1:C:178:PRO:HB3	5:C:638:HOH:O	2.15	0.46
1:F:116:LEU:C	1:F:116:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:LYS:NZ	5:D:621:HOH:O	2.48	0.46
1:E:165:ALA:HB3	1:E:166:PRO:HD3	1.97	0.46
1:C:232[B]:THR:HB	1:C:233:PRO:HD3	1.98	0.46
1:H:437:ARG:H	2:H:502:A1JDZ:C1	2.29	0.46
1:A:116:LEU:HD12	1:A:116:LEU:C	2.40	0.46
1:A:368:THR:OG1	1:A:370:ASP:OD1	2.21	0.46
1:H:116:LEU:HD12	1:H:116:LEU:C	2.41	0.46
1:G:244[B]:MET:HE3	1:H:236:GLU:HG2	1.98	0.45
1:C:180:THR:HB	4:C:505:GOL:H12	1.98	0.45
1:E:338:ILE:HG21	1:E:352:PHE:HB2	1.98	0.45
1:H:236:GLU:OE1	5:H:604:HOH:O	2.20	0.45
1:E:277:PHE:HB3	1:E:322:ILE:HD11	1.98	0.45
1:E:338:ILE:HG23	1:E:364:PHE:CE2	2.52	0.45
1:G:438:GLY:HA2	1:G:439:THR:C	2.42	0.45
1:A:305:LYS:NZ	5:A:619:HOH:O	2.45	0.45
1:B:129[A]:GLU:OE2	1:B:132:SER:OG	2.28	0.45
1:E:134:LYS:NZ	1:G:422:GLU:OE1	2.49	0.45
1:E:438:GLY:HA2	1:E:439:THR:C	2.42	0.45
1:B:155:TYR:OH	1:B:283:ARG:HD2	2.16	0.45
1:B:70[B]:LYS:HG3	5:B:750:HOH:O	2.16	0.45
1:C:165:ALA:HB3	1:C:166:PRO:HD3	1.99	0.45
1:C:250:GLU:OE2	1:C:455[B]:GLN:HG3	2.17	0.45
1:D:325:LEU:HD21	1:D:381:PRO:HD3	1.99	0.45
1:B:414[B]:PHE:HB3	1:B:415:PRO:HD3	1.98	0.44
1:B:367:VAL:HG13	1:B:371[B]:MET:HE2	1.98	0.44
1:D:368:THR:OG1	1:D:370:ASP:OD1	2.18	0.44
5:E:997:HOH:O	1:F:267:LEU:HD22	2.17	0.44
1:C:70:LYS:HG3	5:C:1014:HOH:O	2.17	0.44
1:D:261[B]:GLU:CD	5:D:608:HOH:O	2.59	0.44
4:F:505:GOL:H2	5:F:640:HOH:O	2.17	0.44
1:E:120:GLY:HA3	1:H:122[B]:VAL:HG13	2.00	0.44
1:G:414[B]:PHE:HB3	1:G:415:PRO:HD3	2.00	0.44
1:C:223:VAL:O	1:C:245:ARG:HD2	2.18	0.44
1:H:414[B]:PHE:HB3	1:H:415:PRO:HD3	2.00	0.44
1:D:178:PRO:HB2	1:D:183:SER:HA	2.00	0.43
1:H:232:THR:N	1:H:233[A]:PRO:HD2	2.33	0.43
1:A:392:GLU:N	1:A:392:GLU:CD	2.77	0.43
1:E:284[B]:SER:OG	2:E:501:A1JDZ:O	2.33	0.43
1:A:392:GLU:CD	1:A:392:GLU:H	2.26	0.43
1:A:469[B]:SER:OG	1:B:428:THR:HG23	2.19	0.43
1:B:126:GLY:O	1:C:62[A]:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86[A]:LEU:HD13	1:G:156:PRO:HG2	2.01	0.43
1:G:437:ARG:HD2	2:G:502:A1JDZ:O1	2.19	0.43
1:B:346:ALA:HB2	1:B:371[B]:MET:HE1	2.01	0.43
1:F:70[B]:LYS:HD3	1:F:196:ALA:HA	2.00	0.43
1:C:353[B]:ASN:ND2	5:C:632:HOH:O	2.48	0.43
1:B:438:GLY:HA2	1:B:439:THR:C	2.43	0.43
1:D:153:PHE:CD1	1:D:153:PHE:C	2.97	0.43
1:A:20:ILE:HD11	1:A:209:ARG:HG2	2.01	0.43
1:B:36:ALA:HA	1:B:208:GLY:HA2	2.00	0.42
1:D:86[A]:LEU:HD13	1:D:156:PRO:HG2	2.00	0.42
1:D:232:THR:N	1:D:233[A]:PRO:HD2	2.35	0.42
1:E:120:GLY:HA3	1:H:122[B]:VAL:CG1	2.50	0.42
1:E:122[A]:VAL:HG23	1:H:122[A]:VAL:HG23	2.00	0.42
4:E:504:GOL:H2	5:E:683:HOH:O	2.19	0.42
1:A:402:GLU:OE1	4:A:505:GOL:O1	2.28	0.42
1:D:334:VAL:HG21	1:D:380:GLY:HA3	2.01	0.42
1:F:415:PRO:HG3	1:G:414[A]:PHE:CE2	2.55	0.42
1:A:36:ALA:HA	1:A:208:GLY:HA2	2.01	0.42
1:E:230:GLY:O	1:E:251:LEU:HA	2.20	0.42
1:F:260:LEU:HD22	1:F:391:VAL:HG22	2.01	0.42
1:D:155:TYR:HH	1:D:283:ARG:HD2	1.83	0.41
1:E:295:LYS:NZ	5:E:614:HOH:O	2.39	0.41
1:B:80:GLU:OE2	1:B:94[B]:HIS:NE2	2.45	0.41
1:B:346:ALA:HB2	1:B:371[B]:MET:CE	2.50	0.41
1:B:370:ASP:HB3	1:H:306:THR:HG23	2.02	0.41
1:E:151:SER:O	1:E:179:PRO:HD3	2.20	0.41
1:D:116:LEU:HD12	1:D:116:LEU:C	2.44	0.41
1:E:442:PHE:HA	1:F:123:LEU:HD12	2.01	0.41
1:A:218:VAL:HG13	1:A:226:ILE:HD13	2.02	0.41
1:C:461:ILE:O	1:C:465:THR:HG23	2.20	0.41
1:A:118[A]:MET:CE	5:A:676:HOH:O	2.68	0.41
1:E:418[A]:PHE:CZ	1:F:138[A]:ILE:HD12	2.56	0.41
1:H:232:THR:HB	1:H:233[B]:PRO:HD3	2.02	0.41
1:B:211:SER:OG	3:B:504:SO4:O1	2.33	0.41
1:E:396[A]:LYS:HG3	5:E:748:HOH:O	2.19	0.41
1:G:155:TYR:OH	1:G:283:ARG:HD2	2.21	0.41
1:H:153:PHE:CD1	1:H:153:PHE:C	2.98	0.41
1:B:134:LYS:NZ	1:D:422:GLU:OE1	2.52	0.41
1:B:367:VAL:HG13	1:B:371[B]:MET:CE	2.51	0.41
1:E:459:TYR:OH	1:F:123:LEU:HD11	2.20	0.41
1:F:100:GLU:HG3	1:F:158:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248[A]:MET:HG3	5:F:942:HOH:O	2.20	0.41
1:F:264:ASP:OD1	1:F:264:ASP:C	2.63	0.41
1:F:347[B]:THR:OG1	1:F:365:ASP:HB3	2.21	0.41
1:H:36:ALA:HA	1:H:208:GLY:HA2	2.02	0.41
1:H:118:MET:HG3	5:H:1036:HOH:O	2.19	0.41
1:A:437:ARG:HD2	2:A:502:A1JDZ:O	2.21	0.40
1:E:122[B]:VAL:CG2	1:H:120:GLY:HA3	2.51	0.40
1:H:232:THR:O	1:H:236:GLU:HG3	2.21	0.40
1:B:100:GLU:HG3	1:B:158:ASN:HB2	2.04	0.40
1:D:414[B]:PHE:HB3	1:D:415:PRO:HD3	2.02	0.40
1:B:54:SER:O	1:B:58[B]:THR:HG23	2.20	0.40
1:B:388:VAL:HG21	1:B:394:ALA:HB2	2.03	0.40
1:C:334:VAL:HG21	1:C:380:GLY:HA3	2.03	0.40
1:D:170:ALA:HB1	1:D:465[A]:THR:HG22	2.03	0.40
1:G:225:PHE:CZ	1:G:248[A]:MET:HG3	2.57	0.40
1:D:155:TYR:OH	1:D:283:ARG:HD2	2.20	0.40

All (11) 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)
5:D:742:HOH:O	5:H:681:HOH:O[1_546]	1.98	0.22
5:D:637:HOH:O	5:G:977:HOH:O[1_646]	1.99	0.21
5:C:754:HOH:O	5:G:1027:HOH:O[1_546]	2.01	0.19
5:B:985:HOH:O	5:E:892:HOH:O[1_655]	2.04	0.16
5:D:637:HOH:O	5:G:707:HOH:O[1_646]	2.05	0.15
5:B:1069:HOH:O	5:C:988:HOH:O[1_655]	2.08	0.12
5:C:767:HOH:O	5:G:868:HOH:O[1_546]	2.09	0.11
5:C:851:HOH:O	5:G:1088:HOH:O[1_546]	2.12	0.08
5:E:953:HOH:O	5:G:813:HOH:O[1_556]	2.12	0.08
5:B:674:HOH:O	5:C:637:HOH:O[1_565]	2.15	0.05
5:F:990:HOH:O	5:G:1204:HOH:O[1_545]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/496 (101%)	492 (98%)	9 (2%)	0	100	100
1	B	510/496 (103%)	499 (98%)	11 (2%)	0	100	100
1	C	508/496 (102%)	493 (97%)	15 (3%)	0	100	100
1	D	502/496 (101%)	490 (98%)	12 (2%)	0	100	100
1	E	500/496 (101%)	491 (98%)	9 (2%)	0	100	100
1	F	513/496 (103%)	501 (98%)	12 (2%)	0	100	100
1	G	510/496 (103%)	498 (98%)	12 (2%)	0	100	100
1	H	505/496 (102%)	497 (98%)	8 (2%)	0	100	100
All	All	4049/3968 (102%)	3961 (98%)	88 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	394/388 (102%)	390 (99%)	4 (1%)	73	55
1	B	403/388 (104%)	399 (99%)	4 (1%)	73	55
1	C	404/388 (104%)	398 (98%)	6 (2%)	60	36
1	D	398/388 (103%)	395 (99%)	3 (1%)	79	65
1	E	396/388 (102%)	391 (99%)	5 (1%)	65	42
1	F	407/388 (105%)	403 (99%)	4 (1%)	73	55
1	G	403/388 (104%)	401 (100%)	2 (0%)	86	78
1	H	401/388 (103%)	399 (100%)	2 (0%)	86	78
All	All	3206/3104 (103%)	3176 (99%)	30 (1%)	75	59

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118[A]	MET
1	A	118[B]	MET
1	A	209	ARG
1	A	379	PHE
1	B	12	GLU
1	B	294	ASP
1	B	353	ASN
1	B	379	PHE
1	C	232[A]	THR
1	C	232[B]	THR
1	C	283	ARG
1	C	317[A]	GLU
1	C	317[B]	GLU
1	C	379	PHE
1	D	1	LEU
1	D	118	MET
1	D	379	PHE
1	E	209	ARG
1	E	283	ARG
1	E	379	PHE
1	E	402	GLU
1	E	468	LYS
1	F	244[A]	MET
1	F	244[B]	MET
1	F	379	PHE
1	F	468	LYS
1	G	310	LYS
1	G	379	PHE
1	H	134	LYS
1	H	379	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	B	475	GLN
1	C	4	GLN
1	D	475	GLN
1	E	18	ASN
1	E	353	ASN
1	F	18	ASN
1	H	7	ASN
1	H	18	ASN

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Mol	Chain	Res	Type
1	H	366	HIS

### 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](#)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.14	0
2	A1JDZ	F	501	-	4,7,7	1.86	1 (25%)	1,9,9	1.32	0
4	GOL	A	505	-	5,5,5	0.92	0	5,5,5	0.86	0
2	A1JDZ	B	501	-	4,7,7	1.75	1 (25%)	1,9,9	1.26	0
4	GOL	G	506	-	5,5,5	0.72	0	5,5,5	1.03	0
3	SO4	F	503	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.12	0
2	A1JDZ	B	502	-	4,7,7	1.79	2 (50%)	1,9,9	1.35	0
2	A1JDZ	D	502	-	4,7,7	1.67	1 (25%)	1,9,9	1.17	0
2	A1JDZ	D	501	-	4,7,7	1.85	1 (25%)	1,9,9	1.46	0
2	A1JDZ	H	506	-	4,7,7	1.88	2 (50%)	1,9,9	1.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	504	-	4,4,4	0.12	0	6,6,6	0.15	0
4	GOL	B	505	-	5,5,5	0.77	0	5,5,5	1.04	0
2	A1JDZ	G	501	-	4,7,7	1.75	1 (25%)	1,9,9	1.30	0
3	SO4	H	503	-	4,4,4	0.13	0	6,6,6	0.12	0
2	A1JDZ	E	502	-	4,7,7	1.75	1 (25%)	1,9,9	1.21	0
4	GOL	F	505	-	5,5,5	0.66	0	5,5,5	1.01	0
3	SO4	A	504	-	4,4,4	0.16	0	6,6,6	0.09	0
4	GOL	H	505	-	5,5,5	0.68	0	5,5,5	1.06	0
2	A1JDZ	C	502	-	4,7,7	1.86	2 (50%)	1,9,9	1.54	0
2	A1JDZ	C	501	-	4,7,7	1.64	1 (25%)	1,9,9	0.99	0
2	A1JDZ	E	501	-	4,7,7	1.74	1 (25%)	1,9,9	1.03	0
2	A1JDZ	D	505	-	4,7,7	1.84	1 (25%)	1,9,9	1.07	0
3	SO4	F	504	-	4,4,4	0.15	0	6,6,6	0.06	0
2	A1JDZ	C	503	-	4,7,7	2.00	1 (25%)	1,9,9	1.10	0
4	GOL	C	505	-	5,5,5	0.62	0	5,5,5	0.81	0
4	GOL	B	506	-	5,5,5	0.86	0	5,5,5	1.09	1 (20%)
3	SO4	G	503	-	4,4,4	0.12	0	6,6,6	0.15	0
2	A1JDZ	H	501	-	4,7,7	1.75	1 (25%)	1,9,9	1.33	0
2	A1JDZ	H	502	-	4,7,7	1.87	1 (25%)	1,9,9	0.75	0
3	SO4	E	503	-	4,4,4	0.16	0	6,6,6	0.21	0
3	SO4	H	504	-	4,4,4	0.13	0	6,6,6	0.18	0
2	A1JDZ	A	501	-	4,7,7	1.65	2 (50%)	1,9,9	1.56	0
2	A1JDZ	F	502	-	4,7,7	1.75	1 (25%)	1,9,9	1.16	0
4	GOL	G	505	-	5,5,5	0.92	0	5,5,5	0.98	0
2	A1JDZ	B	503	-	4,7,7	1.96	1 (25%)	1,9,9	0.95	0
4	GOL	E	504	-	5,5,5	0.40	0	5,5,5	0.57	0
2	A1JDZ	A	502	-	4,7,7	1.79	2 (50%)	1,9,9	1.47	0
3	SO4	D	503	-	4,4,4	0.16	0	6,6,6	0.50	0
2	A1JDZ	G	504	-	4,7,7	2.02	1 (25%)	1,9,9	1.00	0
2	A1JDZ	G	502	-	4,7,7	1.68	1 (25%)	1,9,9	1.14	0
3	SO4	A	503	-	4,4,4	0.12	0	6,6,6	0.49	0

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
2	A1JDZ	F	501	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	505	-	-	3/4/4/4	-
4	GOL	G	506	-	-	2/4/4/4	-
2	A1JDZ	B	502	-	-	-	0/1/1/1
2	A1JDZ	G	502	-	-	-	0/1/1/1
2	A1JDZ	D	502	-	-	-	0/1/1/1
2	A1JDZ	D	501	-	-	-	0/1/1/1
2	A1JDZ	H	506	-	-	-	0/1/1/1
4	GOL	B	505	-	-	0/4/4/4	-
4	GOL	F	505	-	-	2/4/4/4	-
2	A1JDZ	G	501	-	-	-	0/1/1/1
2	A1JDZ	E	502	-	-	-	0/1/1/1
4	GOL	H	505	-	-	2/4/4/4	-
2	A1JDZ	C	502	-	-	-	0/1/1/1
2	A1JDZ	C	501	-	-	-	0/1/1/1
2	A1JDZ	E	501	-	-	-	0/1/1/1
2	A1JDZ	D	505	-	-	-	0/1/1/1
2	A1JDZ	C	503	-	-	-	0/1/1/1
4	GOL	C	505	-	-	4/4/4/4	-
4	GOL	B	506	-	-	2/4/4/4	-
2	A1JDZ	H	501	-	-	-	0/1/1/1
2	A1JDZ	H	502	-	-	-	0/1/1/1
2	A1JDZ	A	501	-	-	-	0/1/1/1
2	A1JDZ	F	502	-	-	-	0/1/1/1
4	GOL	G	505	-	-	2/4/4/4	-
2	A1JDZ	B	503	-	-	-	0/1/1/1
4	GOL	E	504	-	-	2/4/4/4	-
2	A1JDZ	A	502	-	-	-	0/1/1/1
2	A1JDZ	G	504	-	-	-	0/1/1/1
2	A1JDZ	B	501	-	-	-	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	504	A1JDZ	C1-N	-2.87	1.32	1.36
2	C	503	A1JDZ	C1-N	-2.79	1.32	1.36
2	B	503	A1JDZ	C1-N	-2.72	1.32	1.36
2	H	502	A1JDZ	C1-N	-2.70	1.32	1.36
2	D	501	A1JDZ	C1-N	-2.65	1.32	1.36
2	D	505	A1JDZ	C1-N	-2.53	1.32	1.36
2	F	502	A1JDZ	C1-N	-2.52	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	A1JDZ	C1-N	-2.42	1.32	1.36
2	C	502	A1JDZ	C1-N	-2.41	1.32	1.36
2	H	506	A1JDZ	C12-N1	-2.38	1.31	1.34
2	H	506	A1JDZ	C1-N	-2.37	1.32	1.36
2	A	502	A1JDZ	C12-N1	-2.34	1.31	1.34
2	B	502	A1JDZ	C1-N	-2.34	1.32	1.36
2	G	501	A1JDZ	C1-N	-2.32	1.32	1.36
2	C	501	A1JDZ	C1-N	-2.29	1.32	1.36
2	H	501	A1JDZ	C1-N	-2.27	1.32	1.36
2	G	502	A1JDZ	C1-N	-2.27	1.32	1.36
2	A	502	A1JDZ	C1-N	-2.23	1.32	1.36
2	C	502	A1JDZ	C12-N1	-2.21	1.31	1.34
2	E	502	A1JDZ	C1-N	-2.21	1.33	1.36
2	D	502	A1JDZ	C1-N	-2.20	1.33	1.36
2	E	501	A1JDZ	C1-N	-2.19	1.33	1.36
2	B	501	A1JDZ	C1-N	-2.16	1.33	1.36
2	A	501	A1JDZ	C12-N1	-2.06	1.31	1.34
2	B	502	A1JDZ	C12-N1	-2.03	1.31	1.34
2	A	501	A1JDZ	C1-N	-2.02	1.33	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	506	GOL	C3-C2-C1	-2.02	103.87	111.70

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	GOL	O1-C1-C2-C3
4	C	505	GOL	O1-C1-C2-C3
4	E	504	GOL	C1-C2-C3-O3
4	F	505	GOL	O1-C1-C2-C3
4	G	505	GOL	C1-C2-C3-O3
4	H	505	GOL	C1-C2-C3-O3
4	H	505	GOL	O2-C2-C3-O3
4	E	504	GOL	O2-C2-C3-O3
4	C	505	GOL	C1-C2-C3-O3
4	C	505	GOL	O1-C1-C2-O2
4	F	505	GOL	O1-C1-C2-O2
4	A	505	GOL	O1-C1-C2-O2
4	G	505	GOL	O2-C2-C3-O3

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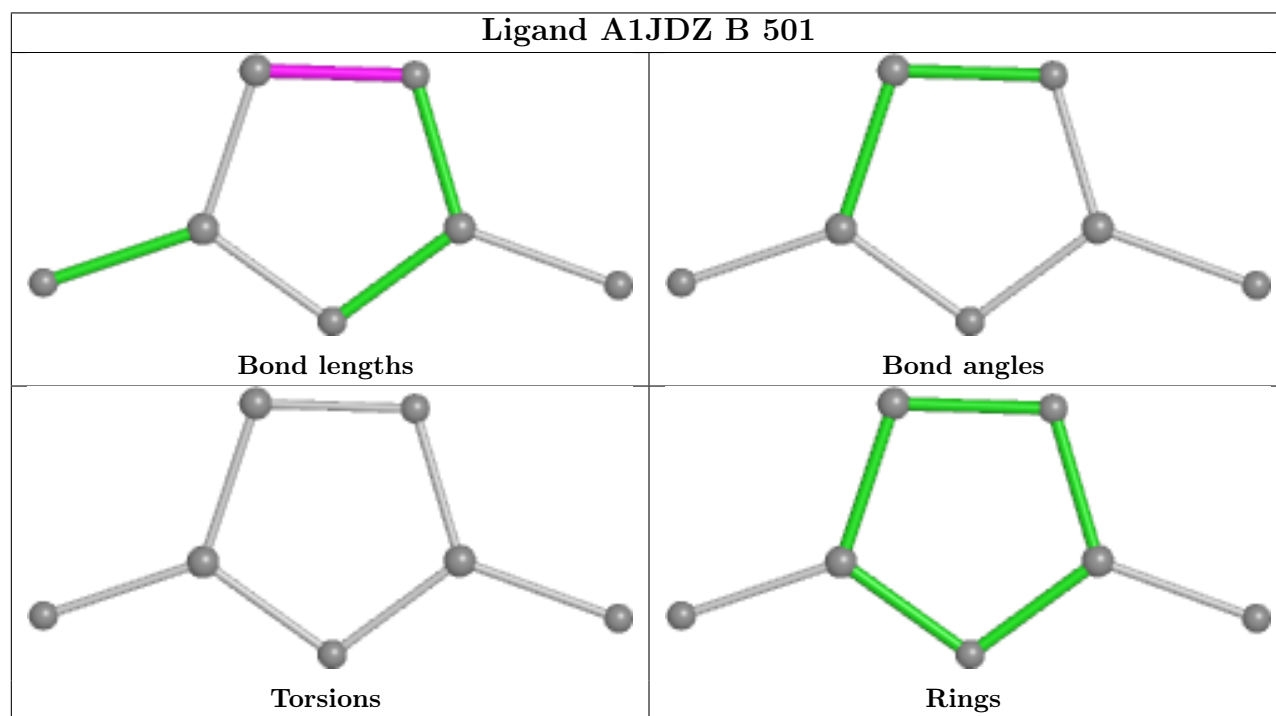
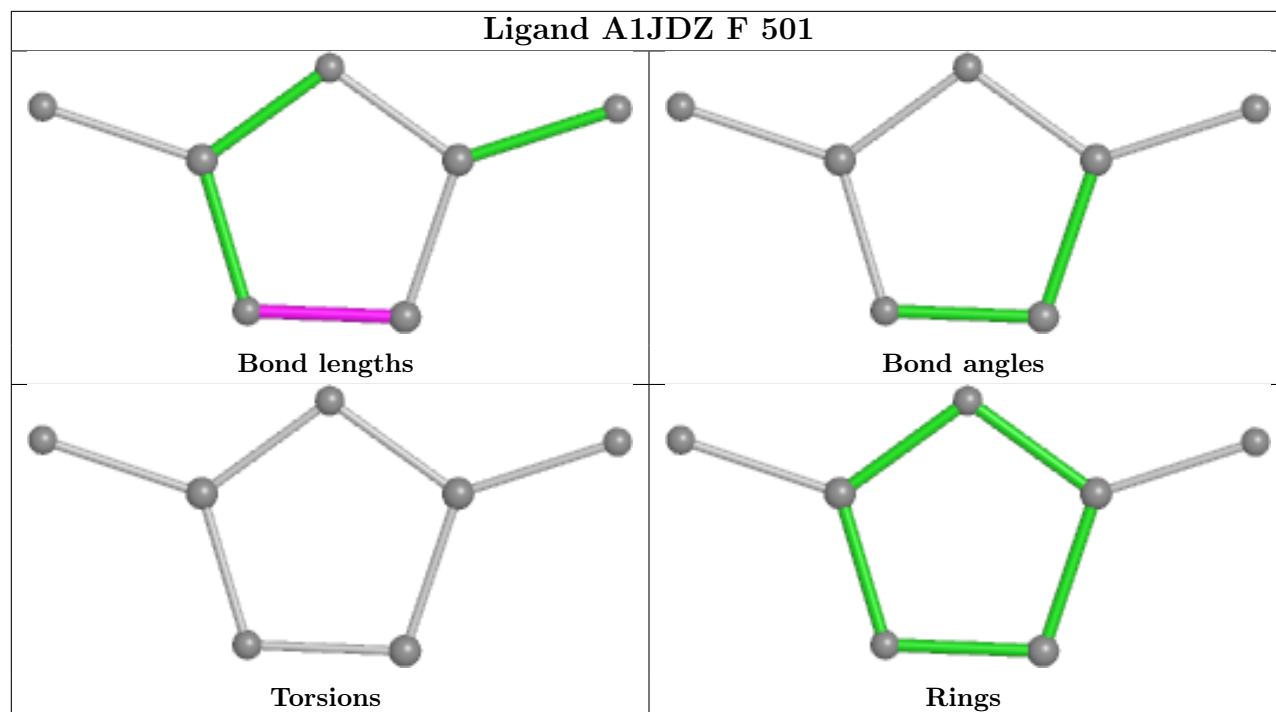
Mol	Chain	Res	Type	Atoms
4	C	505	GOL	O2-C2-C3-O3
4	B	506	GOL	O1-C1-C2-O2
4	G	506	GOL	C1-C2-C3-O3
4	B	506	GOL	O1-C1-C2-C3
4	G	506	GOL	O2-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3

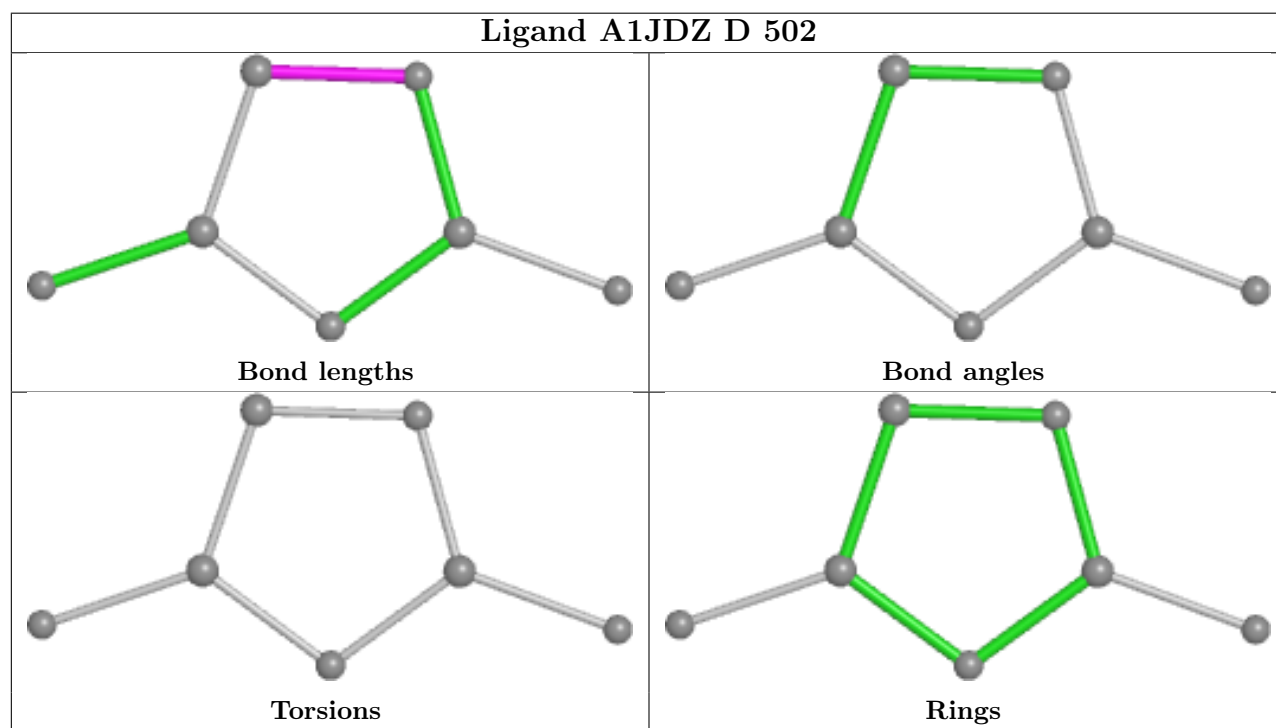
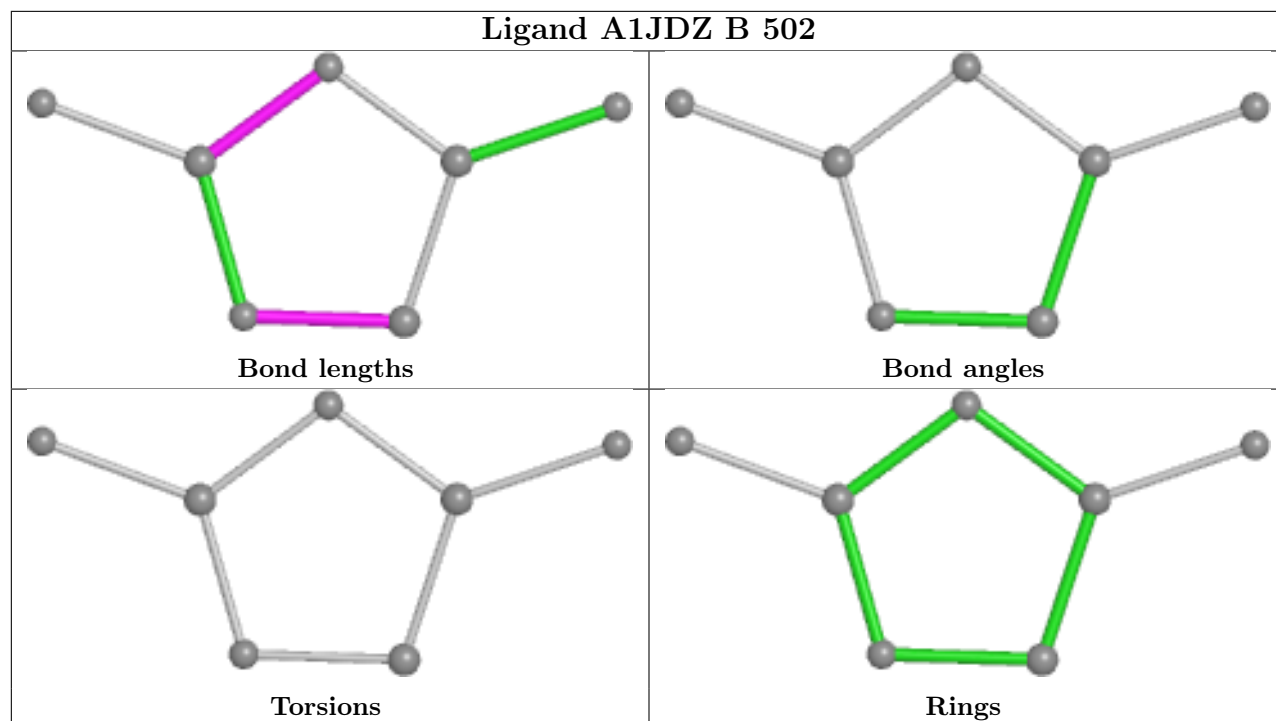
There are no ring outliers.

13 monomers are involved in 15 short contacts:

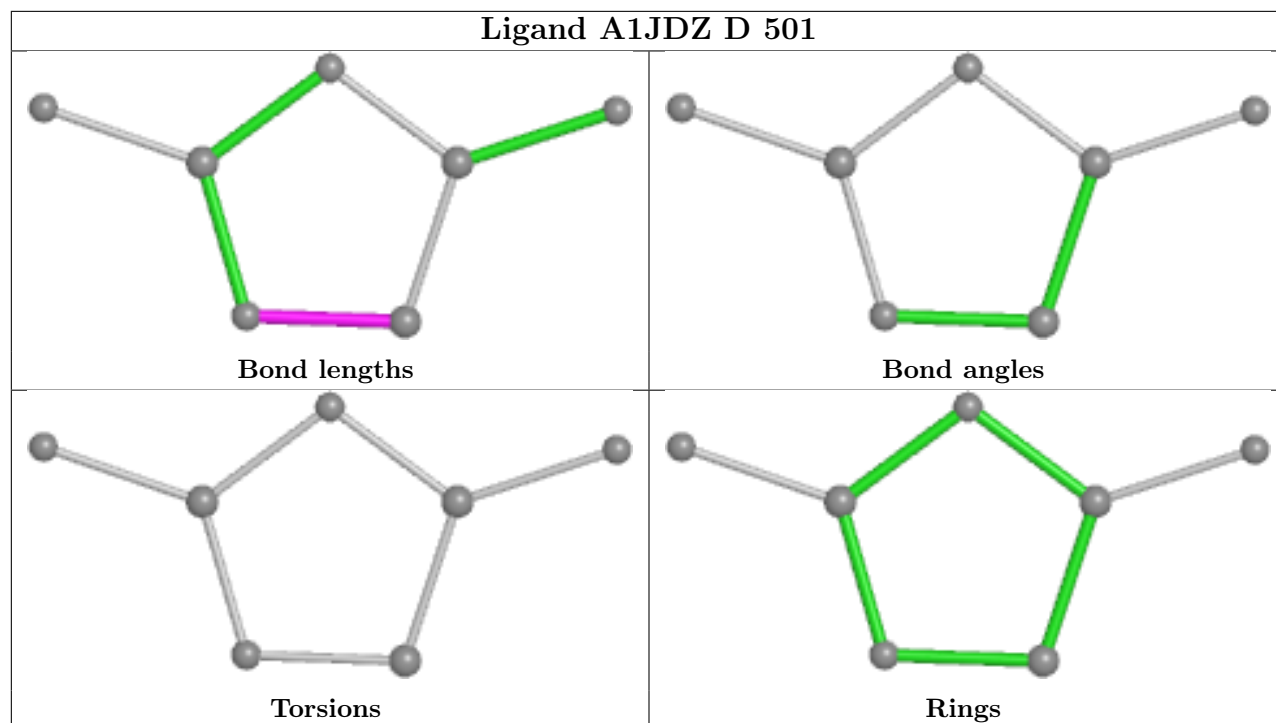
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	A1JDZ	1	0
4	A	505	GOL	1	0
2	D	501	A1JDZ	1	0
3	B	504	SO4	1	0
4	F	505	GOL	1	0
2	E	501	A1JDZ	2	0
4	C	505	GOL	1	0
2	H	502	A1JDZ	1	0
3	E	503	SO4	2	0
4	E	504	GOL	1	0
2	A	502	A1JDZ	1	0
3	D	503	SO4	1	0
2	G	502	A1JDZ	1	0

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.

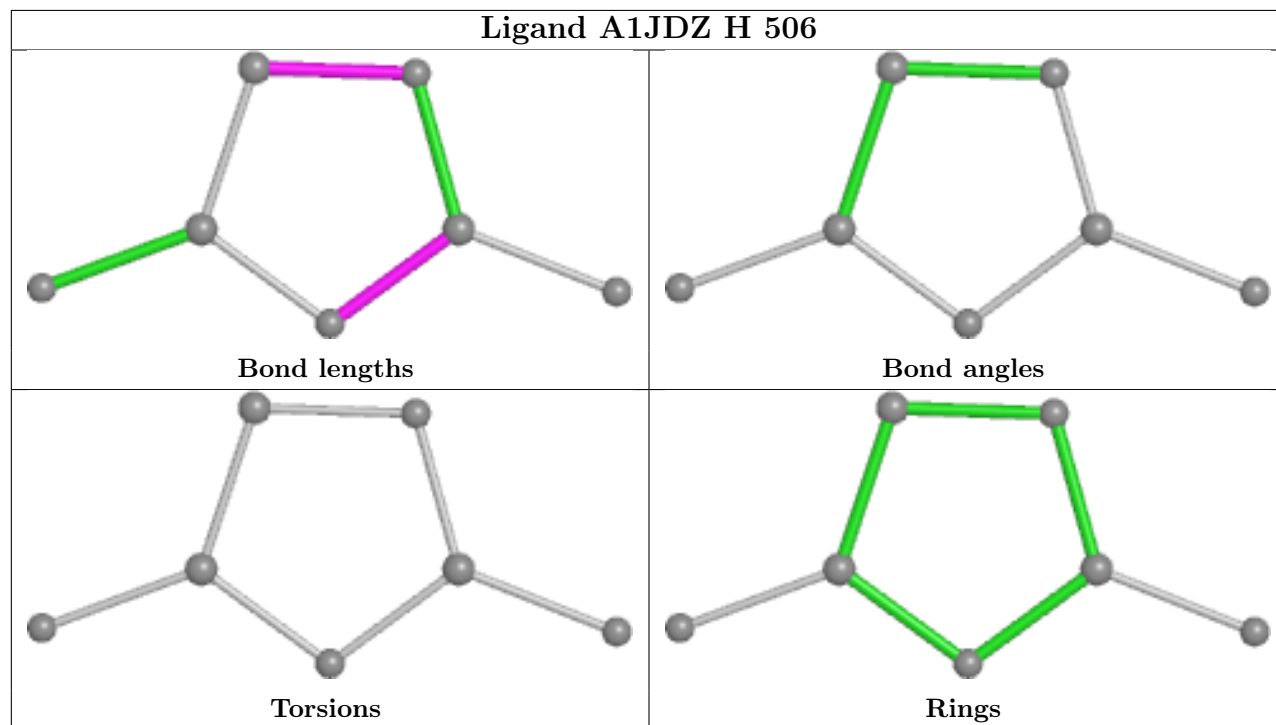




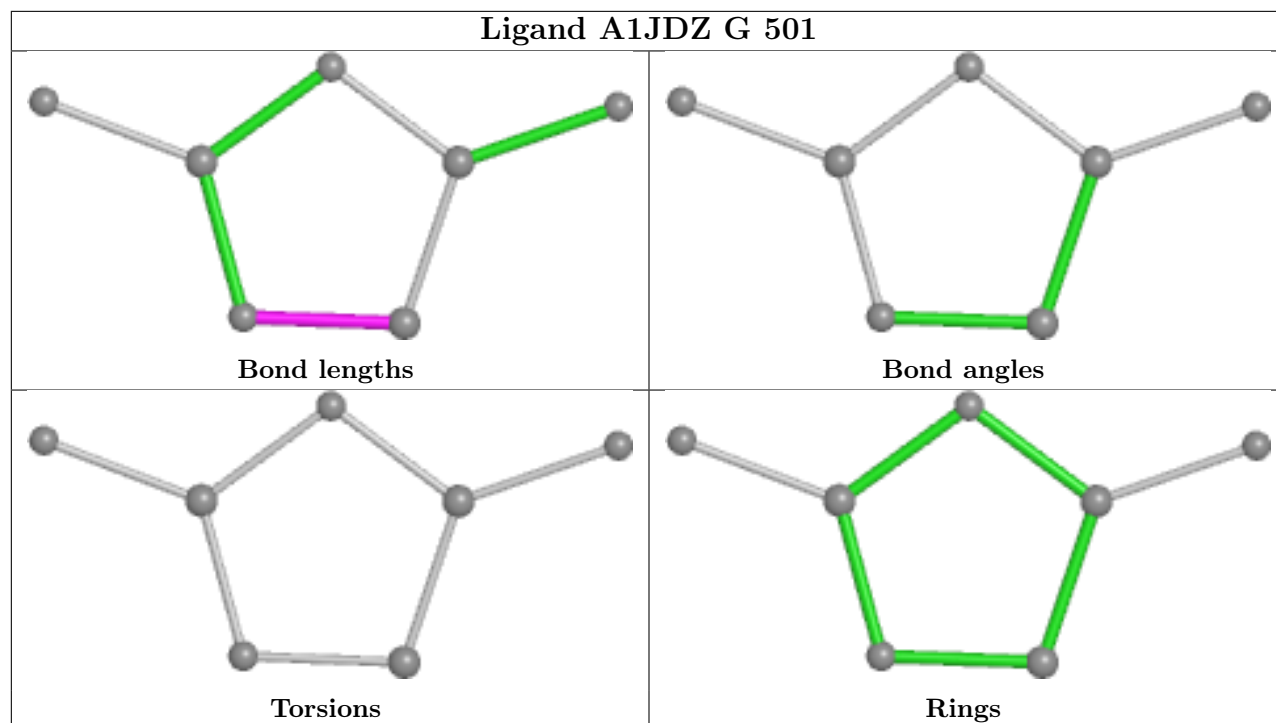
## Ligand A1JDZ D 501



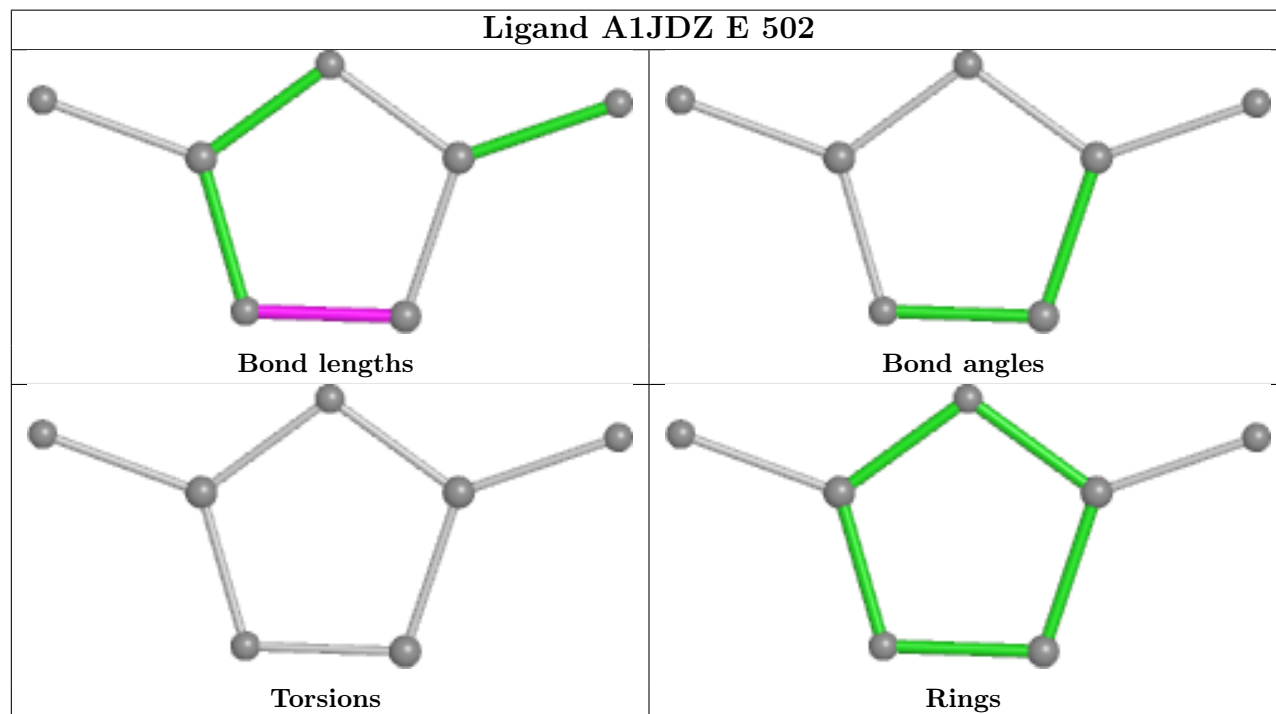
## Ligand A1JDZ H 506

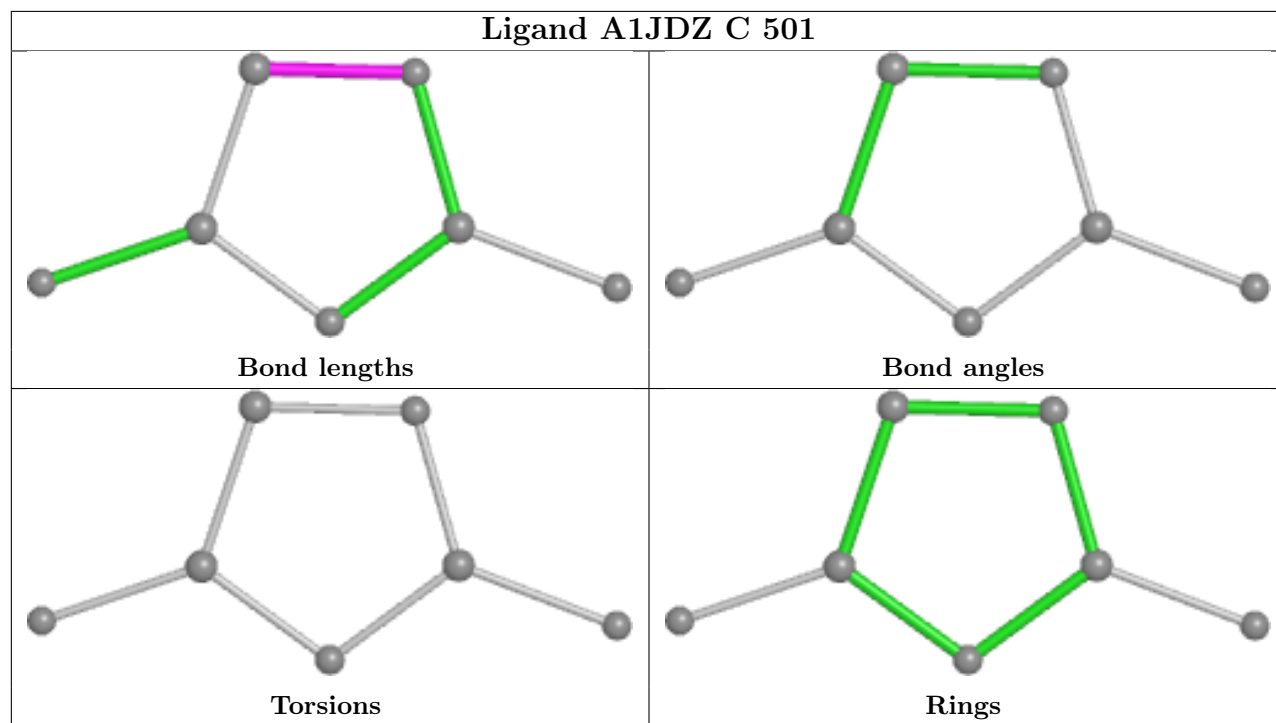
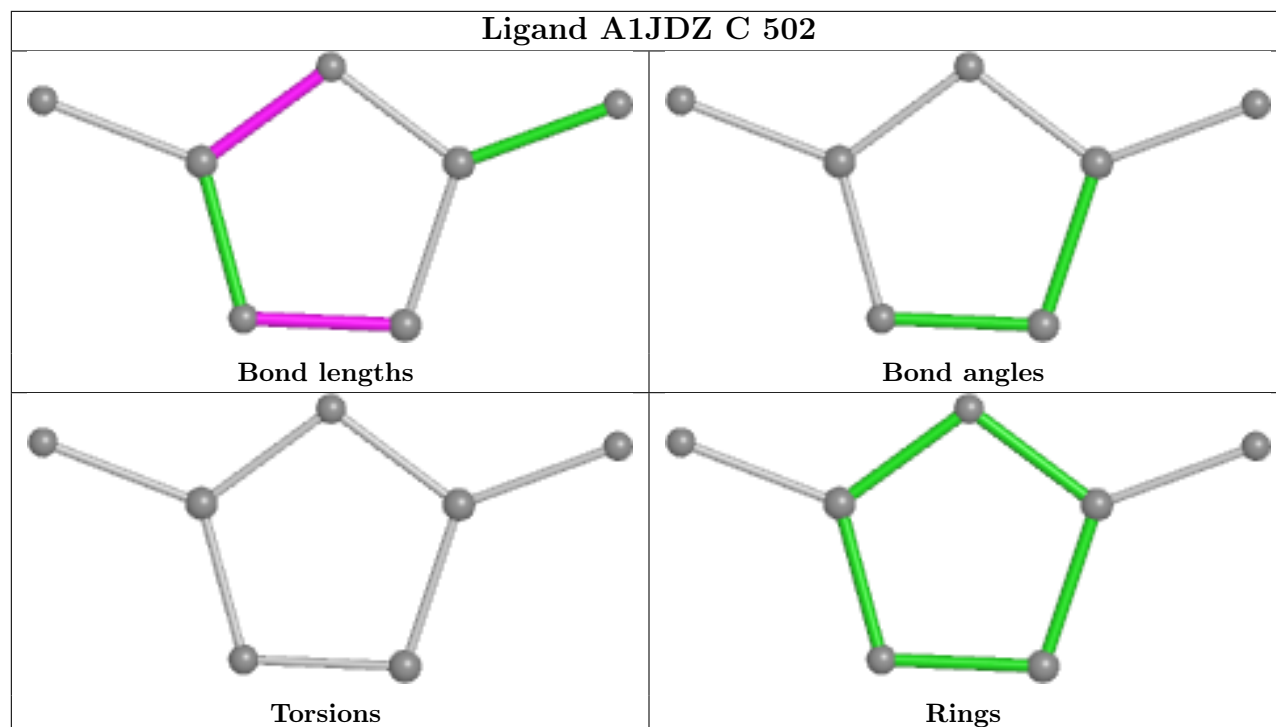


## Ligand A1JDZ G 501



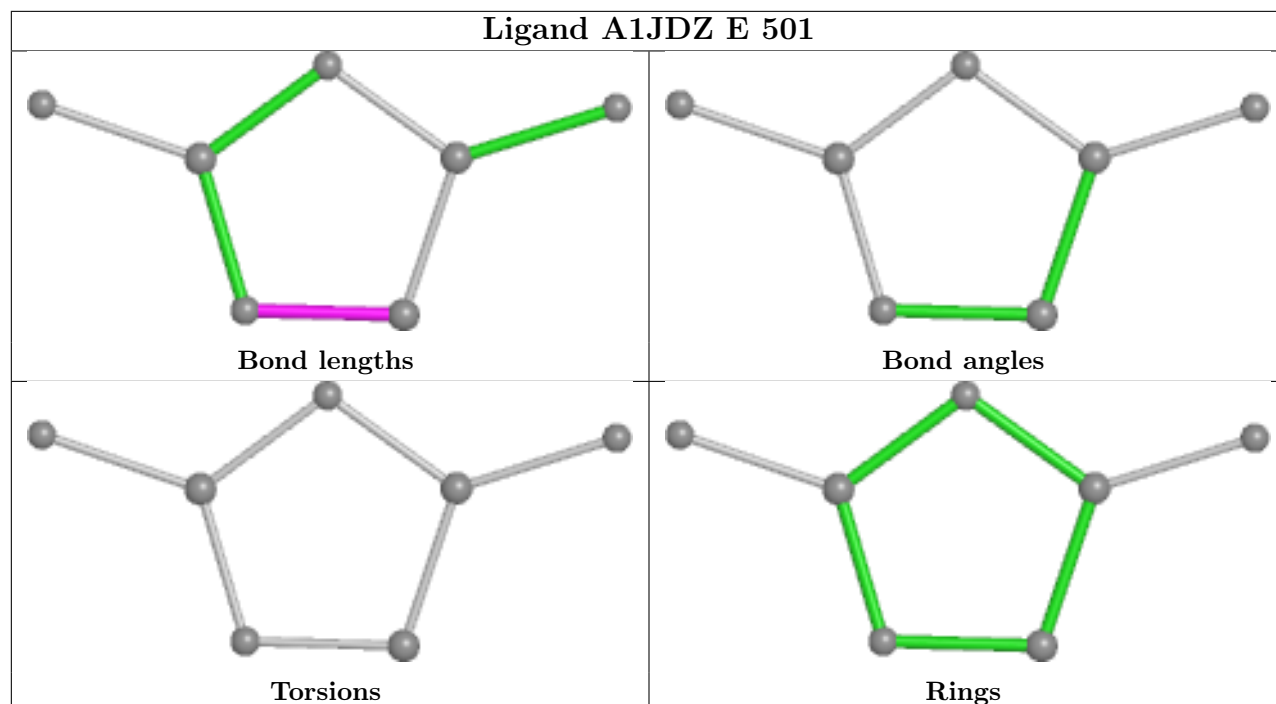
## Ligand A1JDZ E 502



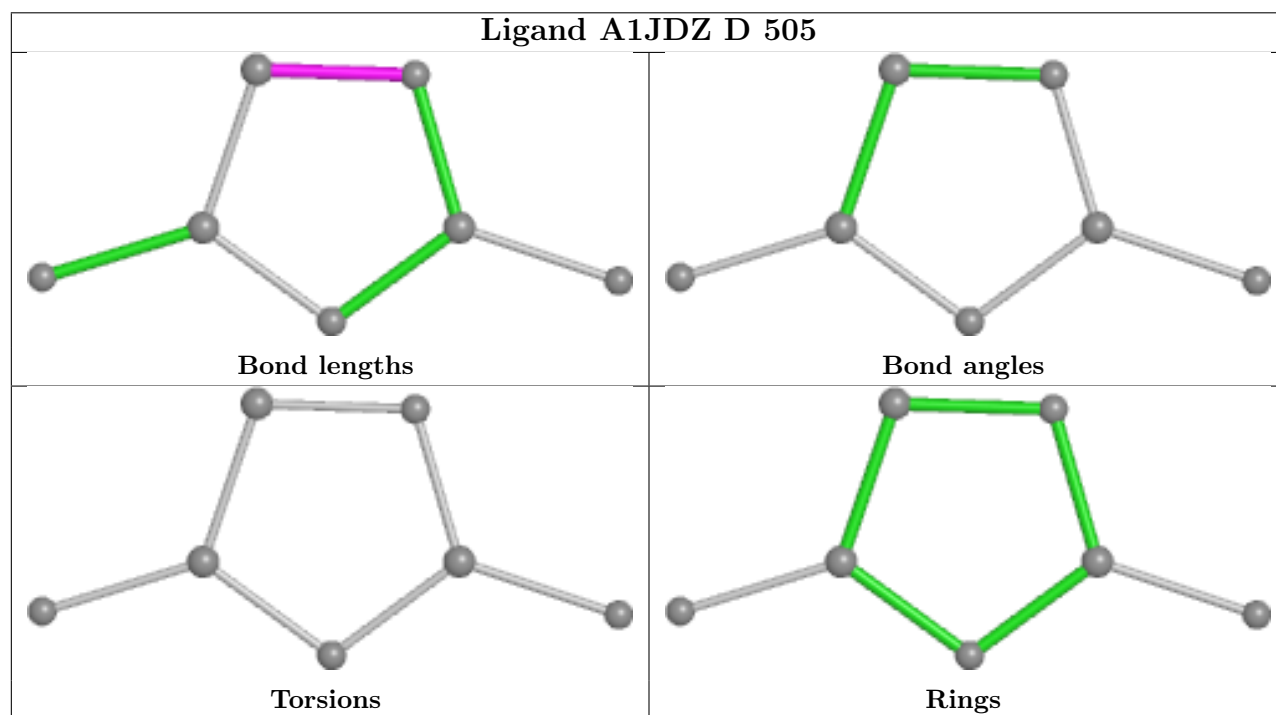


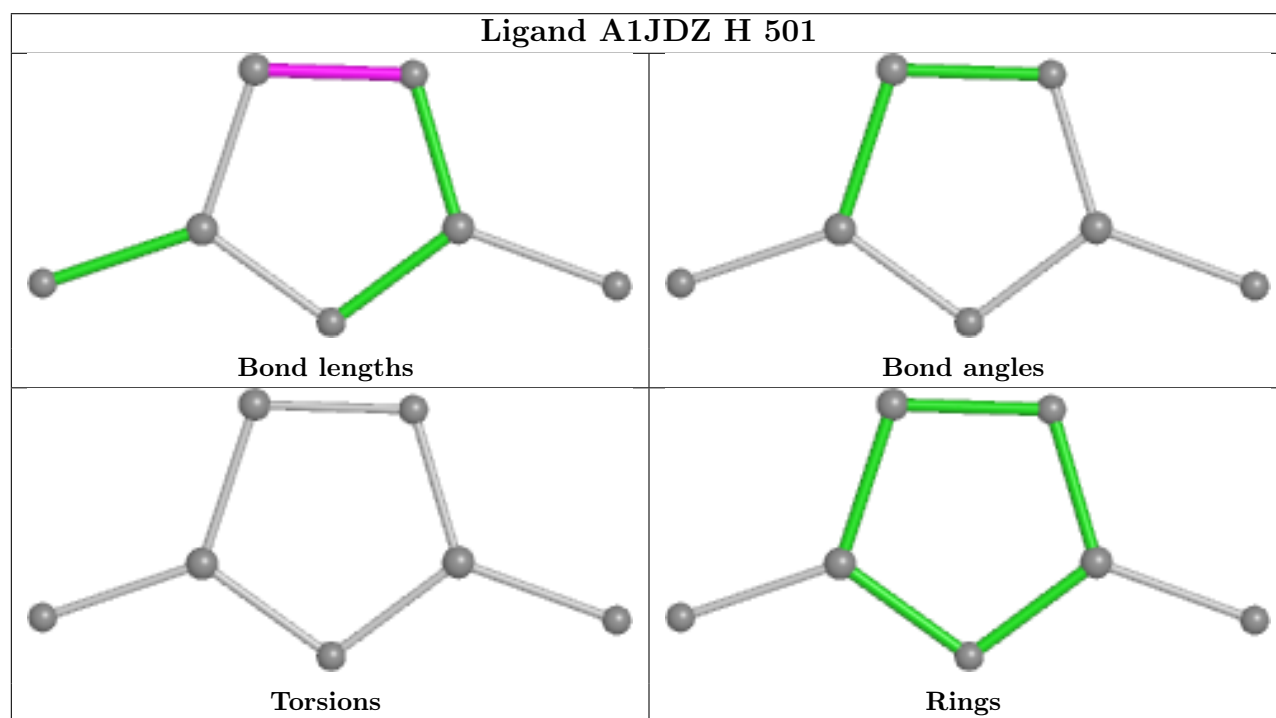
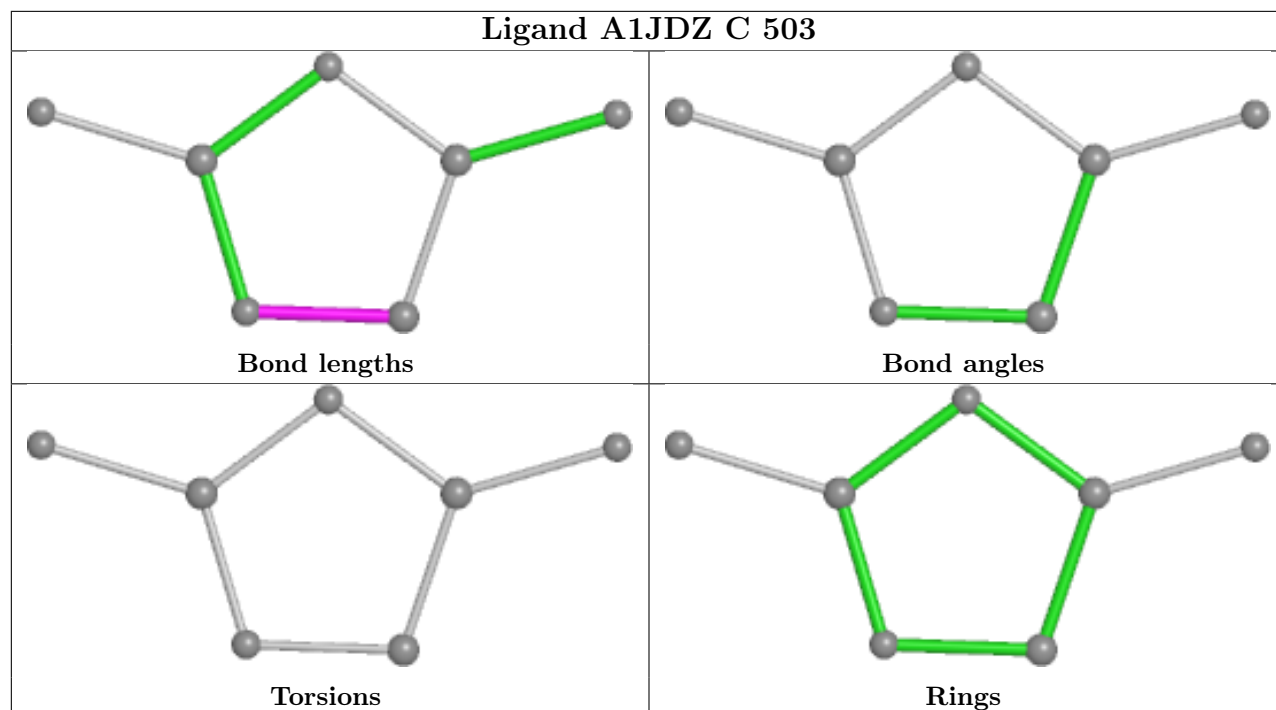


## Ligand A1JDZ E 501

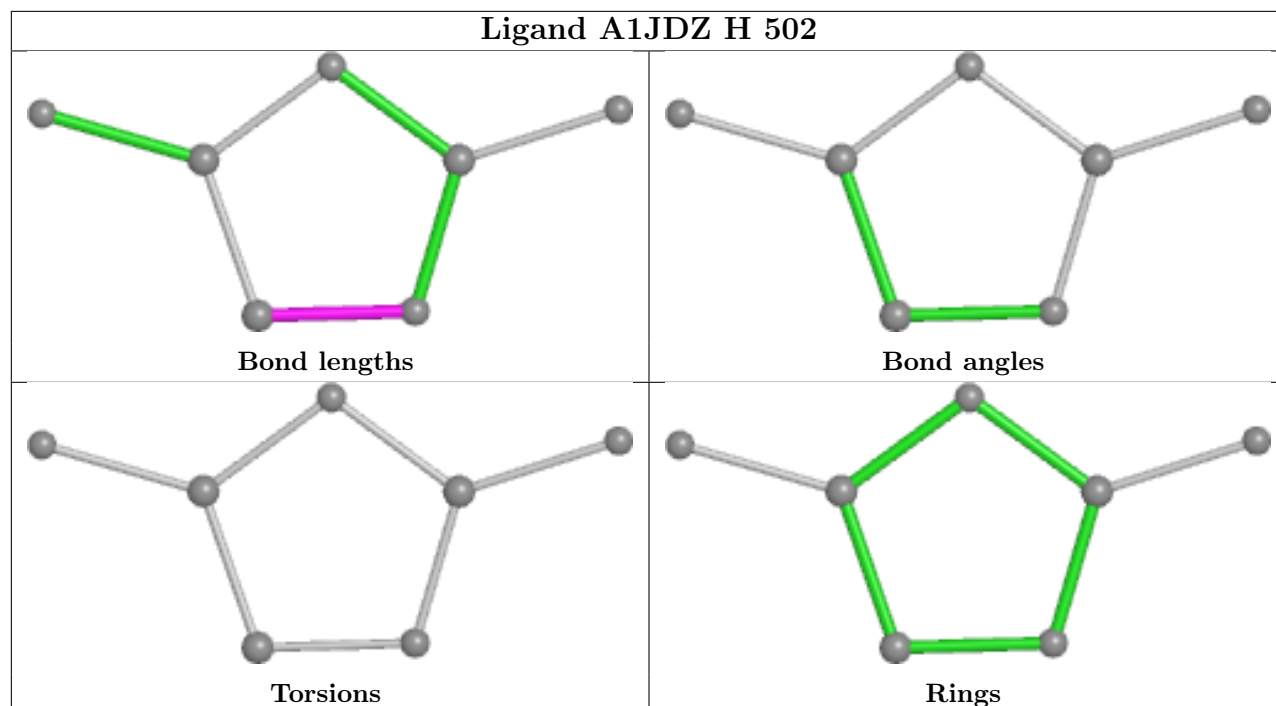


## Ligand A1JDZ D 505

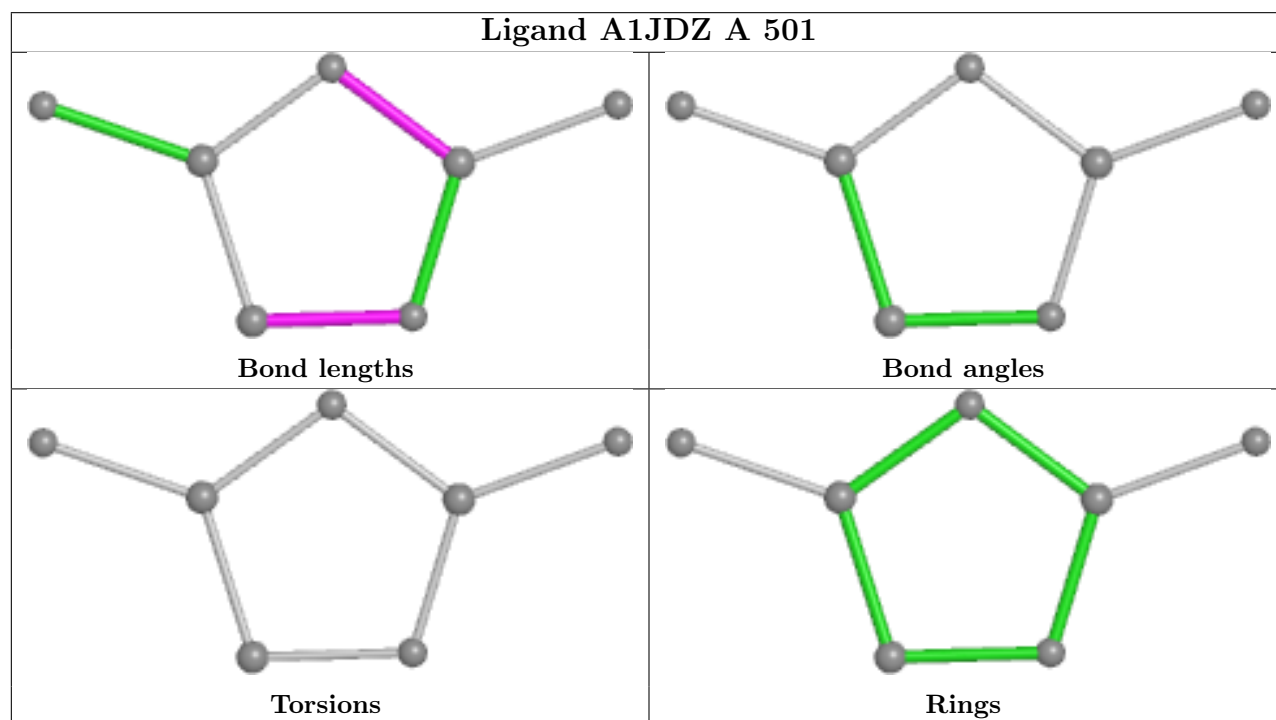


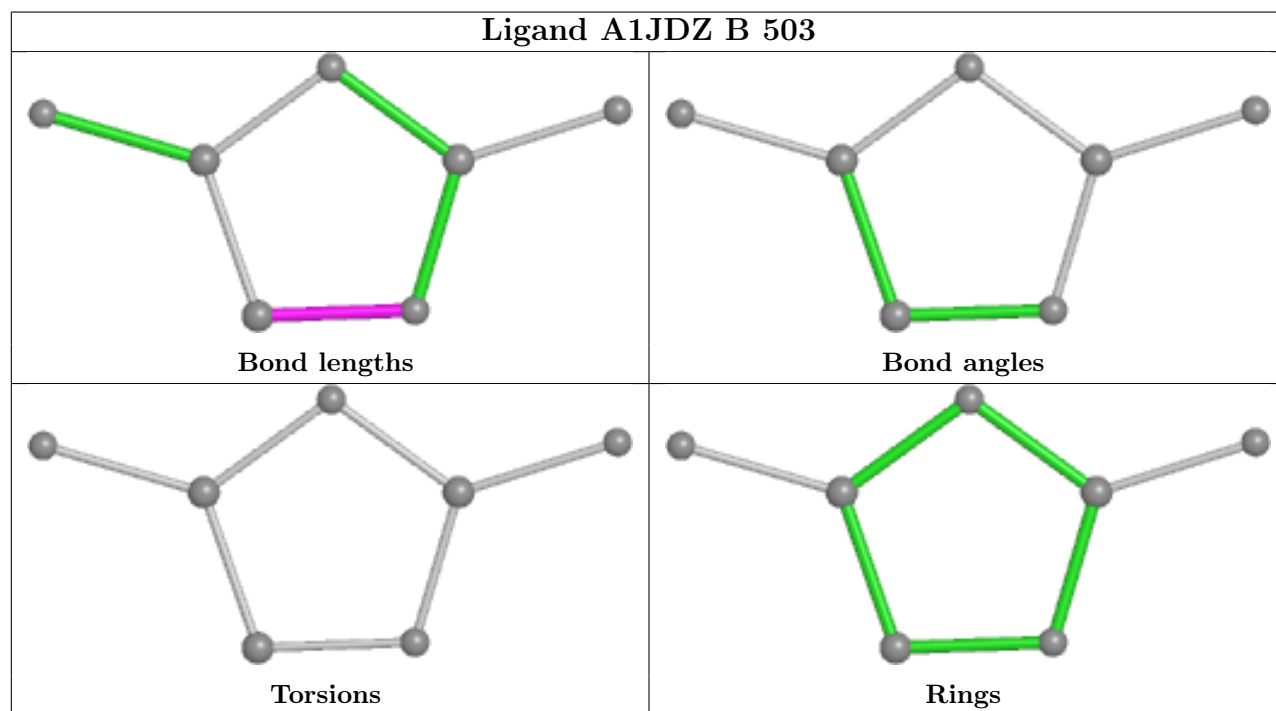
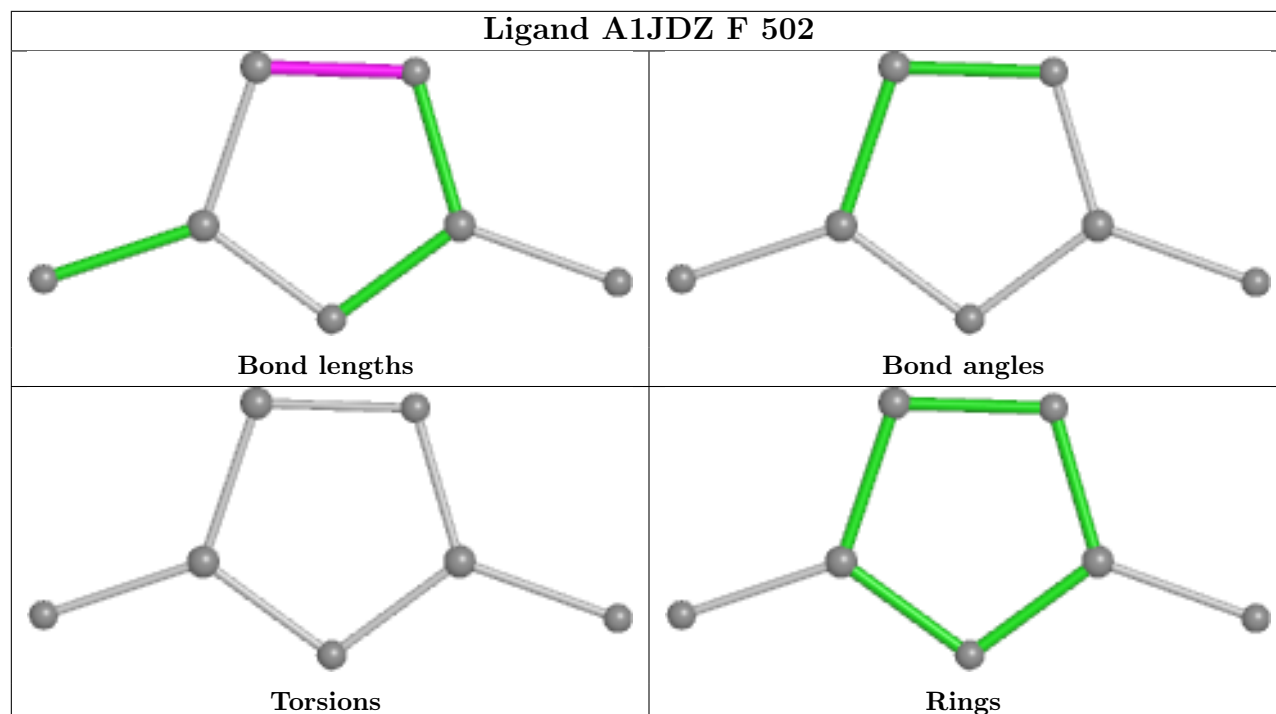


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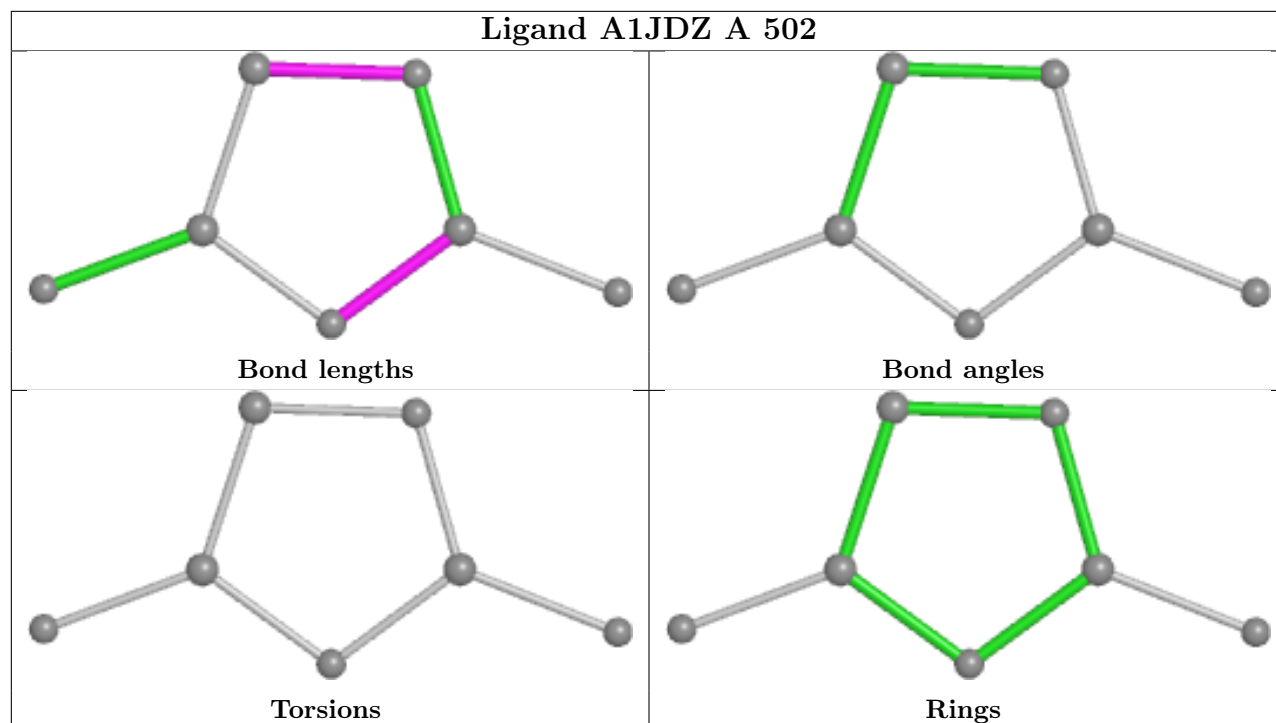


## Ligand A1JDZ A 501

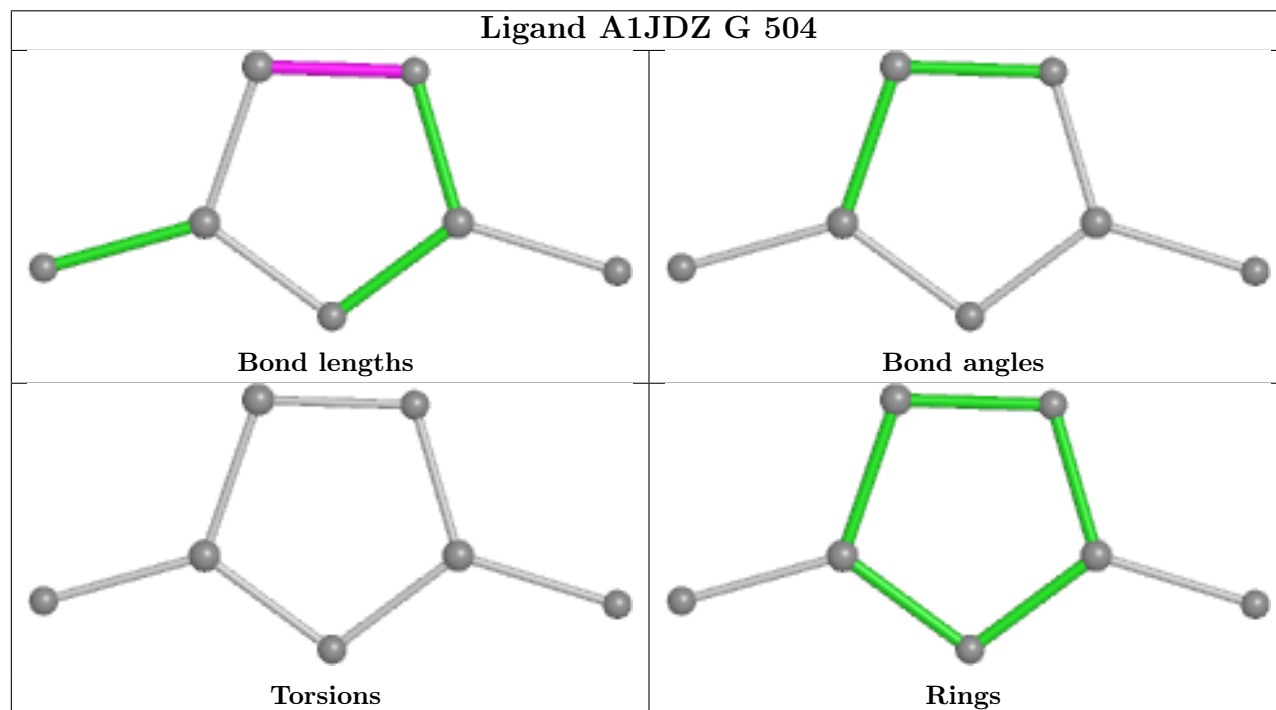


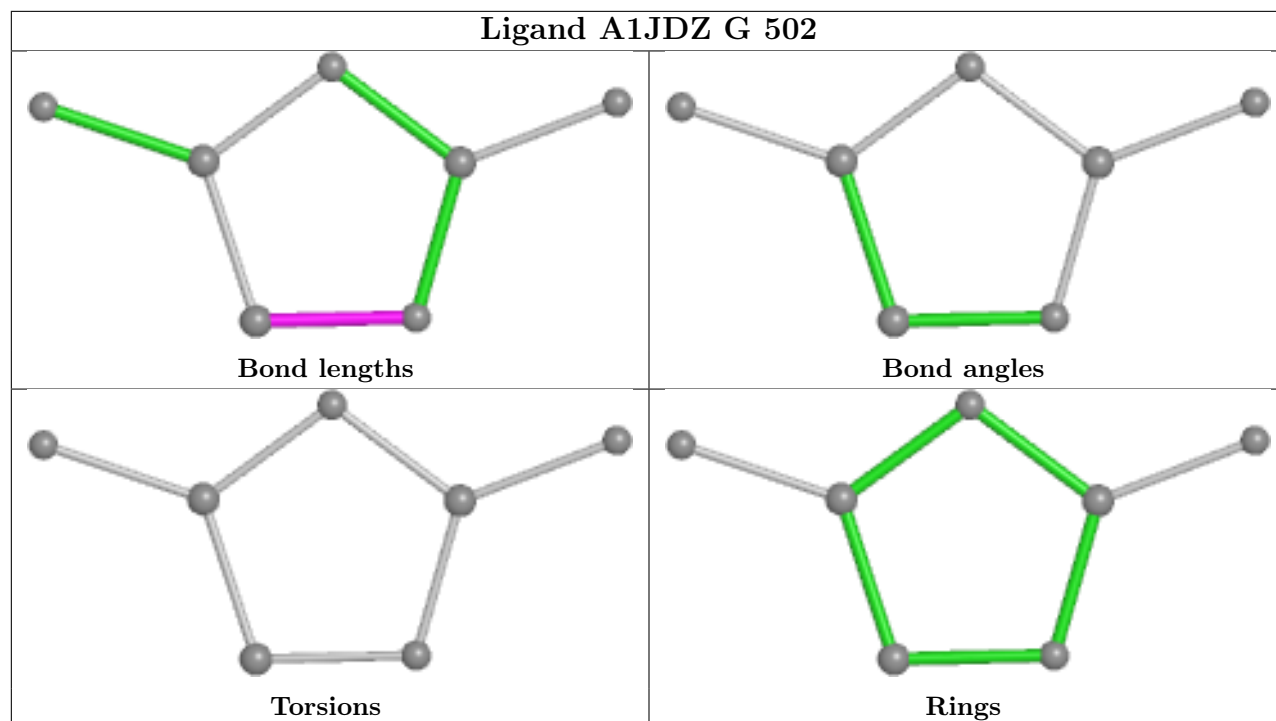


## Ligand A1JDZ A 502



## Ligand A1JDZ G 504





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	474/496 (95%)	-0.53	2 (0%) 89 91	7, 18, 35, 89	25 (5%)
1	B	474/496 (95%)	-0.32	2 (0%) 89 91	6, 21, 40, 78	30 (6%)
1	C	474/496 (95%)	-0.74	0 100 100	6, 14, 26, 50	30 (6%)
1	D	475/496 (95%)	-0.41	2 (0%) 89 91	8, 20, 34, 81	24 (5%)
1	E	474/496 (95%)	-0.24	3 (0%) 85 89	8, 23, 41, 134	25 (5%)
1	F	474/496 (95%)	-0.51	2 (0%) 89 91	7, 18, 30, 53	31 (6%)
1	G	474/496 (95%)	-0.67	2 (0%) 89 91	6, 15, 27, 52	32 (6%)
1	H	480/496 (96%)	-0.23	6 (1%) 74 79	7, 23, 43, 105	24 (5%)
All	All	3799/3968 (95%)	-0.46	19 (0%) 87 90	6, 19, 37, 134	221 (5%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	ALA	4.9
1	A	2	ALA	4.6
1	D	1	LEU	3.7
1	G	2	ALA	3.5
1	H	1	LEU	3.4
1	B	2	ALA	3.1
1	D	2	ALA	2.8
1	E	447	ALA	2.8
1	H	352	PHE	2.7
1	G	118	MET	2.4
1	F	267	LEU	2.4
1	H	-7	ASP	2.4
1	E	13	TRP	2.3
1	H	118	MET	2.3
1	A	118[A]	MET	2.2
1	B	347[A]	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	348	ALA	2.1
1	H	2	ALA	2.0
1	F	118	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1JDZ	C	503	7/7	0.75	0.19	18,32,40,41	0
2	A1JDZ	B	503	7/7	0.76	0.18	28,33,40,42	0
3	SO4	F	504	5/5	0.76	0.12	56,60,72,74	0
4	GOL	E	504	6/6	0.76	0.14	31,45,55,66	0
2	A1JDZ	F	501	7/7	0.78	0.13	27,36,43,46	0
3	SO4	D	503	5/5	0.78	0.15	35,38,43,44	0
4	GOL	G	505	6/6	0.78	0.22	13,30,40,42	14
2	A1JDZ	H	502	7/7	0.79	0.17	25,34,53,55	0
4	GOL	B	506	6/6	0.81	0.14	39,48,59,60	0
4	GOL	H	505	6/6	0.82	0.15	30,49,59,63	0
4	GOL	C	505	6/6	0.83	0.12	34,41,56,65	0
4	GOL	A	505	6/6	0.83	0.13	32,42,47,50	0
2	A1JDZ	D	505	7/7	0.84	0.11	33,42,57,59	0
2	A1JDZ	B	501	7/7	0.84	0.11	26,32,36,39	0
2	A1JDZ	G	504	7/7	0.84	0.17	20,33,42,42	0
4	GOL	G	506	6/6	0.85	0.12	26,39,46,52	0
4	GOL	F	505	6/6	0.85	0.14	27,36,48,50	0
4	GOL	B	505	6/6	0.87	0.12	26,43,57,57	0
3	SO4	D	504	5/5	0.89	0.09	35,44,57,58	0
2	A1JDZ	A	501	7/7	0.89	0.09	15,19,26,31	0

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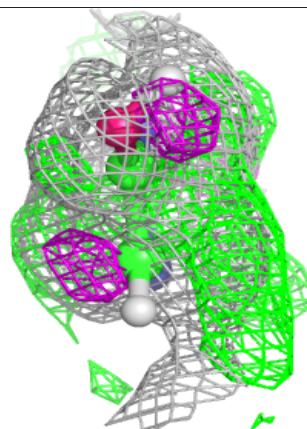
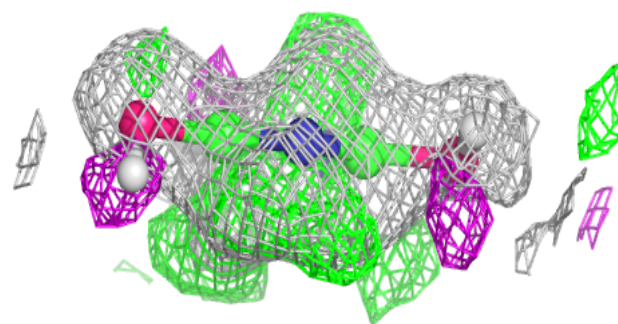
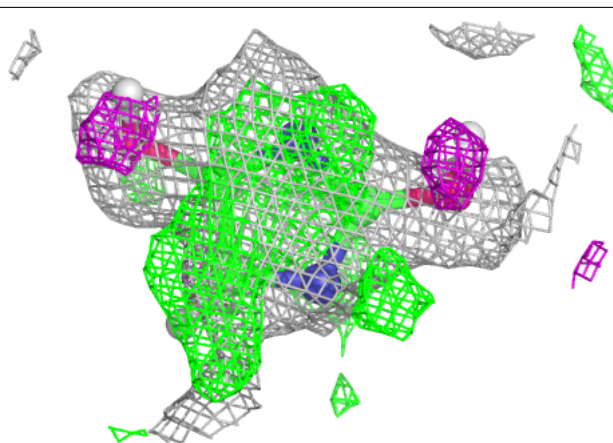
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	H	503	5/5	0.89	0.09	35,43,57,57	0
2	A1JDZ	E	502	7/7	0.89	0.09	24,29,35,35	0
3	SO4	H	504	5/5	0.90	0.11	30,36,41,56	0
2	A1JDZ	D	501	7/7	0.90	0.09	14,19,26,31	0
3	SO4	B	504	5/5	0.91	0.09	32,36,51,51	0
2	A1JDZ	E	501	7/7	0.91	0.09	21,25,35,42	0
3	SO4	A	503	5/5	0.91	0.09	20,24,42,42	0
2	A1JDZ	G	501	7/7	0.92	0.09	14,17,22,23	0
2	A1JDZ	A	502	7/7	0.92	0.08	17,23,26,28	0
3	SO4	F	503	5/5	0.92	0.10	27,33,36,36	0
2	A1JDZ	D	502	7/7	0.92	0.08	19,21,25,27	0
3	SO4	G	503	5/5	0.92	0.09	25,30,41,53	0
2	A1JDZ	B	502	7/7	0.92	0.08	22,25,27,27	0
2	A1JDZ	F	502	7/7	0.92	0.08	21,25,29,32	0
3	SO4	C	504	5/5	0.92	0.07	29,30,44,50	0
2	A1JDZ	H	506	7/7	0.93	0.07	20,24,26,27	0
3	SO4	E	503	5/5	0.93	0.09	30,32,41,45	0
2	A1JDZ	H	501	7/7	0.93	0.07	14,21,25,28	0
3	SO4	A	504	5/5	0.93	0.07	37,46,49,53	0
2	A1JDZ	G	502	7/7	0.94	0.08	11,15,18,21	0
2	A1JDZ	C	501	7/7	0.94	0.08	11,14,20,24	0
2	A1JDZ	C	502	7/7	0.95	0.07	12,15,17,17	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.

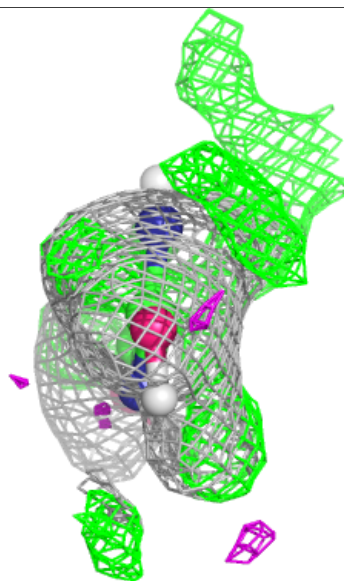
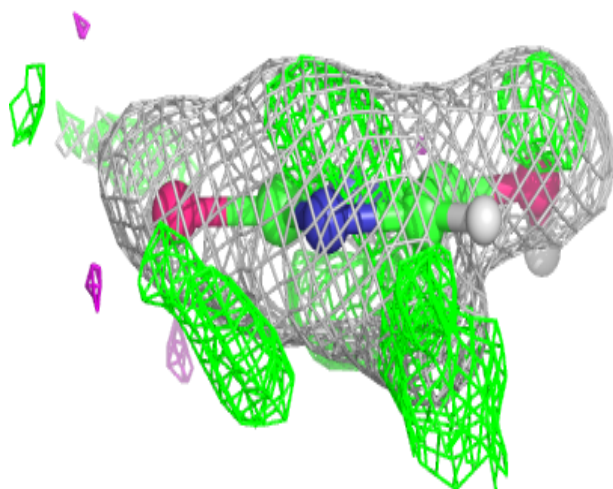
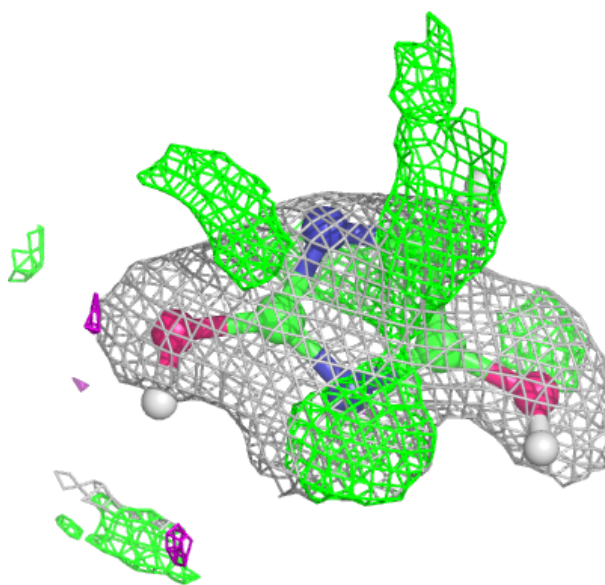
**Electron density around A1JDZ C 503:**

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



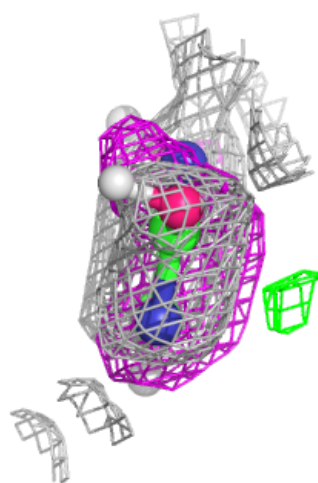
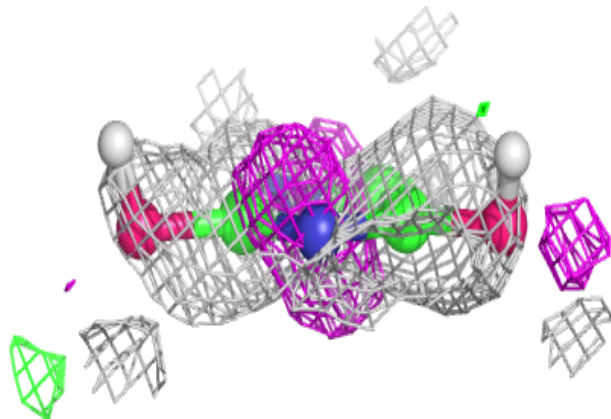
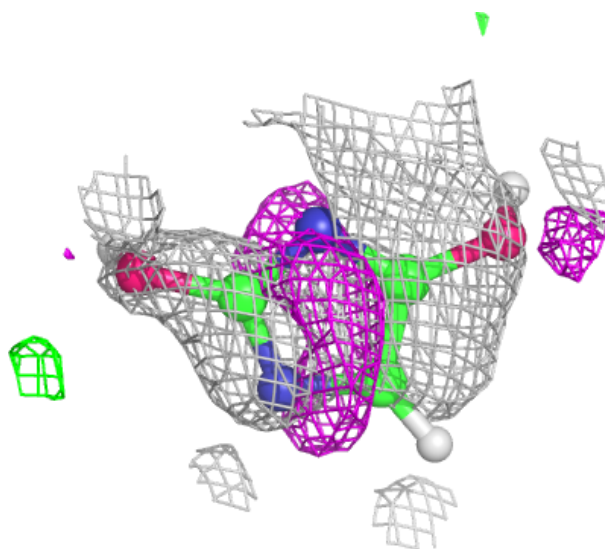
**Electron density around A1JDZ B 503:**

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and green (positive)



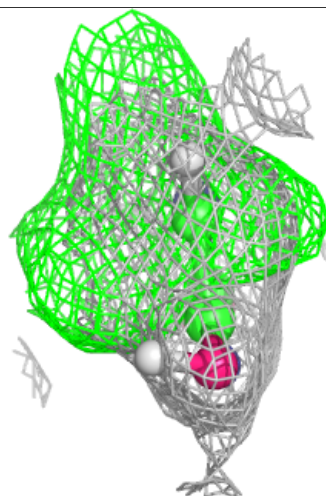
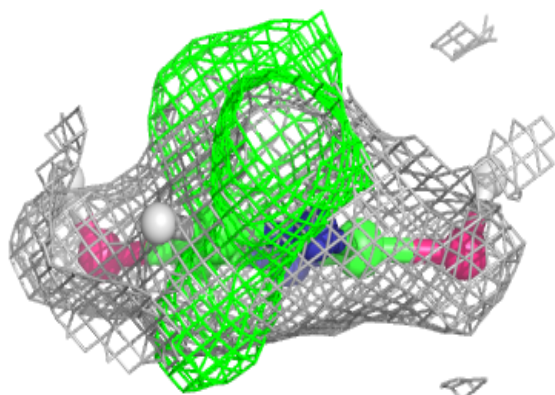
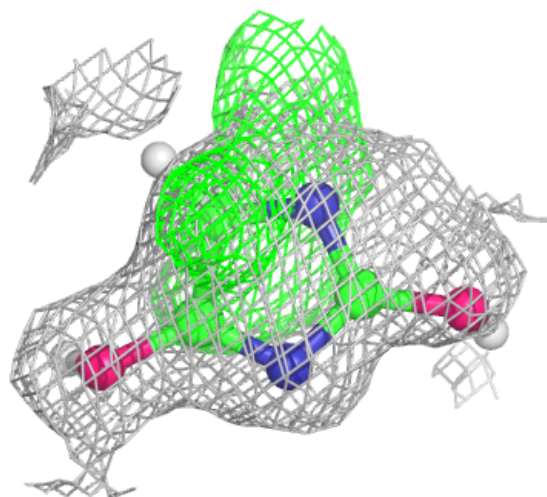
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and green (positive)



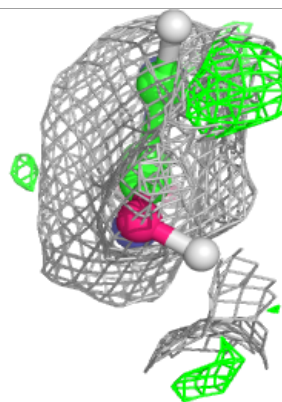
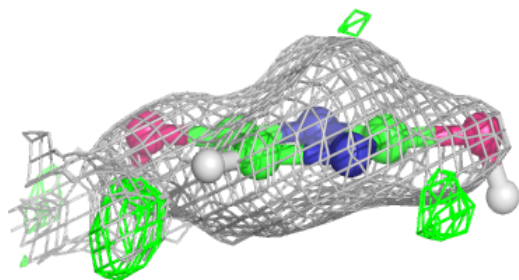
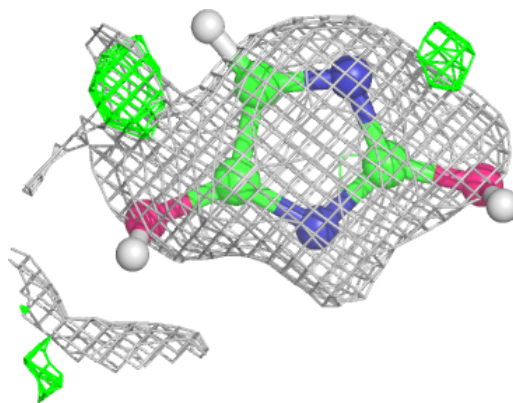
**Electron density around A1JDZ H 502:**

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



**Electron density around A1JDZ D 505:**

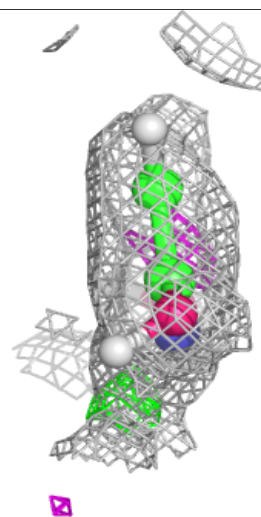
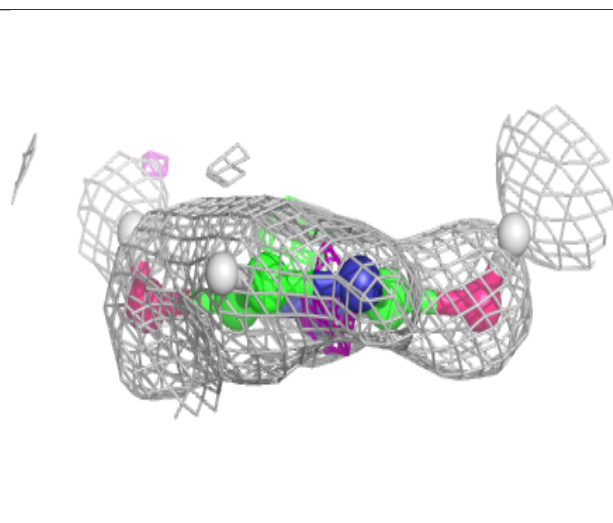
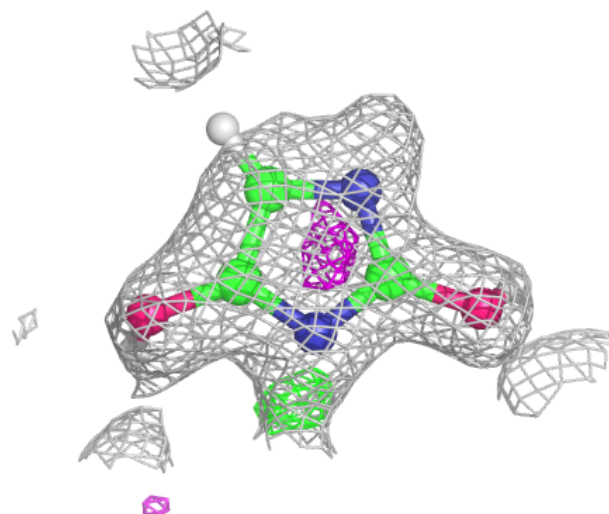
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





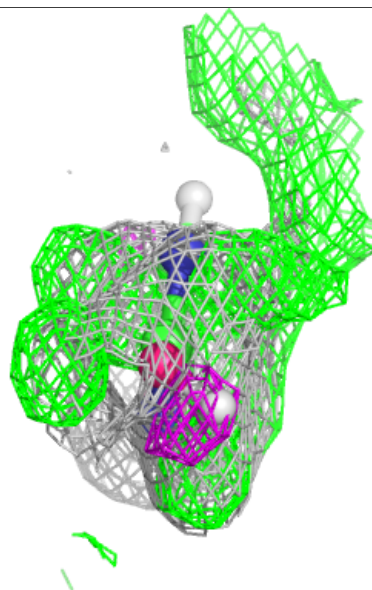
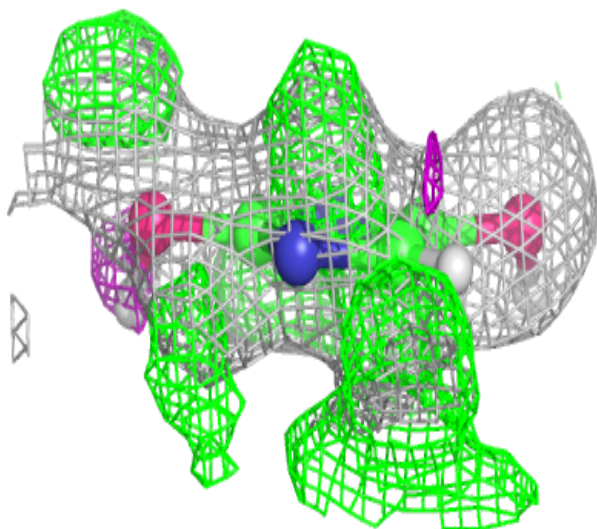
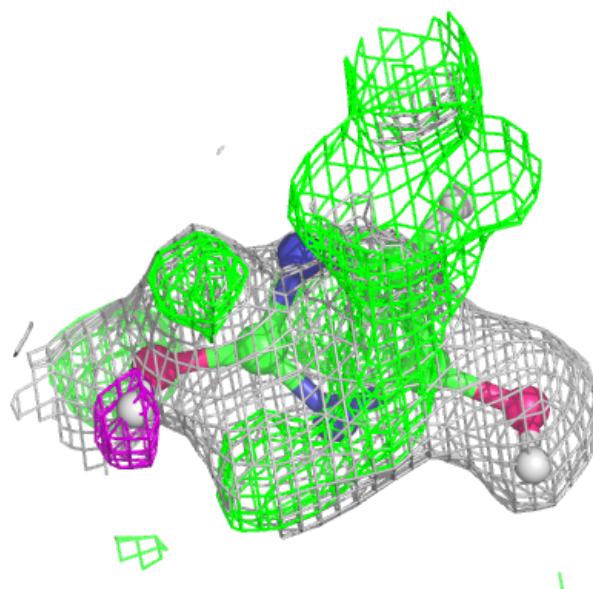
**Electron density around A1JDZ B 501:**

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



**Electron density around A1JDZ G 504:**

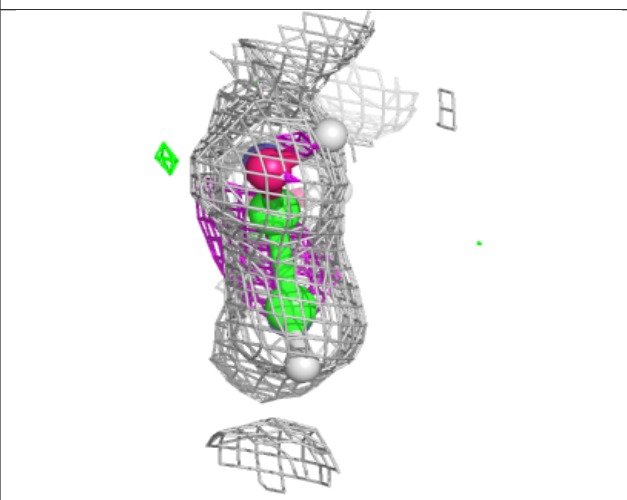
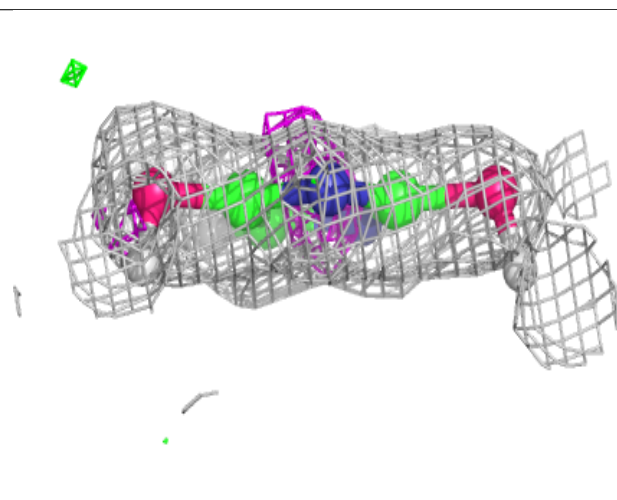
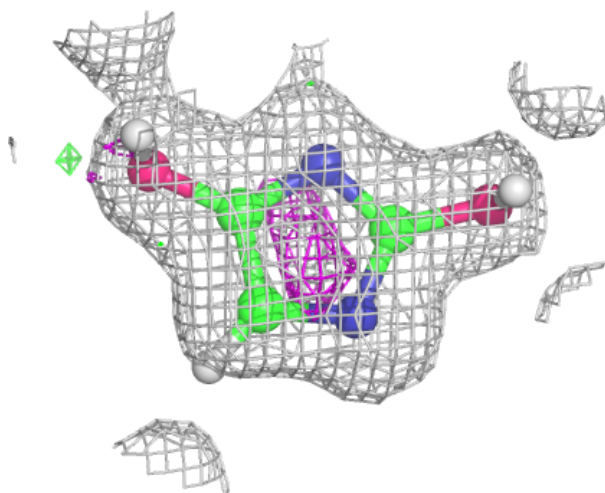
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





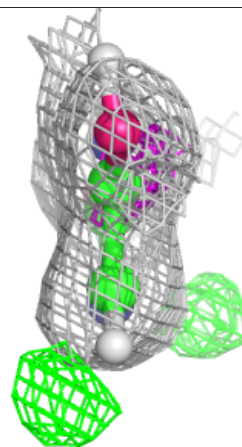
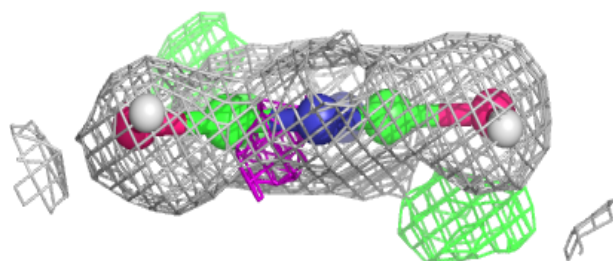
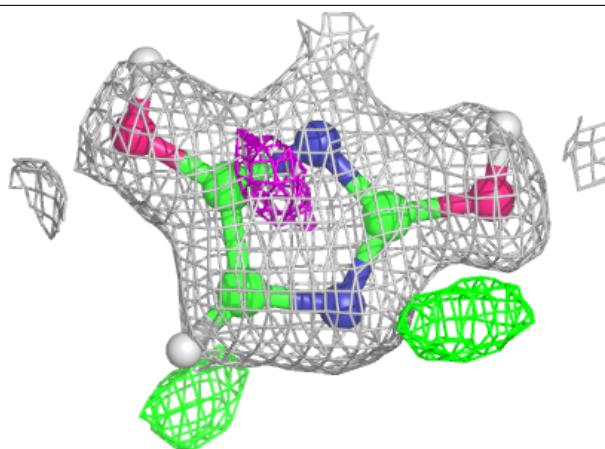
**Electron density around A1JDZ A 501:**

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and green (positive)



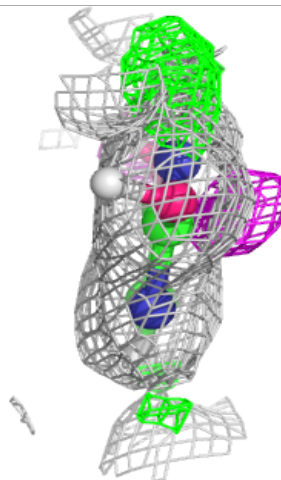
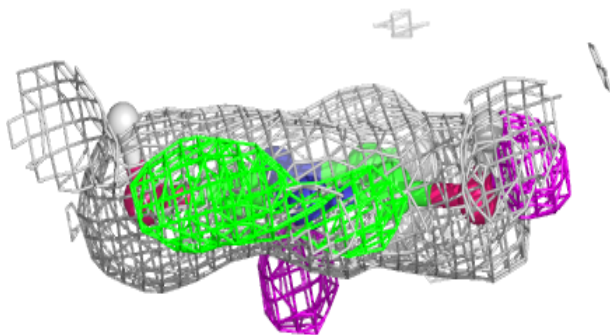
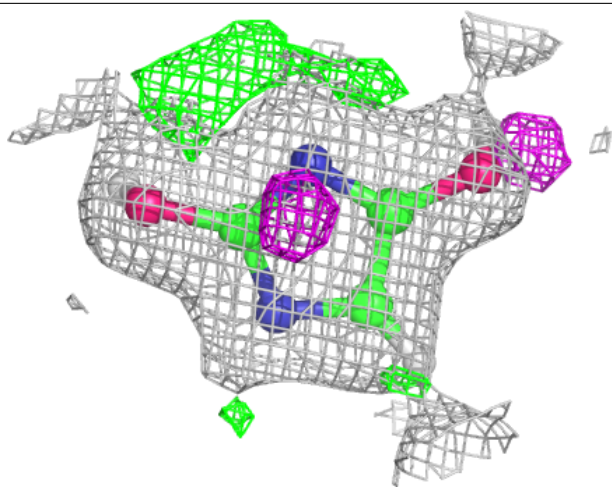
**Electron density around A1JDZ E 502:**

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



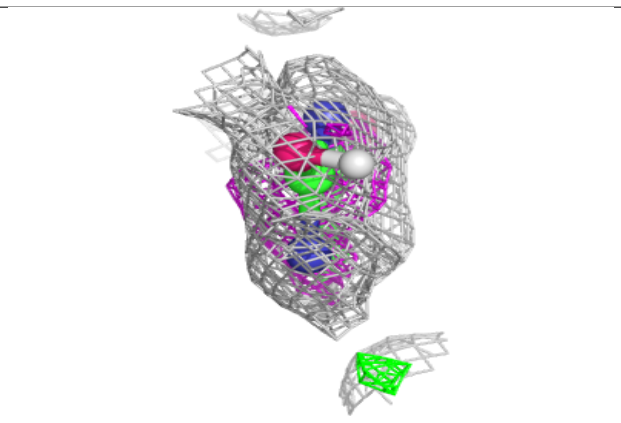
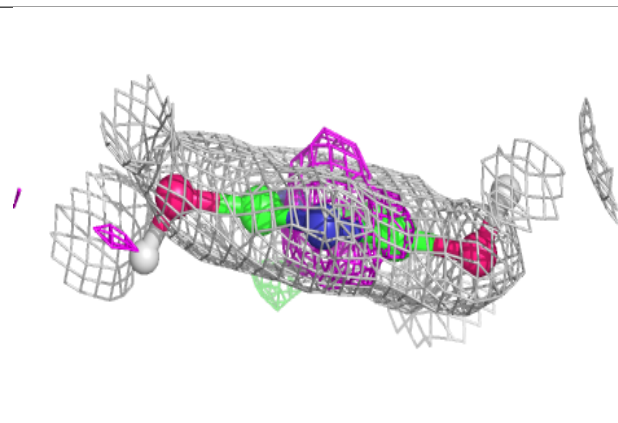
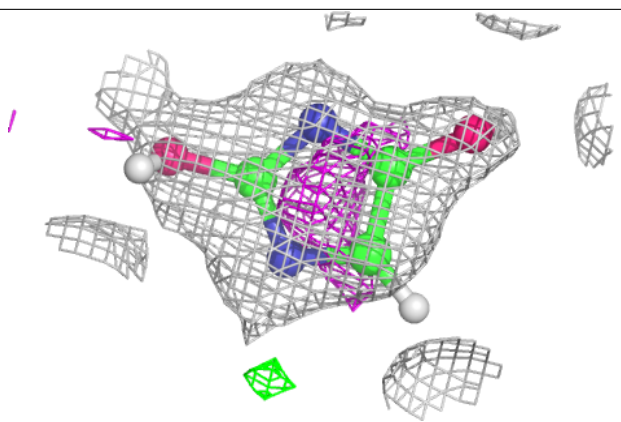
**Electron density around A1JDZ D 501:**

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



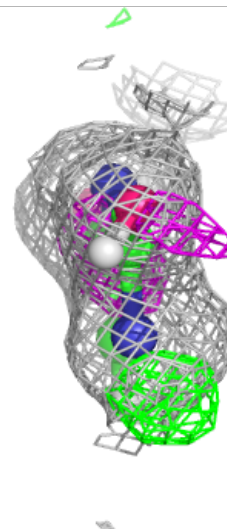
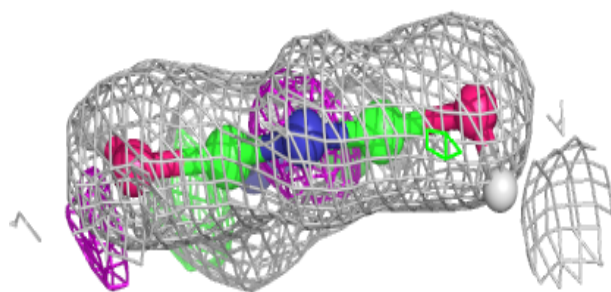
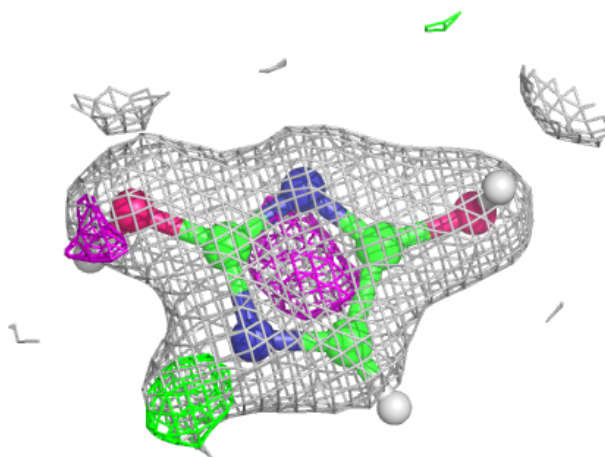
**Electron density around A1JDZ E 501:**

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



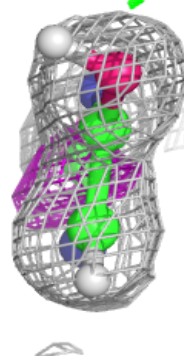
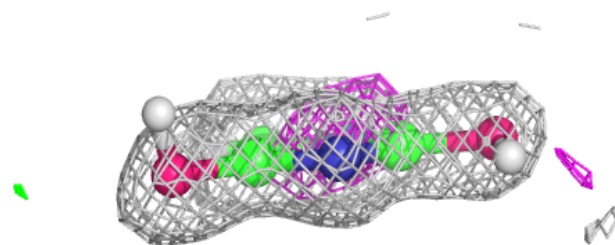
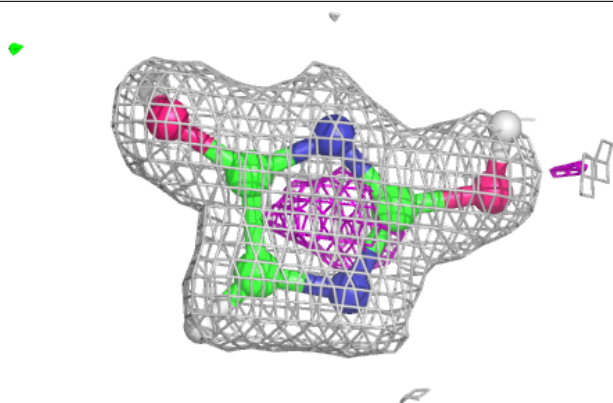
**Electron density around A1JDZ G 501:**

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



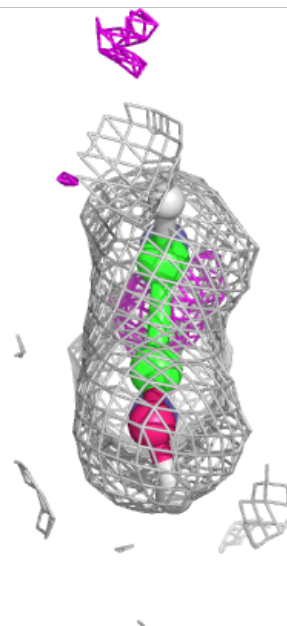
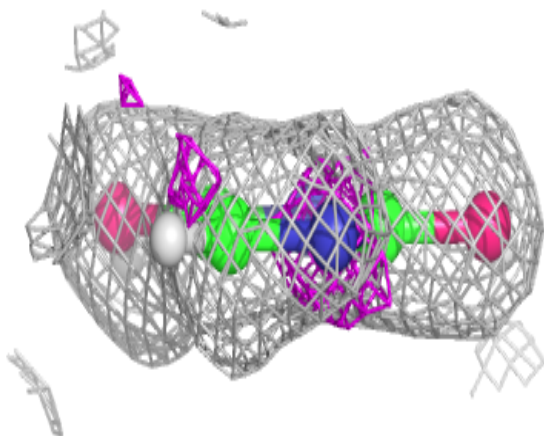
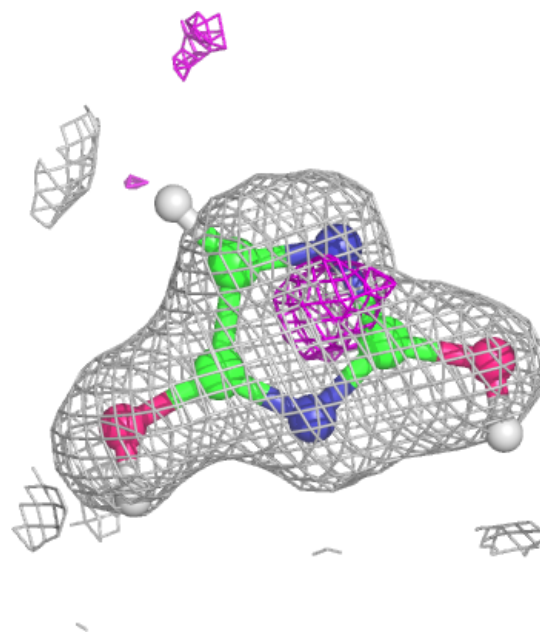
**Electron density around A1JDZ A 502:**

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



**Electron density around A1JDZ D 502:**

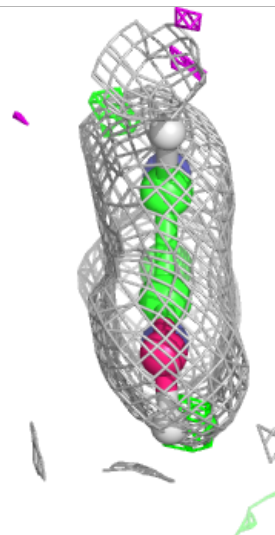
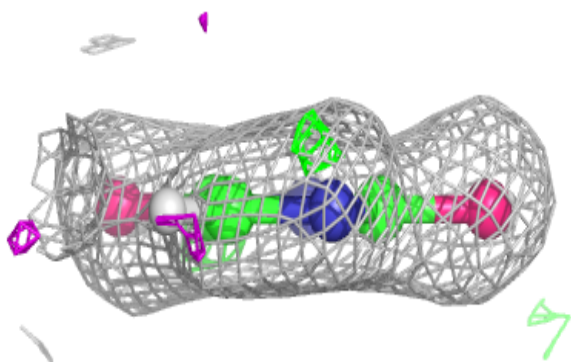
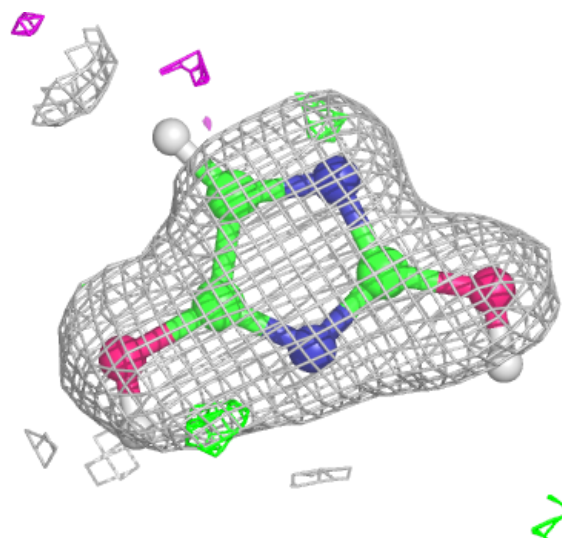
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1JDZ B 502:**

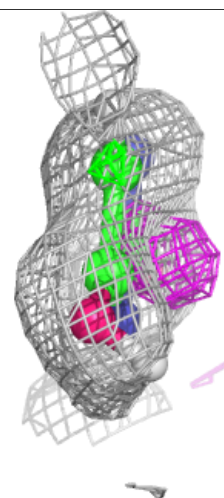
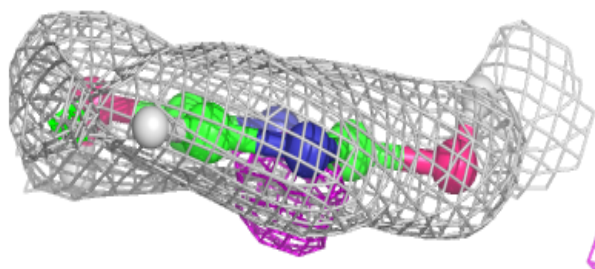
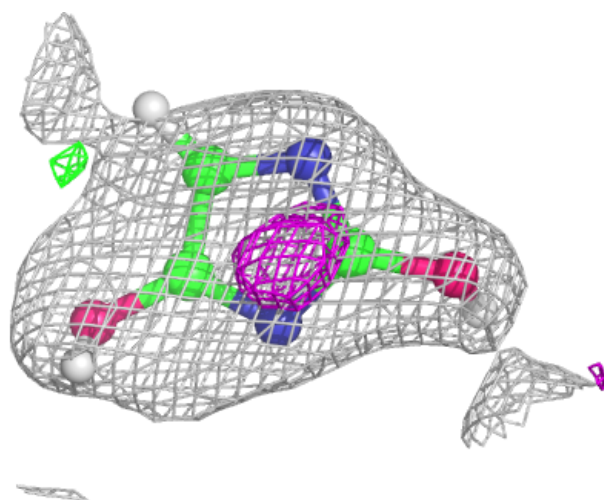
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





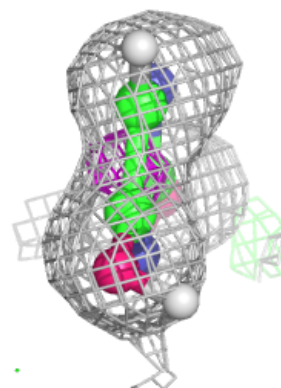
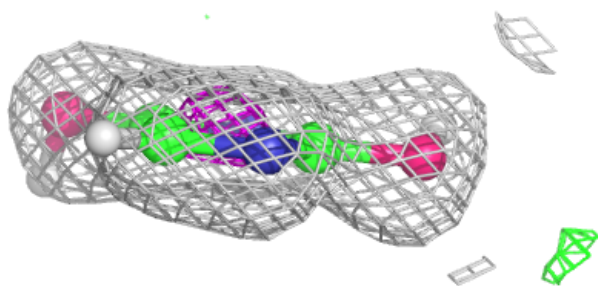
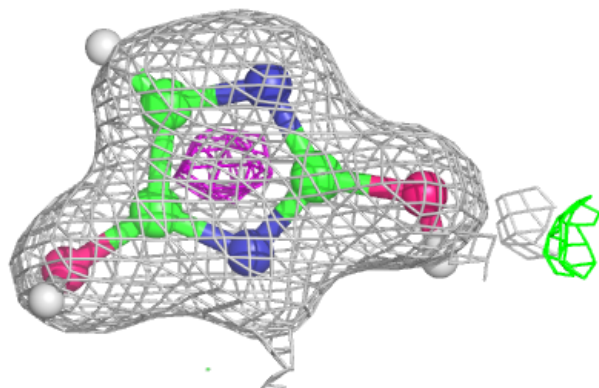
**Electron density around A1JDZ F 502:**

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



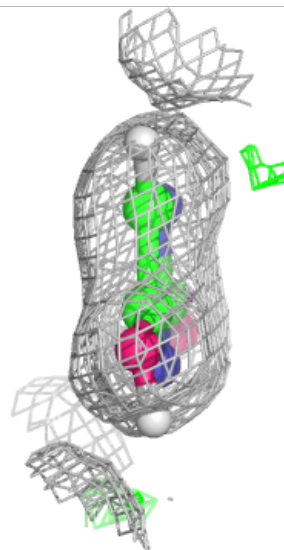
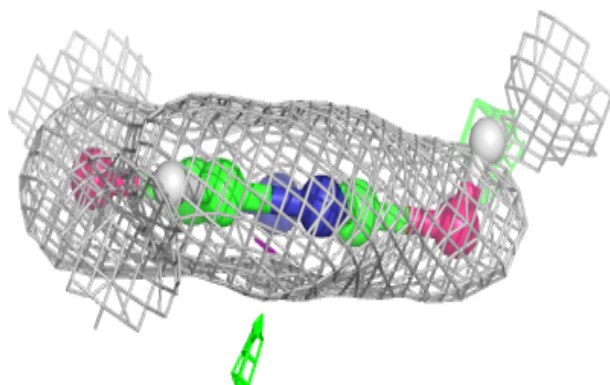
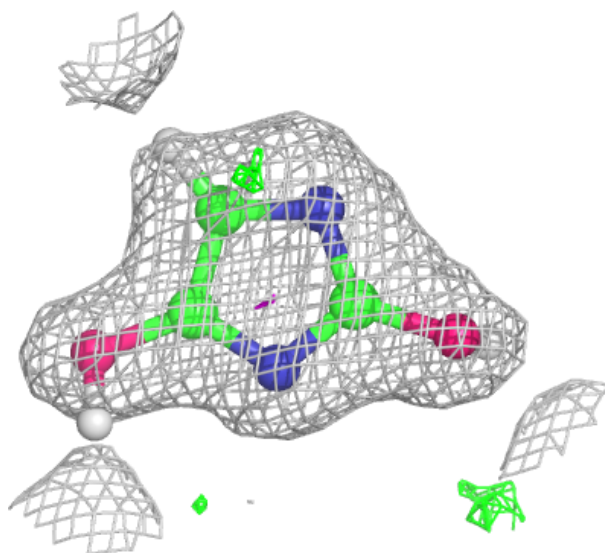
**Electron density around A1JDZ H 506:**

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



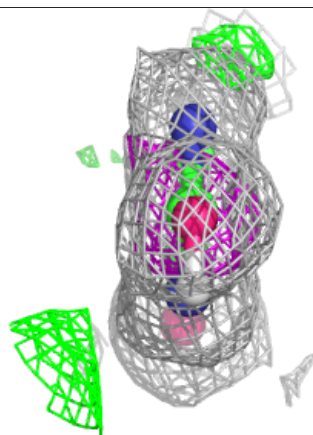
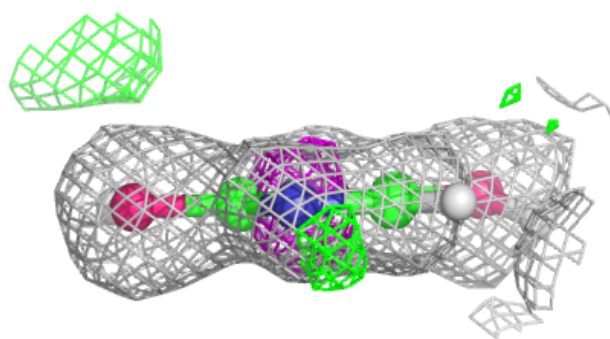
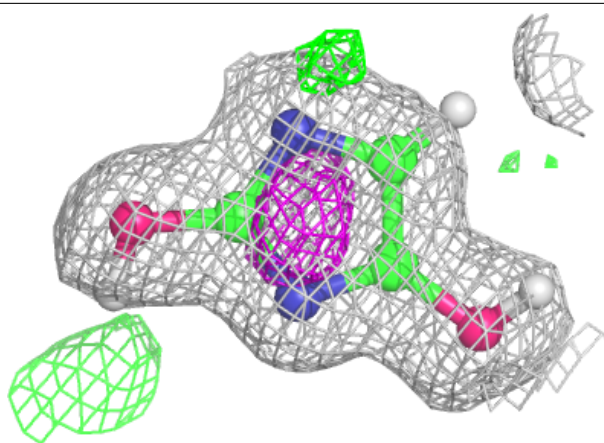
**Electron density around A1JDZ H 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



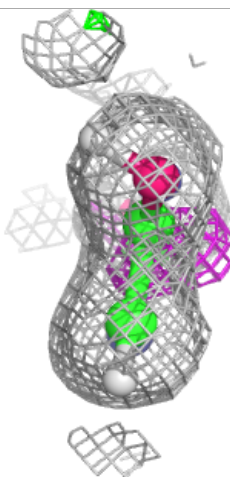
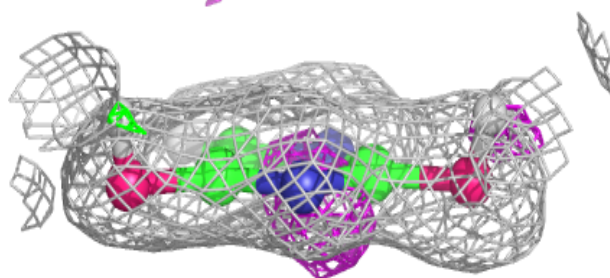
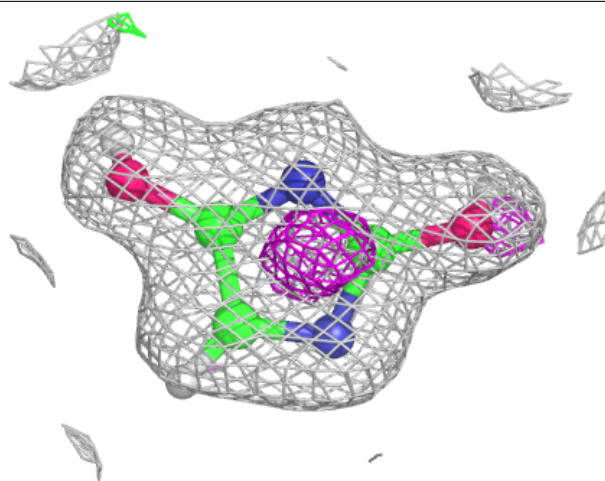
**Electron density around A1JDZ G 502:**

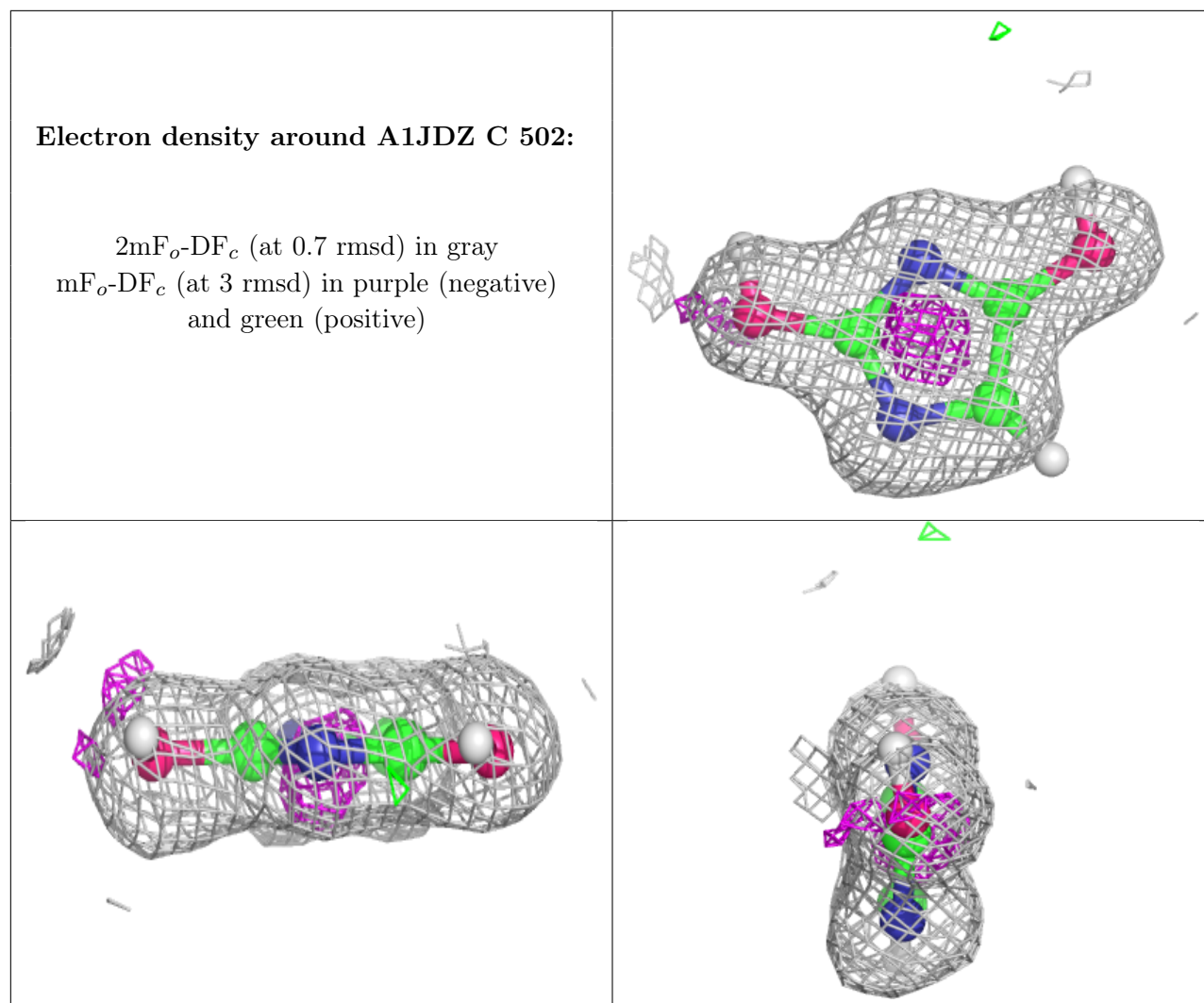
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1JDZ 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.