



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:20 PM UTC

PDB ID : 9RB1 / pdb_00009rb1
Title : Streptococcus pyogenes GapN in complex with 2-cyanoacetamide
Authors : Wirsing, R.; Schindelin, H.
Deposited on : 2025-05-21
Resolution : 1.61 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

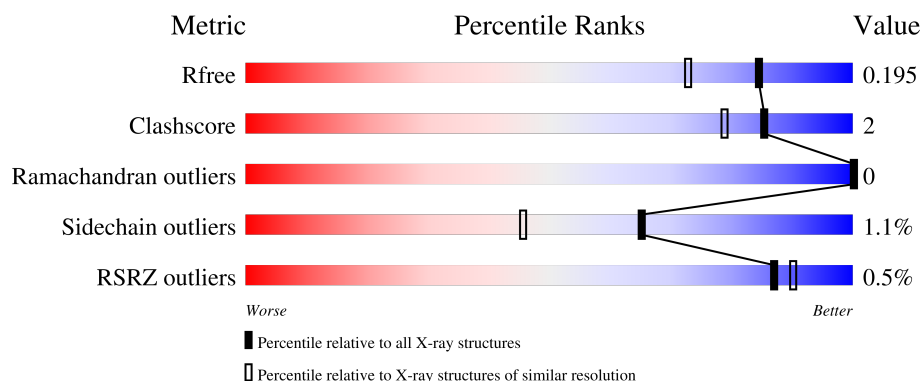
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	496	% 90% 5% . .
1	B	496	89% 6% .
1	C	496	90% 5% .
1	D	496	91% 5% .
1	E	496	91% 5% .

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Mol	Chain	Length	Quality of chain
1	F	496	2%91%5%••
1	G	496	91%5%•
1	H	496	90%6%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 62835 atoms, of which 29464 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	10	0
			7273	2295	3680	592	697	9			
1	B	474	Total	C	H	N	O	S	0	7	0
			7242	2289	3660	592	693	8			
1	C	475	Total	C	H	N	O	S	0	12	0
			7294	2297	3694	596	699	8			
1	D	475	Total	C	H	N	O	S	0	7	0
			7226	2276	3654	592	696	8			
1	E	474	Total	C	H	N	O	S	0	6	0
			7210	2274	3640	591	697	8			
1	F	474	Total	C	H	N	O	S	0	9	0
			7247	2288	3661	592	698	8			
1	G	475	Total	C	H	N	O	S	0	10	0
			7264	2288	3670	600	698	8			
1	H	475	Total	C	H	N	O	S	0	9	0
			7275	2290	3685	596	696	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
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F	-15	PRO	-	expression tag	UNP A0A4U9C786
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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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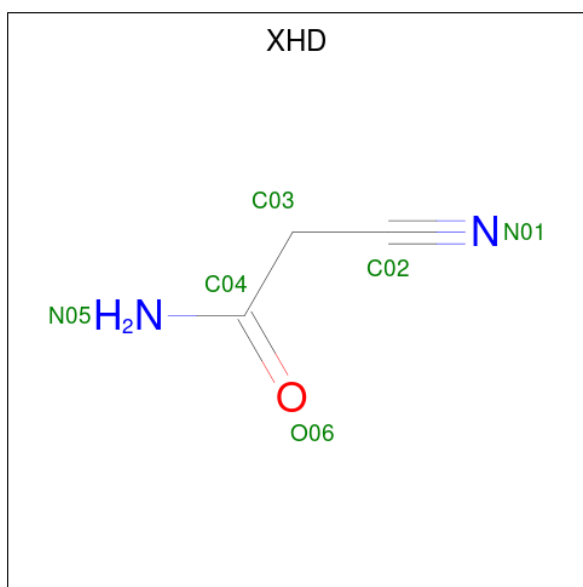
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLU	-	expression tag	UNP A0A4U9C786
F	0	PHE	-	expression tag	UNP A0A4U9C786
F	1	LEU	MET	conflict	UNP A0A4U9C786
F	58	THR	ALA	conflict	UNP A0A4U9C786
F	284	SER	CYS	conflict	UNP A0A4U9C786
G	-20	ALA	-	expression tag	UNP A0A4U9C786
G	-19	SER	-	expression tag	UNP A0A4U9C786
G	-18	TRP	-	expression tag	UNP A0A4U9C786
G	-17	SER	-	expression tag	UNP A0A4U9C786
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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 2-cyanoacetamide (CCD ID: XHD) (formula: $C_3H_4N_2O$) (labeled as "Ligand of Interest" by depositor).



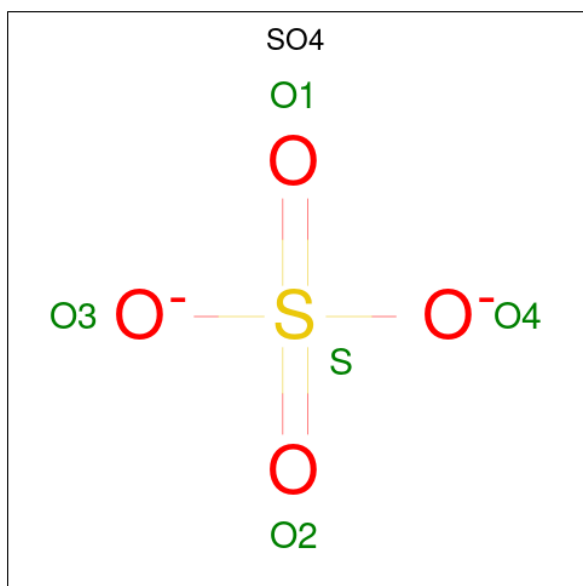
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	B	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	C	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	C	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	D	1	Total	C	H	N	O	0	0
			10	3	4	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	E	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	F	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	G	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	G	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	H	1	Total	C	H	N	O	0	0
			10	3	4	2	1		
2	H	1	Total	C	H	N	O	0	0
			10	3	4	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



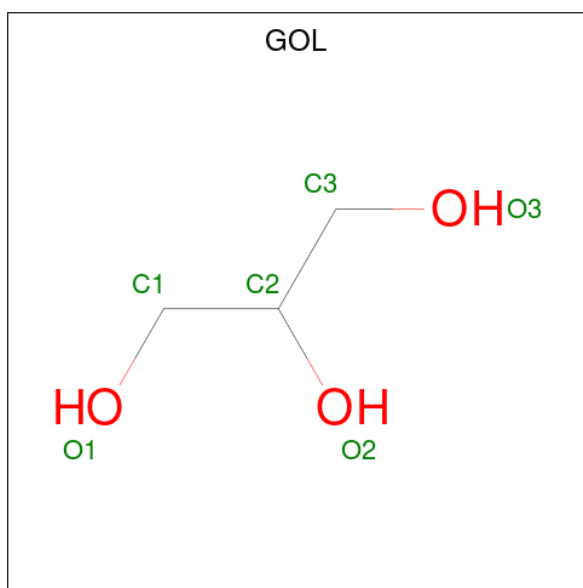
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	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	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	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: $C_3H_8O_3$).



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	D	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		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

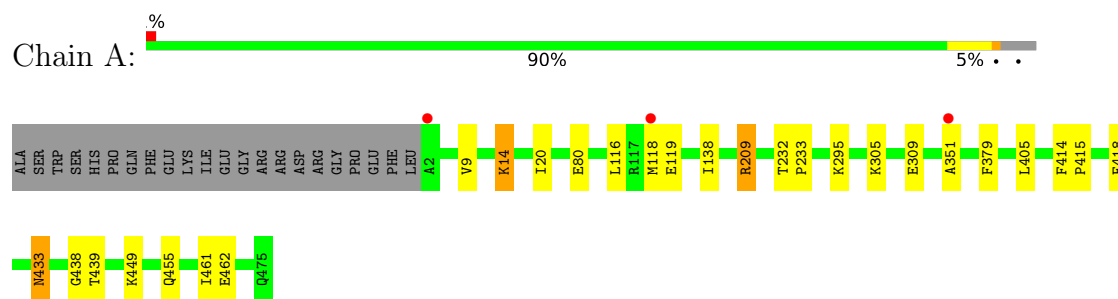
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	524	Total	O	0	0
			524	524		
5	B	554	Total	O	0	0
			554	554		
5	C	614	Total	O	0	2
			616	616		
5	D	595	Total	O	0	0
			595	595		
5	E	496	Total	O	0	0
			496	496		
5	F	472	Total	O	0	0
			472	472		
5	G	609	Total	O	0	1
			610	610		
5	H	611	Total	O	0	0
			611	611		

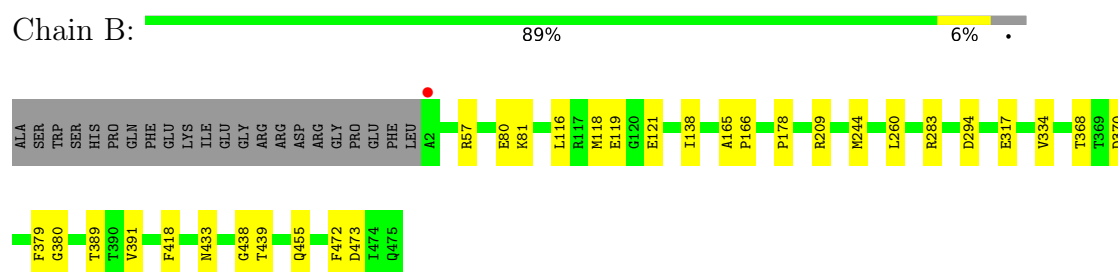
3 Residue-property plots

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.

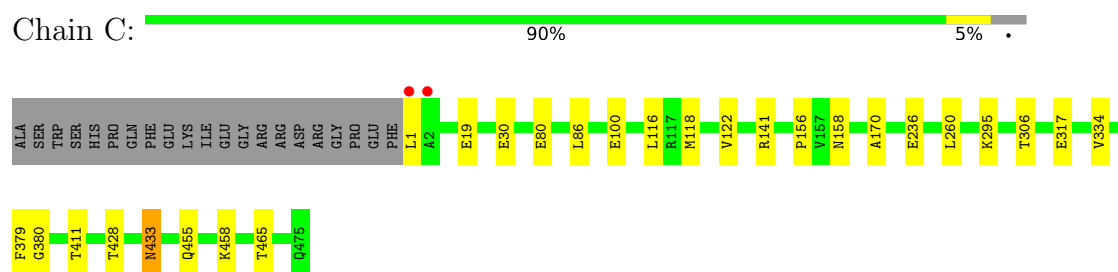
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



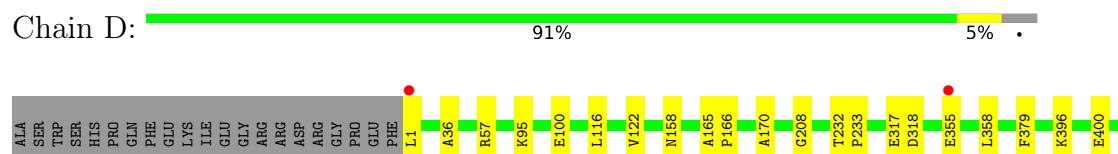
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



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



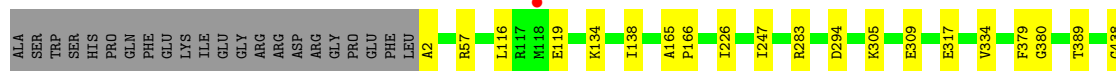
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase





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

Chain E: 91% 5% .



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

Chain F: 91% 2% .



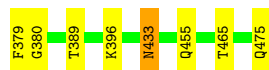
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain G: 91% 5% .



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

Chain H: 90% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.52Å 99.58Å 104.16Å 77.66° 75.94° 67.67°	Depositor
Resolution (Å)	47.92 – 1.61 47.92 – 1.61	Depositor EDS
% Data completeness (in resolution range)	70.3 (47.92-1.61) 70.6 (47.92-1.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.61Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.157 , 0.193 0.161 , 0.195	Depositor DCC
R_{free} test set	16200 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	62835	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XHD, GOL, 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	0/3681	0.40	0/4990
1	B	0.20	0/3662	0.41	0/4966
1	C	0.21	0/3697	0.42	0/5011
1	D	0.20	0/3650	0.43	0/4950
1	E	0.18	0/3645	0.38	0/4942
1	F	0.18	0/3669	0.40	0/4974
1	G	0.20	0/3688	0.43	0/4998
1	H	0.20	0/3675	0.43	0/4980
All	All	0.20	0/29367	0.41	0/39811

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3593	3680	3679	19	0
1	B	3582	3660	3659	20	0
1	C	3600	3694	3681	18	0
1	D	3572	3654	3655	14	0
1	E	3570	3640	3639	14	0
1	F	3586	3661	3656	12	0
1	G	3594	3670	3645	16	0
1	H	3590	3685	3678	19	0
2	A	6	4	0	0	0
2	B	6	4	0	0	0
2	C	12	8	0	0	0
2	D	12	8	0	0	0
2	E	6	4	0	0	0
2	F	6	4	0	0	0
2	G	12	8	0	0	0
2	H	12	8	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0
4	D	6	8	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	6	8	8	0	0
4	F	6	8	8	0	0
4	G	12	16	16	1	0
4	H	12	16	16	0	0
5	A	524	0	0	7	0
5	B	554	0	0	8	1
5	C	616	0	0	10	2
5	D	595	0	0	5	2
5	E	496	0	0	5	0
5	F	472	0	0	5	0
5	G	610	0	0	2	1
5	H	611	0	0	8	2
All	All	33371	29464	29364	125	4

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 (125) 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:D:355:GLU:OE2	5:D:601:HOH:O	1.90	0.88
1:B:433[A]:ASN:OD1	5:B:601:HOH:O	1.92	0.86
1:C:236[A]:GLU:OE1	5:C:601:HOH:O	1.93	0.84
1:H:433:ASN:ND2	5:H:602:HOH:O	2.12	0.83
1:H:475:GLN:OE1	5:H:601:HOH:O	1.98	0.81
1:B:283:ARG:NH2	5:B:604:HOH:O	2.18	0.74
1:E:119:GLU:OE2	5:E:601:HOH:O	2.05	0.74
1:C:236[A]:GLU:OE2	5:C:602:HOH:O	2.04	0.74
1:A:80:GLU:OE1	5:A:601:HOH:O	2.06	0.73
1:C:433:ASN:ND2	5:C:605:HOH:O	2.20	0.73
1:C:236[B]:GLU:OE2	5:C:602:HOH:O	2.06	0.73
1:C:80:GLU:OE1	5:C:603:HOH:O	2.07	0.72
1:B:80:GLU:OE1	5:B:602:HOH:O	2.06	0.72
1:E:462[A]:GLU:OE1	5:E:602:HOH:O	2.08	0.71
1:G:4:GLN:NE2	5:G:602:HOH:O	2.19	0.71
1:D:317:GLU:OE2	5:D:602:HOH:O	2.08	0.70
1:A:351:ALA:O	5:A:602:HOH:O	2.08	0.70
1:C:19:GLU:OE1	5:C:604:HOH:O	2.08	0.70
1:G:17:GLU:OE1	5:G:601:HOH:O	2.11	0.67
1:A:119:GLU:OE2	5:A:603:HOH:O	2.12	0.66
1:F:264:ASP:OD1	5:F:601:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:MET:SD	5:H:906:HOH:O	2.53	0.66
1:F:57:ARG:NH1	5:F:604:HOH:O	2.29	0.65
1:A:433:ASN:OD1	5:A:604:HOH:O	2.14	0.65
1:B:294:ASP:OD2	1:B:389:THR:HG22	1.98	0.64
1:E:57:ARG:NH2	5:E:606:HOH:O	2.30	0.64
1:G:118:MET:HE2	1:G:141[B]:ARG:CZ	2.28	0.64
1:E:283:ARG:NH1	5:E:608:HOH:O	2.34	0.61
1:F:294:ASP:OD2	1:F:389:THR:HG22	2.00	0.61
1:A:14:LYS:NZ	5:A:611:HOH:O	2.32	0.60
1:D:318:ASP:OD1	5:D:603:HOH:O	2.17	0.60
1:F:283:ARG:NH1	5:F:607:HOH:O	2.34	0.60
1:E:305:LYS:NZ	1:E:309:GLU:OE2	2.32	0.58
1:B:119:GLU:OE2	5:B:603:HOH:O	2.17	0.57
1:H:134[A]:LYS:NZ	5:H:610:HOH:O	2.36	0.57
1:C:1:LEU:N	1:C:30:GLU:O	2.37	0.57
1:B:368:THR:OG1	1:B:370:ASP:OD1	2.16	0.56
1:C:306[A]:THR:HG23	5:C:714:HOH:O	2.05	0.54
1:C:170:ALA:HB1	1:C:465:THR:HG22	1.89	0.54
1:G:226:ILE:HB	1:G:247:ILE:HG22	1.90	0.54
1:F:305:LYS:NZ	5:F:611:HOH:O	2.40	0.54
1:A:138:ILE:HG23	1:D:122:VAL:HG21	1.88	0.53
1:A:305:LYS:NZ	1:A:309:GLU:OE2	2.38	0.53
1:B:116[B]:LEU:HD11	5:C:947:HOH:O	2.09	0.52
1:B:138:ILE:HD11	1:B:472:PHE:HE1	1.73	0.52
1:E:2:ALA:N	5:E:610:HOH:O	2.42	0.52
1:A:118[B]:MET:HE3	1:A:461:ILE:HG21	1.90	0.52
1:E:226:ILE:HB	1:E:247:ILE:HG22	1.92	0.52
1:A:433:ASN:ND2	1:B:473:ASP:OD2	2.43	0.52
1:D:396:LYS:NZ	1:D:400:GLU:OE2	2.37	0.52
1:A:9:VAL:HB	1:A:14:LYS:HG3	1.92	0.52
1:H:141:ARG:NH1	5:H:613:HOH:O	2.43	0.51
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.92	0.51
1:A:116:LEU:HD12	1:A:116:LEU:C	2.35	0.50
1:G:119:GLU:O	1:G:141[B]:ARG:NH1	2.44	0.50
1:E:116:LEU:HD12	1:E:116:LEU:C	2.37	0.50
1:B:260:LEU:HD22	1:B:391:VAL:HG12	1.95	0.49
1:A:449:LYS:HA	1:B:244:MET:HE1	1.95	0.49
1:C:116:LEU:C	1:C:116:LEU:HD12	2.38	0.48
1:H:353:ASN:ND2	5:H:608:HOH:O	2.32	0.48
1:B:57:ARG:HD3	5:B:810:HOH:O	2.14	0.48
1:H:226:ILE:HB	1:H:247:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:HG2	5:A:638:HOH:O	2.13	0.47
1:F:317:GLU:OE2	5:F:602:HOH:O	2.20	0.47
1:H:116:LEU:HD12	1:H:116:LEU:C	2.40	0.47
1:D:355:GLU:OE1	1:D:358:LEU:HD23	2.15	0.47
1:E:134:LYS:NZ	1:G:422:GLU:OE1	2.47	0.46
1:C:100:GLU:HG3	1:C:158:ASN:HB2	1.98	0.46
1:G:438:GLY:HA3	4:G:505:GOL:H2	1.96	0.46
1:F:4:GLN:NE2	1:F:19:GLU:OE1	2.49	0.46
1:H:212:VAL:HG12	1:H:213:ILE:HG23	1.97	0.46
1:G:303:GLU:O	1:G:306:THR:HG22	2.16	0.45
1:G:116:LEU:C	1:G:116:LEU:HD12	2.41	0.45
1:B:317[B]:GLU:H	1:B:317[B]:GLU:CD	2.23	0.45
1:D:116:LEU:HD12	1:D:116:LEU:C	2.41	0.45
1:G:86:LEU:HG	1:G:97:ALA:HB1	1.99	0.45
1:A:414[B]:PHE:HB3	1:A:415:PRO:HD3	1.98	0.45
1:D:57:ARG:HD3	5:D:998:HOH:O	2.16	0.45
1:C:428:THR:HG23	1:D:469[B]:SER:OG	2.17	0.45
1:E:138:ILE:HG23	1:H:122:VAL:HG21	1.98	0.45
1:H:165:ALA:HB3	1:H:166:PRO:HD3	1.98	0.44
1:A:20:ILE:HD11	1:A:209:ARG:HG2	1.99	0.44
1:F:368:THR:OG1	1:F:370:ASP:OD1	2.28	0.44
1:F:218:VAL:HG13	1:F:226:ILE:HD13	1.98	0.44
1:G:170:ALA:HB1	1:G:465:THR:HG22	1.99	0.44
1:G:449:LYS:HA	1:H:244:MET:HE1	2.00	0.44
1:E:165:ALA:HB3	1:E:166:PRO:HD3	2.00	0.44
1:H:170:ALA:HB1	1:H:465:THR:HG22	2.00	0.43
1:H:118:MET:HE3	1:H:141:ARG:CZ	2.48	0.43
1:C:317:GLU:OE1	5:C:606:HOH:O	2.21	0.43
1:G:165:ALA:HB3	1:G:166:PRO:HD3	1.99	0.43
1:B:178:PRO:HB3	5:B:691:HOH:O	2.18	0.43
1:F:226:ILE:HB	1:F:247:ILE:HG22	2.01	0.43
1:G:9:VAL:HB	1:G:14:LYS:HD3	2.00	0.43
1:G:86:LEU:C	1:G:86:LEU:HD12	2.43	0.43
1:D:100:GLU:HG3	1:D:158:ASN:HB2	2.00	0.42
1:C:141:ARG:NH1	5:C:628:HOH:O	2.52	0.42
1:H:334:VAL:HG21	1:H:380:GLY:HA3	2.00	0.42
1:B:118:MET:HB3	5:B:1082:HOH:O	2.19	0.42
1:C:334:VAL:HG21	1:C:380:GLY:HA3	2.02	0.42
1:E:334:VAL:HG21	1:E:380:GLY:HA3	2.02	0.42
1:E:438:GLY:HA2	1:E:439:THR:C	2.45	0.42
1:F:438:GLY:HA2	1:F:439:THR:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:MET:HE1	1:H:389:THR:O	2.19	0.42
1:B:81:LYS:HD3	5:B:616:HOH:O	2.19	0.41
1:F:100:GLU:HG3	1:F:158:ASN:HB2	2.02	0.41
1:B:438:GLY:HA2	1:B:439:THR:C	2.45	0.41
1:G:86:LEU:HD12	1:G:86:LEU:O	2.21	0.41
1:C:86:LEU:HD13	1:C:156:PRO:HG2	2.03	0.41
1:D:232:THR:N	1:D:233:PRO:HD2	2.36	0.41
1:E:294[A]:ASP:OD2	1:E:389:THR:HG22	2.20	0.41
1:A:438:GLY:HA2	1:A:439:THR:C	2.46	0.41
4:D:505:GOL:H2	5:D:767:HOH:O	2.21	0.41
1:H:223:VAL:O	1:H:245:ARG:HD2	2.21	0.41
1:D:170:ALA:HB1	1:D:465:THR:HG22	2.03	0.40
1:D:36:ALA:HA	1:D:208:GLY:HA2	2.03	0.40
1:D:165:ALA:HB3	1:D:166:PRO:HD3	2.03	0.40
1:H:57:ARG:HD3	5:H:972:HOH:O	2.20	0.40
1:B:334:VAL:HG21	1:B:380:GLY:HA3	2.04	0.40
1:H:295:LYS:NZ	5:H:632:HOH:O	2.55	0.40
1:A:462[A]:GLU:HG3	5:A:834:HOH:O	2.21	0.40
1:C:260:LEU:HD12	1:C:411:THR:HB	2.03	0.40
1:A:119:GLU:OE2	1:C:458:LYS:NZ	2.48	0.40
1:A:232:THR:N	1:A:233:PRO:HD2	2.36	0.40

All (4) 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:C:1100:HOH:O	5:G:1151:HOH:O[1_466]	1.97	0.23
5:D:936:HOH:O	5:H:661:HOH:O[1_456]	2.07	0.13
5:D:1011:HOH:O	5:H:910:HOH:O[1_456]	2.08	0.12
5:B:695:HOH:O	5:C:650:HOH:O[1_655]	2.15	0.05

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	482/496 (97%)	471 (98%)	11 (2%)	0	100	100
1	B	479/496 (97%)	468 (98%)	11 (2%)	0	100	100
1	C	485/496 (98%)	471 (97%)	14 (3%)	0	100	100
1	D	480/496 (97%)	469 (98%)	11 (2%)	0	100	100
1	E	478/496 (96%)	465 (97%)	13 (3%)	0	100	100
1	F	481/496 (97%)	470 (98%)	11 (2%)	0	100	100
1	G	483/496 (97%)	469 (97%)	14 (3%)	0	100	100
1	H	482/496 (97%)	470 (98%)	12 (2%)	0	100	100
All	All	3850/3968 (97%)	3753 (98%)	97 (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	379/388 (98%)	373 (98%)	6 (2%)	55	32
1	B	376/388 (97%)	372 (99%)	4 (1%)	65	46
1	C	382/388 (98%)	377 (99%)	5 (1%)	61	39
1	D	377/388 (97%)	374 (99%)	3 (1%)	73	59
1	E	375/388 (97%)	372 (99%)	3 (1%)	73	59
1	F	377/388 (97%)	373 (99%)	4 (1%)	65	46
1	G	379/388 (98%)	375 (99%)	4 (1%)	65	46
1	H	379/388 (98%)	375 (99%)	4 (1%)	65	46
All	All	3024/3104 (97%)	2991 (99%)	33 (1%)	65	46

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	209	ARG
1	A	379	PHE
1	A	405	LEU
1	A	418	PHE
1	A	433	ASN
1	B	121	GLU
1	B	209	ARG
1	B	379	PHE
1	B	418	PHE
1	C	118	MET
1	C	122	VAL
1	C	295	LYS
1	C	379	PHE
1	C	433	ASN
1	D	1	LEU
1	D	95	LYS
1	D	379	PHE
1	E	317	GLU
1	E	379	PHE
1	E	475	GLN
1	F	209	ARG
1	F	379	PHE
1	F	418	PHE
1	F	467	VAL
1	G	1	LEU
1	G	70	LYS
1	G	86	LEU
1	G	379	PHE
1	H	1	LEU
1	H	379	PHE
1	H	396	LYS
1	H	433	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	HIS
1	B	18	ASN
1	B	353	ASN
1	C	18	ASN
1	C	353	ASN
1	C	475	GLN

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Mol	Chain	Res	Type
1	D	18	ASN
1	D	423	GLN
1	D	475	GLN
1	E	4	GLN
1	E	433	ASN
1	F	433	ASN
1	F	475	GLN
1	G	423	GLN
1	H	4	GLN
1	H	366	HIS
1	H	423	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

37 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	$\# Z > 2$
4	GOL	A	503	-	5,5,5	0.67	0	5,5,5	0.83	0
3	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.11	0
2	XHD	G	501	-	5,5,5	2.41	2 (40%)	5,5,5	1.69	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XHD	D	501	-	5,5,5	2.58	2 (40%)	5,5,5	1.14	0
4	GOL	B	504	-	5,5,5	0.83	0	5,5,5	1.19	1 (20%)
3	SO4	C	503	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	F	503	-	4,4,4	0.23	0	6,6,6	0.12	0
4	GOL	E	504	-	5,5,5	0.97	0	5,5,5	1.16	0
2	XHD	C	504	-	5,5,5	2.51	2 (40%)	5,5,5	1.03	0
3	SO4	G	502	-	4,4,4	0.25	0	6,6,6	0.17	0
2	XHD	B	501	-	5,5,5	2.60	2 (40%)	5,5,5	1.55	1 (20%)
3	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	H	502	-	4,4,4	0.29	0	6,6,6	0.08	0
4	GOL	H	505	-	5,5,5	0.89	0	5,5,5	1.03	0
4	GOL	G	505	-	5,5,5	1.14	0	5,5,5	1.31	1 (20%)
2	XHD	A	501	-	5,5,5	2.47	2 (40%)	5,5,5	1.29	0
3	SO4	E	503	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.13	0
4	GOL	F	504	-	5,5,5	0.65	0	5,5,5	0.82	0
3	SO4	E	502	-	4,4,4	0.22	0	6,6,6	0.20	0
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.14	0
4	GOL	D	505	-	5,5,5	0.89	0	5,5,5	0.86	0
2	XHD	F	501	-	5,5,5	2.43	2 (40%)	5,5,5	1.27	0
3	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.14	0
4	GOL	H	506	-	5,5,5	0.85	0	5,5,5	1.10	0
3	SO4	H	503	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	G	503	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	F	502	-	4,4,4	0.25	0	6,6,6	0.13	0
2	XHD	H	501	-	5,5,5	2.40	2 (40%)	5,5,5	1.13	0
2	XHD	C	501	-	5,5,5	2.52	2 (40%)	5,5,5	0.93	0
2	XHD	H	504	-	5,5,5	2.67	2 (40%)	5,5,5	1.39	1 (20%)
2	XHD	G	504	-	5,5,5	2.58	2 (40%)	5,5,5	1.52	2 (40%)
2	XHD	D	504	-	5,5,5	2.62	2 (40%)	5,5,5	1.66	1 (20%)
2	XHD	E	501	-	5,5,5	2.52	2 (40%)	5,5,5	1.19	0
3	SO4	D	502	-	4,4,4	0.22	0	6,6,6	0.17	0
4	GOL	G	506	-	5,5,5	0.67	0	5,5,5	0.98	0
3	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.07	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
4	GOL	A	503	-	-	0/4/4/4	-
2	XHD	G	501	-	-	1/3/3/3	-
2	XHD	D	501	-	-	0/3/3/3	-
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	E	504	-	-	1/4/4/4	-
2	XHD	C	504	-	-	1/3/3/3	-
2	XHD	B	501	-	-	0/3/3/3	-
4	GOL	H	505	-	-	2/4/4/4	-
4	GOL	G	505	-	-	1/4/4/4	-
2	XHD	A	501	-	-	0/3/3/3	-
4	GOL	F	504	-	-	4/4/4/4	-
4	GOL	D	505	-	-	0/4/4/4	-
2	XHD	F	501	-	-	1/3/3/3	-
4	GOL	H	506	-	-	0/4/4/4	-
2	XHD	H	501	-	-	0/3/3/3	-
2	XHD	C	501	-	-	0/3/3/3	-
2	XHD	H	504	-	-	2/3/3/3	-
2	XHD	G	504	-	-	0/3/3/3	-
2	XHD	D	504	-	-	2/3/3/3	-
4	GOL	G	506	-	-	2/4/4/4	-
2	XHD	E	501	-	-	0/3/3/3	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	XHD	C04-N05	4.07	1.46	1.32
2	C	504	XHD	C04-N05	4.02	1.45	1.32
2	C	501	XHD	C04-N05	3.98	1.45	1.32
2	D	504	XHD	C04-N05	3.98	1.45	1.32
2	G	504	XHD	C04-N05	3.97	1.45	1.32
2	D	504	XHD	C03-C02	3.96	1.53	1.45
2	B	501	XHD	C03-C02	3.91	1.53	1.45
2	H	504	XHD	C03-C02	3.90	1.53	1.45
2	D	501	XHD	C04-N05	3.88	1.45	1.32
2	D	501	XHD	C03-C02	3.87	1.53	1.45
2	H	504	XHD	C04-N05	3.81	1.45	1.32
2	E	501	XHD	C04-N05	3.80	1.45	1.32
2	F	501	XHD	C04-N05	3.76	1.45	1.32
2	C	501	XHD	C03-C02	3.73	1.52	1.45
2	A	501	XHD	C04-N05	3.73	1.44	1.32
2	G	504	XHD	C03-C02	3.72	1.52	1.45
2	H	501	XHD	C04-N05	3.71	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	XHD	C04-N05	3.68	1.44	1.32
2	A	501	XHD	C03-C02	3.68	1.52	1.45
2	G	501	XHD	C03-C02	3.64	1.52	1.45
2	E	501	XHD	C03-C02	3.62	1.52	1.45
2	C	504	XHD	C03-C02	3.59	1.52	1.45
2	F	501	XHD	C03-C02	3.48	1.52	1.45
2	H	501	XHD	C03-C02	3.44	1.52	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	XHD	C03-C04-N05	3.39	120.57	116.48
2	G	501	XHD	C02-C03-C04	-2.81	108.43	111.24
4	G	505	GOL	C3-C2-C1	-2.66	102.05	111.80
2	G	504	XHD	C02-C03-C04	-2.32	108.91	111.24
2	H	504	XHD	C03-C04-N05	2.31	119.27	116.48
2	B	501	XHD	C03-C04-N05	2.31	119.26	116.48
2	G	504	XHD	C03-C04-N05	2.20	119.14	116.48
2	G	501	XHD	C03-C04-N05	2.14	119.06	116.48
4	B	504	GOL	C3-C2-C1	-2.11	104.07	111.80

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	504	XHD	N01-C02-C03-C04
2	F	501	XHD	N01-C02-C03-C04
2	G	501	XHD	N01-C02-C03-C04
4	B	504	GOL	C1-C2-C3-O3
4	F	504	GOL	O1-C1-C2-C3
4	F	504	GOL	C1-C2-C3-O3
4	G	506	GOL	O1-C1-C2-C3
4	H	505	GOL	O1-C1-C2-O2
4	E	504	GOL	O1-C1-C2-C3
4	H	505	GOL	O1-C1-C2-C3
4	B	504	GOL	O2-C2-C3-O3
4	F	504	GOL	O1-C1-C2-O2
4	F	504	GOL	O2-C2-C3-O3
4	G	506	GOL	O1-C1-C2-O2
2	D	504	XHD	C02-C03-C04-O06
2	H	504	XHD	C02-C03-C04-O06
2	D	504	XHD	C02-C03-C04-N05

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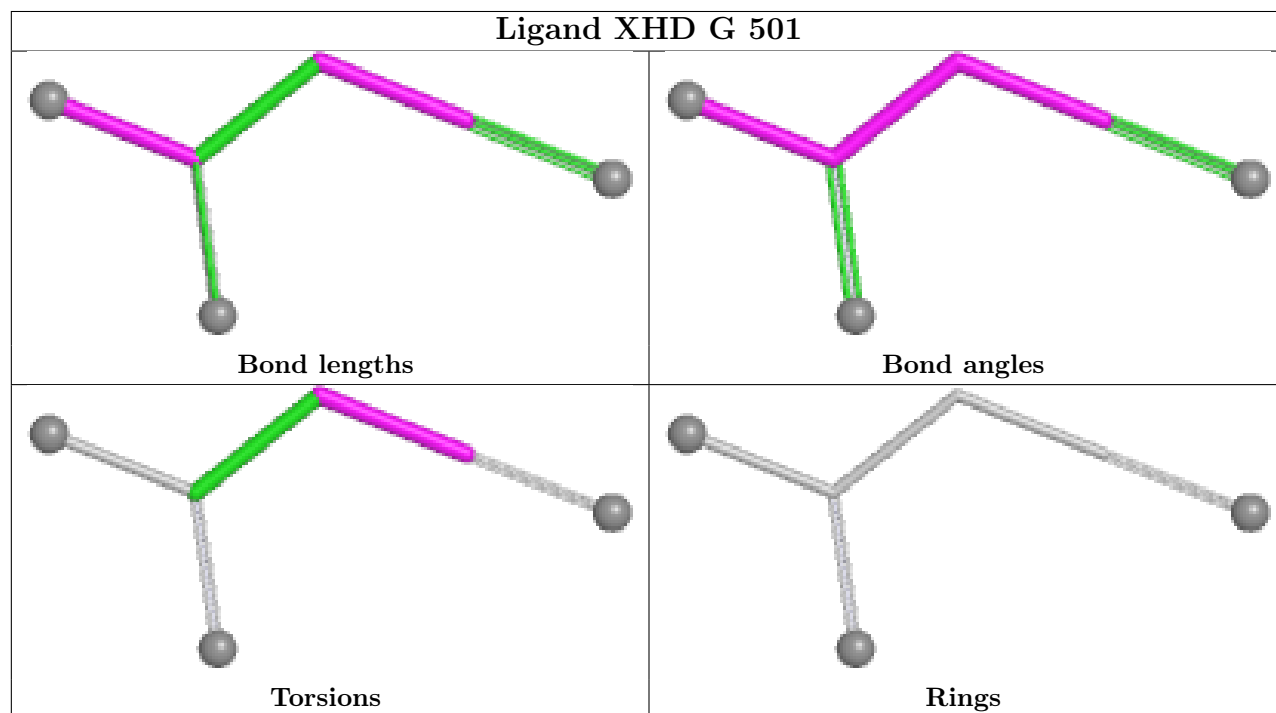
Mol	Chain	Res	Type	Atoms
4	G	505	GOL	O1-C1-C2-O2
2	H	504	XHD	C02-C03-C04-N05

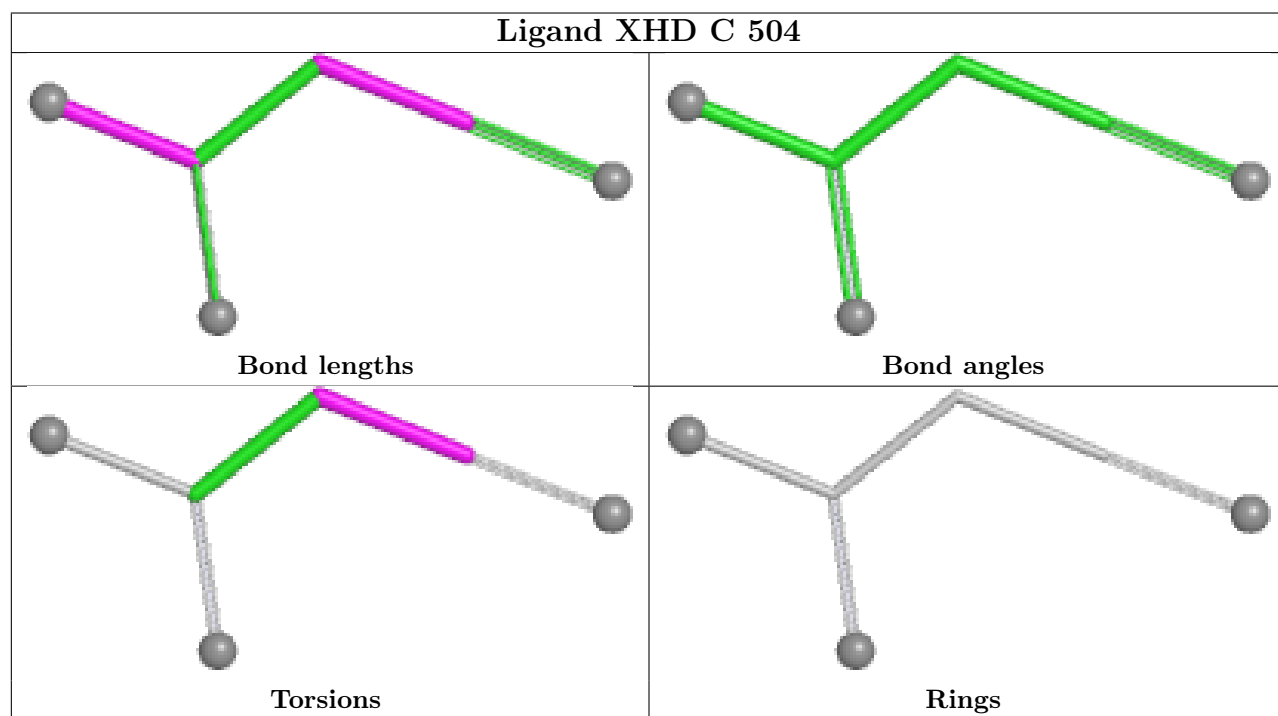
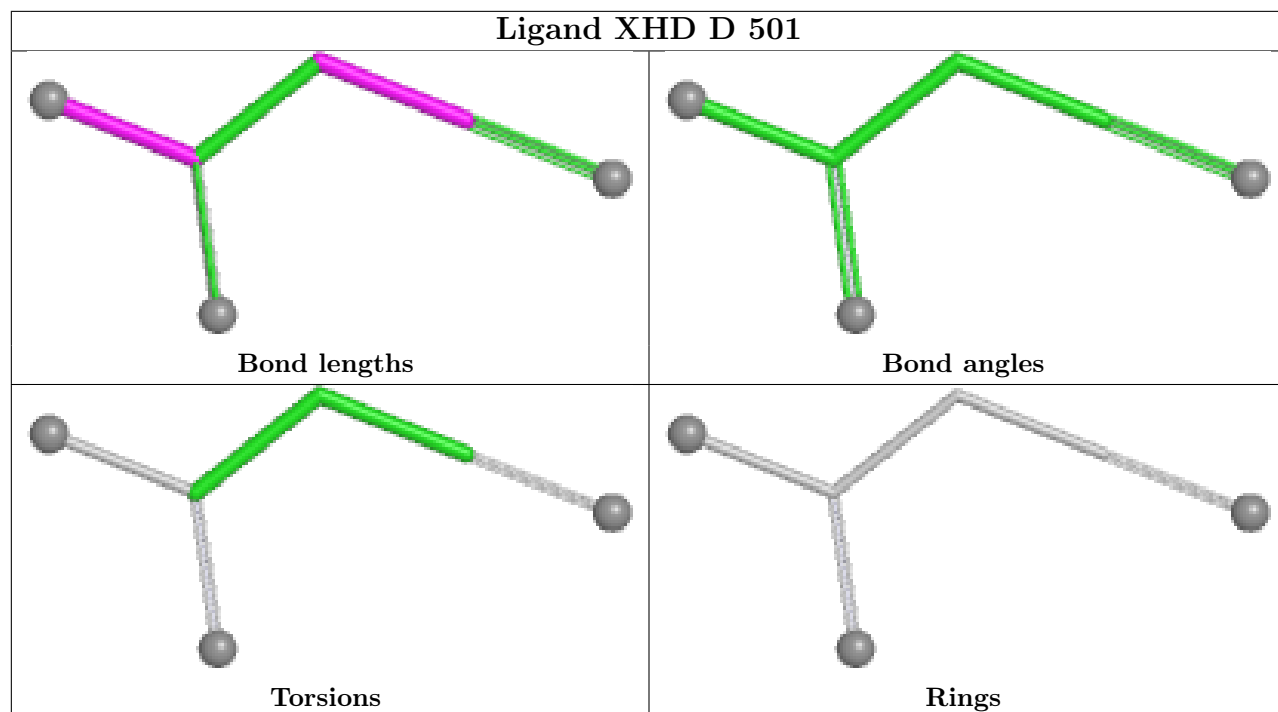
There are no ring outliers.

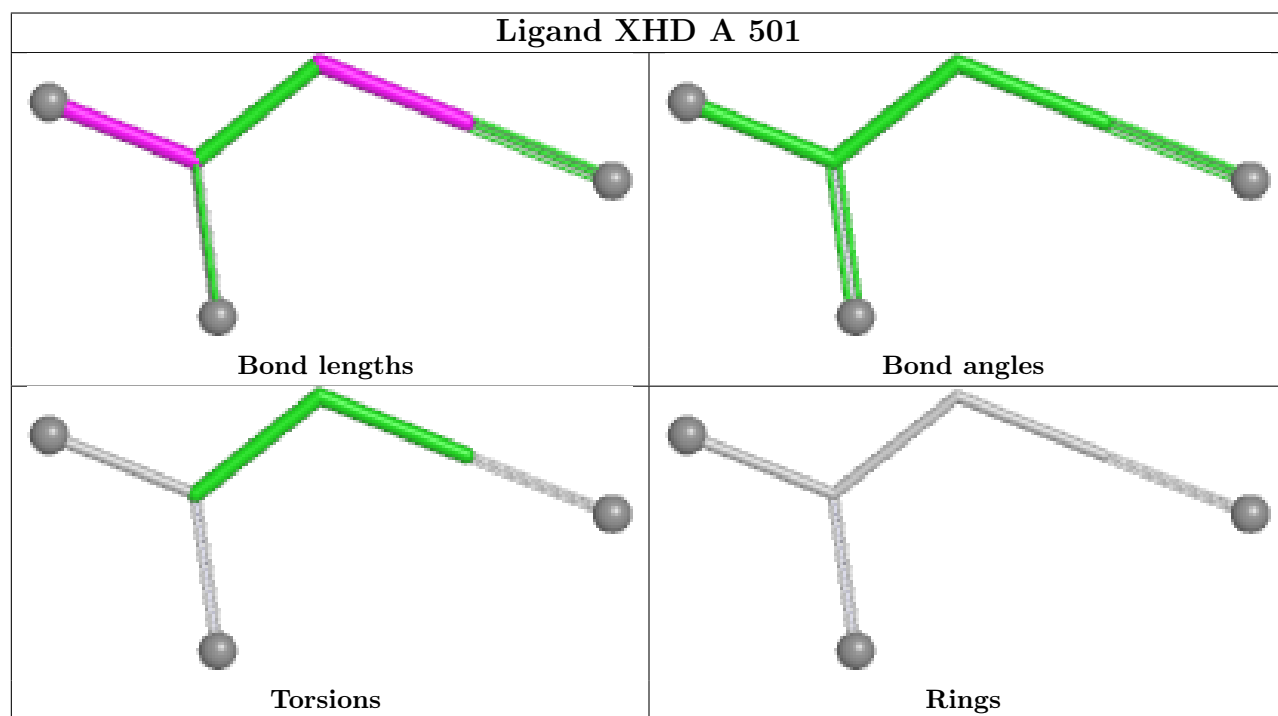
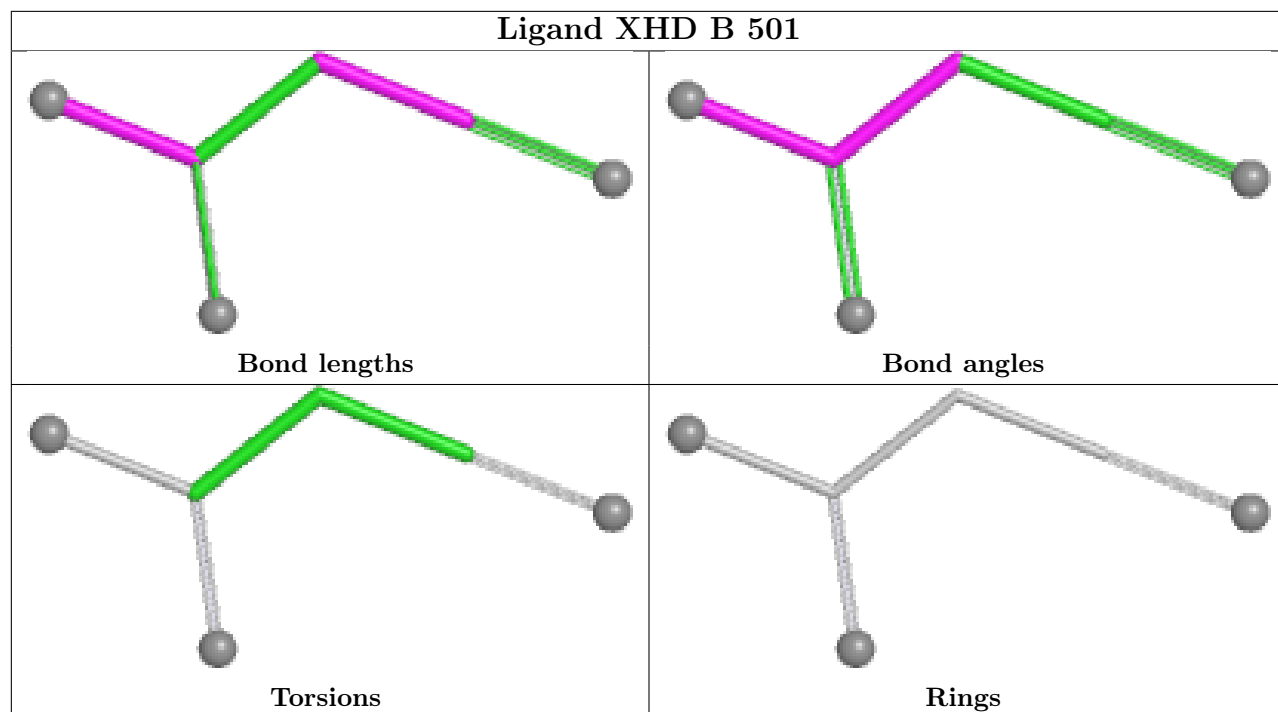
2 monomers are involved in 2 short contacts:

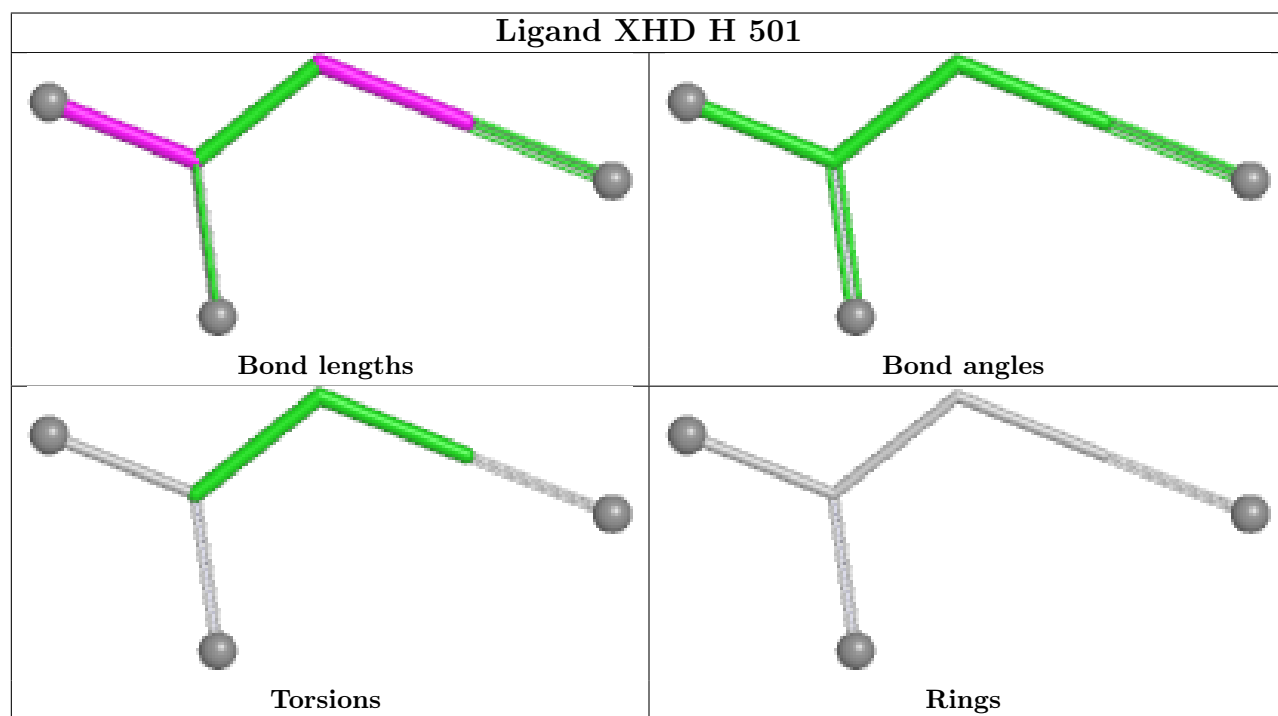
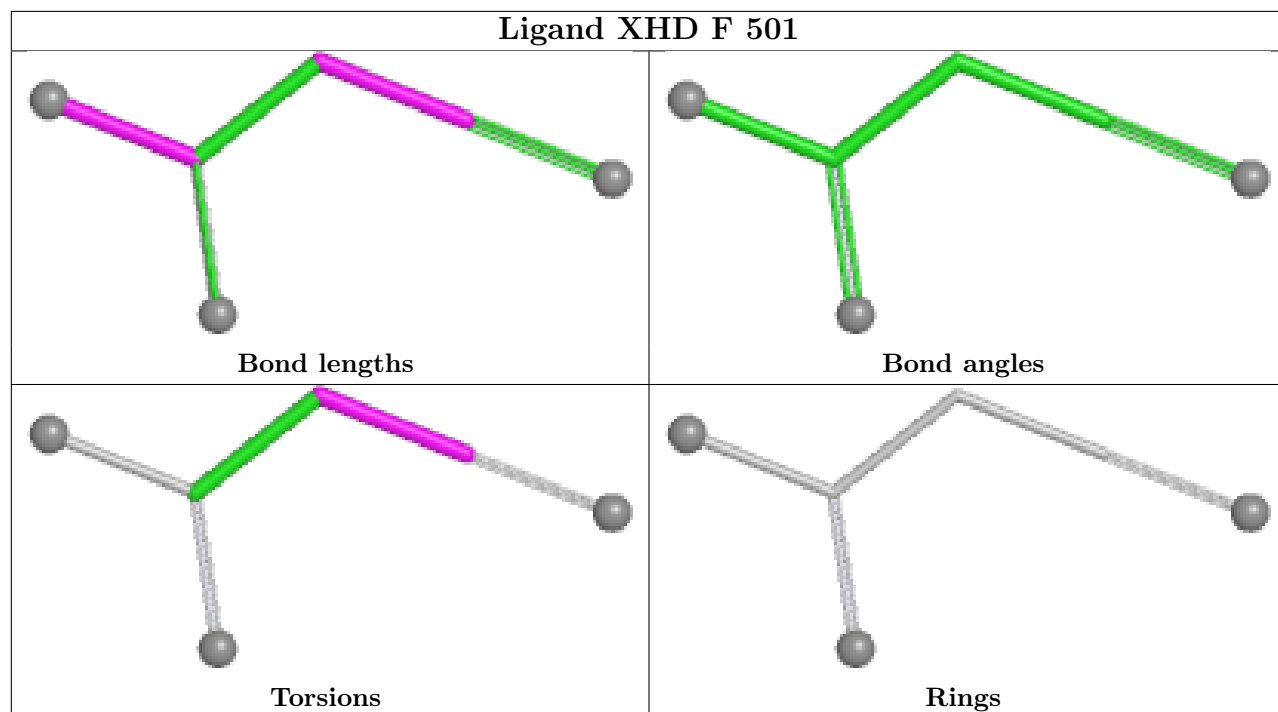
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	505	GOL	1	0
4	D	505	GOL	1	0

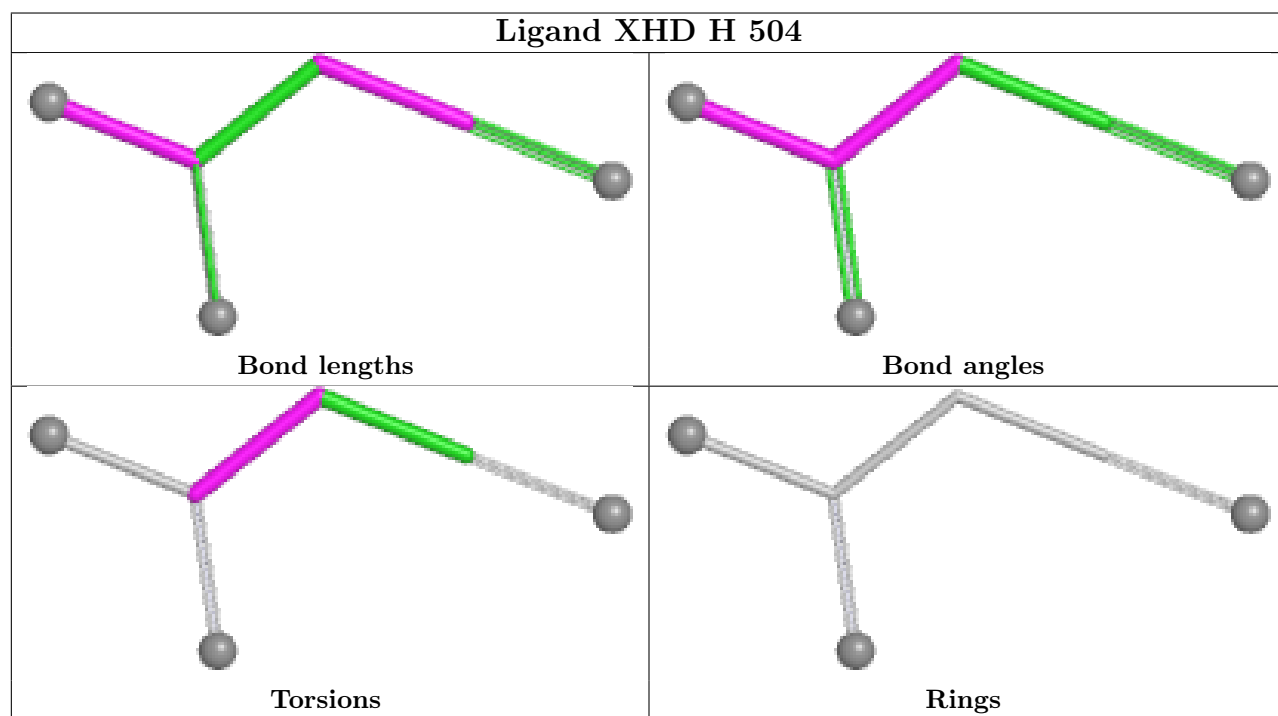
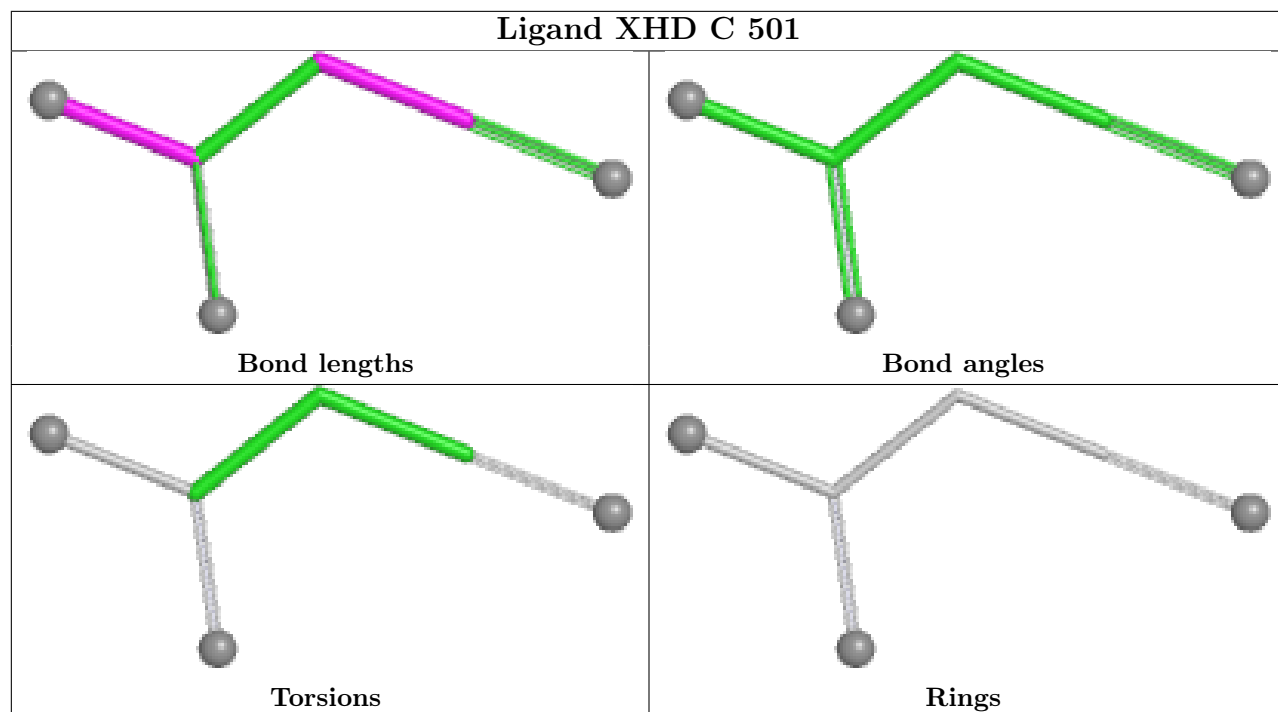
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

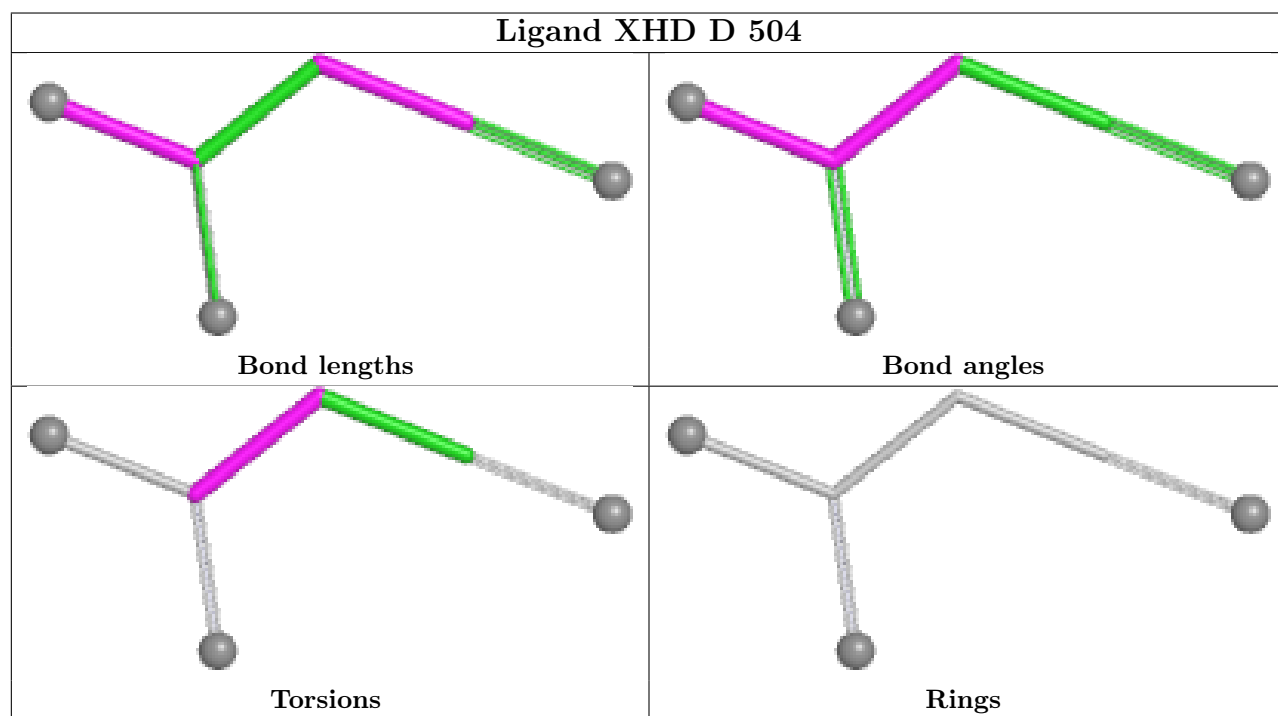
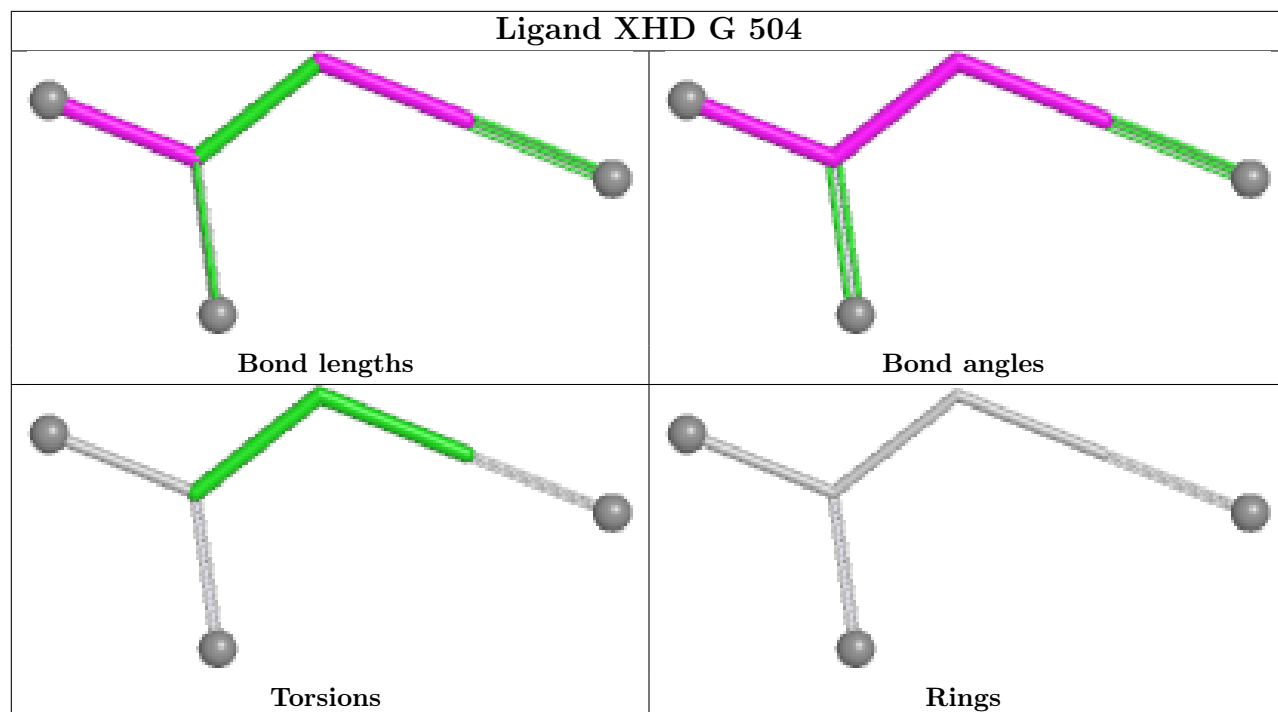


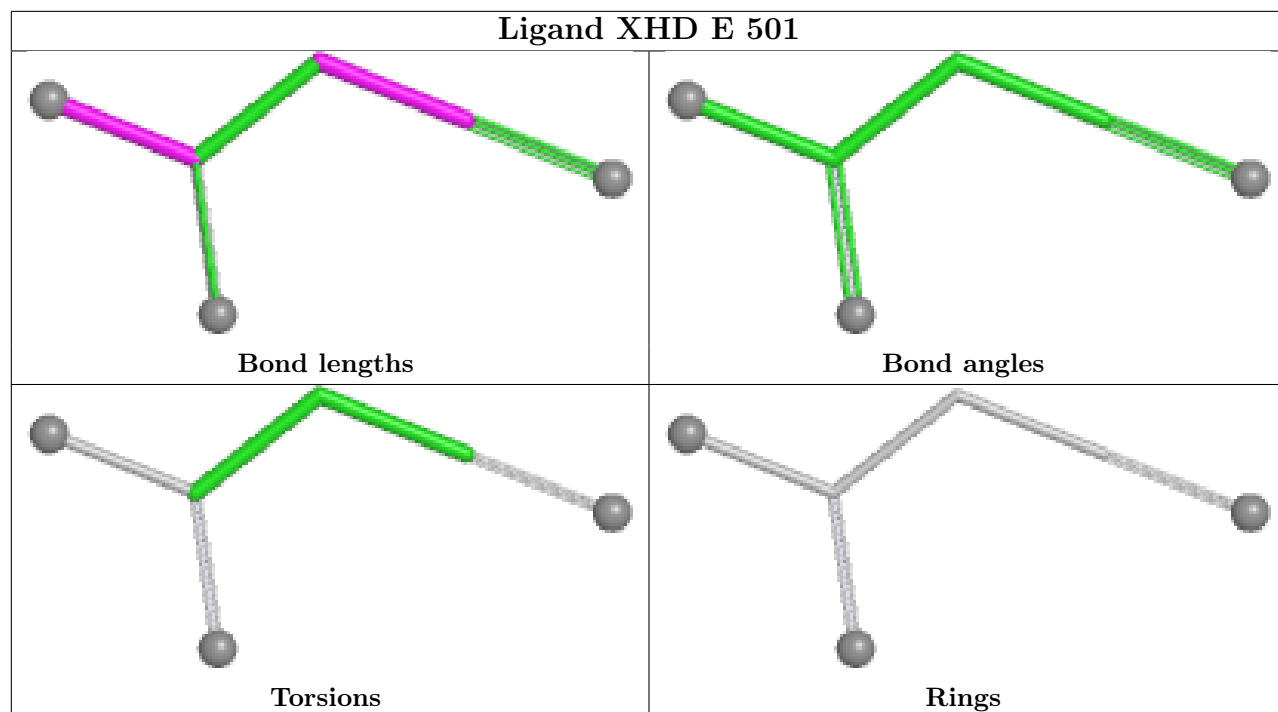












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/496 (95%)	-0.44	3 (0%) 85 89	10, 23, 39, 80	10 (2%)
1	B	474/496 (95%)	-0.53	1 (0%) 91 92	9, 21, 38, 73	7 (1%)
1	C	475/496 (95%)	-0.57	2 (0%) 88 91	9, 20, 31, 114	11 (2%)
1	D	475/496 (95%)	-0.55	2 (0%) 88 91	9, 21, 32, 60	7 (1%)
1	E	474/496 (95%)	-0.34	1 (0%) 91 92	11, 25, 43, 70	6 (1%)
1	F	474/496 (95%)	-0.30	8 (1%) 69 73	10, 24, 50, 95	8 (1%)
1	G	475/496 (95%)	-0.59	1 (0%) 91 92	9, 20, 30, 63	7 (1%)
1	H	475/496 (95%)	-0.55	1 (0%) 91 92	10, 20, 32, 56	8 (1%)
All	All	3796/3968 (95%)	-0.48	19 (0%) 87 90	9, 22, 38, 114	64 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	LEU	7.4
1	C	2	ALA	5.0
1	D	1	LEU	4.2
1	G	1	LEU	4.2
1	F	2	ALA	4.0
1	F	238	ILE	3.4
1	F	237[A]	GLY	2.8
1	B	2	ALA	2.7
1	E	118	MET	2.5
1	H	1	LEU	2.5
1	F	17[A]	GLU	2.4
1	D	355	GLU	2.4
1	F	239	GLY	2.3
1	A	351	ALA	2.3
1	A	118[A]	MET	2.1
1	F	3	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.1
1	F	212	VAL	2.0
1	F	210	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	E	504	6/6	0.61	0.20	33,50,59,60	0
3	SO4	A	504	5/5	0.67	0.16	43,48,52,55	5
3	SO4	E	503	5/5	0.70	0.14	83,94,102,117	0
4	GOL	D	505	6/6	0.71	0.17	41,53,64,72	0
3	SO4	B	503	5/5	0.72	0.13	69,80,90,95	0
4	GOL	G	506	6/6	0.73	0.16	37,44,53,53	14
4	GOL	H	506	6/6	0.73	0.16	32,47,62,75	0
3	SO4	F	503	5/5	0.74	0.15	88,89,93,96	0
4	GOL	G	505	6/6	0.74	0.18	16,29,31,37	14
4	GOL	A	503	6/6	0.79	0.13	35,53,63,63	0
4	GOL	H	505	6/6	0.80	0.15	31,51,62,62	0
4	GOL	F	504	6/6	0.82	0.14	41,56,71,71	0
4	GOL	B	504	6/6	0.85	0.13	23,35,41,49	14
3	SO4	D	503	5/5	0.88	0.09	34,39,57,58	0
2	XHD	G	504	6/6	0.88	0.10	25,32,42,42	0
3	SO4	H	503	5/5	0.89	0.09	32,35,53,53	0
2	XHD	C	504	6/6	0.89	0.11	35,45,54,54	0
2	XHD	D	504	6/6	0.91	0.07	25,31,37,37	0
2	XHD	H	504	6/6	0.92	0.07	25,31,38,38	0
3	SO4	C	503	5/5	0.94	0.07	32,36,46,48	0

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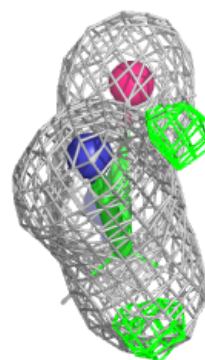
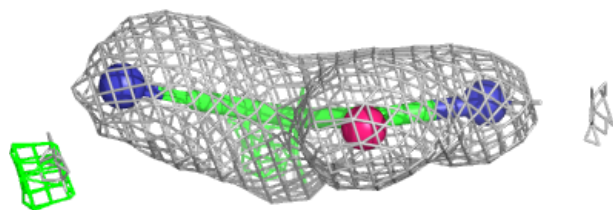
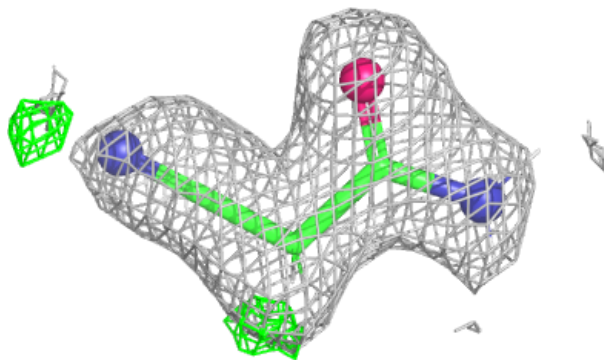
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XHD	F	501	6/6	0.96	0.06	18,20,24,24	0
3	SO4	G	503	5/5	0.96	0.06	26,29,44,46	0
2	XHD	G	501	6/6	0.96	0.06	14,18,21,21	0
2	XHD	A	501	6/6	0.96	0.07	18,21,23,23	0
2	XHD	H	501	6/6	0.96	0.06	15,19,23,23	0
2	XHD	E	501	6/6	0.96	0.07	19,22,24,24	0
2	XHD	C	501	6/6	0.97	0.05	14,15,18,18	0
2	XHD	B	501	6/6	0.97	0.04	17,19,25,25	0
2	XHD	D	501	6/6	0.97	0.05	16,20,26,26	0
3	SO4	D	502	5/5	0.99	0.04	17,18,21,23	0
3	SO4	G	502	5/5	0.99	0.03	16,17,19,22	0
3	SO4	C	502	5/5	0.99	0.03	14,16,20,21	0
3	SO4	H	502	5/5	0.99	0.04	16,18,23,23	0
3	SO4	E	502	5/5	0.99	0.03	20,21,24,25	0
3	SO4	A	502	5/5	0.99	0.03	19,20,23,24	0
3	SO4	F	502	5/5	0.99	0.04	17,18,22,25	0
3	SO4	B	502	5/5	1.00	0.03	16,19,24,27	0

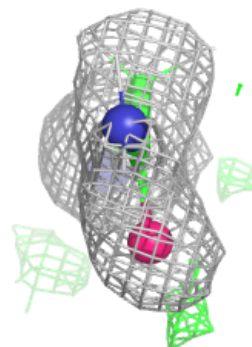
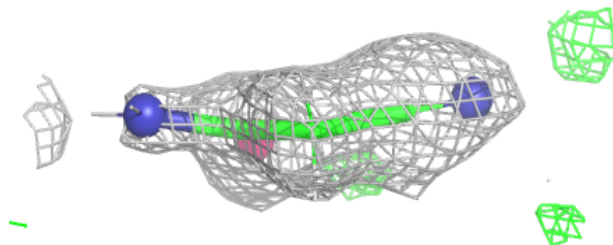
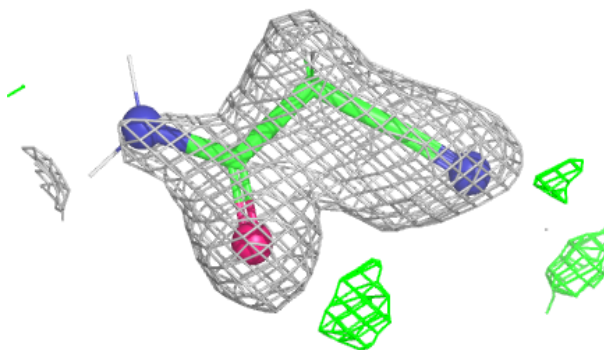
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XHD G 504:

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

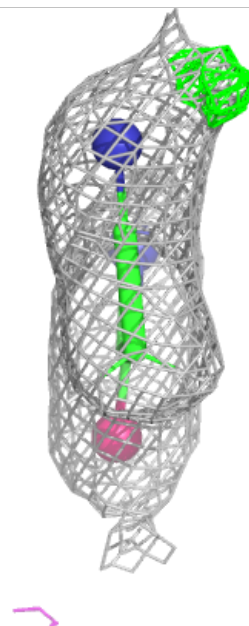
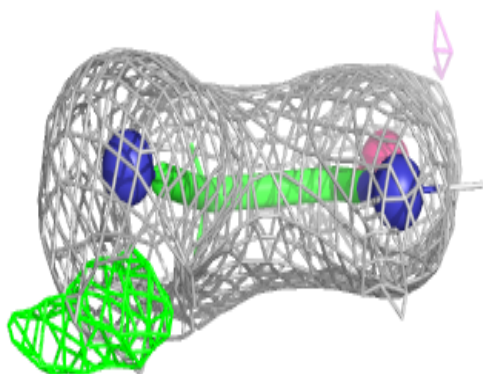
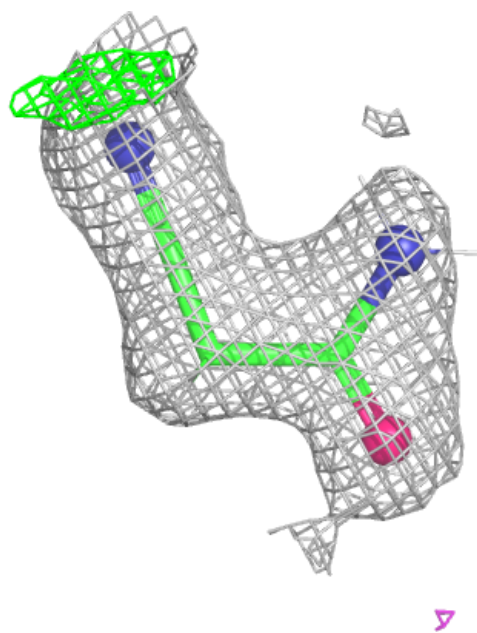
**Electron density around XHD C 504:**

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



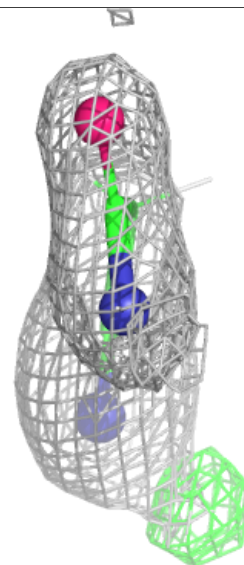
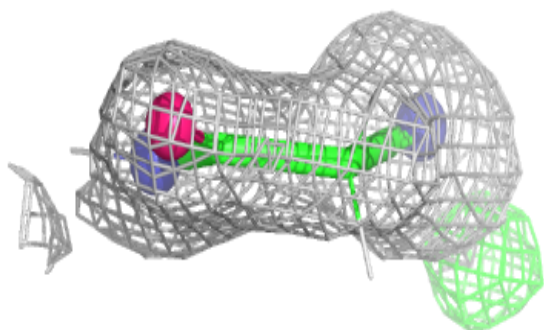
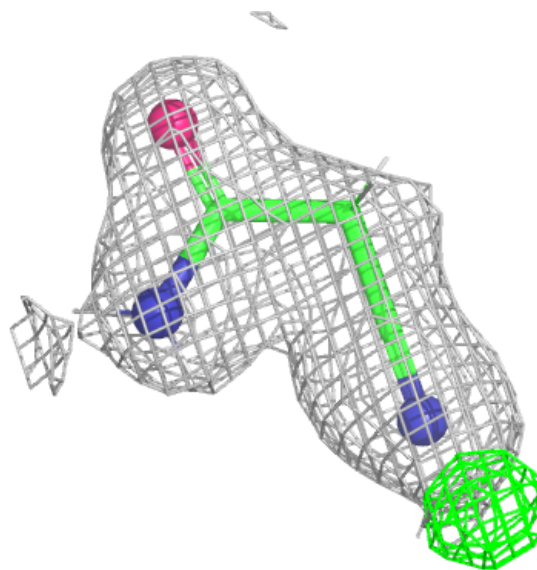
Electron density around XHD D 504:

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



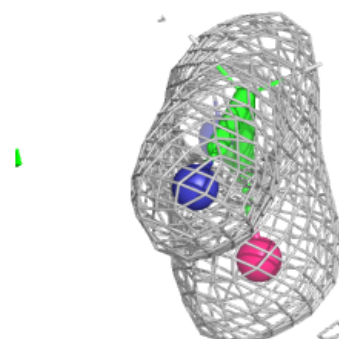
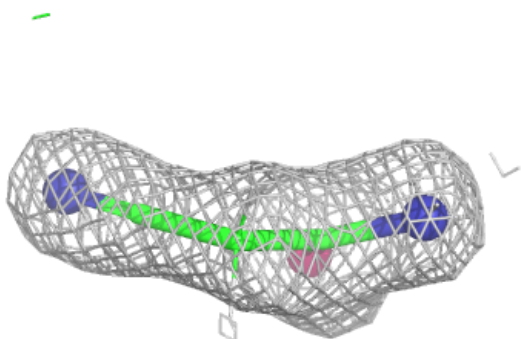
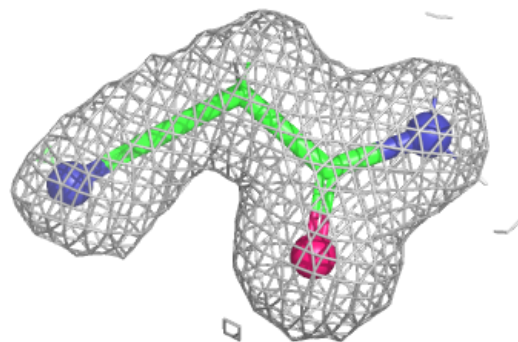
Electron density around XHD H 504:

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

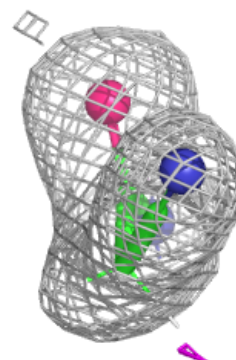
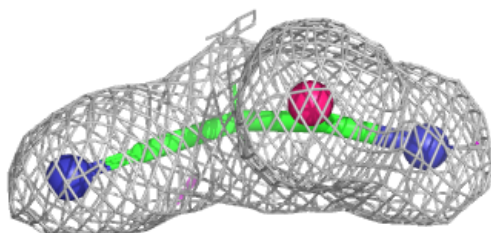
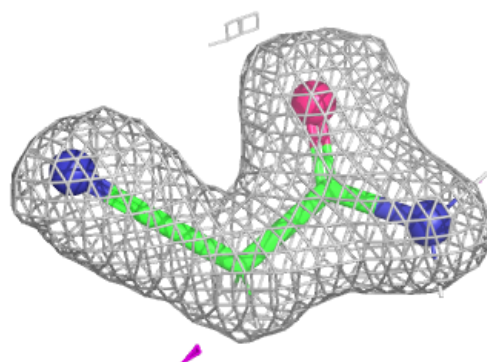


Electron density around XHD F 501:

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

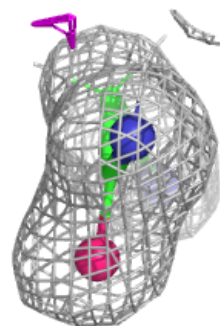
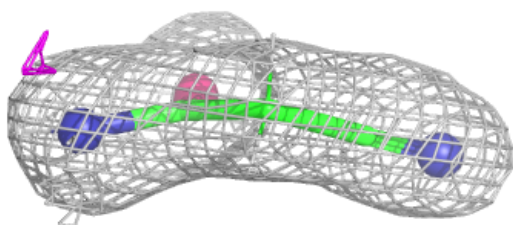
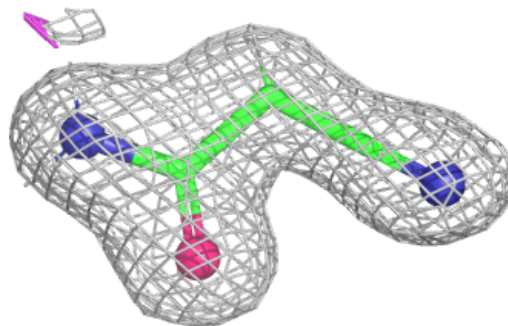
**Electron density around XHD G 501:**

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

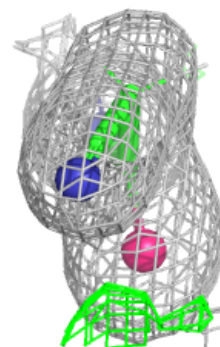
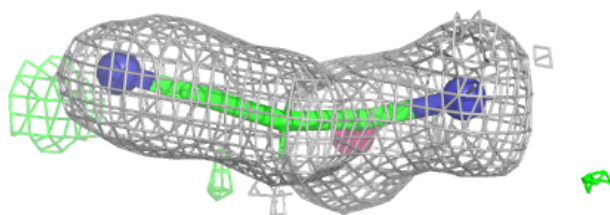
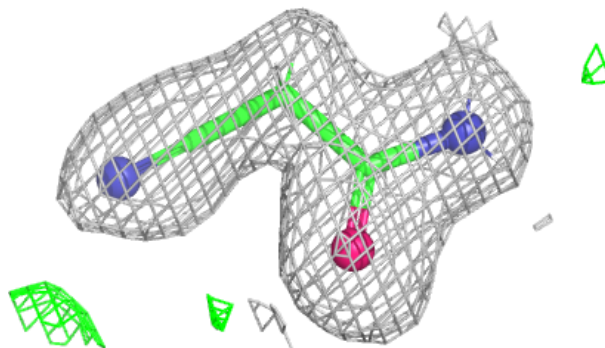


Electron density around XHD A 501:

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

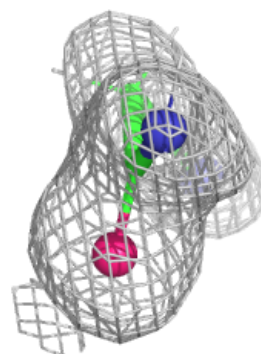
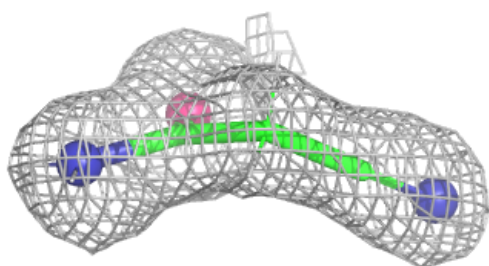
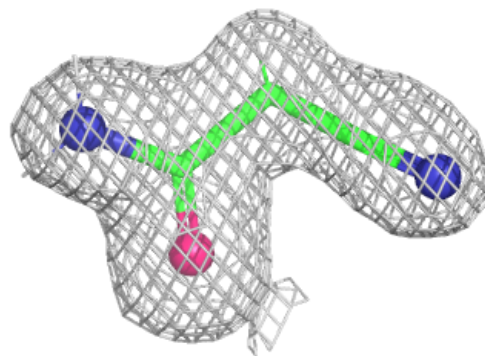
**Electron density around XHD H 501:**

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

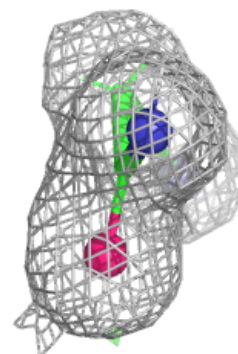
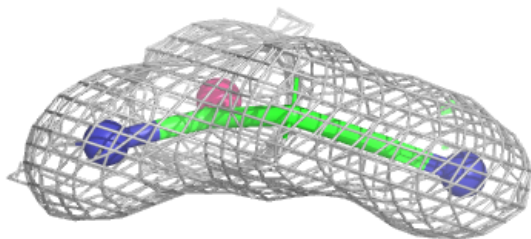
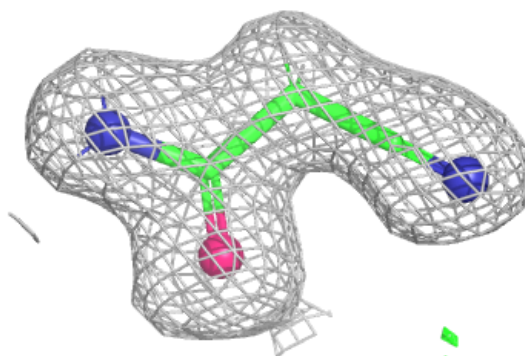


Electron density around XHD E 501:

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

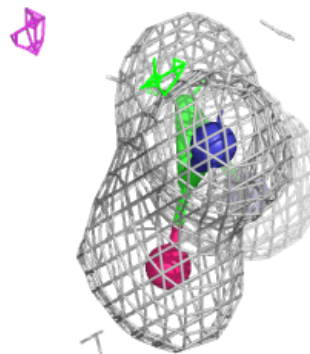
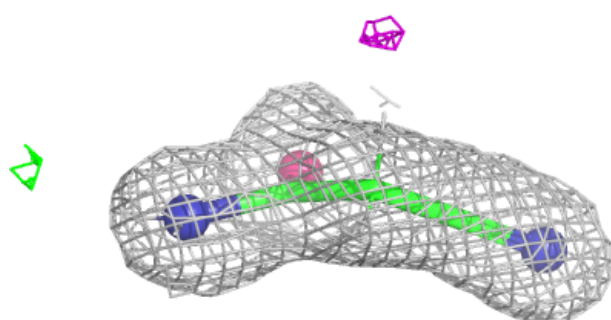
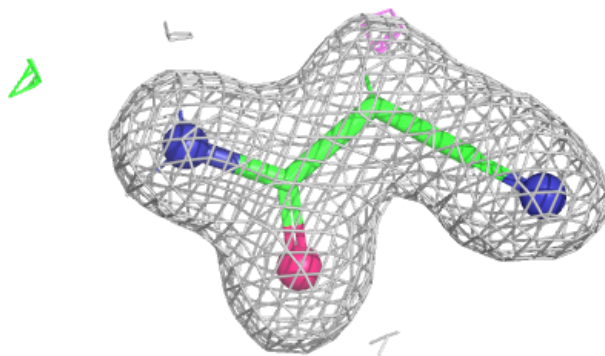
**Electron density around XHD C 501:**

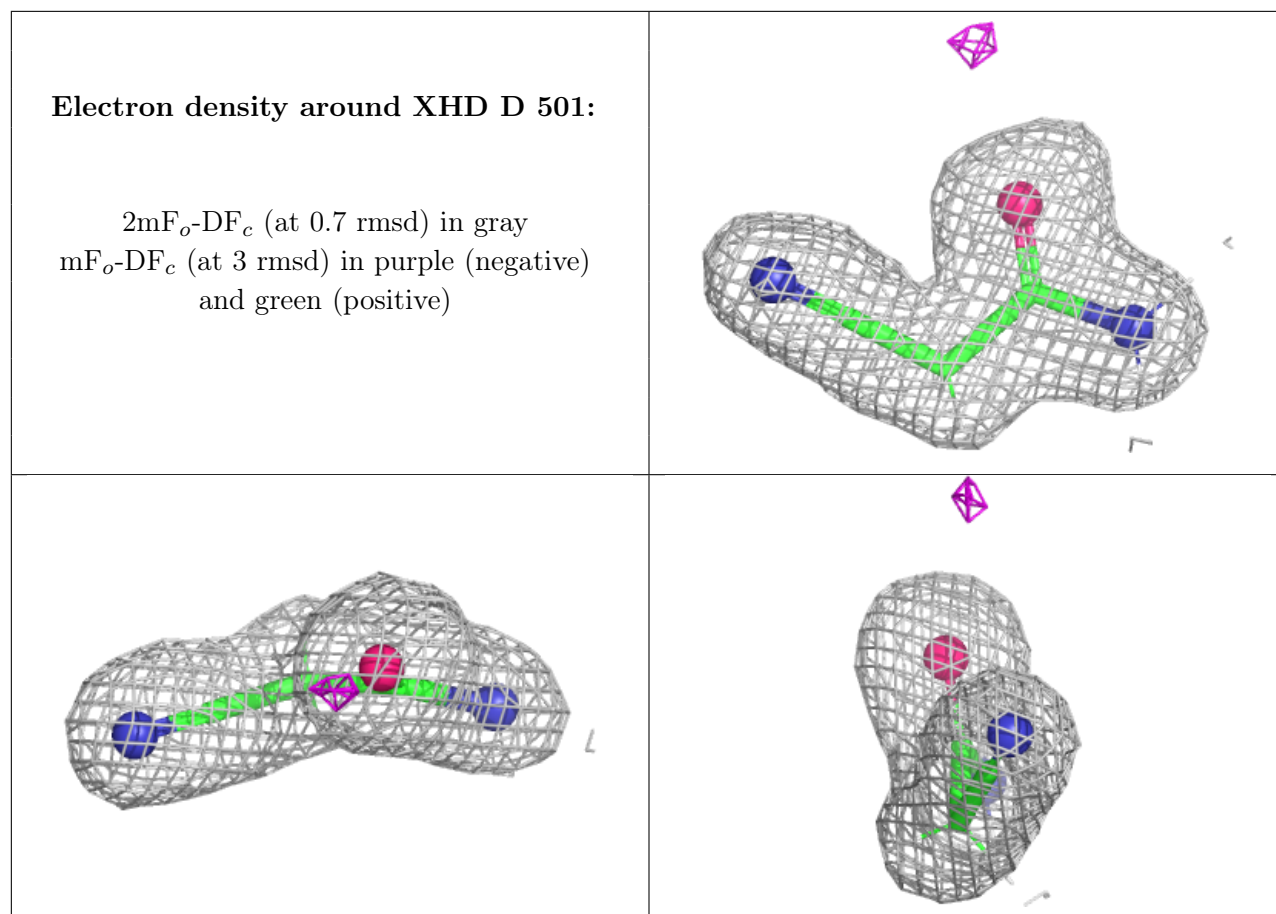
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XHD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.