



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 23, 2025 – 04:33 pm BST

PDB ID : 9RAU / pdb\_00009rau  
Title : Streptococcus pyogenes GapN in complex with pyrimidine-5-amine  
Authors : Wirsing, R.; Schindelin, H.  
Deposited on : 2025-05-21  
Resolution : 1.77 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 Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

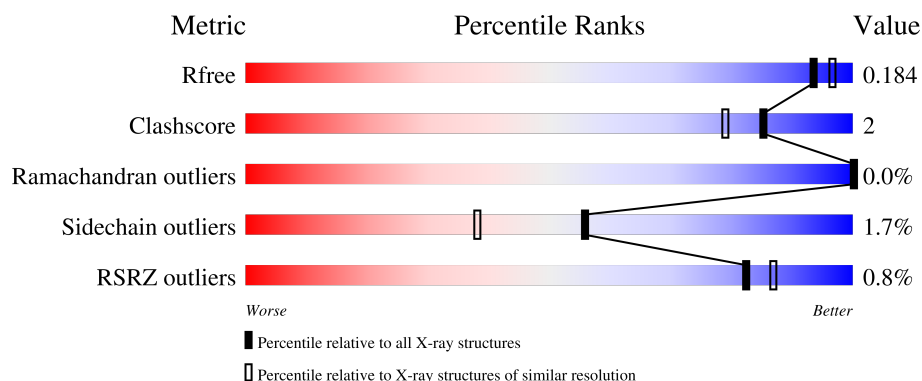
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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.



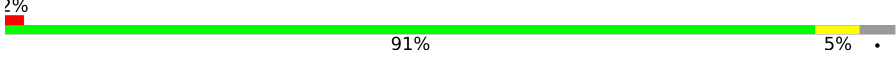


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	 91% 5% •
1	G	496	 91% 5% •
1	H	496	 92% • •

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 61356 atoms, of which 29477 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	2	0
			7173	2263	3620	591	691	8			
1	B	474	Total	C	H	N	O	S	0	10	0
			7263	2296	3666	593	700	8			
1	C	475	Total	C	H	N	O	S	0	8	0
			7232	2280	3650	597	697	8			
1	D	475	Total	C	H	N	O	S	0	8	0
			7233	2280	3651	595	699	8			
1	E	474	Total	C	H	N	O	S	0	2	0
			7173	2263	3620	591	691	8			
1	F	474	Total	C	H	N	O	S	0	9	0
			7255	2294	3661	593	699	8			
1	G	475	Total	C	H	N	O	S	0	9	0
			7251	2285	3663	598	696	9			
1	H	475	Total	C	H	N	O	S	0	3	0
			7194	2268	3634	592	692	8			

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
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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	-20	ALA	-	expression tag	UNP A0A4U9C786
H	-19	SER	-	expression tag	UNP A0A4U9C786
H	-18	TRP	-	expression tag	UNP A0A4U9C786
H	-17	SER	-	expression tag	UNP A0A4U9C786
H	-16	HIS	-	expression tag	UNP A0A4U9C786
H	-15	PRO	-	expression tag	UNP A0A4U9C786
H	-14	GLN	-	expression tag	UNP A0A4U9C786
H	-13	PHE	-	expression tag	UNP A0A4U9C786
H	-12	GLU	-	expression tag	UNP A0A4U9C786
H	-11	LYS	-	expression tag	UNP A0A4U9C786
H	-10	ILE	-	expression tag	UNP A0A4U9C786
H	-9	GLU	-	expression tag	UNP A0A4U9C786
H	-8	GLY	-	expression tag	UNP A0A4U9C786

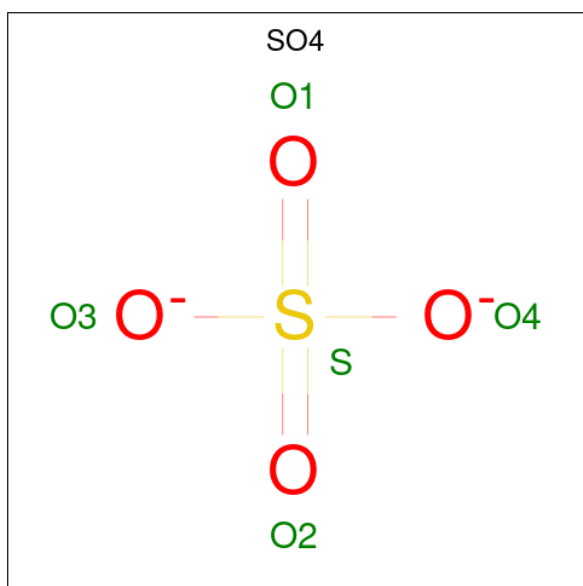
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ARG	-	expression tag	UNP A0A4U9C786
H	-6	ARG	-	expression tag	UNP A0A4U9C786
H	-5	ASP	-	expression tag	UNP A0A4U9C786
H	-4	ARG	-	expression tag	UNP A0A4U9C786
H	-3	GLY	-	expression tag	UNP A0A4U9C786
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 SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



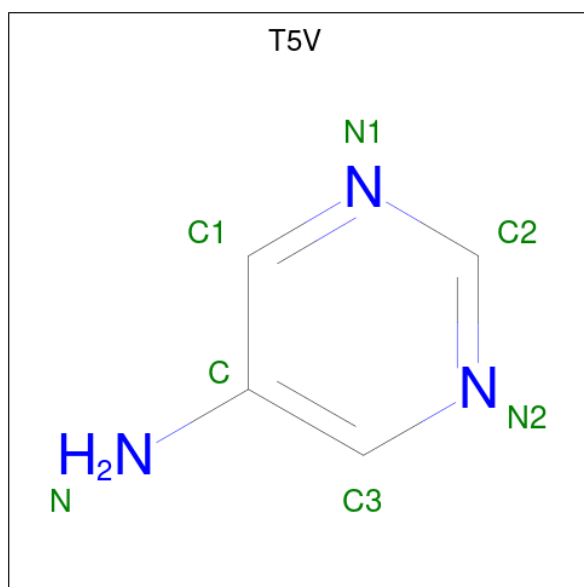
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is pyrimidin-5-amine (CCD ID: T5V) (formula:  $C_4H_5N_3$ ) (labeled as "Ligand of Interest" by depositor).



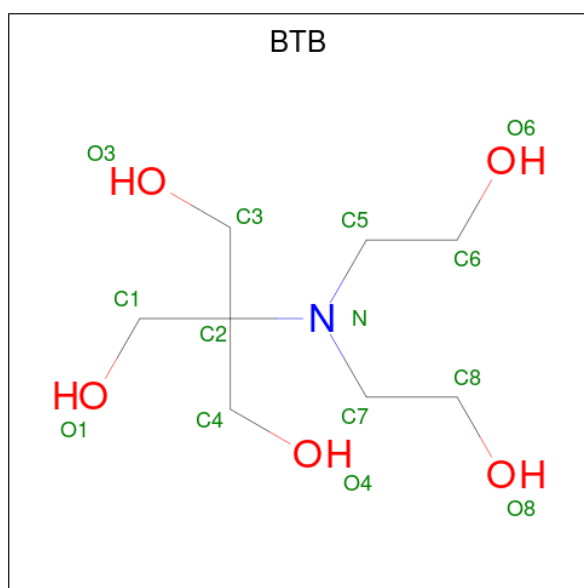
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			12	4	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	N	0	0
			12	4	5	3		
3	C	1	Total	C	H	N	0	0
			12	4	5	3		
3	D	1	Total	C	H	N	0	0
			12	4	5	3		
3	E	1	Total	C	H	N	0	1
			24	8	10	6		
3	F	1	Total	C	H	N	0	0
			12	4	5	3		
3	G	1	Total	C	H	N	0	0
			12	4	5	3		
3	H	1	Total	C	H	N	0	0
			12	4	5	3		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula:  $C_8H_{19}NO_5$ ).



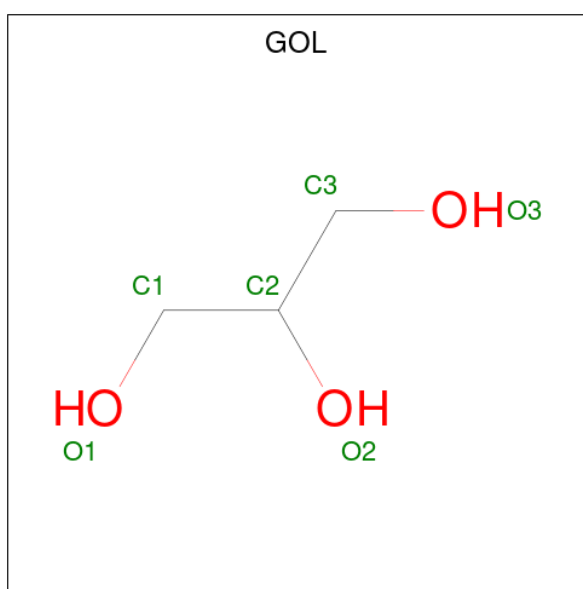
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
4	B	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
4	C	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
4	D	1	Total	C	H	N	O	0	0
			33	8	19	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
4	F	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
4	G	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
4	H	1	Total	C	H	N	O	0	0
			33	8	19	1	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



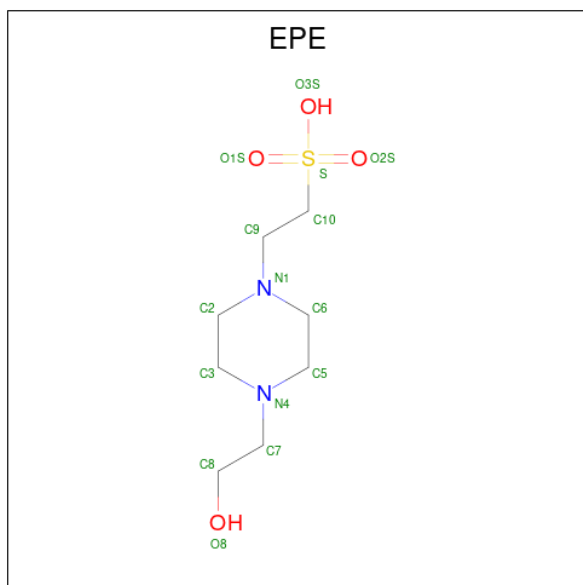
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	G	1	Total	C	H	O	0	0
			14	3	8	3		
5	H	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	D	1	Total	C	H	N	O	S	0	1
			64	16	34	4	8	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	307	Total	O	0	0
			307	307		
8	B	412	Total	O	0	0
			412	412		

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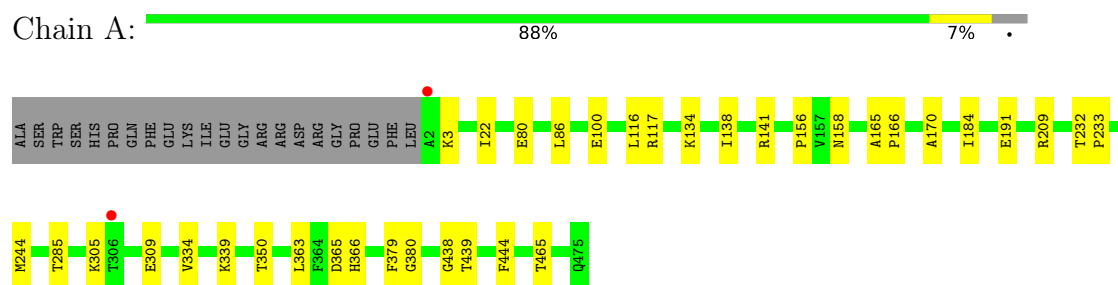
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	431	Total 431	O 431	0	0
8	D	357	Total 358	O 358	0	1
8	E	227	Total 227	O 227	0	0
8	F	326	Total 326	O 326	0	0
8	G	420	Total 420	O 420	0	0
8	H	440	Total 440	O 440	0	0

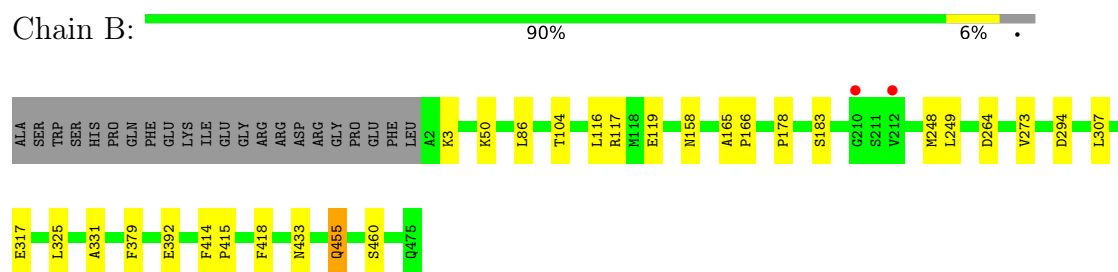
### 3 Residue-property plots [i](#)

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.

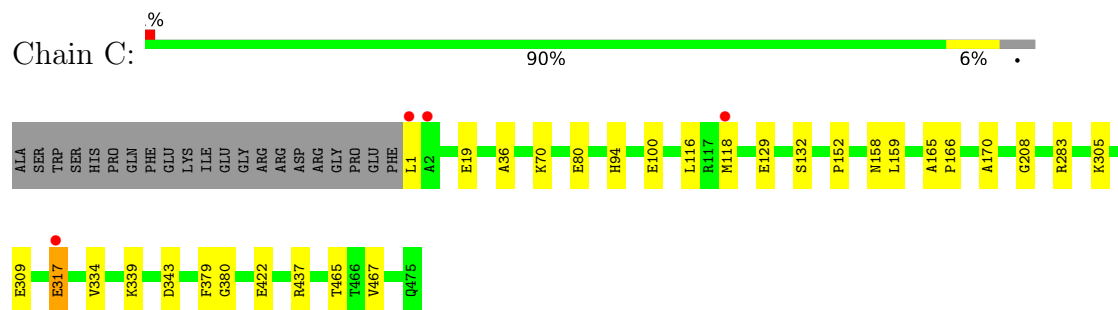
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



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



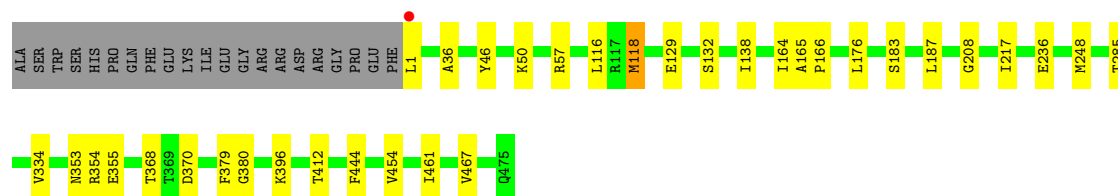
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



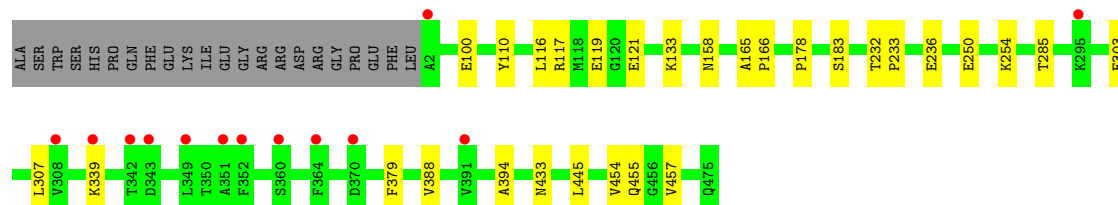
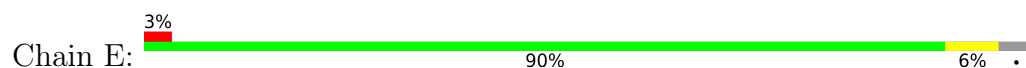
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



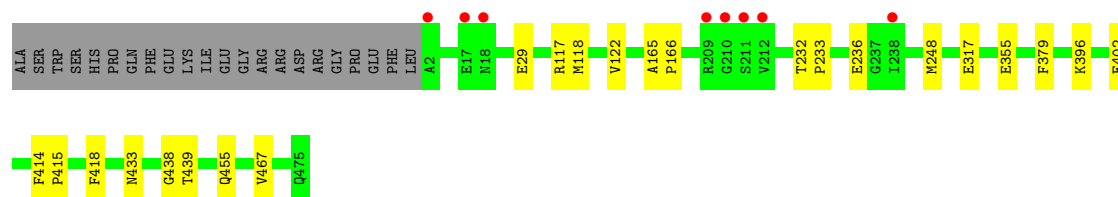
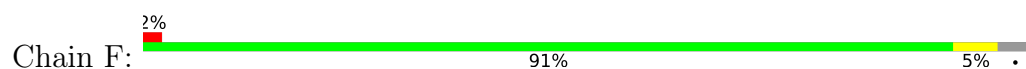




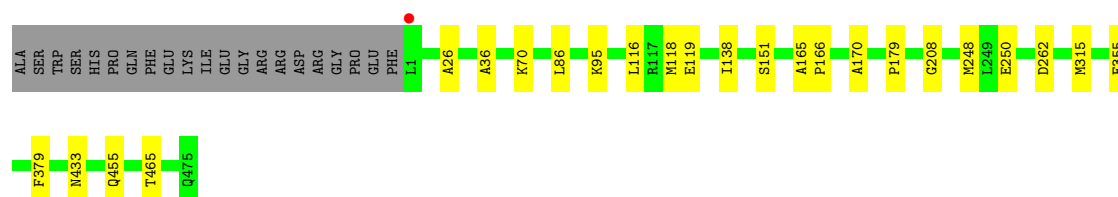
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



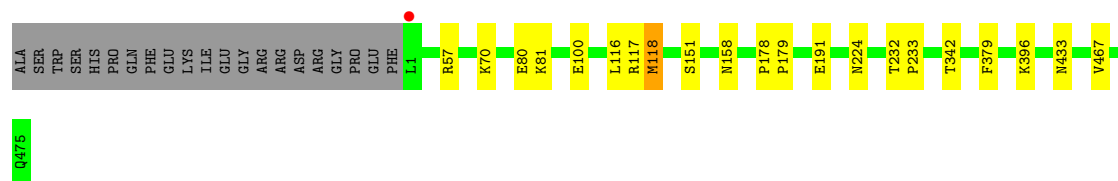
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- 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, $\alpha$ , $\beta$ , $\gamma$	97.76Å 98.95Å 103.03Å 78.04° 75.63° 67.01°	Depositor
Resolution (Å)	44.22 – 1.77 44.22 – 1.77	Depositor EDS
% Data completeness (in resolution range)	67.0 (44.22-1.77) 67.5 (44.22-1.77)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 1.76Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.175 , 0.219 0.182 , 0.184	Depositor DCC
$R_{free}$ test set	16365 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	61356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, SO4, EPE, T5V, BTB, CL

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	0.18	0/3616	0.33	0/4903
1	B	0.18	0/3689	0.36	0/5001
1	C	0.19	0/3672	0.36	0/4978
1	D	0.19	0/3659	0.35	0/4962
1	E	0.15	0/3616	0.28	0/4903
1	F	0.16	0/3683	0.32	0/4993
1	G	0.18	0/3683	0.34	0/4992
1	H	0.19	0/3626	0.35	0/4917
All	All	0.18	0/29244	0.34	0/39649

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	ARG	Sidechain

## 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	3553	3620	3619	21	0
1	B	3597	3666	3651	17	0
1	C	3582	3650	3625	18	0
1	D	3582	3651	3636	19	0
1	E	3553	3620	3619	15	0
1	F	3594	3661	3646	11	0
1	G	3588	3663	3630	12	0
1	H	3560	3634	3635	12	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	15	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
3	A	7	5	0	0	0
3	B	7	5	0	0	0
3	C	7	5	0	0	0
3	D	7	5	0	0	0
3	E	14	10	0	0	0
3	F	7	5	0	0	0
3	G	7	5	0	0	0
3	H	7	5	0	0	0
4	A	14	19	19	0	0
4	B	14	19	19	0	0
4	C	14	19	19	0	0
4	D	14	19	19	0	0
4	E	14	19	19	0	0
4	F	14	19	19	0	0
4	G	14	19	19	0	0
4	H	14	19	19	0	0
5	A	6	8	8	0	0
5	C	6	8	8	0	0
5	E	6	8	8	0	0
5	F	12	16	16	1	0
5	G	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	12	16	16	0	0
6	B	15	17	17	0	0
6	D	30	34	34	1	0
7	H	1	0	0	0	0
8	A	307	0	0	4	0
8	B	412	0	0	5	1
8	C	431	0	0	8	2
8	D	358	0	0	3	3
8	E	227	0	0	6	0
8	F	326	0	0	4	1
8	G	420	0	0	3	3
8	H	440	0	0	8	2
All	All	31879	29477	29328	122	6

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 2.

All (122) 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:H:70:LYS:NZ	8:H:601:HOH:O	1.97	0.94
1:B:392:GLU:OE1	8:B:601:HOH:O	1.99	0.80
1:D:236:GLU:OE2	8:D:601:HOH:O	1.98	0.80
1:E:303:GLU:OE1	8:E:601:HOH:O	2.00	0.78
1:C:80:GLU:OE1	8:C:601:HOH:O	2.03	0.76
1:H:224:ASN:ND2	8:H:605:HOH:O	2.20	0.74
1:E:254:LYS:NZ	8:E:605:HOH:O	2.21	0.73
1:H:118:MET:SD	8:H:1013:HOH:O	2.48	0.71
1:H:342:THR:O	8:H:602:HOH:O	2.11	0.68
1:E:236:GLU:O	8:E:602:HOH:O	2.12	0.68
1:B:119:GLU:OE2	8:B:602:HOH:O	2.13	0.66
1:D:217:ILE:HD11	6:D:505[B]:EPE:H32	1.78	0.66
1:E:307:LEU:O	8:E:603:HOH:O	2.14	0.65
1:A:285:THR:HG21	1:A:444:PHE:HE1	1.62	0.64
1:G:262:ASP:OD2	8:G:601:HOH:O	2.15	0.64
1:D:118:MET:HE1	1:D:461:ILE:HG22	1.78	0.64
1:A:80:GLU:OE1	8:A:601:HOH:O	2.15	0.63
1:E:388:VAL:HG21	1:E:394:ALA:HB2	1.82	0.61
1:F:29:GLU:OE2	8:F:601:HOH:O	2.16	0.61
1:C:170:ALA:HB1	1:C:465:THR:HG22	1.82	0.61
1:A:244:MET:HG2	1:B:249:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ARG:NH2	8:C:613:HOH:O	2.35	0.59
1:A:305:LYS:NZ	1:A:309:GLU:OE2	2.35	0.59
1:F:236:GLU:OE2	8:F:602:HOH:O	2.17	0.59
1:G:455[B]:GLN:NE2	8:G:607:HOH:O	2.36	0.59
1:C:19:GLU:OE1	8:C:602:HOH:O	2.17	0.57
1:B:264:ASP:OD1	8:B:604:HOH:O	2.17	0.57
1:F:317[A]:GLU:OE2	8:F:603:HOH:O	2.17	0.56
1:A:141:ARG:NH2	8:A:612:HOH:O	2.40	0.55
1:B:455:GLN:NE2	8:B:603:HOH:O	2.15	0.55
1:C:343:ASP:OD1	8:C:603:HOH:O	2.18	0.54
1:A:191:GLU:OE2	8:A:602:HOH:O	2.19	0.54
1:H:191:GLU:OE2	8:H:603:HOH:O	2.19	0.53
1:D:412:THR:O	8:D:602:HOH:O	2.18	0.53
1:A:285:THR:HG21	1:A:444:PHE:CE1	2.43	0.53
1:G:119:GLU:OE2	8:G:602:HOH:O	2.19	0.52
1:A:134:LYS:NZ	1:C:422:GLU:OE1	2.43	0.51
1:E:133:LYS:NZ	8:E:618:HOH:O	2.43	0.51
1:H:80:GLU:OE1	8:H:604:HOH:O	2.19	0.51
1:E:119:GLU:OE2	8:E:604:HOH:O	2.19	0.51
1:C:283:ARG:NH1	8:C:622:HOH:O	2.43	0.50
1:E:100:GLU:HG3	1:E:158:ASN:HB2	1.94	0.50
1:C:334:VAL:HG21	1:C:380:GLY:HA3	1.94	0.49
1:F:165:ALA:HB3	1:F:166:PRO:HD3	1.93	0.48
1:A:3:LYS:NZ	8:A:602:HOH:O	2.46	0.47
1:C:100:GLU:HG3	1:C:158:ASN:HB2	1.96	0.47
1:B:455:GLN:NE2	1:B:460:SER:OG	2.48	0.47
1:D:334:VAL:HG21	1:D:380:GLY:HA3	1.96	0.47
1:D:129:GLU:OE2	1:D:132:SER:OG	2.32	0.46
1:B:414[B]:PHE:HB3	1:B:415:PRO:HD3	1.98	0.46
1:D:165:ALA:HB3	1:D:166:PRO:HD3	1.97	0.46
1:F:402[B]:GLU:OE1	5:F:506:GOL:O3	2.24	0.46
1:C:305:LYS:NZ	1:C:309:GLU:OE2	2.48	0.46
1:F:414[B]:PHE:HB3	1:F:415:PRO:HD3	1.98	0.46
1:E:110:TYR:HD1	1:E:457:VAL:HG11	1.80	0.45
1:A:365:ASP:OD1	1:A:366:HIS:N	2.46	0.45
1:D:285[B]:THR:HG21	1:D:444:PHE:CE1	2.51	0.45
1:D:164:ILE:HD11	1:D:176:LEU:HD22	1.98	0.45
1:C:116:LEU:C	1:C:116:LEU:HD12	2.42	0.45
1:H:116:LEU:HD12	1:H:116:LEU:C	2.42	0.45
1:C:339:LYS:NZ	8:C:607:HOH:O	2.26	0.44
1:F:438:GLY:HA2	1:F:439:THR:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD12	1:A:116:LEU:C	2.42	0.44
1:G:165:ALA:HB3	1:G:166:PRO:HD3	1.99	0.44
1:D:116:LEU:HD12	1:D:116:LEU:C	2.43	0.44
1:A:22[A]:ILE:HD12	1:A:184:ILE:HG13	1.99	0.44
1:B:248:MET:SD	1:B:455:GLN:HG2	2.57	0.44
1:C:159:LEU:HD22	8:C:613:HOH:O	2.17	0.43
1:C:317[A]:GLU:H	1:C:317[A]:GLU:CD	2.25	0.43
1:E:250:GLU:OE2	1:E:455:GLN:HG3	2.18	0.43
1:A:100:GLU:HG3	1:A:158:ASN:HB2	2.01	0.43
1:A:438:GLY:HA2	1:A:439:THR:C	2.43	0.43
1:F:122:VAL:HG21	1:G:138:ILE:HG23	2.01	0.43
1:B:104:THR:OG1	1:B:158:ASN:HA	2.19	0.43
1:B:273:VAL:HG21	1:B:307:LEU:HB2	2.01	0.43
1:C:36:ALA:HA	1:C:208:GLY:HA2	2.01	0.43
1:D:138:ILE:HD12	1:D:138:ILE:N	2.34	0.43
1:E:232:THR:N	1:E:233:PRO:HD2	2.34	0.43
1:C:129:GLU:OE2	1:C:132:SER:OG	2.34	0.42
1:D:353:ASN:OD1	1:D:354:ARG:N	2.52	0.42
1:G:116:LEU:C	1:G:116:LEU:HD12	2.44	0.42
1:D:36:ALA:HA	1:D:208:GLY:HA2	2.01	0.42
1:F:396:LYS:NZ	8:F:628:HOH:O	2.52	0.42
1:E:178:PRO:HB2	1:E:183:SER:HA	2.01	0.42
1:E:445:LEU:HD13	1:E:454:VAL:HG22	2.01	0.42
1:H:151:SER:O	1:H:179:PRO:HD3	2.20	0.42
1:A:138:ILE:HD12	1:A:138:ILE:N	2.34	0.42
1:A:232:THR:N	1:A:233:PRO:HD2	2.34	0.42
1:F:232:THR:N	1:F:233:PRO:HD2	2.35	0.42
1:B:50:LYS:NZ	8:B:617:HOH:O	2.40	0.42
1:G:250:GLU:OE2	1:G:455[B]:GLN:HG3	2.20	0.42
1:E:165:ALA:HB3	1:E:166:PRO:HD3	2.02	0.42
1:D:46:TYR:O	1:D:50:LYS:HG2	2.20	0.41
1:D:183:SER:O	1:D:187:LEU:HG	2.20	0.41
1:A:86:LEU:HD13	1:A:156:PRO:HG2	2.02	0.41
1:B:86:LEU:HD23	1:B:86:LEU:C	2.45	0.41
1:E:116:LEU:C	1:E:116:LEU:HD12	2.46	0.41
1:H:100:GLU:HG3	1:H:158:ASN:HB2	2.02	0.41
1:H:178:PRO:HB3	8:H:616:HOH:O	2.20	0.41
1:A:165:ALA:HB3	1:A:166:PRO:HD3	2.01	0.41
1:B:317[B]:GLU:H	1:B:317[B]:GLU:CD	2.28	0.41
1:C:94[A]:HIS:NE2	8:C:601:HOH:O	2.31	0.41
1:G:26:ALA:HB1	1:G:315:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:SER:O	1:G:179:PRO:HD3	2.20	0.41
1:A:334:VAL:HG21	1:A:380:GLY:HA3	2.02	0.41
1:B:116:LEU:C	1:B:116:LEU:HD12	2.46	0.41
1:D:57:ARG:HD3	8:D:733:HOH:O	2.21	0.41
1:B:178:PRO:HB2	1:B:183:SER:HA	2.03	0.41
1:H:57:ARG:HD3	8:H:954:HOH:O	2.20	0.41
1:F:317[B]:GLU:CD	1:F:317[B]:GLU:H	2.28	0.41
1:B:165:ALA:HB3	1:B:166:PRO:HD3	2.01	0.41
1:B:325:LEU:HD12	1:B:331:ALA:HA	2.02	0.41
1:G:86:LEU:HD23	1:G:86:LEU:C	2.45	0.41
1:G:170:ALA:HB1	1:G:465:THR:HG22	2.03	0.41
1:D:412:THR:O	1:D:412:THR:HG22	2.21	0.41
1:H:232:THR:N	1:H:233:PRO:HD2	2.36	0.41
1:D:248:MET:HE1	1:D:454:VAL:O	2.21	0.40
1:D:368:THR:OG1	1:D:370:ASP:OD1	2.33	0.40
1:C:165:ALA:HB3	1:C:166:PRO:HD3	2.02	0.40
1:G:36:ALA:HA	1:G:208:GLY:HA2	2.04	0.40
1:A:170:ALA:HB1	1:A:465:THR:CG2	2.51	0.40
1:A:350:THR:OG1	1:A:363:LEU:N	2.50	0.40

All (6) 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)
8:C:933:HOH:O	8:G:922:HOH:O[1_456]	2.11	0.09
8:C:642:HOH:O	8:H:619:HOH:O[1_466]	2.13	0.07
8:B:742:HOH:O	8:G:768:HOH:O[1_556]	2.14	0.06
8:D:920:HOH:O	8:G:883:HOH:O[1_456]	2.14	0.06
8:D:655:HOH:O	8:F:636:HOH:O[1_556]	2.16	0.04
8:D:786:HOH:O	8:H:838:HOH:O[1_456]	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	474/496 (96%)	462 (98%)	12 (2%)	0	100	100
1	B	482/496 (97%)	470 (98%)	12 (2%)	0	100	100
1	C	481/496 (97%)	467 (97%)	13 (3%)	1 (0%)	44	29
1	D	481/496 (97%)	468 (97%)	13 (3%)	0	100	100
1	E	474/496 (96%)	459 (97%)	15 (3%)	0	100	100
1	F	481/496 (97%)	467 (97%)	14 (3%)	0	100	100
1	G	482/496 (97%)	469 (97%)	13 (3%)	0	100	100
1	H	476/496 (96%)	465 (98%)	11 (2%)	0	100	100
All	All	3831/3968 (96%)	3727 (97%)	103 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	PRO

### 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	371/388 (96%)	368 (99%)	3 (1%)	79	70
1	B	379/388 (98%)	370 (98%)	9 (2%)	44	24
1	C	378/388 (97%)	371 (98%)	7 (2%)	52	33
1	D	375/388 (97%)	368 (98%)	7 (2%)	52	33
1	E	371/388 (96%)	365 (98%)	6 (2%)	58	41
1	F	378/388 (97%)	368 (97%)	10 (3%)	41	21
1	G	379/388 (98%)	370 (98%)	9 (2%)	44	24
1	H	373/388 (96%)	366 (98%)	7 (2%)	52	33
All	All	3004/3104 (97%)	2946 (98%)	58 (2%)	56	33

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	339	LYS
1	A	379	PHE
1	B	3	LYS
1	B	117	ARG
1	B	294[A]	ASP
1	B	294[B]	ASP
1	B	379	PHE
1	B	418	PHE
1	B	433[A]	ASN
1	B	433[B]	ASN
1	B	455	GLN
1	C	1	LEU
1	C	70	LYS
1	C	118	MET
1	C	317[A]	GLU
1	C	317[B]	GLU
1	C	379	PHE
1	C	467	VAL
1	D	1	LEU
1	D	118	MET
1	D	355[A]	GLU
1	D	355[B]	GLU
1	D	379	PHE
1	D	396	LYS
1	D	467	VAL
1	E	117	ARG
1	E	121	GLU
1	E	285	THR
1	E	339	LYS
1	E	379	PHE
1	E	433	ASN
1	F	117	ARG
1	F	118	MET
1	F	248	MET
1	F	355	GLU
1	F	379	PHE
1	F	418	PHE
1	F	433[A]	ASN
1	F	433[B]	ASN
1	F	455	GLN
1	F	467	VAL

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Mol	Chain	Res	Type
1	G	70	LYS
1	G	95[A]	LYS
1	G	95[B]	LYS
1	G	118	MET
1	G	248[A]	MET
1	G	248[B]	MET
1	G	355	GLU
1	G	379	PHE
1	G	433	ASN
1	H	81	LYS
1	H	117	ARG
1	H	118	MET
1	H	379	PHE
1	H	396	LYS
1	H	433	ASN
1	H	467	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	B	353	ASN
1	C	18	ASN
1	C	423	GLN
1	D	10	ASN
1	D	366	HIS
1	E	94	HIS
1	F	423	GLN
1	G	271	ASN
1	G	353	ASN
1	G	433	ASN
1	H	423	GLN
1	H	475	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 1 is monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	GOL	C	503	-	5,5,5	0.82	0	5,5,5	0.99	0
6	EPE	D	505[B]	-	15,15,15	0.83	1 (6%)	18,20,20	1.44	3 (16%)
2	SO4	D	503	-	4,4,4	0.15	0	6,6,6	0.07	0
3	T5V	H	501	-	7,7,7	0.97	1 (14%)	8,8,8	2.78	5 (62%)
5	GOL	G	505	-	5,5,5	0.94	0	5,5,5	0.86	0
5	GOL	E	504	-	5,5,5	0.80	0	5,5,5	1.15	0
6	EPE	D	505[A]	-	15,15,15	0.81	1 (6%)	18,20,20	1.61	3 (16%)
3	T5V	G	501	-	7,7,7	0.89	0	8,8,8	2.83	5 (62%)
3	T5V	C	501	-	7,7,7	0.91	0	8,8,8	2.83	5 (62%)
2	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.11	0
5	GOL	F	506	-	5,5,5	0.91	0	5,5,5	0.95	0
2	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.06	0
3	T5V	D	502	-	7,7,7	0.89	1 (14%)	8,8,8	2.79	5 (62%)
4	BTB	F	504	-	13,13,13	0.85	0	7,16,16	0.74	0
4	BTB	H	504	-	13,13,13	0.98	0	7,16,16	0.91	0
4	BTB	A	503	-	13,13,13	0.90	0	7,16,16	0.78	0
4	BTB	G	504	-	13,13,13	0.88	0	7,16,16	0.81	0
4	BTB	E	503	-	13,13,13	0.84	0	7,16,16	0.61	0
5	GOL	F	505	-	5,5,5	0.82	0	5,5,5	0.97	0
3	T5V	E	501[B]	-	7,7,7	0.95	1 (14%)	8,8,8	2.78	5 (62%)
2	SO4	H	502	-	4,4,4	0.15	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	502	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	E	502	-	4,4,4	0.14	0	6,6,6	0.17	0
3	T5V	B	501	-	7,7,7	0.93	1 (14%)	8,8,8	2.74	5 (62%)
2	SO4	F	503	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	D	504	-	4,4,4	0.21	0	6,6,6	0.19	0
3	T5V	A	502	-	7,7,7	0.89	1 (14%)	8,8,8	2.67	5 (62%)
5	GOL	H	505	-	5,5,5	0.85	0	5,5,5	0.93	0
2	SO4	G	502	-	4,4,4	0.12	0	6,6,6	0.12	0
3	T5V	E	501[A]	-	7,7,7	0.95	1 (14%)	8,8,8	2.75	5 (62%)
2	SO4	H	503	-	4,4,4	0.16	0	6,6,6	0.20	0
5	GOL	A	504	-	5,5,5	0.76	0	5,5,5	1.11	0
2	SO4	G	503	-	4,4,4	0.12	0	6,6,6	0.09	0
4	BTB	B	504	-	13,13,13	0.91	0	7,16,16	0.86	0
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.20	0
4	BTB	D	506	-	13,13,13	0.84	0	7,16,16	0.62	0
4	BTB	C	504	-	13,13,13	0.95	0	7,16,16	0.61	0
5	GOL	H	506	-	5,5,5	0.77	0	5,5,5	0.88	0
2	SO4	F	502	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	B	503	-	4,4,4	0.12	0	6,6,6	0.14	0
3	T5V	F	501	-	7,7,7	0.95	1 (14%)	8,8,8	2.80	5 (62%)
6	EPE	B	505	-	15,15,15	0.82	1 (6%)	18,20,20	1.52	4 (22%)
2	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.09	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
5	GOL	C	503	-	-	2/4/4/4	-
6	EPE	D	505[B]	-	-	2/9/19/19	0/1/1/1
3	T5V	H	501	-	-	-	0/1/1/1
5	GOL	G	505	-	-	0/4/4/4	-
5	GOL	E	504	-	-	2/4/4/4	-
6	EPE	D	505[A]	-	-	3/9/19/19	0/1/1/1
3	T5V	G	501	-	-	-	0/1/1/1
3	T5V	C	501	-	-	-	0/1/1/1
5	GOL	F	506	-	-	2/4/4/4	-
4	BTB	F	504	-	-	3/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	H	504	-	-	3/21/21/21	-
3	T5V	D	502	-	-	-	0/1/1/1
4	BTB	A	503	-	-	5/21/21/21	-
4	BTB	G	504	-	-	1/21/21/21	-
5	GOL	F	505	-	-	4/4/4/4	-
3	T5V	E	501[B]	-	-	-	0/1/1/1
3	T5V	B	501	-	-	-	0/1/1/1
5	GOL	H	505	-	-	2/4/4/4	-
3	T5V	A	502	-	-	-	0/1/1/1
3	T5V	E	501[A]	-	-	-	0/1/1/1
5	GOL	A	504	-	-	0/4/4/4	-
4	BTB	B	504	-	-	6/21/21/21	-
4	BTB	D	506	-	-	5/21/21/21	-
4	BTB	C	504	-	-	4/21/21/21	-
5	GOL	H	506	-	-	3/4/4/4	-
6	EPE	B	505	-	-	4/9/19/19	0/1/1/1
3	T5V	F	501	-	-	-	0/1/1/1
4	BTB	E	503	-	-	7/21/21/21	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	505[A]	EPE	C10-S	2.69	1.81	1.77
6	D	505[B]	EPE	C10-S	2.62	1.81	1.77
6	B	505	EPE	C10-S	2.52	1.81	1.77
3	B	501	T5V	C-N	2.10	1.45	1.38
3	A	502	T5V	C-N	2.08	1.45	1.38
3	E	501[B]	T5V	C-N	2.08	1.45	1.38
3	F	501	T5V	C-N	2.07	1.45	1.38
3	E	501[A]	T5V	C-N	2.06	1.45	1.38
3	H	501	T5V	C-N	2.02	1.45	1.38
3	D	502	T5V	C-N	2.02	1.45	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	T5V	C3-N2-C2	4.57	121.65	115.80
3	H	501	T5V	C3-N2-C2	4.55	121.62	115.80
3	E	501[B]	T5V	C3-N2-C2	4.52	121.58	115.80
3	D	502	T5V	C3-N2-C2	4.47	121.53	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	T5V	C3-N2-C2	4.46	121.51	115.80
3	E	501[A]	T5V	C3-N2-C2	4.46	121.50	115.80
3	C	501	T5V	C3-N2-C2	4.40	121.44	115.80
6	D	505[A]	EPE	C5-N4-C3	4.35	118.61	108.83
3	F	501	T5V	C3-N2-C2	4.34	121.36	115.80
3	A	502	T5V	C3-N2-C2	4.31	121.32	115.80
3	F	501	T5V	C1-N1-C2	3.85	120.72	115.80
3	C	501	T5V	C1-N1-C2	3.83	120.70	115.80
3	H	501	T5V	C-C3-N2	-3.73	118.79	123.25
3	G	501	T5V	C-C3-N2	-3.73	118.79	123.25
3	E	501[A]	T5V	C-C3-N2	-3.72	118.80	123.25
3	G	501	T5V	C1-N1-C2	3.71	120.55	115.80
3	D	502	T5V	C-C3-N2	-3.69	118.83	123.25
3	D	502	T5V	C1-N1-C2	3.69	120.52	115.80
3	E	501[B]	T5V	C-C3-N2	-3.68	118.85	123.25
3	C	501	T5V	C-C3-N2	-3.67	118.86	123.25
3	A	502	T5V	C-C3-N2	-3.64	118.90	123.25
3	B	501	T5V	C1-N1-C2	3.63	120.44	115.80
3	E	501[B]	T5V	C1-N1-C2	3.59	120.39	115.80
3	F	501	T5V	C-C3-N2	-3.57	118.98	123.25
3	H	501	T5V	C1-N1-C2	3.55	120.34	115.80
3	B	501	T5V	C-C3-N2	-3.50	119.06	123.25
3	E	501[A]	T5V	C1-N1-C2	3.50	120.28	115.80
3	A	502	T5V	C1-N1-C2	3.44	120.20	115.80
6	B	505	EPE	C7-N4-C5	3.19	119.40	111.23
6	D	505[A]	EPE	C7-N4-C5	3.01	118.93	111.23
3	F	501	T5V	C-C1-N1	-2.95	119.73	123.25
3	C	501	T5V	C-C1-N1	-2.94	119.74	123.25
6	D	505[B]	EPE	O3S-S-C10	2.83	110.34	105.77
3	G	501	T5V	C-C1-N1	-2.78	119.92	123.25
3	G	501	T5V	N2-C2-N1	-2.76	121.21	126.61
3	B	501	T5V	C-C1-N1	-2.76	119.95	123.25
3	E	501[A]	T5V	C-C1-N1	-2.75	119.97	123.25
3	H	501	T5V	C-C1-N1	-2.74	119.97	123.25
3	E	501[B]	T5V	C-C1-N1	-2.74	119.97	123.25
3	D	502	T5V	C-C1-N1	-2.74	119.98	123.25
3	C	501	T5V	N2-C2-N1	-2.73	121.26	126.61
3	D	502	T5V	N2-C2-N1	-2.73	121.27	126.61
3	F	501	T5V	N2-C2-N1	-2.73	121.28	126.61
3	H	501	T5V	N2-C2-N1	-2.69	121.35	126.61
3	E	501[B]	T5V	N2-C2-N1	-2.68	121.36	126.61
3	B	501	T5V	N2-C2-N1	-2.67	121.38	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501[A]	T5V	N2-C2-N1	-2.60	121.52	126.61
6	D	505[B]	EPE	C7-N4-C5	2.59	117.85	111.23
3	A	502	T5V	C-C1-N1	-2.58	120.16	123.25
3	A	502	T5V	N2-C2-N1	-2.55	121.63	126.61
6	B	505	EPE	C7-N4-C3	2.52	117.67	111.23
6	D	505[A]	EPE	O3S-S-C10	2.49	109.80	105.77
6	B	505	EPE	C5-N4-C3	2.48	114.40	108.83
6	D	505[B]	EPE	C5-N4-C3	2.46	114.36	108.83
6	B	505	EPE	C6-N1-C2	2.18	113.75	108.83

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	BTB	C1-C2-C3-O3
4	A	503	BTB	C4-C2-C3-O3
4	A	503	BTB	N-C2-C3-O3
4	B	504	BTB	C1-C2-C4-O4
4	B	504	BTB	C3-C2-C4-O4
4	B	504	BTB	N-C2-C4-O4
4	D	506	BTB	O1-C1-C2-C3
4	D	506	BTB	C4-C2-C3-O3
4	E	503	BTB	C1-C2-C4-O4
4	E	503	BTB	C3-C2-C4-O4
4	E	503	BTB	N-C2-C4-O4
4	F	504	BTB	O1-C1-C2-C3
4	F	504	BTB	O1-C1-C2-N
4	H	504	BTB	O1-C1-C2-C3
4	H	504	BTB	O1-C1-C2-C4
4	H	504	BTB	O1-C1-C2-N
5	C	503	GOL	C1-C2-C3-O3
5	E	504	GOL	C1-C2-C3-O3
5	E	504	GOL	O2-C2-C3-O3
5	F	505	GOL	O1-C1-C2-C3
5	F	505	GOL	O2-C2-C3-O3
5	H	505	GOL	O1-C1-C2-O2
5	H	505	GOL	O1-C1-C2-C3
5	H	506	GOL	O1-C1-C2-C3
6	D	505[A]	EPE	C8-C7-N4-C5
6	D	505[A]	EPE	S-C10-C9-N1
6	B	505	EPE	C8-C7-N4-C5
4	G	504	BTB	N-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	E	503	BTB	N-C7-C8-O8
4	A	503	BTB	N-C7-C8-O8
5	F	505	GOL	C1-C2-C3-O3
5	F	506	GOL	C1-C2-C3-O3
5	H	506	GOL	C1-C2-C3-O3
4	B	504	BTB	N-C7-C8-O8
5	C	503	GOL	O2-C2-C3-O3
5	F	505	GOL	O1-C1-C2-O2
5	F	506	GOL	O2-C2-C3-O3
5	H	506	GOL	O1-C1-C2-O2
4	C	504	BTB	N-C7-C8-O8
6	D	505[B]	EPE	C10-C9-N1-C2
6	D	505[B]	EPE	C10-C9-N1-C6
4	B	504	BTB	O1-C1-C2-C4
4	E	503	BTB	O1-C1-C2-C3
4	C	504	BTB	N-C2-C3-O3
4	D	506	BTB	O1-C1-C2-N
4	D	506	BTB	N-C2-C3-O3
4	E	503	BTB	O1-C1-C2-N
4	A	503	BTB	N-C5-C6-O6
6	B	505	EPE	N4-C7-C8-O8
4	B	504	BTB	N-C5-C6-O6
4	E	503	BTB	N-C5-C6-O6
6	D	505[A]	EPE	C9-C10-S-O3S
6	B	505	EPE	S-C10-C9-N1
4	C	504	BTB	O1-C1-C2-C4
4	C	504	BTB	C1-C2-C3-O3
4	D	506	BTB	O1-C1-C2-C4
4	F	504	BTB	O1-C1-C2-C4
6	B	505	EPE	C9-C10-S-O1S

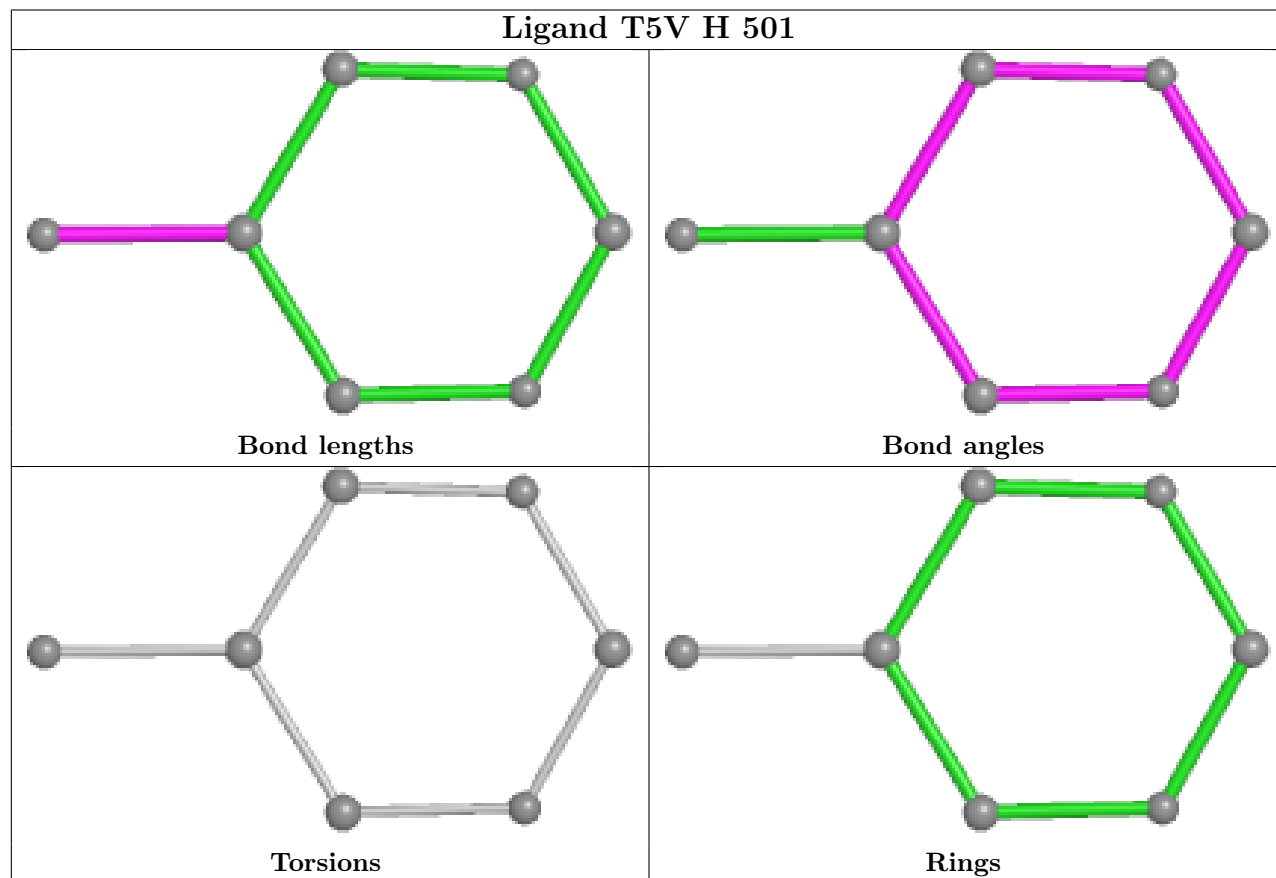
There are no ring outliers.

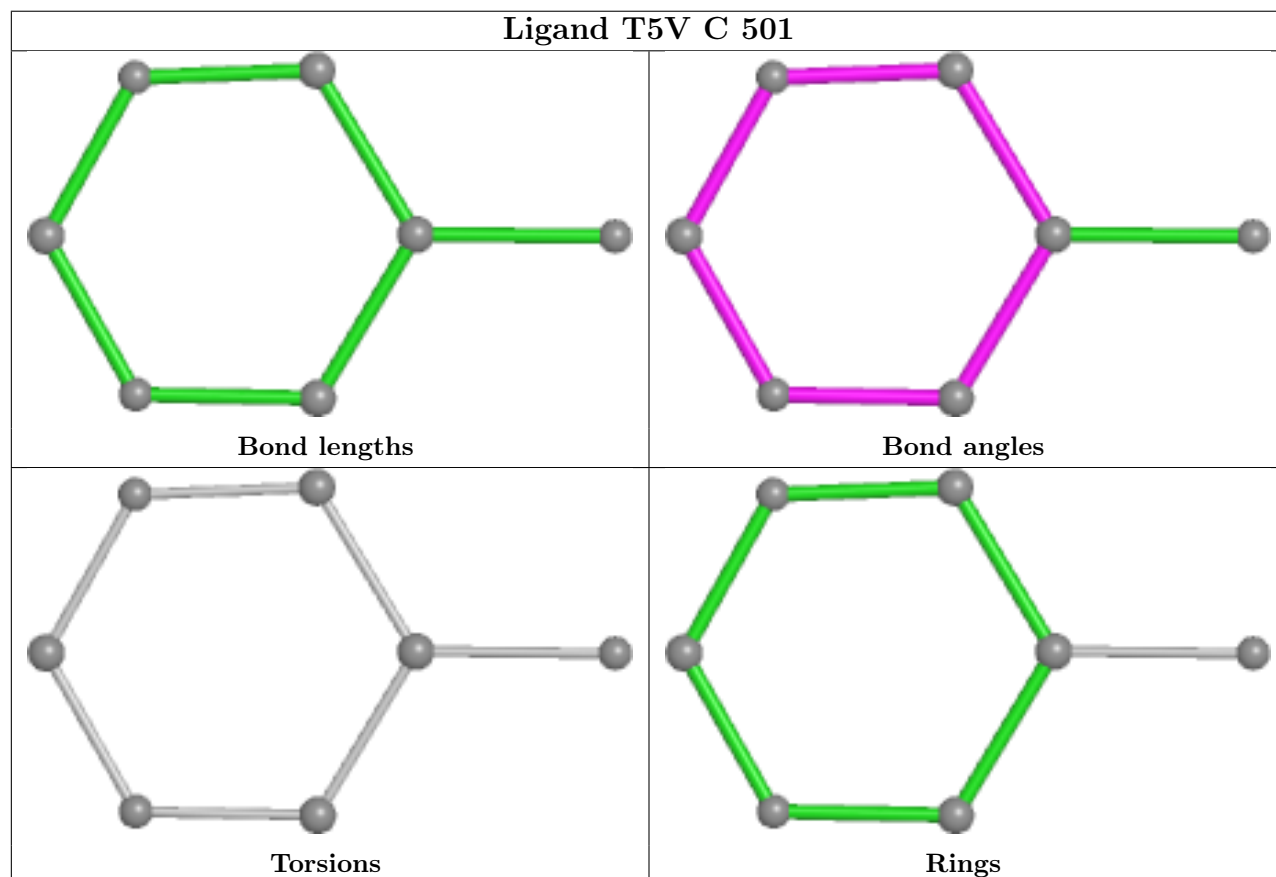
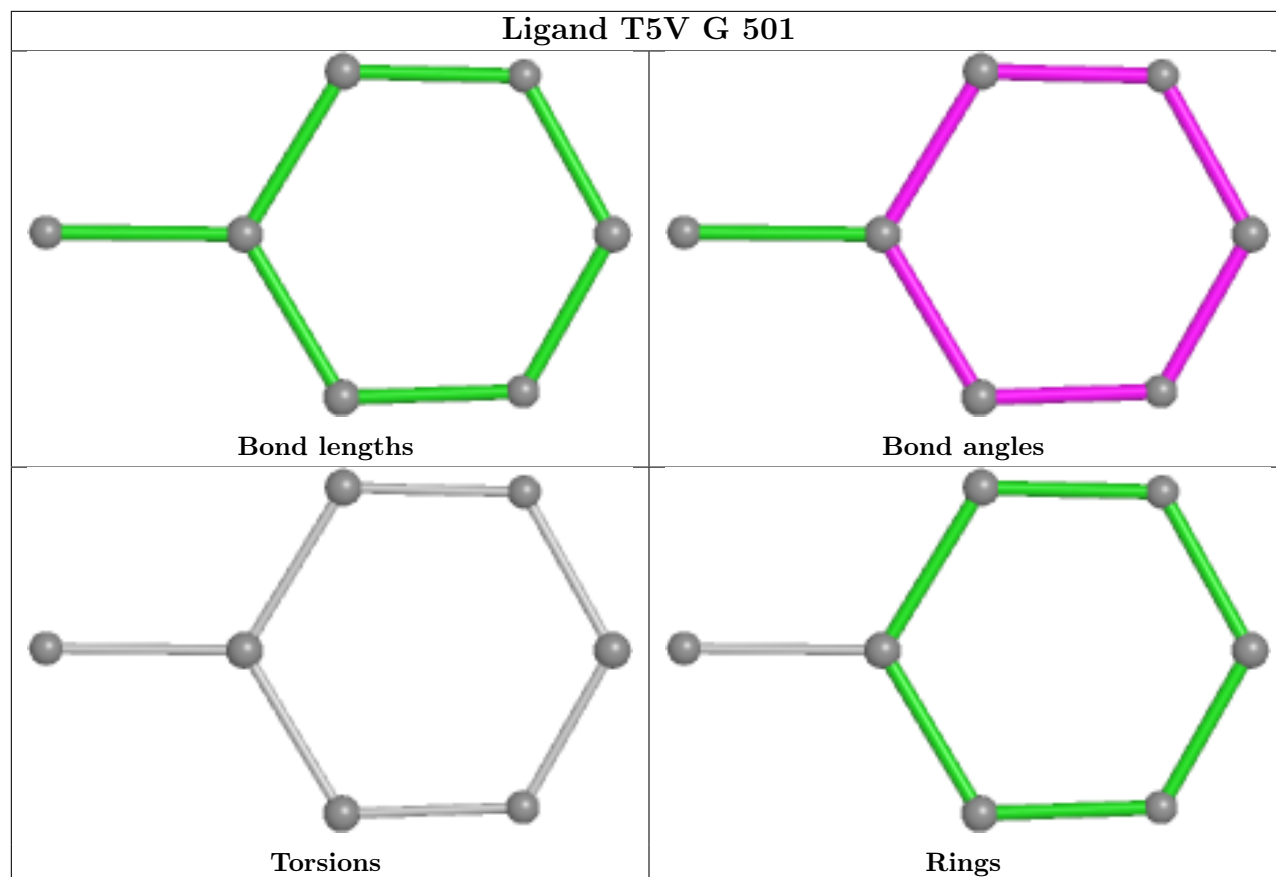
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	505[B]	EPE	1	0
5	F	506	GOL	1	0

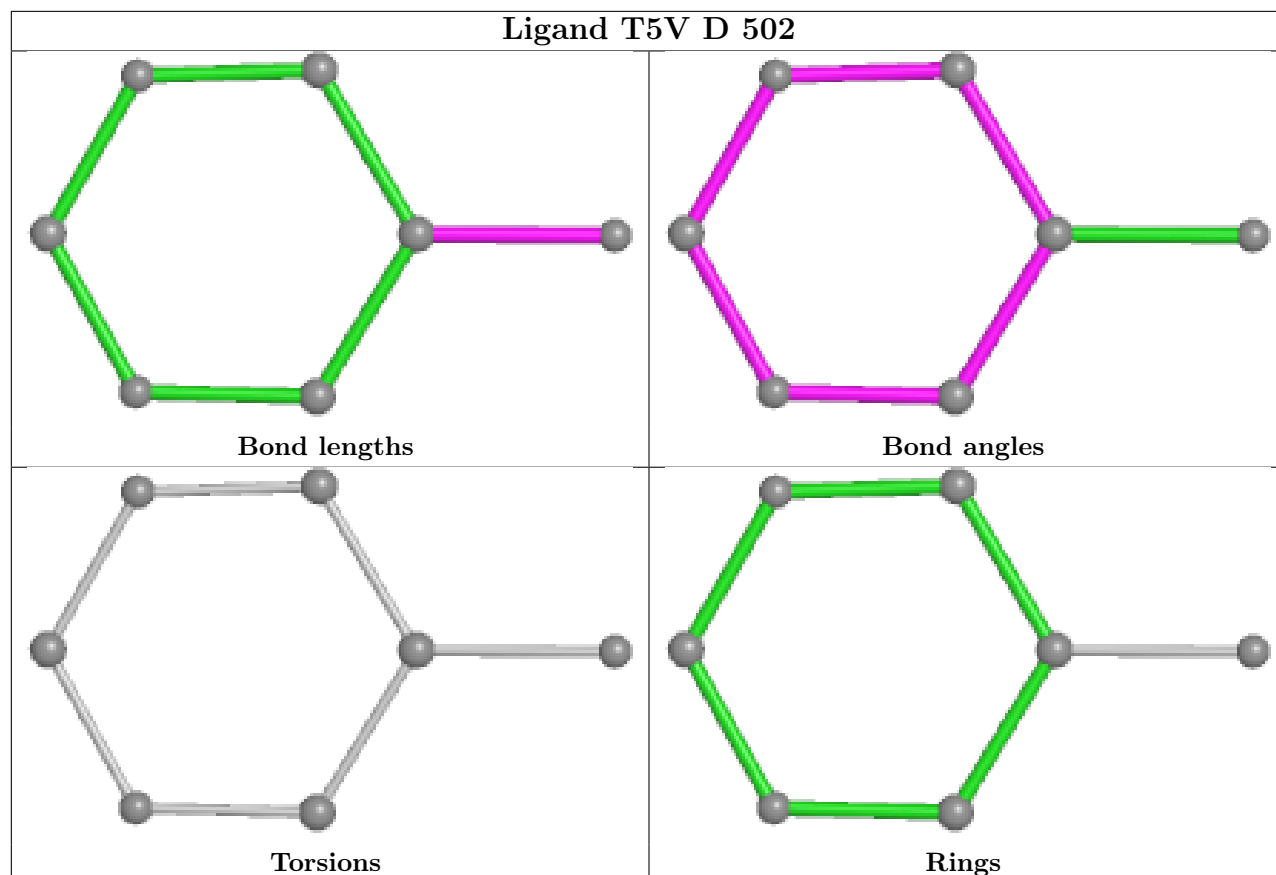
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

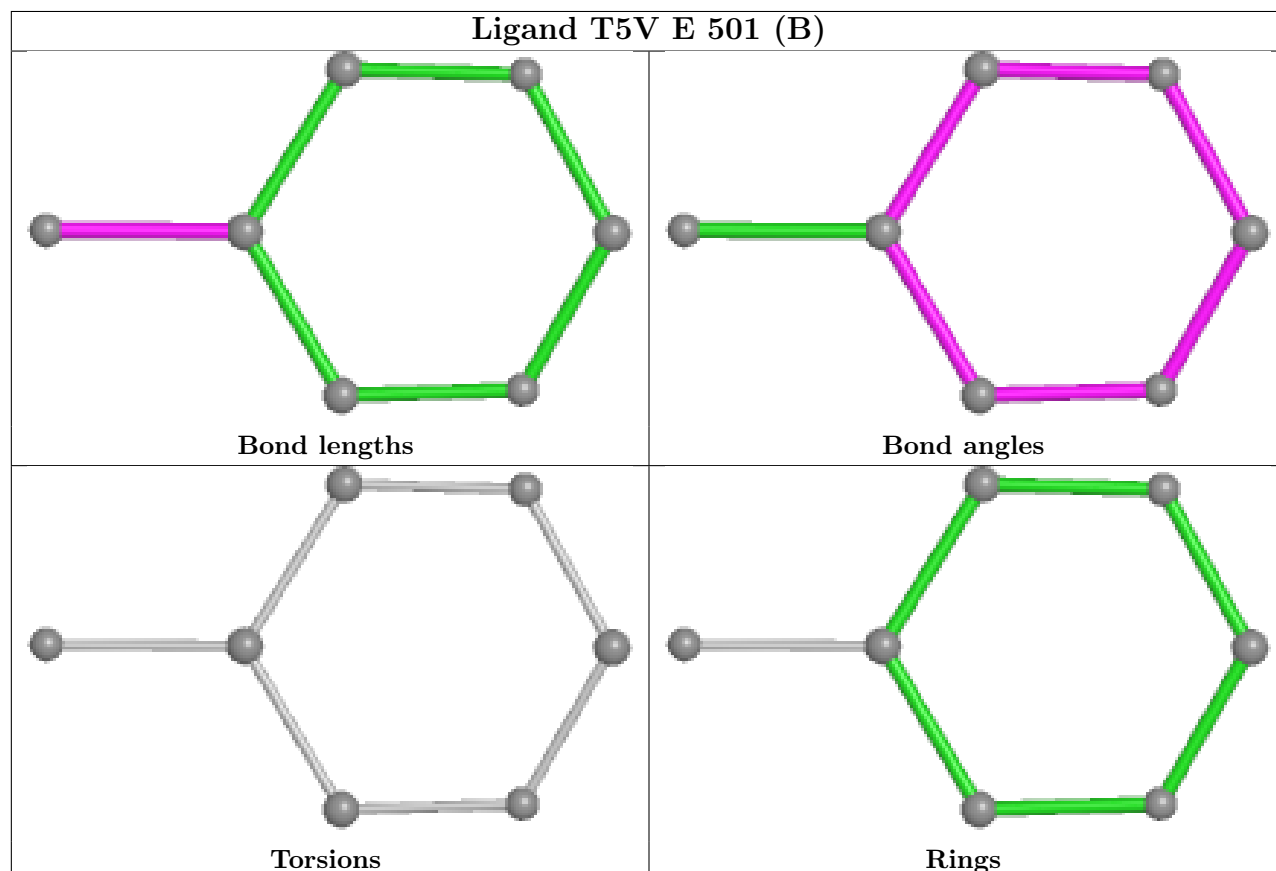




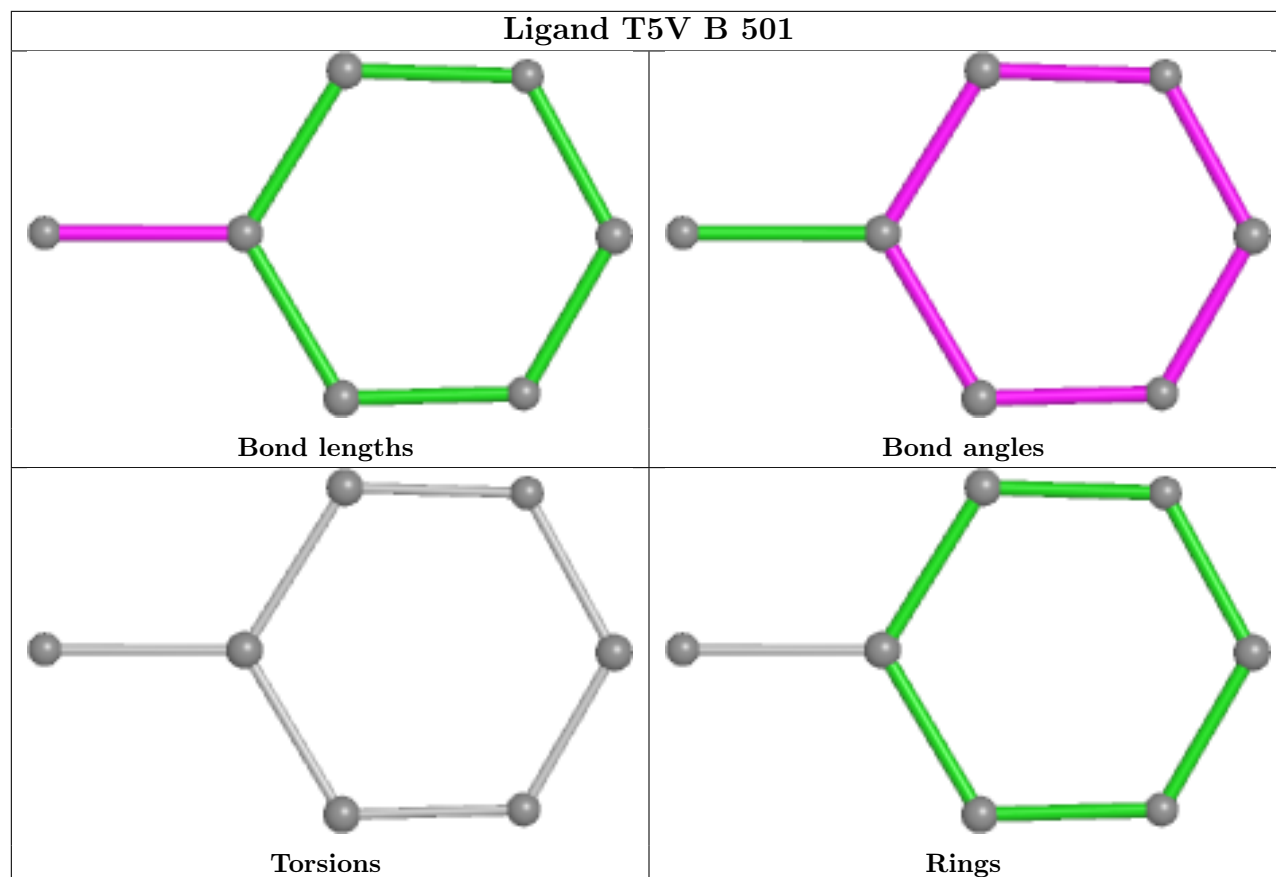
## Ligand T5V D 502



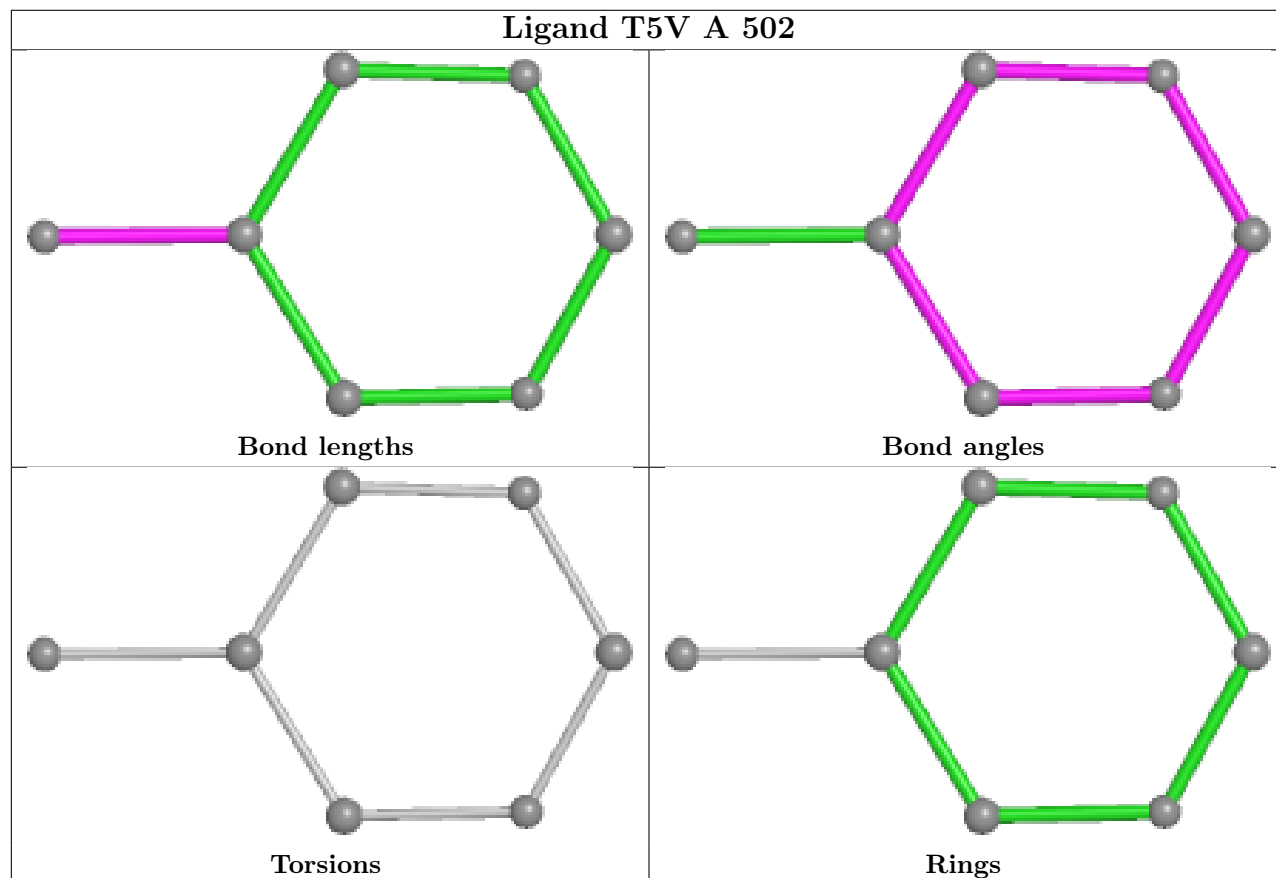
## Ligand T5V E 501 (B)



## Ligand T5V B 501

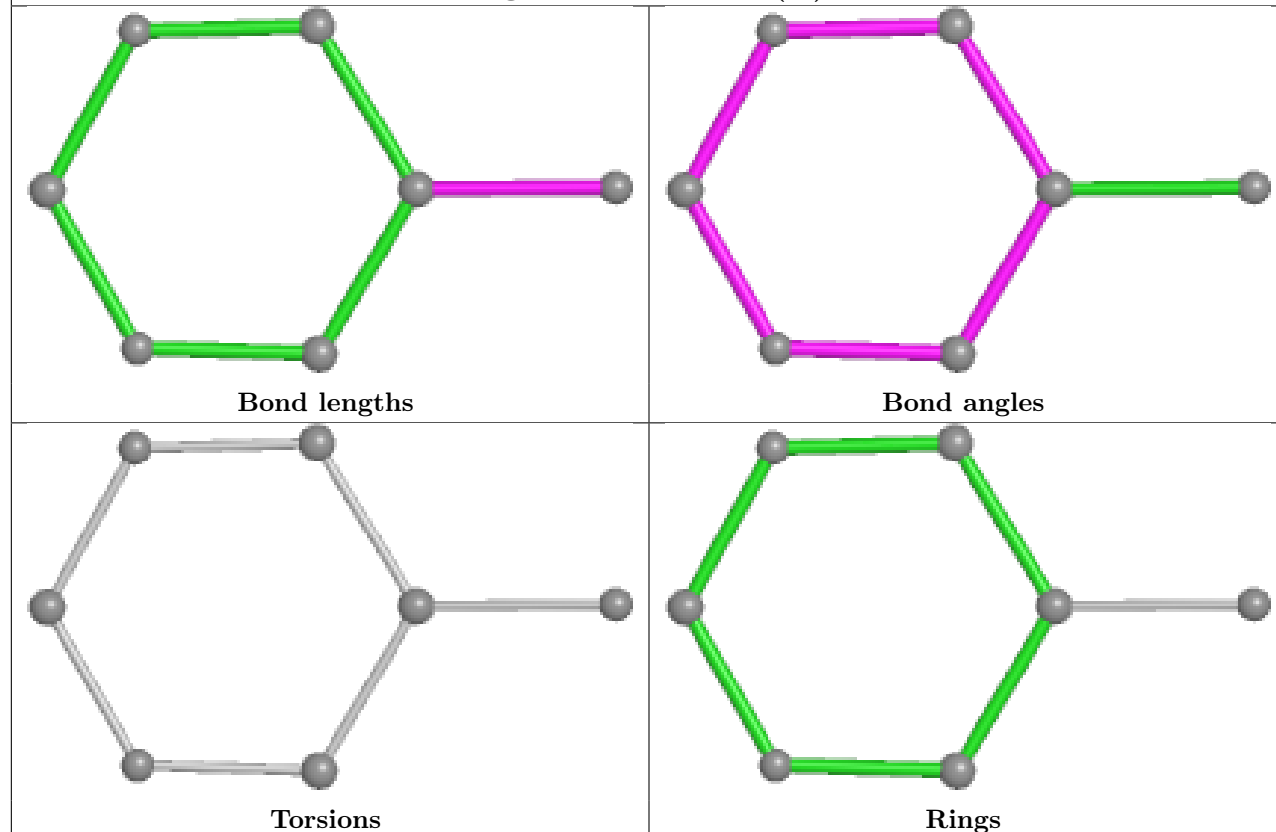


## Ligand T5V A 502

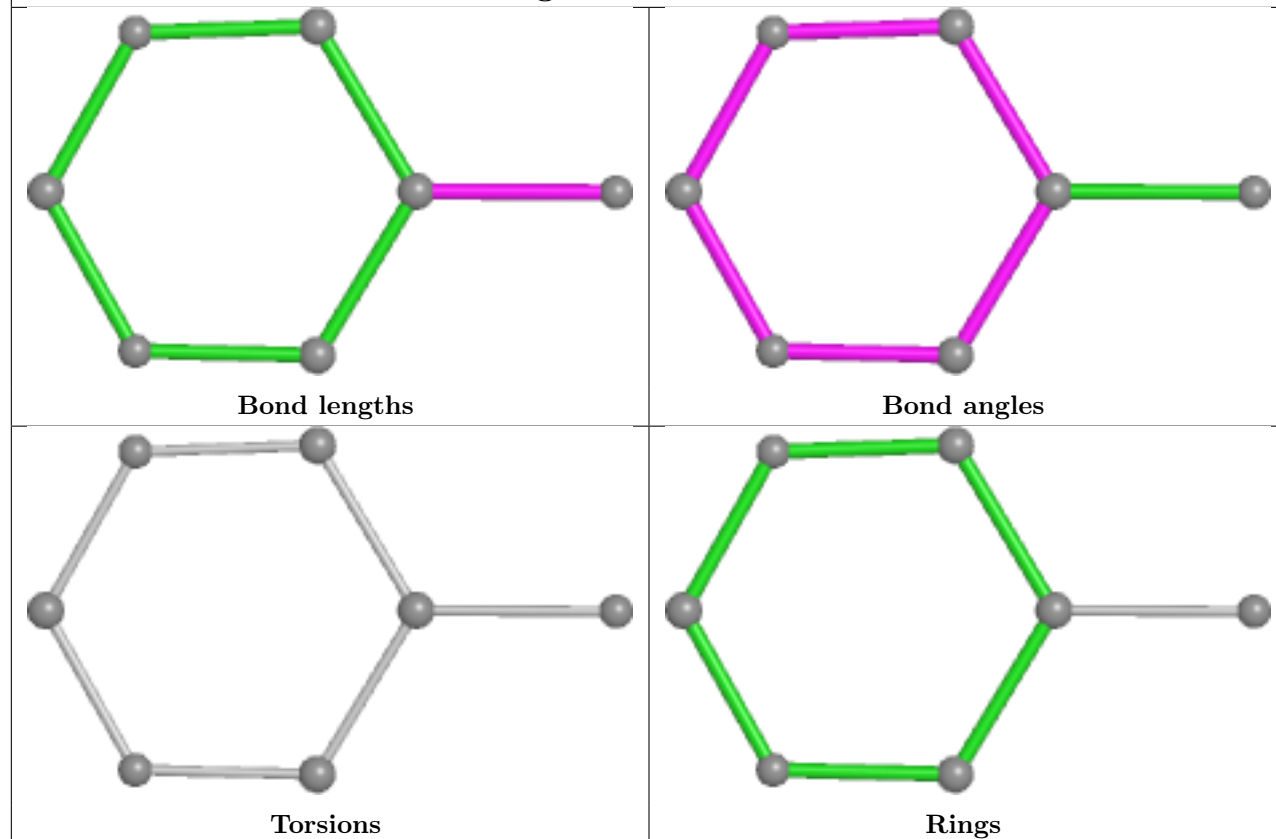




## Ligand T5V E 501 (A)



## Ligand T5V F 501



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.22	2 (0%) 89 92	13, 25, 41, 74	2 (0%)
1	B	474/496 (95%)	-0.48	2 (0%) 89 92	8, 19, 32, 64	9 (1%)
1	C	475/496 (95%)	-0.54	4 (0%) 82 87	9, 19, 30, 71	5 (1%)
1	D	475/496 (95%)	-0.46	1 (0%) 92 94	9, 20, 33, 54	5 (1%)
1	E	474/496 (95%)	0.22	13 (2%) 56 62	14, 34, 58, 90	2 (0%)
1	F	474/496 (95%)	-0.19	8 (1%) 69 75	9, 24, 48, 98	8 (1%)
1	G	475/496 (95%)	-0.50	1 (0%) 92 94	10, 19, 31, 83	6 (1%)
1	H	475/496 (95%)	-0.50	1 (0%) 92 94	9, 19, 32, 60	3 (0%)
All	All	3796/3968 (95%)	-0.33	32 (0%) 82 87	8, 21, 44, 98	40 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	212	VAL	4.8
1	F	210	GLY	4.6
1	G	1	LEU	4.2
1	B	212	VAL	3.7
1	C	1	LEU	3.7
1	B	210	GLY	3.6
1	E	370	ASP	3.6
1	D	1	LEU	3.3
1	F	18	ASN	3.2
1	C	2	ALA	3.0
1	E	2	ALA	3.0
1	E	339	LYS	2.7
1	F	209	ARG	2.7
1	E	295	LYS	2.7
1	E	308	VAL	2.7
1	E	364	PHE	2.7

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	E	351	ALA	2.6
1	E	360	SER	2.6
1	E	349	LEU	2.5
1	F	238	ILE	2.5
1	E	391	VAL	2.5
1	F	17[A]	GLU	2.5
1	F	211	SER	2.5
1	C	317[A]	GLU	2.4
1	C	118	MET	2.3
1	H	1	LEU	2.3
1	F	2	ALA	2.2
1	E	342	THR	2.2
1	E	352	PHE	2.2
1	A	306	THR	2.1
1	E	343	ASP	2.0
1	A	2	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EPE	D	505[A]	15/15	0.63	0.22	25,32,37,38	32
6	EPE	D	505[B]	15/15	0.63	0.22	15,30,35,36	32
6	EPE	B	505	15/15	0.65	0.17	23,31,45,49	32
5	GOL	E	504	6/6	0.71	0.17	28,34,38,46	14
2	SO4	F	502	5/5	0.75	0.13	53,55,56,60	0
2	SO4	A	505	5/5	0.77	0.13	26,29,33,35	5
5	GOL	F	506	6/6	0.78	0.12	27,36,47,48	0

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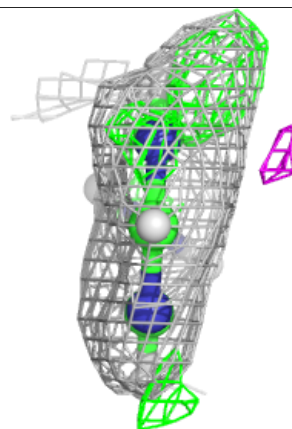
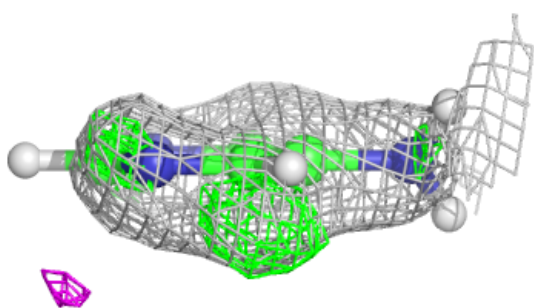
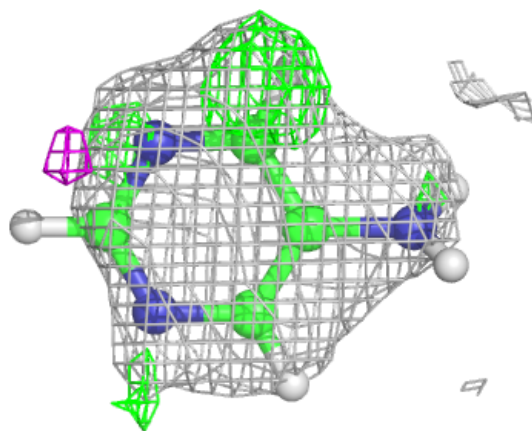
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	F	505	6/6	0.78	0.13	23,33,39,42	14
5	GOL	H	505	6/6	0.79	0.14	28,34,45,54	0
2	SO4	D	501	5/5	0.80	0.12	29,36,41,52	5
5	GOL	A	504	6/6	0.81	0.12	26,32,40,48	0
4	BTB	E	503	14/14	0.81	0.14	26,38,46,56	33
5	GOL	H	506	6/6	0.83	0.12	28,34,39,43	14
4	BTB	A	503	14/14	0.83	0.11	28,37,50,50	33
5	GOL	G	505	6/6	0.83	0.11	31,37,48,57	0
5	GOL	C	503	6/6	0.83	0.10	30,39,52,52	0
2	SO4	D	503	5/5	0.84	0.08	42,46,53,56	0
2	SO4	C	505	5/5	0.87	0.09	30,33,34,46	5
3	T5V	E	501[A]	7/7	0.87	0.29	75,76,91,91	12
4	BTB	F	504	14/14	0.87	0.10	25,37,57,57	0
4	BTB	H	504	14/14	0.87	0.10	18,28,41,48	0
3	T5V	E	501[B]	7/7	0.87	0.29	75,76,91,91	12
4	BTB	C	504	14/14	0.88	0.10	18,30,46,51	0
4	BTB	B	504	14/14	0.89	0.10	20,32,47,48	0
3	T5V	A	502	7/7	0.91	0.09	22,26,32,32	0
2	SO4	G	502	5/5	0.91	0.09	36,38,51,55	0
4	BTB	G	504	14/14	0.91	0.08	18,31,39,47	0
2	SO4	H	502	5/5	0.92	0.08	34,36,42,44	0
2	SO4	B	502	5/5	0.92	0.10	42,46,51,52	0
2	SO4	B	503	5/5	0.93	0.08	24,27,35,37	0
3	T5V	F	501	7/7	0.93	0.07	21,28,33,35	0
4	BTB	D	506	14/14	0.94	0.06	19,27,37,45	0
2	SO4	A	501	5/5	0.94	0.08	28,30,36,37	0
2	SO4	E	502	5/5	0.94	0.07	31,34,41,44	0
3	T5V	D	502	7/7	0.94	0.06	15,17,21,21	0
3	T5V	G	501	7/7	0.96	0.05	15,19,21,24	0
2	SO4	F	503	5/5	0.96	0.07	29,31,35,36	0
3	T5V	B	501	7/7	0.96	0.05	18,22,24,27	0
2	SO4	H	503	5/5	0.96	0.07	24,24,31,39	0
7	CL	H	507	1/1	0.96	0.13	36,36,36,36	0
2	SO4	G	503	5/5	0.97	0.06	19,28,29,35	0
2	SO4	D	504	5/5	0.97	0.05	16,19,27,29	0
3	T5V	H	501	7/7	0.98	0.05	15,18,22,23	0
3	T5V	C	501	7/7	0.98	0.04	15,19,22,23	0
2	SO4	C	502	5/5	0.98	0.06	19,22,28,33	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.

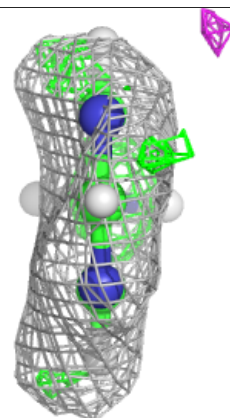
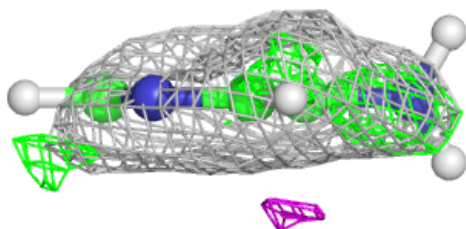
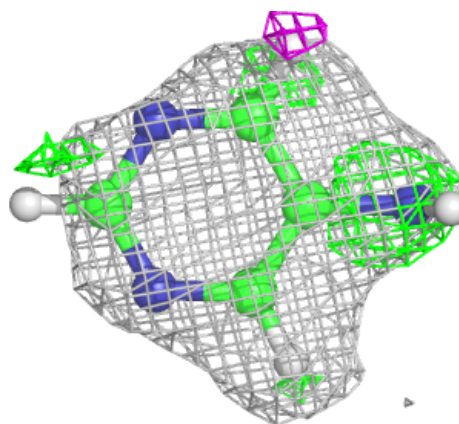
**Electron density around T5V E 501 (A):**

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



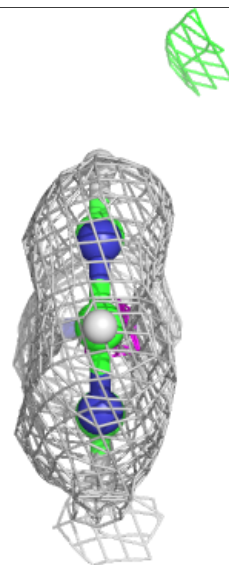
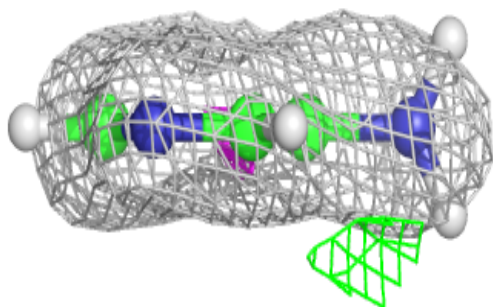
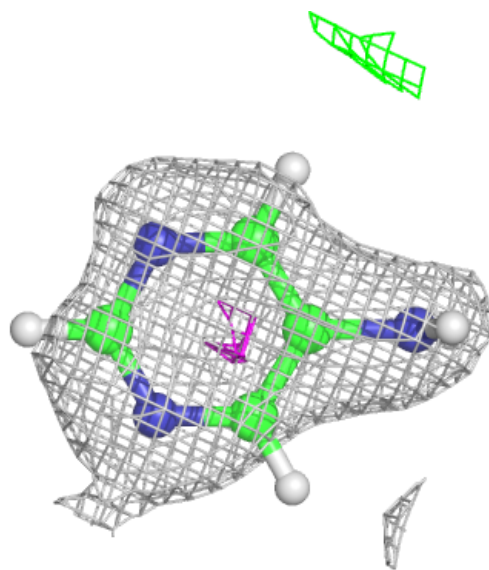
**Electron density around T5V E 501 (B):**

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and green (positive)



**Electron density around T5V A 502:**

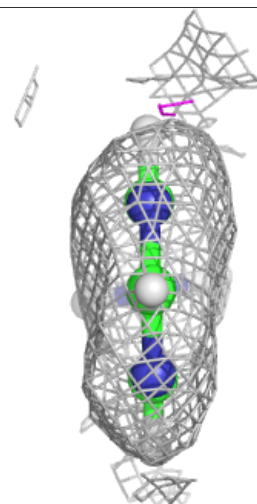
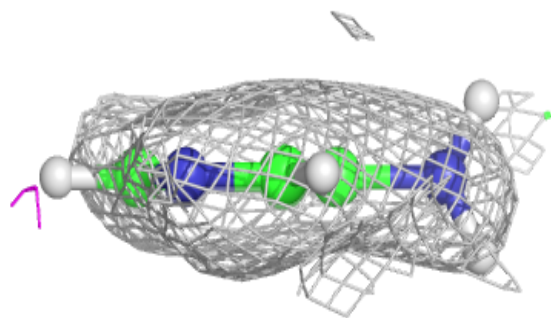
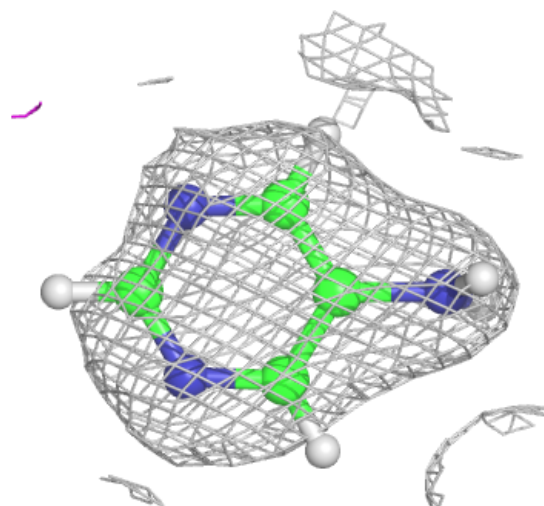
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





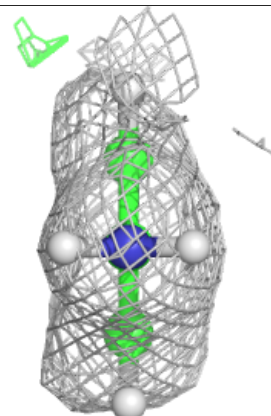
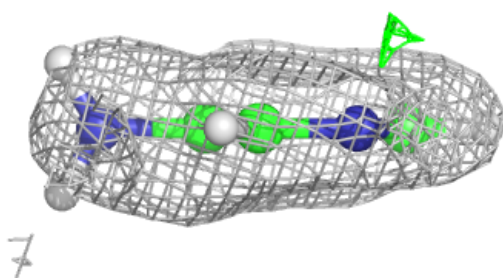
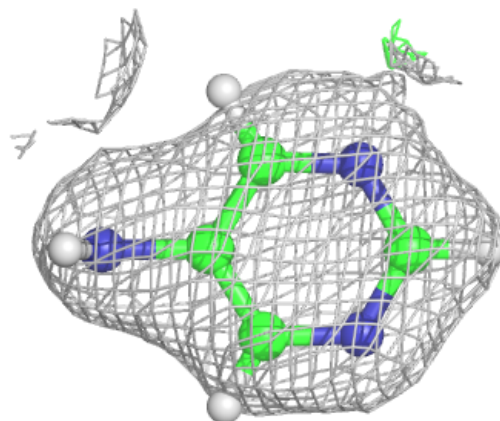
**Electron density around T5V F 501:**

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and green (positive)



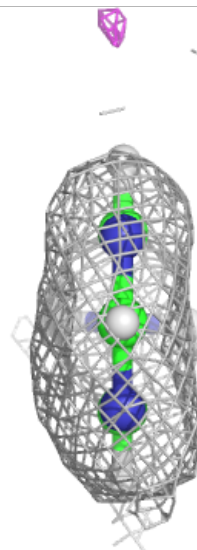
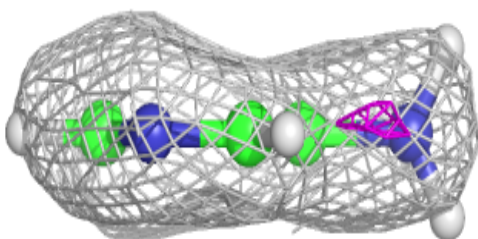
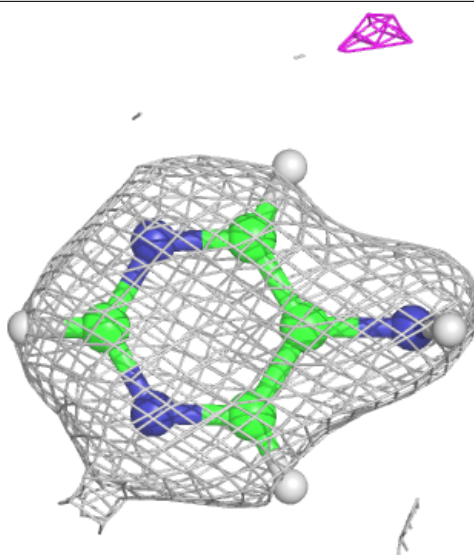
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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



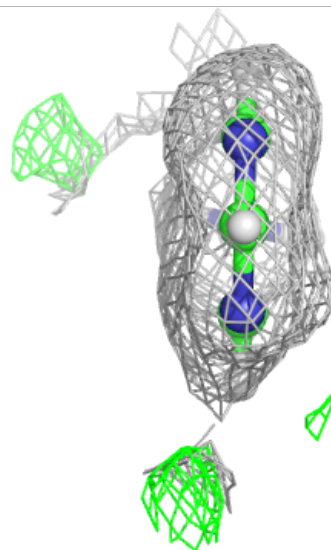
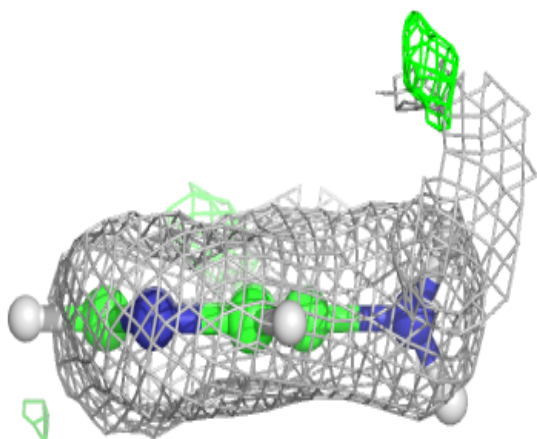
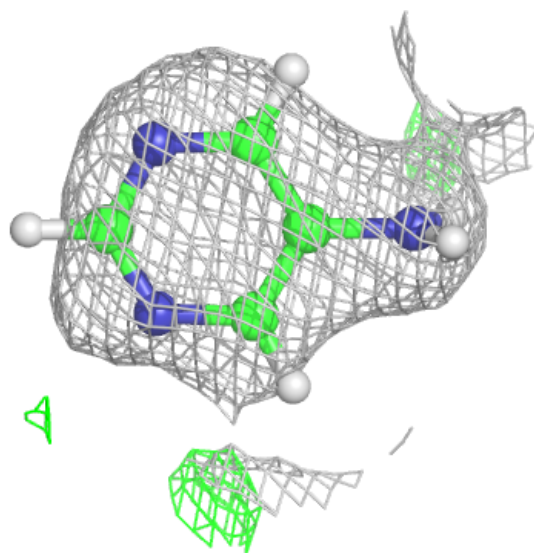
**Electron density around T5V G 501:**

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and green (positive)



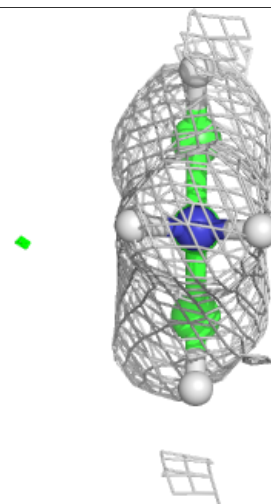
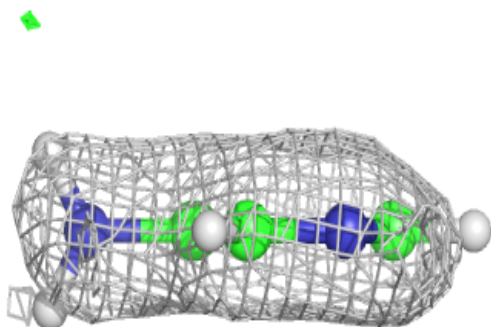
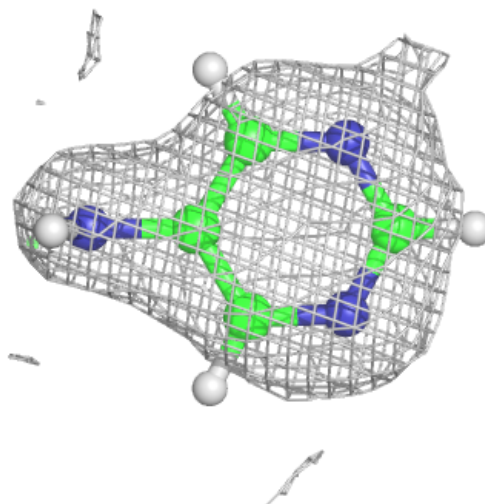
**Electron density around T5V B 501:**

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and green (positive)



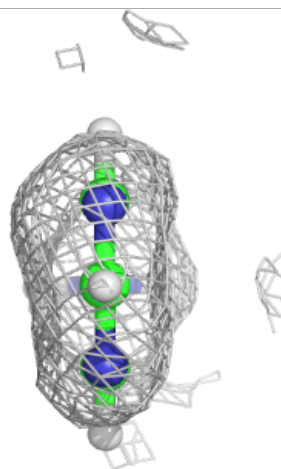
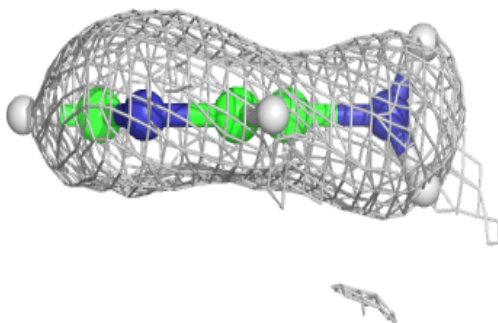
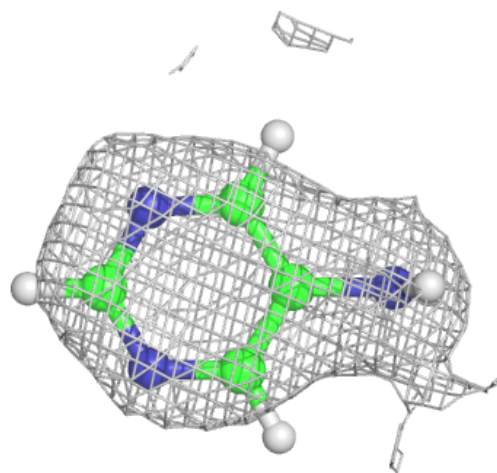
**Electron density around T5V H 501:**

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



**Electron density around T5V 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.