



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:45 PM UTC

PDB ID : 7P76 / pdb_00007p76
Title : Re-engineered 2-deoxy-D-ribose-5-phosphate aldolase catalysing asymmetric Michael addition reactions, Schiff base complex with cinnamaldehyde
Authors : Thunnissen, A.M.W.H.; Rozeboom, H.J.; Kunzendorf, A.; Poelarends, G.J.
Deposited on : 2021-07-19
Resolution : 1.90 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

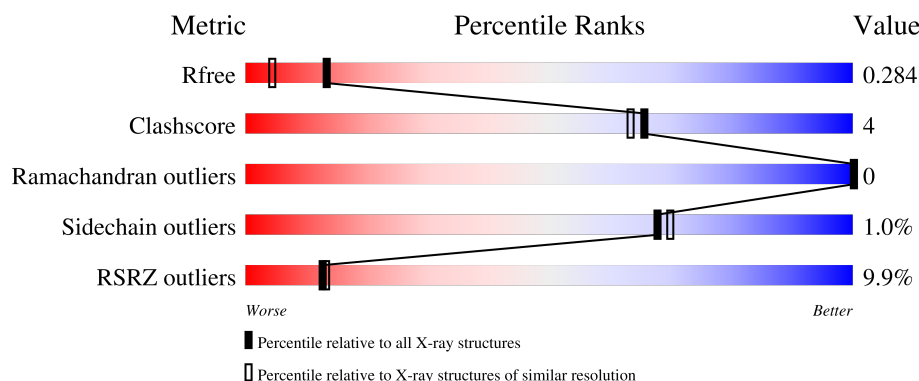
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	267	10% 83% 10% 7%
1	B	267	5% 83% 9% 7%
1	C	267	8% 85% 7% 7%
1	D	267	13% 84% 8% 7%
1	E	267	7% 83% 9% 7%

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Mol	Chain	Length	Quality of chain
1	F	267	
1	G	267	
1	H	267	
1	I	267	
1	J	267	
1	K	267	
1	L	267	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23612 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Deoxyribose-phosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1851	1168	320	355	8			
1	B	247	Total	C	N	O	S	0	0	0
			1850	1166	319	357	8			
1	C	248	Total	C	N	O	S	0	0	0
			1859	1172	321	358	8			
1	D	247	Total	C	N	O	S	0	1	0
			1855	1168	321	358	8			
1	E	248	Total	C	N	O	S	0	0	0
			1855	1170	321	356	8			
1	F	248	Total	C	N	O	S	0	1	0
			1870	1178	325	359	8			
1	G	248	Total	C	N	O	S	0	0	0
			1859	1172	321	358	8			
1	H	246	Total	C	N	O	S	0	0	0
			1843	1162	318	355	8			
1	I	246	Total	C	N	O	S	0	0	0
			1843	1162	318	355	8			
1	J	246	Total	C	N	O	S	0	0	0
			1846	1164	318	356	8			
1	K	247	Total	C	N	O	S	0	0	0
			1849	1166	318	357	8			
1	L	246	Total	C	N	O	S	0	0	0
			1843	1161	318	356	8			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	THR	engineered mutation	UNP V0AAC4
A	22	GLY	ASP	engineered mutation	UNP V0AAC4
A	24	TYR	ASP	engineered mutation	UNP V0AAC4
A	47	SER	CYS	engineered mutation	UNP V0AAC4
A	52	SER	PHE	engineered mutation	UNP V0AAC4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	THR	engineered mutation	UNP V0AAC4
A	172	LEU	LYS	engineered mutation	UNP V0AAC4
A	197	SER	THR	engineered mutation	UNP V0AAC4
A	202	VAL	PRO	engineered mutation	UNP V0AAC4
A	203	THR	ALA	engineered mutation	UNP V0AAC4
A	206	ALA	VAL	engineered mutation	UNP V0AAC4
A	239	GLY	SER	engineered mutation	UNP V0AAC4
A	260	LEU	-	expression tag	UNP V0AAC4
A	261	GLU	-	expression tag	UNP V0AAC4
A	262	HIS	-	expression tag	UNP V0AAC4
A	263	HIS	-	expression tag	UNP V0AAC4
A	264	HIS	-	expression tag	UNP V0AAC4
A	265	HIS	-	expression tag	UNP V0AAC4
A	266	HIS	-	expression tag	UNP V0AAC4
A	267	HIS	-	expression tag	UNP V0AAC4
B	18	SER	THR	engineered mutation	UNP V0AAC4
B	22	GLY	ASP	engineered mutation	UNP V0AAC4
B	24	TYR	ASP	engineered mutation	UNP V0AAC4
B	47	SER	CYS	engineered mutation	UNP V0AAC4
B	52	SER	PHE	engineered mutation	UNP V0AAC4
B	142	SER	THR	engineered mutation	UNP V0AAC4
B	172	LEU	LYS	engineered mutation	UNP V0AAC4
B	197	SER	THR	engineered mutation	UNP V0AAC4
B	202	VAL	PRO	engineered mutation	UNP V0AAC4
B	203	THR	ALA	engineered mutation	UNP V0AAC4
B	206	ALA	VAL	engineered mutation	UNP V0AAC4
B	239	GLY	SER	engineered mutation	UNP V0AAC4
B	260	LEU	-	expression tag	UNP V0AAC4
B	261	GLU	-	expression tag	UNP V0AAC4
B	262	HIS	-	expression tag	UNP V0AAC4
B	263	HIS	-	expression tag	UNP V0AAC4
B	264	HIS	-	expression tag	UNP V0AAC4
B	265	HIS	-	expression tag	UNP V0AAC4
B	266	HIS	-	expression tag	UNP V0AAC4
B	267	HIS	-	expression tag	UNP V0AAC4
C	18	SER	THR	engineered mutation	UNP V0AAC4
C	22	GLY	ASP	engineered mutation	UNP V0AAC4
C	24	TYR	ASP	engineered mutation	UNP V0AAC4
C	47	SER	CYS	engineered mutation	UNP V0AAC4
C	52	SER	PHE	engineered mutation	UNP V0AAC4
C	142	SER	THR	engineered mutation	UNP V0AAC4
C	172	LEU	LYS	engineered mutation	UNP V0AAC4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	197	SER	THR	engineered mutation	UNP V0AAC4
C	202	VAL	PRO	engineered mutation	UNP V0AAC4
C	203	THR	ALA	engineered mutation	UNP V0AAC4
C	206	ALA	VAL	engineered mutation	UNP V0AAC4
C	239	GLY	SER	engineered mutation	UNP V0AAC4
C	260	LEU	-	expression tag	UNP V0AAC4
C	261	GLU	-	expression tag	UNP V0AAC4
C	262	HIS	-	expression tag	UNP V0AAC4
C	263	HIS	-	expression tag	UNP V0AAC4
C	264	HIS	-	expression tag	UNP V0AAC4
C	265	HIS	-	expression tag	UNP V0AAC4
C	266	HIS	-	expression tag	UNP V0AAC4
C	267	HIS	-	expression tag	UNP V0AAC4
D	18	SER	THR	engineered mutation	UNP V0AAC4
D	22	GLY	ASP	engineered mutation	UNP V0AAC4
D	24	TYR	ASP	engineered mutation	UNP V0AAC4
D	47	SER	CYS	engineered mutation	UNP V0AAC4
D	52	SER	PHE	engineered mutation	UNP V0AAC4
D	142	SER	THR	engineered mutation	UNP V0AAC4
D	172	LEU	LYS	engineered mutation	UNP V0AAC4
D	197	SER	THR	engineered mutation	UNP V0AAC4
D	202	VAL	PRO	engineered mutation	UNP V0AAC4
D	203	THR	ALA	engineered mutation	UNP V0AAC4
D	206	ALA	VAL	engineered mutation	UNP V0AAC4
D	239	GLY	SER	engineered mutation	UNP V0AAC4
D	260	LEU	-	expression tag	UNP V0AAC4
D	261	GLU	-	expression tag	UNP V0AAC4
D	262	HIS	-	expression tag	UNP V0AAC4
D	263	HIS	-	expression tag	UNP V0AAC4
D	264	HIS	-	expression tag	UNP V0AAC4
D	265	HIS	-	expression tag	UNP V0AAC4
D	266	HIS	-	expression tag	UNP V0AAC4
D	267	HIS	-	expression tag	UNP V0AAC4
E	18	SER	THR	engineered mutation	UNP V0AAC4
E	22	GLY	ASP	engineered mutation	UNP V0AAC4
E	24	TYR	ASP	engineered mutation	UNP V0AAC4
E	47	SER	CYS	engineered mutation	UNP V0AAC4
E	52	SER	PHE	engineered mutation	UNP V0AAC4
E	142	SER	THR	engineered mutation	UNP V0AAC4
E	172	LEU	LYS	engineered mutation	UNP V0AAC4
E	197	SER	THR	engineered mutation	UNP V0AAC4
E	202	VAL	PRO	engineered mutation	UNP V0AAC4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	203	THR	ALA	engineered mutation	UNP V0AAC4
E	206	ALA	VAL	engineered mutation	UNP V0AAC4
E	239	GLY	SER	engineered mutation	UNP V0AAC4
E	260	LEU	-	expression tag	UNP V0AAC4
E	261	GLU	-	expression tag	UNP V0AAC4
E	262	HIS	-	expression tag	UNP V0AAC4
E	263	HIS	-	expression tag	UNP V0AAC4
E	264	HIS	-	expression tag	UNP V0AAC4
E	265	HIS	-	expression tag	UNP V0AAC4
E	266	HIS	-	expression tag	UNP V0AAC4
E	267	HIS	-	expression tag	UNP V0AAC4
F	18	SER	THR	engineered mutation	UNP V0AAC4
F	22	GLY	ASP	engineered mutation	UNP V0AAC4
F	24	TYR	ASP	engineered mutation	UNP V0AAC4
F	47	SER	CYS	engineered mutation	UNP V0AAC4
F	52	SER	PHE	engineered mutation	UNP V0AAC4
F	142	SER	THR	engineered mutation	UNP V0AAC4
F	172	LEU	LYS	engineered mutation	UNP V0AAC4
F	197	SER	THR	engineered mutation	UNP V0AAC4
F	202	VAL	PRO	engineered mutation	UNP V0AAC4
F	203	THR	ALA	engineered mutation	UNP V0AAC4
F	206	ALA	VAL	engineered mutation	UNP V0AAC4
F	239	GLY	SER	engineered mutation	UNP V0AAC4
F	260	LEU	-	expression tag	UNP V0AAC4
F	261	GLU	-	expression tag	UNP V0AAC4
F	262	HIS	-	expression tag	UNP V0AAC4
F	263	HIS	-	expression tag	UNP V0AAC4
F	264	HIS	-	expression tag	UNP V0AAC4
F	265	HIS	-	expression tag	UNP V0AAC4
F	266	HIS	-	expression tag	UNP V0AAC4
F	267	HIS	-	expression tag	UNP V0AAC4
G	18	SER	THR	engineered mutation	UNP V0AAC4
G	22	GLY	ASP	engineered mutation	UNP V0AAC4
G	24	TYR	ASP	engineered mutation	UNP V0AAC4
G	47	SER	CYS	engineered mutation	UNP V0AAC4
G	52	SER	PHE	engineered mutation	UNP V0AAC4
G	142	SER	THR	engineered mutation	UNP V0AAC4
G	172	LEU	LYS	engineered mutation	UNP V0AAC4
G	197	SER	THR	engineered mutation	UNP V0AAC4
G	202	VAL	PRO	engineered mutation	UNP V0AAC4
G	203	THR	ALA	engineered mutation	UNP V0AAC4
G	206	ALA	VAL	engineered mutation	UNP V0AAC4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	239	GLY	SER	engineered mutation	UNP V0AAC4
G	260	LEU	-	expression tag	UNP V0AAC4
G	261	GLU	-	expression tag	UNP V0AAC4
G	262	HIS	-	expression tag	UNP V0AAC4
G	263	HIS	-	expression tag	UNP V0AAC4
G	264	HIS	-	expression tag	UNP V0AAC4
G	265	HIS	-	expression tag	UNP V0AAC4
G	266	HIS	-	expression tag	UNP V0AAC4
G	267	HIS	-	expression tag	UNP V0AAC4
H	18	SER	THR	engineered mutation	UNP V0AAC4
H	22	GLY	ASP	engineered mutation	UNP V0AAC4
H	24	TYR	ASP	engineered mutation	UNP V0AAC4
H	47	SER	CYS	engineered mutation	UNP V0AAC4
H	52	SER	PHE	engineered mutation	UNP V0AAC4
H	142	SER	THR	engineered mutation	UNP V0AAC4
H	172	LEU	LYS	engineered mutation	UNP V0AAC4
H	197	SER	THR	engineered mutation	UNP V0AAC4
H	202	VAL	PRO	engineered mutation	UNP V0AAC4
H	203	THR	ALA	engineered mutation	UNP V0AAC4
H	206	ALA	VAL	engineered mutation	UNP V0AAC4
H	239	GLY	SER	engineered mutation	UNP V0AAC4
H	260	LEU	-	expression tag	UNP V0AAC4
H	261	GLU	-	expression tag	UNP V0AAC4
H	262	HIS	-	expression tag	UNP V0AAC4
H	263	HIS	-	expression tag	UNP V0AAC4
H	264	HIS	-	expression tag	UNP V0AAC4
H	265	HIS	-	expression tag	UNP V0AAC4
H	266	HIS	-	expression tag	UNP V0AAC4
H	267	HIS	-	expression tag	UNP V0AAC4
I	18	SER	THR	engineered mutation	UNP V0AAC4
I	22	GLY	ASP	engineered mutation	UNP V0AAC4
I	24	TYR	ASP	engineered mutation	UNP V0AAC4
I	47	SER	CYS	engineered mutation	UNP V0AAC4
I	52	SER	PHE	engineered mutation	UNP V0AAC4
I	142	SER	THR	engineered mutation	UNP V0AAC4
I	172	LEU	LYS	engineered mutation	UNP V0AAC4
I	197	SER	THR	engineered mutation	UNP V0AAC4
I	202	VAL	PRO	engineered mutation	UNP V0AAC4
I	203	THR	ALA	engineered mutation	UNP V0AAC4
I	206	ALA	VAL	engineered mutation	UNP V0AAC4
I	239	GLY	SER	engineered mutation	UNP V0AAC4
I	260	LEU	-	expression tag	UNP V0AAC4

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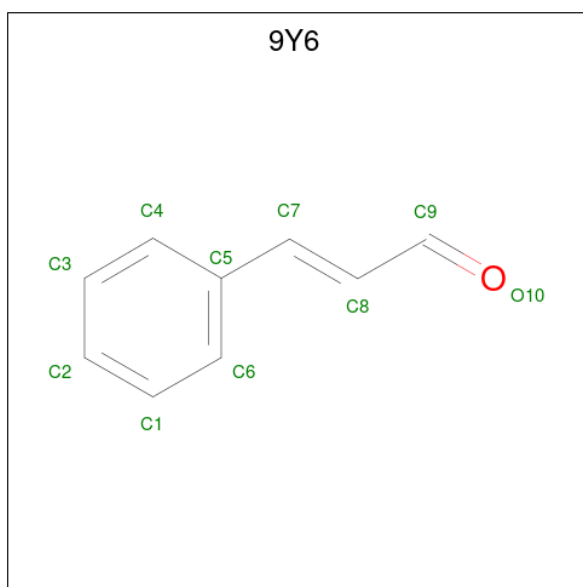
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I	262	HIS	-	expression tag	UNP V0AAC4
I	263	HIS	-	expression tag	UNP V0AAC4
I	264	HIS	-	expression tag	UNP V0AAC4
I	265	HIS	-	expression tag	UNP V0AAC4
I	266	HIS	-	expression tag	UNP V0AAC4
I	267	HIS	-	expression tag	UNP V0AAC4
J	18	SER	THR	engineered mutation	UNP V0AAC4
J	22	GLY	ASP	engineered mutation	UNP V0AAC4
J	24	TYR	ASP	engineered mutation	UNP V0AAC4
J	47	SER	CYS	engineered mutation	UNP V0AAC4
J	52	SER	PHE	engineered mutation	UNP V0AAC4
J	142	SER	THR	engineered mutation	UNP V0AAC4
J	172	LEU	LYS	engineered mutation	UNP V0AAC4
J	197	SER	THR	engineered mutation	UNP V0AAC4
J	202	VAL	PRO	engineered mutation	UNP V0AAC4
J	203	THR	ALA	engineered mutation	UNP V0AAC4
J	206	ALA	VAL	engineered mutation	UNP V0AAC4
J	239	GLY	SER	engineered mutation	UNP V0AAC4
J	260	LEU	-	expression tag	UNP V0AAC4
J	261	GLU	-	expression tag	UNP V0AAC4
J	262	HIS	-	expression tag	UNP V0AAC4
J	263	HIS	-	expression tag	UNP V0AAC4
J	264	HIS	-	expression tag	UNP V0AAC4
J	265	HIS	-	expression tag	UNP V0AAC4
J	266	HIS	-	expression tag	UNP V0AAC4
J	267	HIS	-	expression tag	UNP V0AAC4
K	18	SER	THR	engineered mutation	UNP V0AAC4
K	22	GLY	ASP	engineered mutation	UNP V0AAC4
K	25	TYR	ASP	engineered mutation	UNP V0AAC4
K	47	SER	CYS	engineered mutation	UNP V0AAC4
K	52	SER	PHE	engineered mutation	UNP V0AAC4
K	142	SER	THR	engineered mutation	UNP V0AAC4
K	172	LEU	LYS	engineered mutation	UNP V0AAC4
K	197	SER	THR	engineered mutation	UNP V0AAC4
K	202	VAL	PRO	engineered mutation	UNP V0AAC4
K	203	THR	ALA	engineered mutation	UNP V0AAC4
K	206	ALA	VAL	engineered mutation	UNP V0AAC4
K	239	GLY	SER	engineered mutation	UNP V0AAC4
K	260	LEU	-	expression tag	UNP V0AAC4
K	261	GLU	-	expression tag	UNP V0AAC4
K	262	HIS	-	expression tag	UNP V0AAC4

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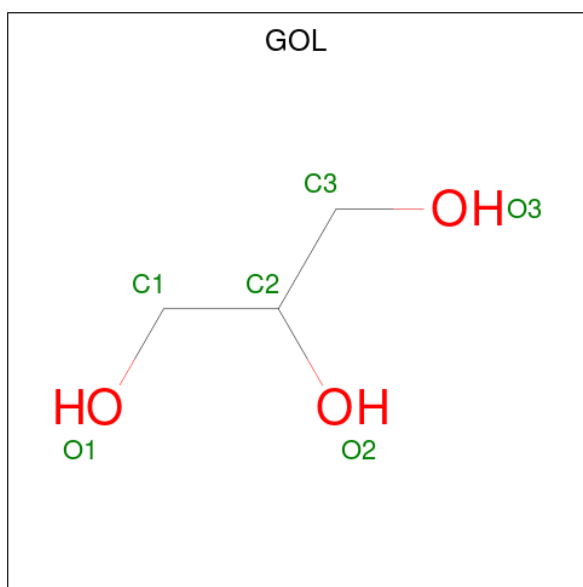
Chain	Residue	Modelled	Actual	Comment	Reference
K	263	HIS	-	expression tag	UNP V0AAC4
K	264	HIS	-	expression tag	UNP V0AAC4
K	265	HIS	-	expression tag	UNP V0AAC4
K	266	HIS	-	expression tag	UNP V0AAC4
K	267	HIS	-	expression tag	UNP V0AAC4
L	18	SER	THR	engineered mutation	UNP V0AAC4
L	22	GLY	ASP	engineered mutation	UNP V0AAC4
L	24	TYR	ASP	engineered mutation	UNP V0AAC4
L	47	SER	CYS	engineered mutation	UNP V0AAC4
L	52	SER	PHE	engineered mutation	UNP V0AAC4
L	142	SER	THR	engineered mutation	UNP V0AAC4
L	172	LEU	LYS	engineered mutation	UNP V0AAC4
L	197	SER	THR	engineered mutation	UNP V0AAC4
L	202	VAL	PRO	engineered mutation	UNP V0AAC4
L	203	THR	ALA	engineered mutation	UNP V0AAC4
L	206	ALA	VAL	engineered mutation	UNP V0AAC4
L	239	GLY	SER	engineered mutation	UNP V0AAC4
L	260	LEU	-	expression tag	UNP V0AAC4
L	261	GLU	-	expression tag	UNP V0AAC4
L	262	HIS	-	expression tag	UNP V0AAC4
L	263	HIS	-	expression tag	UNP V0AAC4
L	264	HIS	-	expression tag	UNP V0AAC4
L	265	HIS	-	expression tag	UNP V0AAC4
L	266	HIS	-	expression tag	UNP V0AAC4
L	267	HIS	-	expression tag	UNP V0AAC4

- Molecule 2 is (2E)-3-phenylprop-2-enal (CCD ID: 9Y6) (formula: C₉H₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9 9	0	0
2	B	1	Total C 9 9	0	0
2	C	1	Total C 9 9	0	0
2	D	1	Total C 9 9	0	0
2	E	1	Total C 9 9	0	0
2	F	1	Total C 9 9	0	0
2	G	1	Total C 9 9	0	0
2	H	1	Total C 9 9	0	0
2	I	1	Total C 9 9	0	0
2	J	1	Total C 9 9	0	0
2	K	1	Total C 9 9	0	0
2	L	1	Total C 9 9	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	104	Total	O	0	0
			104	104		
4	C	121	Total	O	0	0
			121	121		
4	D	83	Total	O	0	0
			83	83		
4	E	126	Total	O	0	0
			126	126		
4	F	144	Total	O	0	0
			144	144		
4	G	117	Total	O	0	0
			117	117		
4	H	74	Total	O	0	0
			74	74		
4	I	85	Total	O	0	0
			85	85		
4	J	94	Total	O	0	0
			94	94		
4	K	116	Total	O	0	0
			116	116		

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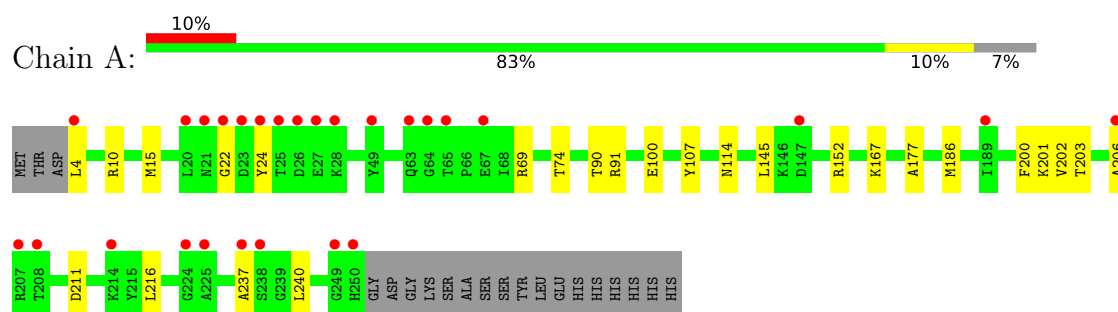
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	97	Total	O	0	0
			97	97		

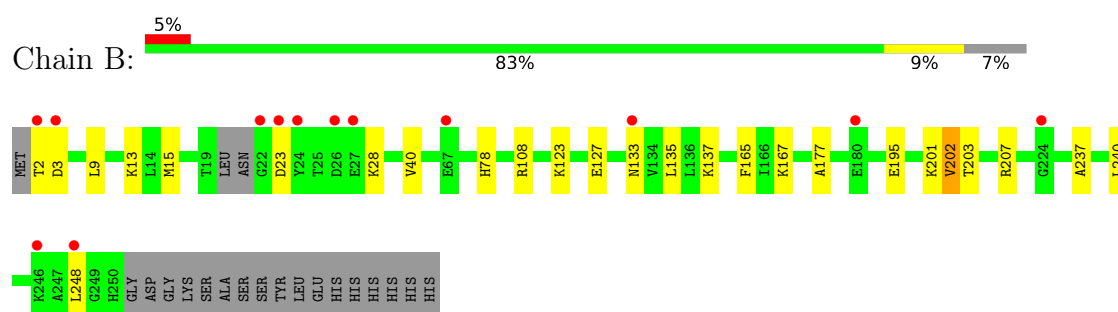
3 Residue-property plots

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.

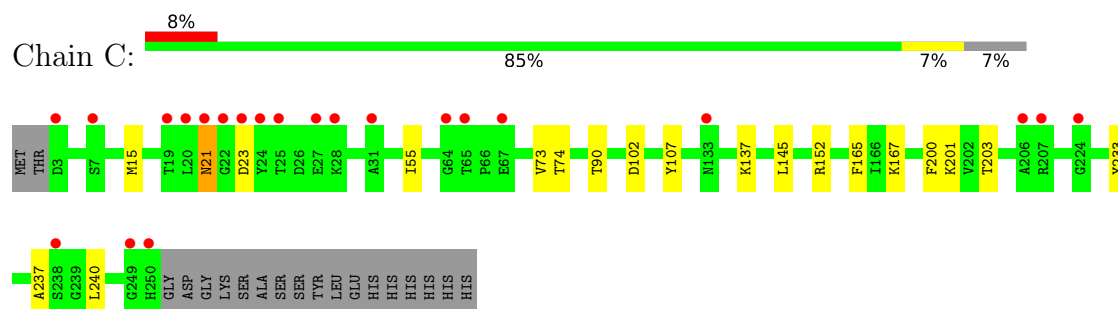
• Molecule 1: Deoxyribose-phosphate aldolase



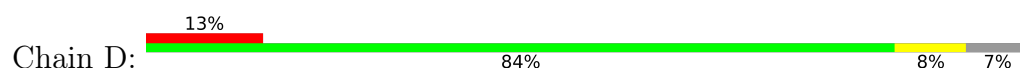
• Molecule 1: Deoxyribose-phosphate aldolase



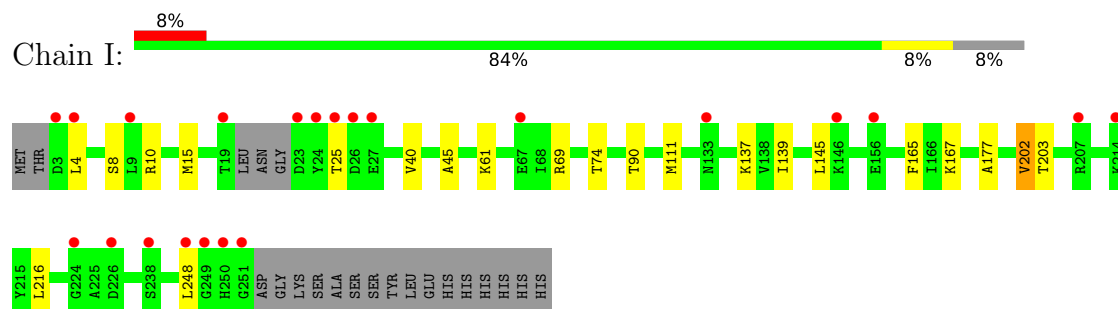
• Molecule 1: Deoxyribose-phosphate aldolase



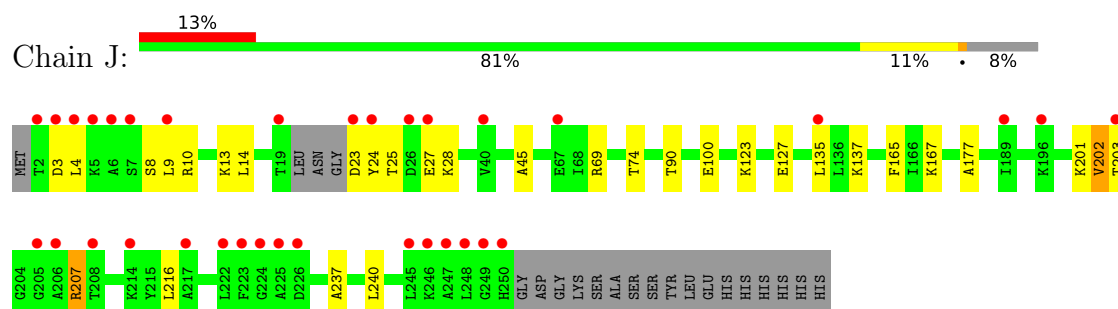
• Molecule 1: Deoxyribose-phosphate aldolase



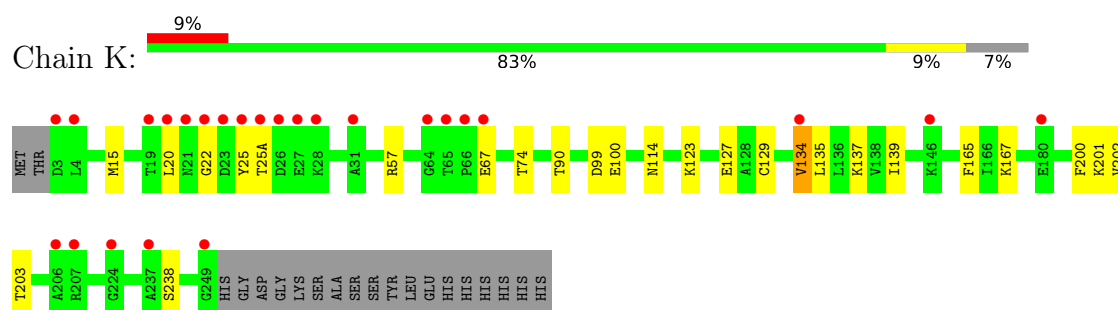
- Molecule 1: Deoxyribose-phosphate aldolase



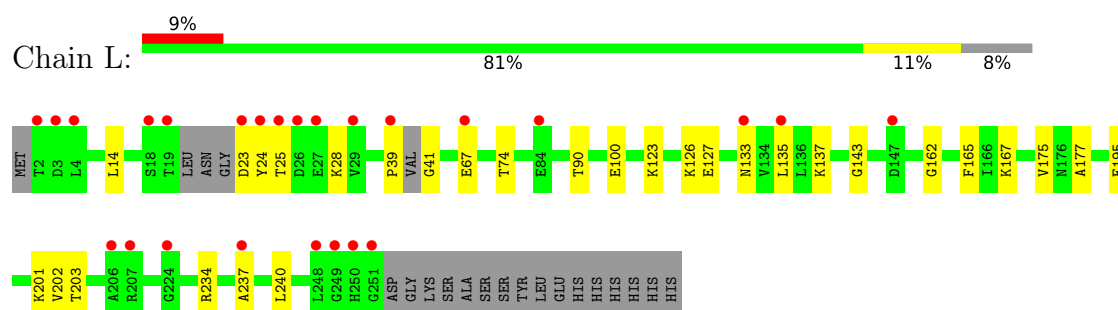
- Molecule 1: Deoxyribose-phosphate aldolase



- Molecule 1: Deoxyribose-phosphate aldolase



- Molecule 1: Deoxyribose-phosphate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.27Å 92.79Å 106.89Å 88.96° 88.83° 89.08°	Depositor
Resolution (Å)	80.24 – 1.90 80.24 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (80.24-1.90) 94.3 (80.24-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.235 , 0.283 0.236 , 0.284	Depositor DCC
R_{free} test set	11336 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	1.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23612	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9675e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9Y6, GOL

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	0.38	0/1876	0.58	0/2536
1	B	0.32	0/1874	0.53	0/2532
1	C	0.33	0/1884	0.53	0/2547
1	D	0.32	0/1879	0.54	0/2538
1	E	0.36	0/1880	0.57	0/2541
1	F	0.32	0/1895	0.53	0/2561
1	G	0.36	0/1884	0.55	0/2547
1	H	0.34	0/1867	0.52	0/2522
1	I	0.30	0/1867	0.51	0/2522
1	J	0.34	0/1870	0.54	0/2527
1	K	0.37	0/1873	0.57	0/2532
1	L	0.34	0/1866	0.52	0/2519
All	All	0.34	0/22515	0.54	0/30424

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1851	0	1892	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1850	0	1885	16	0
1	C	1859	0	1896	13	0
1	D	1855	0	1886	15	0
1	E	1855	0	1895	15	0
1	F	1870	0	1908	13	0
1	G	1859	0	1896	10	0
1	H	1843	0	1878	14	0
1	I	1843	0	1878	14	0
1	J	1846	0	1882	20	0
1	K	1849	0	1889	15	0
1	L	1843	0	1875	18	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	0	0
2	E	9	0	0	0	0
2	F	9	0	0	0	0
2	G	9	0	0	0	0
2	H	9	0	0	0	0
2	I	9	0	0	0	0
2	J	9	0	0	0	0
2	K	9	0	0	0	0
2	L	9	0	0	0	0
3	I	6	0	8	0	0
4	A	114	0	0	3	0
4	B	104	0	0	1	1
4	C	121	0	0	1	1
4	D	83	0	0	1	0
4	E	126	0	0	1	0
4	F	144	0	0	3	0
4	G	117	0	0	1	1
4	H	74	0	0	0	0
4	I	85	0	0	1	0
4	J	94	0	0	2	0
4	K	116	0	0	1	0
4	L	97	0	0	2	1
All	All	23612	0	22668	173	2

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 4.

All (173) 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:123:LYS:NZ	1:H:127:GLU:OE2	2.18	0.77
1:L:123:LYS:NZ	1:L:127:GLU:OE2	2.19	0.76
1:B:123:LYS:NZ	1:B:127:GLU:OE2	2.19	0.74
1:G:123:LYS:NZ	1:G:127:GLU:OE2	2.20	0.70
1:I:111:MET:HE2	1:I:145:LEU:HA	1.76	0.68
1:B:195:GLU:OE2	1:J:207:ARG:NH1	2.15	0.68
1:B:23:ASP:HB3	1:B:28:LYS:HG3	1.78	0.64
1:L:100:GLU:HG2	1:L:135:LEU:HB2	1.80	0.64
1:D:123:LYS:NZ	1:D:127:GLU:OE2	2.31	0.64
1:L:23:ASP:HB3	1:L:28:LYS:HG3	1.79	0.64
1:L:133:ASN:ND2	4:L:401:HOH:O	2.30	0.63
1:F:23:ASP:HB3	1:F:28:LYS:HG3	1.82	0.61
1:E:23:ASP:HB3	1:E:28:LYS:HG3	1.82	0.61
1:H:80:ASN:OD1	1:H:108:ARG:NH2	2.25	0.61
1:D:167:LYS:HE3	1:D:203:THR:OG1	2.01	0.60
1:J:167:LYS:HE3	1:J:203:THR:OG1	2.02	0.59
1:F:91:ARG:NH1	4:F:401:HOH:O	2.23	0.59
1:B:207:ARG:NH1	1:L:195:GLU:OE2	2.24	0.59
1:D:127:GLU:O	4:D:401:HOH:O	2.17	0.59
1:L:167:LYS:HE3	1:L:203:THR:OG1	2.02	0.58
1:L:39:PRO:O	1:L:41:GLY:N	2.37	0.58
1:A:4:LEU:N	4:A:402:HOH:O	2.37	0.57
1:K:123:LYS:NZ	1:K:127:GLU:OE2	2.28	0.57
1:B:167:LYS:HE3	1:B:203:THR:OG1	2.05	0.57
1:H:167:LYS:HE3	1:H:203:THR:OG1	2.04	0.57
1:J:100:GLU:HG2	1:J:135:LEU:HB2	1.88	0.56
1:F:207[B]:ARG:NH2	4:F:404:HOH:O	2.39	0.55
1:D:3:ASP:HB2	1:D:210:GLU:CD	2.32	0.54
1:E:177:ALA:CB	1:E:202:VAL:HG23	2.38	0.54
1:J:123:LYS:NZ	1:J:127:GLU:OE2	2.33	0.54
1:E:167:LYS:HE3	1:E:203:THR:OG1	2.07	0.54
1:C:21:ASN:OD1	1:C:21:ASN:N	2.40	0.54
1:H:23:ASP:HB3	1:H:28:LYS:HG3	1.89	0.54
1:I:167:LYS:HE3	1:I:203:THR:OG1	2.07	0.53
1:A:167:LYS:HD2	1:A:201:LYS:HD3	1.91	0.53
1:B:133:ASN:ND2	1:J:27:GLU:OE1	2.41	0.53
1:G:137:LYS:HG2	1:G:165:PHE:HB2	1.91	0.53
1:C:167:LYS:HE3	1:C:203:THR:OG1	2.09	0.52
1:F:167:LYS:HE3	1:F:203:THR:OG1	2.08	0.52
1:A:200:PHE:CE2	1:A:202:VAL:HG23	2.45	0.52
1:G:167:LYS:HD2	1:G:201:LYS:HD3	1.92	0.52
1:D:74:THR:HG21	1:D:90:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:THR:HG21	1:J:90:THR:HA	1.93	0.51
1:A:167:LYS:HE3	1:A:203:THR:OG1	2.12	0.50
1:H:42:ASN:ND2	1:H:67:GLU:OE2	2.44	0.50
1:K:167:LYS:HD2	1:K:201:LYS:HD3	1.94	0.50
1:G:167:LYS:HE3	1:G:203:THR:OG1	2.12	0.50
1:H:100:GLU:HG2	1:H:135:LEU:HB2	1.94	0.50
1:G:200:PHE:CE2	1:G:202:VAL:HG22	2.48	0.48
1:E:167:LYS:HD2	1:E:201:LYS:HD3	1.94	0.48
1:L:67:GLU:OE1	1:L:67:GLU:N	2.31	0.48
1:H:137:LYS:HG2	1:H:165:PHE:HB2	1.95	0.48
1:L:167:LYS:HD2	1:L:201:LYS:HD3	1.94	0.48
1:B:167:LYS:HD2	1:B:201:LYS:HD3	1.94	0.48
1:E:207:ARG:HD2	1:F:133:ASN:OD1	2.13	0.48
1:H:246:LYS:HA	1:H:251:GLY:H	1.79	0.48
1:F:15:MET:HE3	1:F:15:MET:HB2	1.74	0.47
1:F:123:LYS:NZ	1:F:127:GLU:OE2	2.32	0.47
1:K:100:GLU:HG2	1:K:135:LEU:HB2	1.96	0.47
1:D:3:ASP:HB2	1:D:210:GLU:HG3	1.95	0.47
1:A:74:THR:HG21	1:A:90:THR:HA	1.96	0.47
1:I:74:THR:HG21	1:I:90:THR:HA	1.97	0.47
1:K:200:PHE:CE2	1:K:202:VAL:HG22	2.49	0.47
1:L:25:THR:HG23	4:L:418:HOH:O	2.13	0.47
1:K:57:ARG:HH22	1:K:99:ASP:CG	2.23	0.47
1:B:2:THR:HA	4:B:481:HOH:O	2.14	0.47
1:J:23:ASP:HB3	1:J:28:LYS:HG3	1.97	0.47
1:K:15:MET:HE3	1:K:15:MET:HB2	1.74	0.47
1:E:74:THR:HG21	1:E:90:THR:HA	1.96	0.46
1:K:137:LYS:HG2	1:K:165:PHE:HB2	1.97	0.46
1:L:24:TYR:C	1:L:24:TYR:CD2	2.93	0.46
1:B:78:HIS:O	1:B:108:ARG:NH1	2.39	0.46
1:A:152:ARG:NH1	4:A:408:HOH:O	2.47	0.46
1:C:137:LYS:HG2	1:C:165:PHE:HB2	1.98	0.46
1:J:10:ARG:HD3	1:J:216:LEU:HD13	1.97	0.46
1:I:137:LYS:HG2	1:I:165:PHE:HB2	1.98	0.46
1:H:177:ALA:CB	1:H:202:VAL:HG23	2.46	0.46
1:A:69:ARG:HD3	1:A:100:GLU:OE2	2.15	0.45
1:J:237:ALA:HB1	1:J:240:LEU:HB3	1.97	0.45
1:B:40:VAL:HG21	1:B:248:LEU:HD13	1.98	0.45
1:K:167:LYS:HE3	1:K:203:THR:OG1	2.16	0.45
1:E:57:ARG:NH2	1:E:97:GLY:O	2.47	0.45
1:C:167:LYS:HD2	1:C:201:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:ARG:HD3	1:F:100:GLU:OE2	2.15	0.45
1:B:137:LYS:HG2	1:B:165:PHE:HB2	1.99	0.45
1:E:107:TYR:HB2	1:E:145:LEU:HD21	1.99	0.45
1:J:45:ALA:HB2	1:J:69:ARG:HB2	1.98	0.45
1:D:40:VAL:HG21	1:D:248:LEU:HD13	1.99	0.45
1:F:167:LYS:HD2	1:F:201:LYS:HD3	1.98	0.45
1:F:74:THR:HG21	1:F:90:THR:HA	1.99	0.45
1:B:15:MET:HE3	1:B:15:MET:HB2	1.90	0.45
1:E:15:MET:HE3	1:E:15:MET:HB2	1.73	0.44
1:K:74:THR:HG21	1:K:90:THR:HA	1.99	0.44
1:L:143:GLY:HA3	1:L:175:VAL:O	2.17	0.44
1:J:24:TYR:OH	4:J:401:HOH:O	2.15	0.44
1:L:137:LYS:HG2	1:L:165:PHE:HB2	2.00	0.44
1:I:10:ARG:HD3	1:I:216:LEU:HD13	1.99	0.44
1:L:126:LYS:NZ	1:L:162:GLY:O	2.44	0.44
1:E:213:GLN:NE2	4:E:401:HOH:O	2.22	0.44
1:G:15:MET:HE3	1:G:15:MET:HB2	1.74	0.44
1:H:74:THR:HG21	1:H:90:THR:HA	2.00	0.44
1:A:177:ALA:CB	1:A:202:VAL:HG13	2.47	0.44
1:D:100:GLU:HG2	1:D:135:LEU:HB2	1.98	0.44
1:A:15:MET:HE3	1:A:15:MET:HB2	1.82	0.44
1:I:15:MET:HE3	1:I:15:MET:HB2	1.87	0.44
1:I:61:LYS:HG3	4:I:476:HOH:O	2.18	0.43
1:J:177:ALA:CB	1:J:202:VAL:HG23	2.47	0.43
1:G:22:GLY:HA2	4:G:474:HOH:O	2.17	0.43
1:F:152:ARG:NH1	4:F:411:HOH:O	2.50	0.43
1:K:67:GLU:OE1	1:K:67:GLU:N	2.41	0.43
1:L:237:ALA:HB1	1:L:240:LEU:HB3	1.99	0.43
1:A:206:ALA:HA	1:A:211:ASP:HB3	2.00	0.43
1:I:139:ILE:HG12	1:I:167:LYS:HD3	2.00	0.43
1:B:133:ASN:OD1	1:J:28:LYS:NZ	2.51	0.43
1:G:23:ASP:HB3	1:G:28:LYS:HG3	2.01	0.43
1:H:62:GLU:HB3	1:K:114:ASN:HA	1.99	0.43
1:D:137:LYS:HG2	1:D:165:PHE:HB2	2.01	0.43
1:J:9:LEU:HD11	1:J:13:LYS:HE3	2.00	0.43
1:I:111:MET:CE	1:I:145:LEU:HD23	2.49	0.43
1:J:24:TYR:CD2	1:J:24:TYR:C	2.97	0.43
1:J:137:LYS:HG2	1:J:165:PHE:HB2	2.01	0.43
1:A:91:ARG:NH1	4:A:405:HOH:O	2.39	0.43
1:F:177:ALA:CB	1:F:202:VAL:HG23	2.49	0.43
1:L:74:THR:HG21	1:L:90:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:VAL:HA	1:C:102:ASP:O	2.19	0.42
1:K:139:ILE:HG12	1:K:167:LYS:HD3	2.00	0.42
1:D:186:MET:HE2	1:D:200:PHE:CE2	2.54	0.42
1:E:245:LEU:HD23	1:E:245:LEU:HA	1.89	0.42
1:A:10:ARG:HD3	1:A:216:LEU:HD13	2.01	0.42
1:D:45:ALA:HB2	1:D:69:ARG:HB2	2.01	0.42
1:H:15:MET:HE3	1:H:15:MET:HB2	1.86	0.42
1:K:22:GLY:HA2	4:K:493:HOH:O	2.18	0.42
1:B:9:LEU:HD11	1:B:13:LYS:HE3	2.02	0.42
1:C:200:PHE:O	1:C:233:TYR:HA	2.20	0.42
1:B:237:ALA:HB1	1:B:240:LEU:HB3	2.01	0.42
1:I:40:VAL:HG21	1:I:248:LEU:HD13	2.02	0.42
1:J:10:ARG:O	1:J:14:LEU:HG	2.19	0.42
1:L:14:LEU:O	1:L:234:ARG:HA	2.20	0.42
1:J:4:LEU:O	1:J:8:SER:OG	2.35	0.42
1:J:25:THR:HG23	4:J:446:HOH:O	2.20	0.42
1:C:74:THR:HG21	1:C:90:THR:HA	2.02	0.42
1:E:7:SER:OG	1:E:213:GLN:HG3	2.20	0.42
1:G:237:ALA:HB1	1:G:240:LEU:HB3	2.01	0.42
1:C:15:MET:HE3	1:C:15:MET:HB2	1.88	0.41
1:E:26:ASP:O	1:E:30:ILE:HG13	2.19	0.41
1:I:111:MET:HE3	1:I:145:LEU:HD23	2.01	0.41
1:D:200:PHE:CE2	1:D:202:VAL:HG22	2.55	0.41
1:J:167:LYS:HD2	1:J:201:LYS:HD3	2.01	0.41
1:G:74:THR:HG21	1:G:90:THR:HA	2.02	0.41
1:H:53:ILE:HD13	1:H:98:ALA:HB2	2.02	0.41
1:K:129:CYS:HB3	1:K:134:VAL:HG22	2.03	0.41
1:F:14:LEU:O	1:F:234:ARG:HA	2.21	0.41
1:L:177:ALA:CB	1:L:202:VAL:HG23	2.50	0.41
1:C:237:ALA:HB1	1:C:240:LEU:HB3	2.02	0.41
1:K:20:LEU:HA	1:K:238:SER:OG	2.20	0.41
1:A:22:GLY:O	1:A:24:TYR:CE1	2.73	0.41
1:A:107:TYR:HB2	1:A:145:LEU:HD21	2.03	0.41
1:I:45:ALA:HB2	1:I:69:ARG:HB2	2.03	0.41
1:A:186:MET:HE2	1:A:200:PHE:CE2	2.56	0.41
1:C:152:ARG:NH1	4:C:409:HOH:O	2.52	0.41
1:D:3:ASP:HB2	1:D:210:GLU:CG	2.51	0.41
1:A:114:ASN:HA	1:D:62:GLU:HB3	2.02	0.40
1:C:55:ILE:HD12	1:C:55:ILE:HA	1.94	0.40
1:H:139:ILE:HG12	1:H:167:LYS:HD3	2.02	0.40
1:I:177:ALA:CB	1:I:202:VAL:HG23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASP:N	1:C:23:ASP:OD1	2.55	0.40
1:E:10:ARG:HD3	1:E:216:LEU:HD13	2.03	0.40
1:E:200:PHE:O	1:E:233:TYR:HA	2.20	0.40
1:B:177:ALA:CB	1:B:202:VAL:HG23	2.51	0.40
1:C:107:TYR:HB2	1:C:145:LEU:HD21	2.03	0.40
1:A:237:ALA:HB1	1:A:240:LEU:HB3	2.03	0.40
1:D:246:LYS:HA	1:D:251:GLY:H	1.85	0.40
1:I:4:LEU:O	1:I:8:SER:OG	2.33	0.40

All (2) 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)
4:B:481:HOH:O	4:C:476:HOH:O[1_655]	2.14	0.06
4:G:424:HOH:O	4:L:479:HOH:O[1_565]	2.19	0.01

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	245/267 (92%)	239 (98%)	6 (2%)	0	100	100
1	B	243/267 (91%)	238 (98%)	5 (2%)	0	100	100
1	C	246/267 (92%)	239 (97%)	7 (3%)	0	100	100
1	D	244/267 (91%)	239 (98%)	5 (2%)	0	100	100
1	E	246/267 (92%)	238 (97%)	8 (3%)	0	100	100
1	F	247/267 (92%)	241 (98%)	6 (2%)	0	100	100
1	G	246/267 (92%)	241 (98%)	5 (2%)	0	100	100
1	H	242/267 (91%)	237 (98%)	5 (2%)	0	100	100
1	I	242/267 (91%)	236 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	242/267 (91%)	237 (98%)	5 (2%)	0	100	100
1	K	245/267 (92%)	240 (98%)	5 (2%)	0	100	100
1	L	240/267 (90%)	235 (98%)	5 (2%)	0	100	100
All	All	2928/3204 (91%)	2860 (98%)	68 (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	190/207 (92%)	190 (100%)	0	100	100
1	B	190/207 (92%)	187 (98%)	3 (2%)	55	54
1	C	191/207 (92%)	190 (100%)	1 (0%)	81	84
1	D	190/207 (92%)	190 (100%)	0	100	100
1	E	190/207 (92%)	186 (98%)	4 (2%)	47	44
1	F	192/207 (93%)	190 (99%)	2 (1%)	68	70
1	G	191/207 (92%)	189 (99%)	2 (1%)	68	70
1	H	189/207 (91%)	186 (98%)	3 (2%)	55	54
1	I	189/207 (91%)	187 (99%)	2 (1%)	65	67
1	J	190/207 (92%)	187 (98%)	3 (2%)	55	54
1	K	190/207 (92%)	187 (98%)	3 (2%)	55	54
1	L	189/207 (91%)	189 (100%)	0	100	100
All	All	2281/2484 (92%)	2258 (99%)	23 (1%)	68	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	ASP
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	202	VAL
1	C	21	ASN
1	E	24	TYR
1	E	135	LEU
1	E	202	VAL
1	E	207	ARG
1	F	135	LEU
1	F	202	VAL
1	G	3	ASP
1	G	24	TYR
1	H	25	THR
1	H	61	LYS
1	H	202	VAL
1	I	25	THR
1	I	202	VAL
1	J	3	ASP
1	J	202	VAL
1	J	207	ARG
1	K	25	TYR
1	K	25(A)	THR
1	K	134	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	E	250	HIS
1	F	213	GLN
1	H	42	ASN
1	J	213	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
2	9Y6	K	301	1	9,9,10	0.35	0	10,10,11	0.46	0
2	9Y6	B	301	1	9,9,10	0.35	0	10,10,11	0.49	0
2	9Y6	J	301	1	9,9,10	0.30	0	10,10,11	0.48	0
2	9Y6	E	301	1	9,9,10	0.29	0	10,10,11	0.48	0
2	9Y6	I	301	1	9,9,10	0.30	0	10,10,11	0.44	0
2	9Y6	L	301	1	9,9,10	0.28	0	10,10,11	0.51	0
2	9Y6	A	301	1	9,9,10	0.34	0	10,10,11	0.52	0
2	9Y6	F	301	1	9,9,10	0.34	0	10,10,11	0.49	0
2	9Y6	D	301	1	9,9,10	0.29	0	10,10,11	0.46	0
2	9Y6	H	301	1	9,9,10	0.30	0	10,10,11	0.41	0
2	9Y6	G	301	1	9,9,10	0.30	0	10,10,11	0.46	0
2	9Y6	C	301	1	9,9,10	0.35	0	10,10,11	0.47	0
3	GOL	I	302	-	5,5,5	0.91	0	5,5,5	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9Y6	K	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	B	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	J	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	E	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	I	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	L	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	A	301	1	-	0/3/3/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9Y6	F	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	D	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	H	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	G	301	1	-	0/3/3/4	0/1/1/1
2	9Y6	C	301	1	-	0/3/3/4	0/1/1/1
3	GOL	I	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

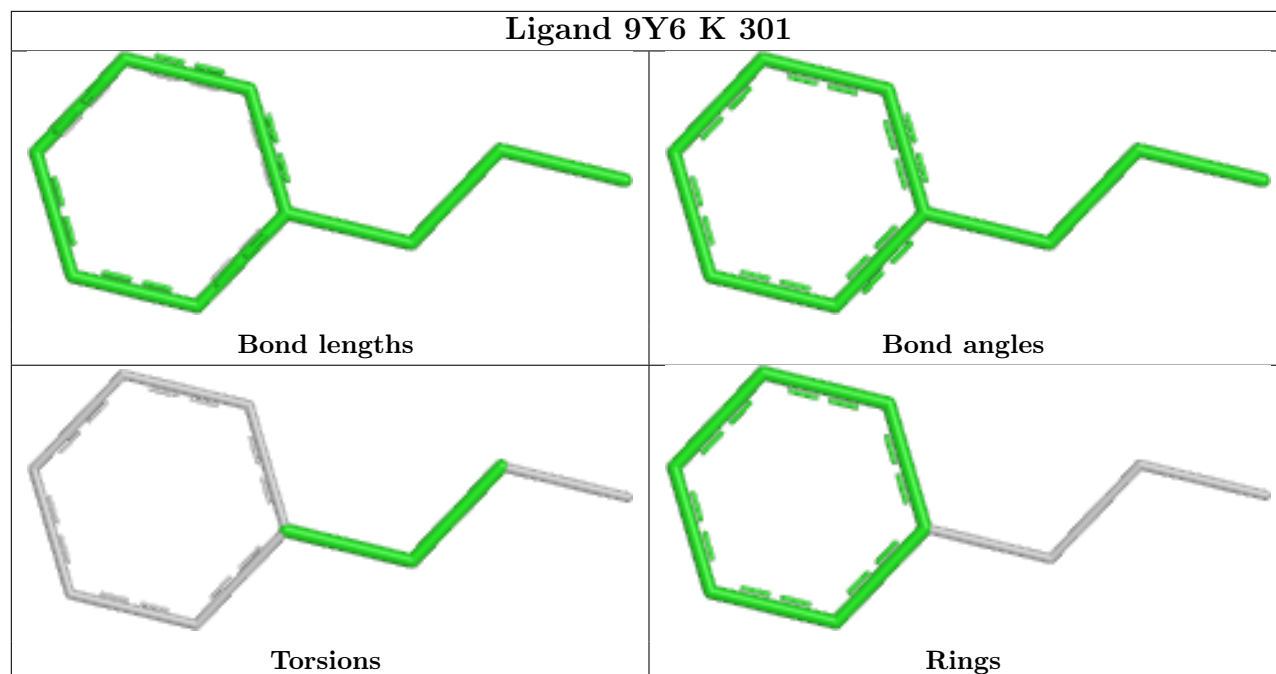
There are no torsion outliers.

There are no ring outliers.

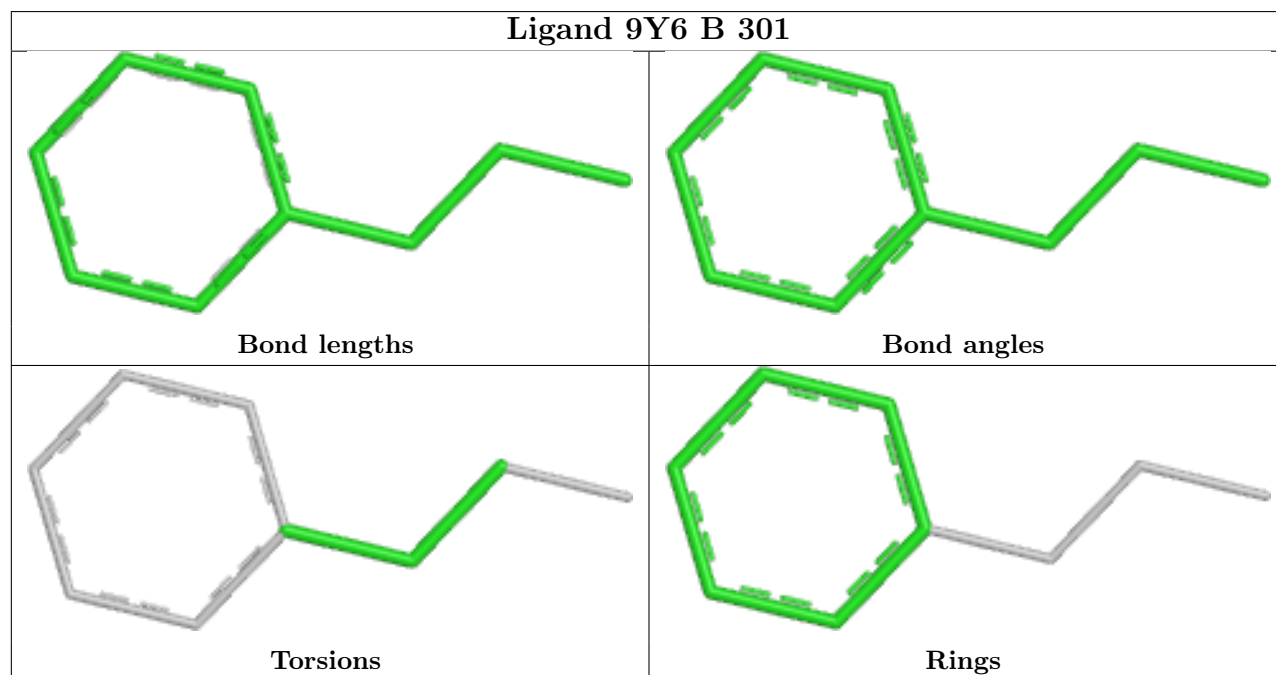
No monomer is involved in short contacts.

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.

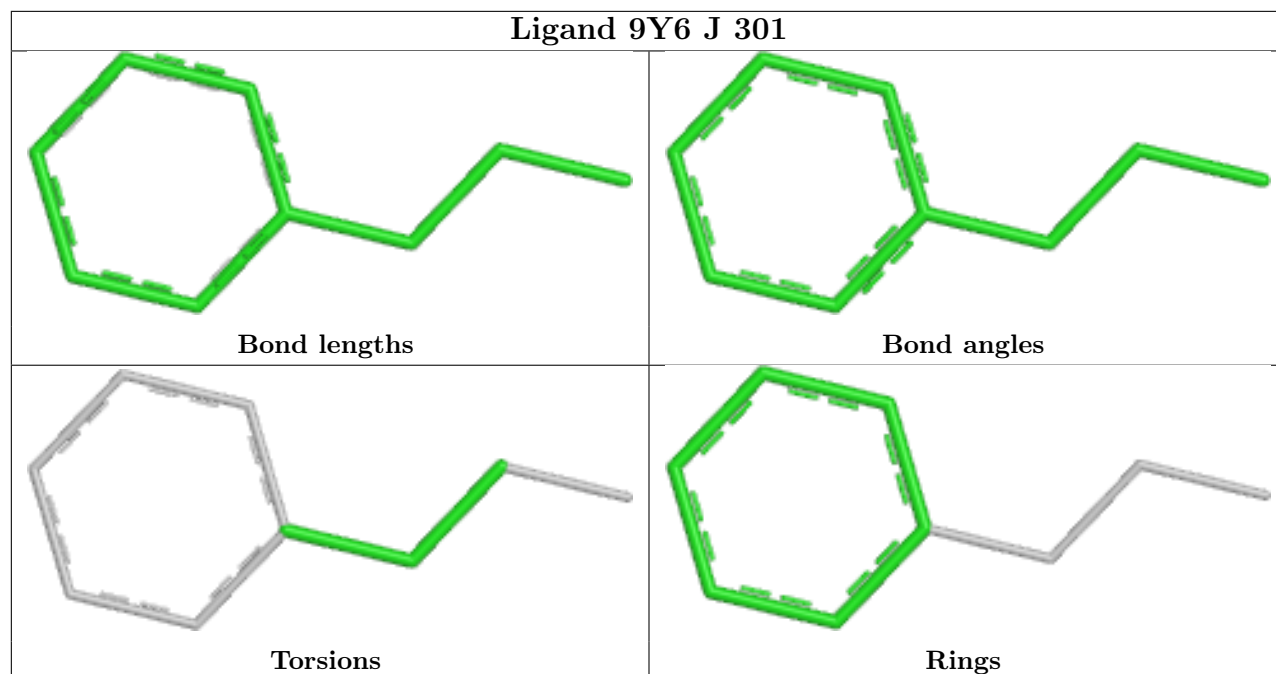
Ligand 9Y6 K 301



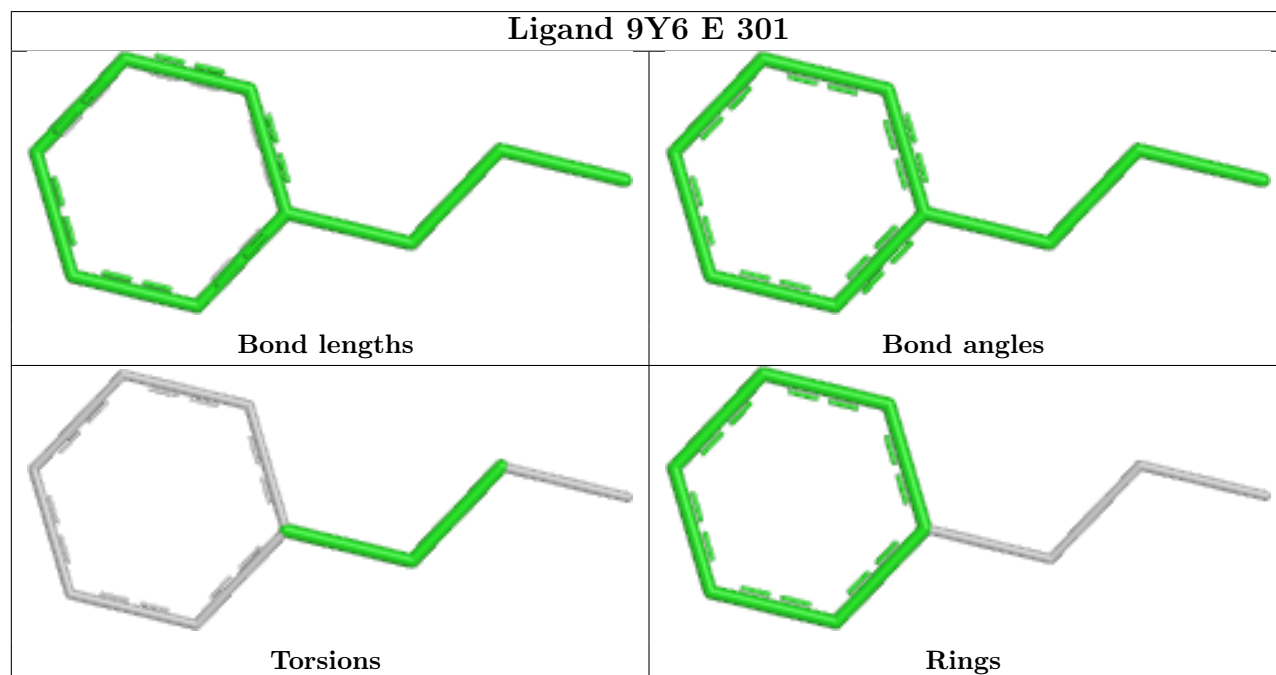
Ligand 9Y6 B 301



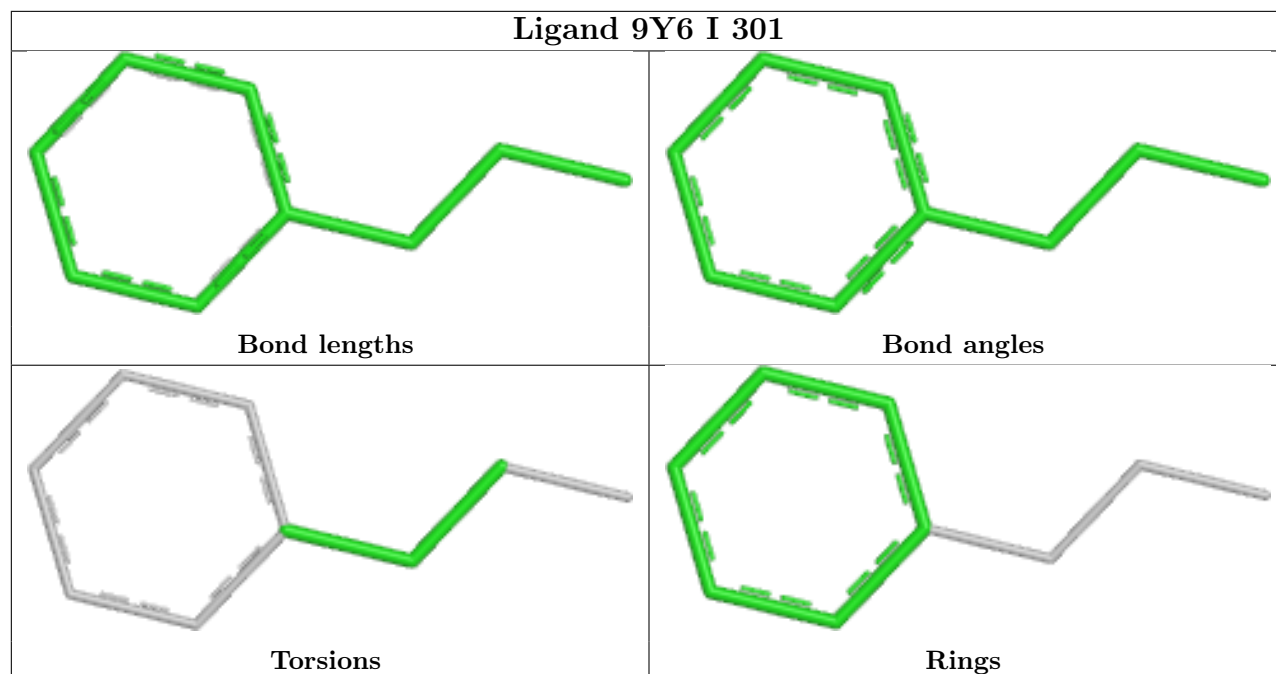
Ligand 9Y6 J 301



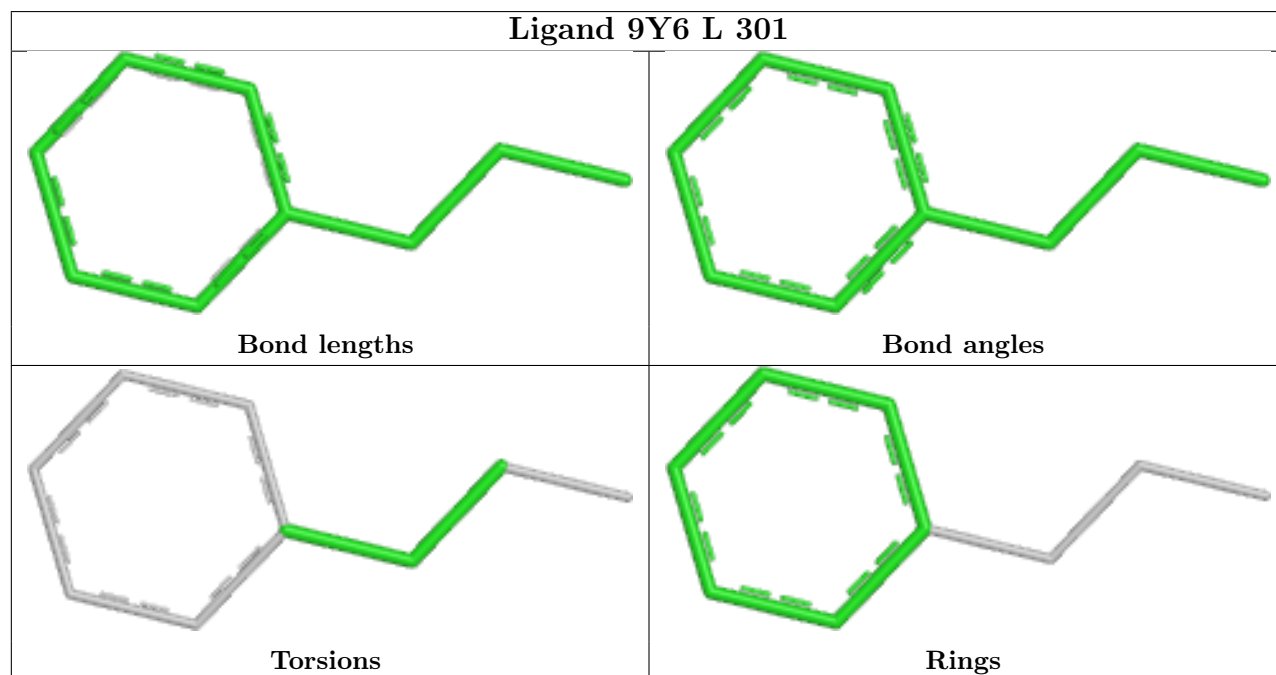
Ligand 9Y6 E 301



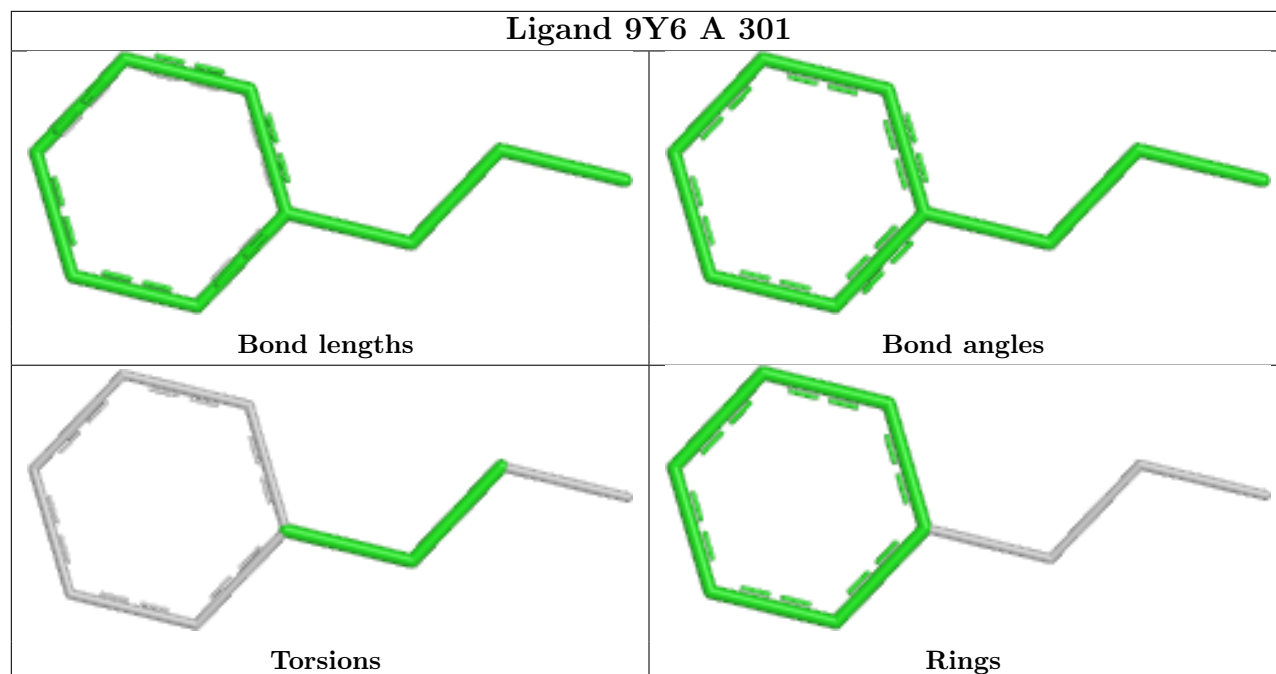
Ligand 9Y6 I 301



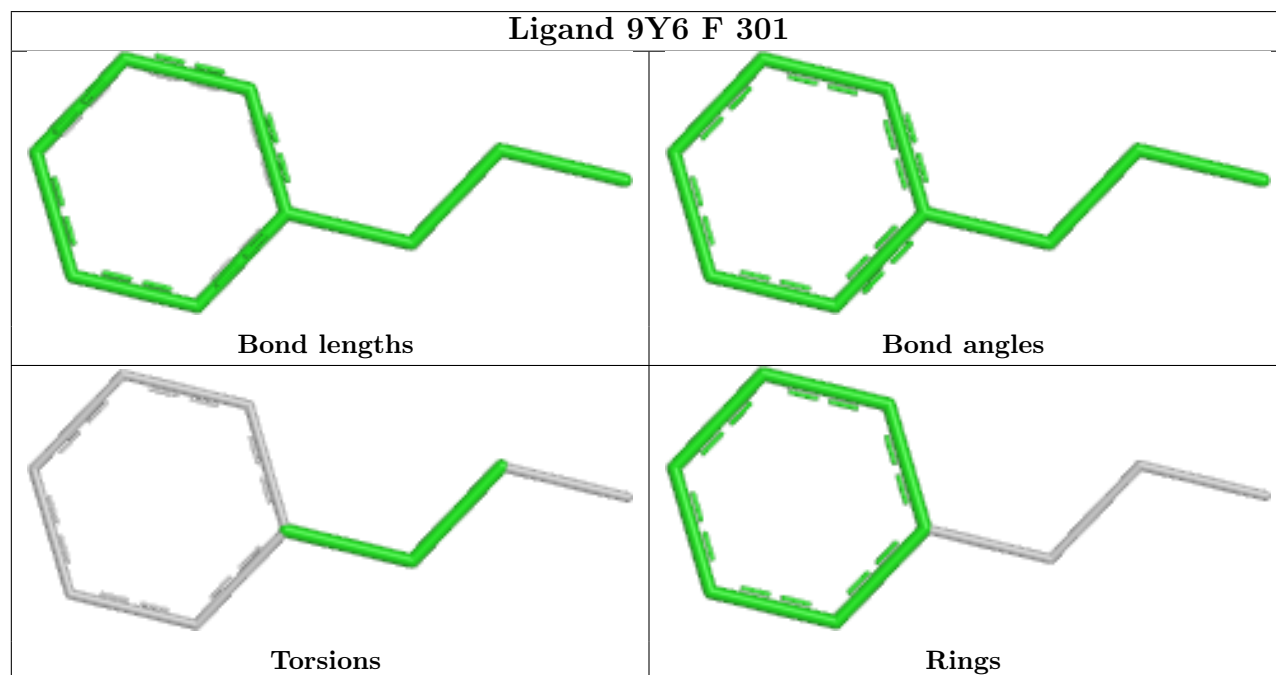
Ligand 9Y6 L 301



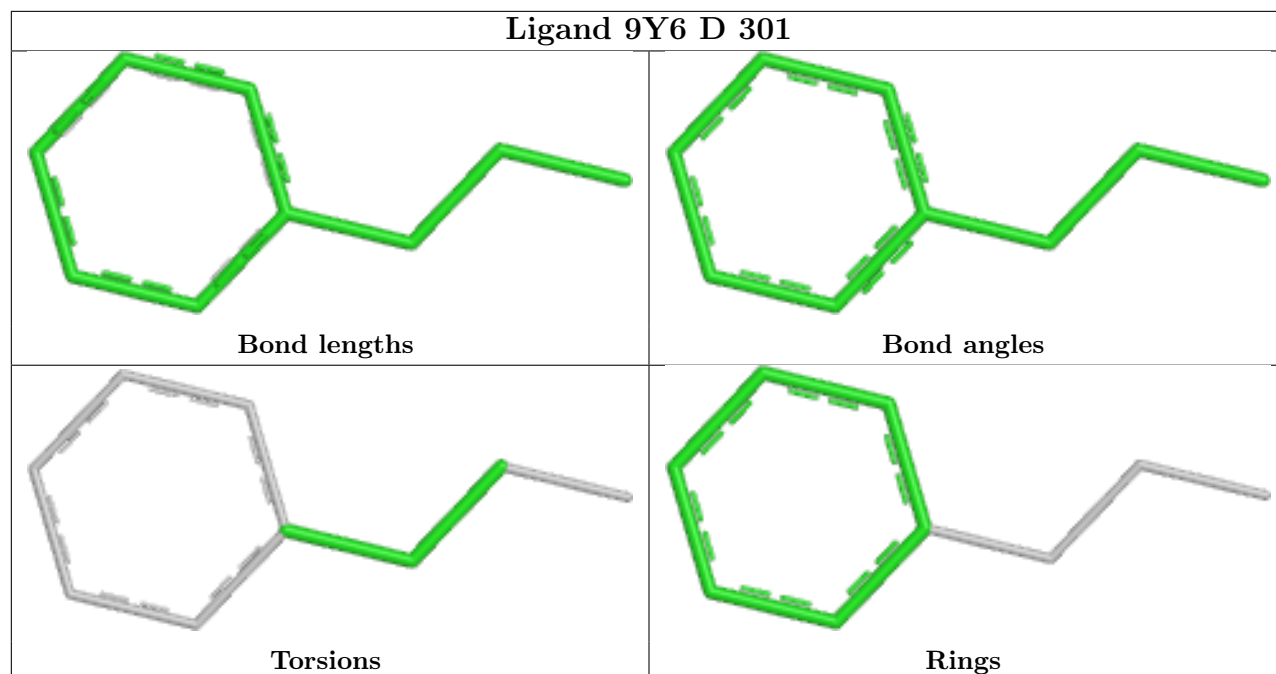
Ligand 9Y6 A 301



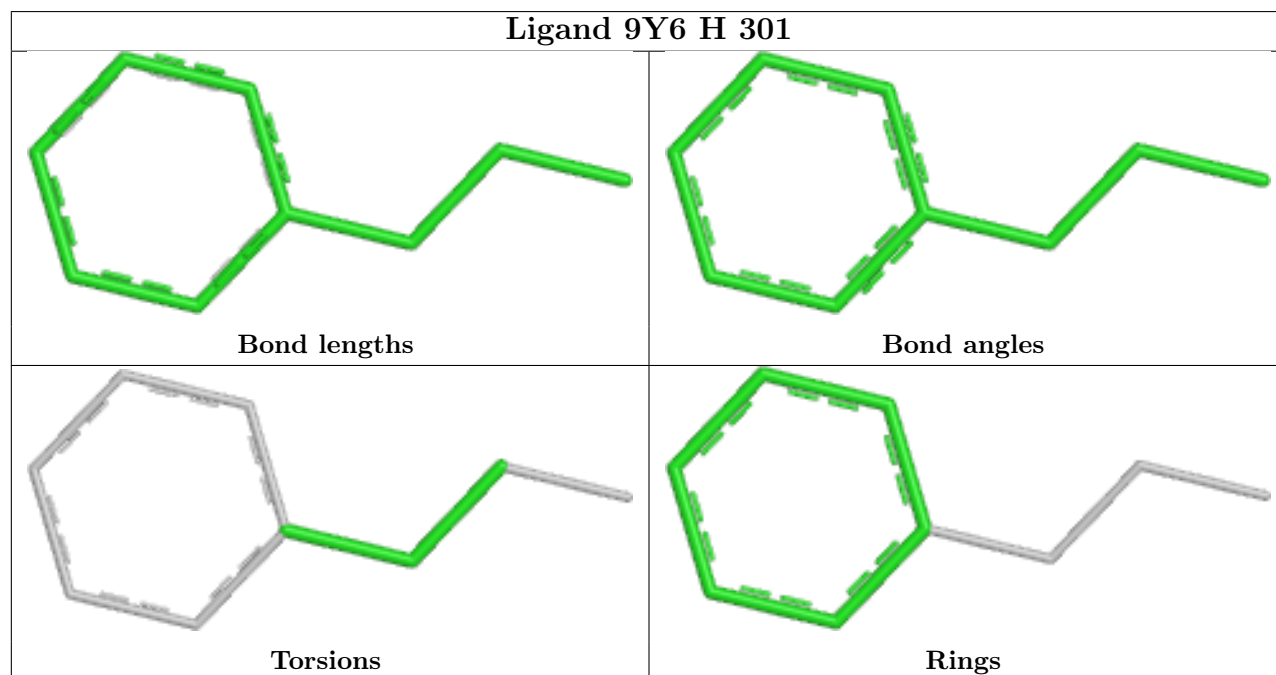
Ligand 9Y6 F 301

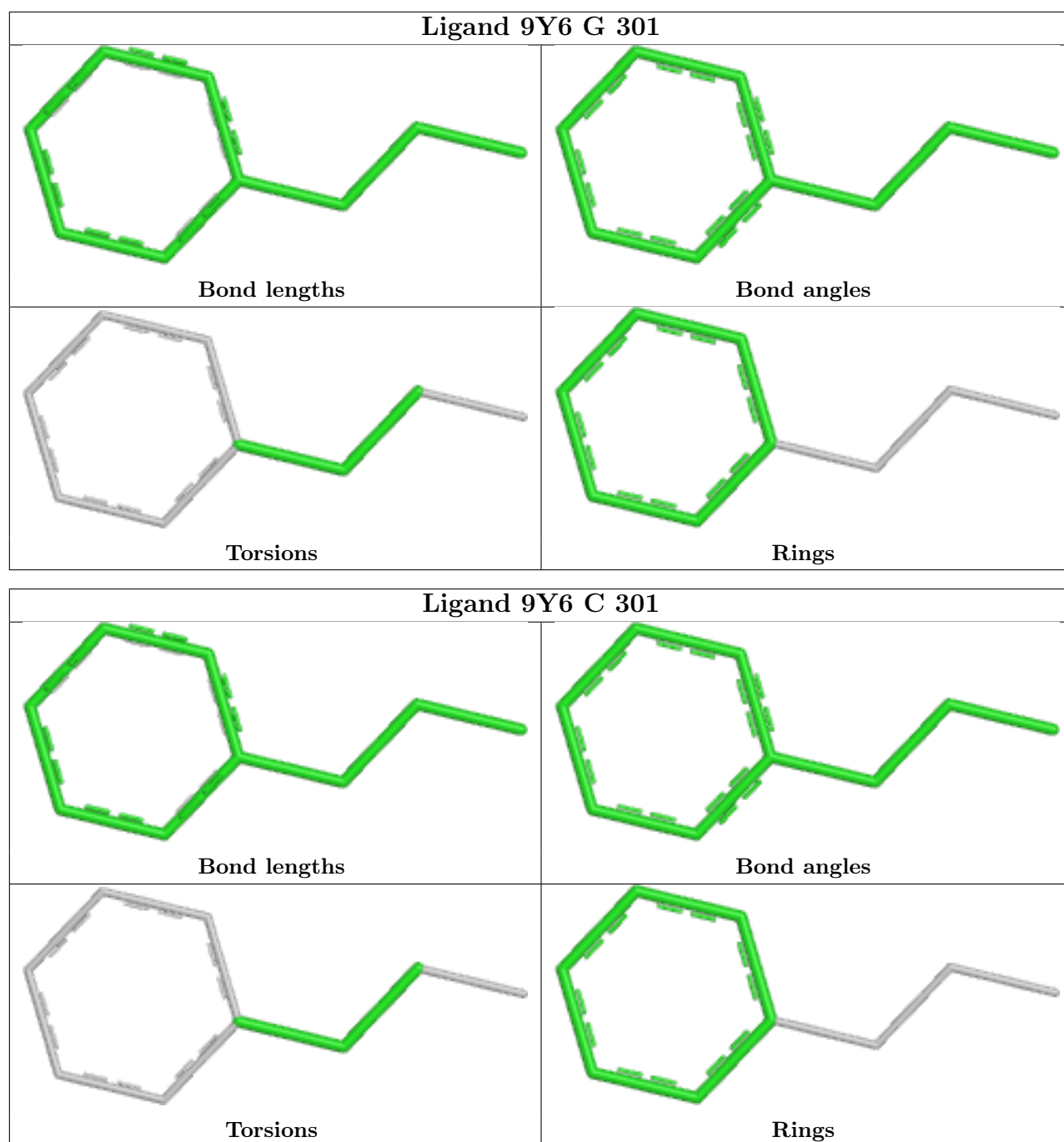


Ligand 9Y6 D 301



Ligand 9Y6 H 301





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	247/267 (92%)	0.80	27 (10%) 10 11	7, 17, 33, 45	0
1	B	247/267 (92%)	0.21	13 (5%) 32 34	7, 16, 30, 44	0
1	C	248/267 (92%)	0.33	22 (8%) 15 16	7, 14, 31, 47	0
1	D	247/267 (92%)	1.06	36 (14%) 6 6	10, 22, 36, 48	1 (0%)
1	E	248/267 (92%)	0.64	19 (7%) 19 21	7, 17, 32, 41	0
1	F	248/267 (92%)	0.18	12 (4%) 35 38	7, 14, 28, 42	1 (0%)
1	G	248/267 (92%)	0.89	32 (12%) 7 7	7, 18, 35, 49	0
1	H	246/267 (92%)	0.92	27 (10%) 10 11	10, 22, 36, 50	0
1	I	246/267 (92%)	0.42	22 (8%) 15 16	7, 19, 33, 46	0
1	J	246/267 (92%)	0.92	34 (13%) 6 6	9, 20, 34, 44	0
1	K	247/267 (92%)	0.80	25 (10%) 12 13	7, 18, 35, 49	0
1	L	246/267 (92%)	0.89	25 (10%) 12 12	9, 20, 34, 50	0
All	All	2964/3204 (92%)	0.67	294 (9%) 13 13	7, 18, 34, 50	2 (0%)

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	ASP	9.9
1	F	24	TYR	9.6
1	A	24	TYR	9.3
1	C	24	TYR	9.2
1	L	24	TYR	9.2
1	H	24	TYR	8.0
1	C	20	LEU	7.8
1	G	24	TYR	7.1
1	D	23	ASP	7.0
1	I	23	ASP	7.0
1	I	24	TYR	6.6

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Mol	Chain	Res	Type	RSRZ
1	G	22	GLY	6.5
1	B	2	THR	6.5
1	G	21	ASN	6.5
1	L	251	GLY	6.3
1	L	23	ASP	6.1
1	D	22	GLY	6.1
1	K	25	TYR	6.1
1	L	2	THR	6.1
1	H	23	ASP	6.1
1	B	24	TYR	6.0
1	G	20	LEU	6.0
1	D	249	GLY	5.9
1	E	24	TYR	5.9
1	C	249	GLY	5.8
1	C	22	GLY	5.7
1	K	21	ASN	5.7
1	K	20	LEU	5.7
1	J	249	GLY	5.6
1	J	24	TYR	5.5
1	F	22	GLY	5.5
1	D	4	LEU	5.4
1	C	64	GLY	5.3
1	E	251	GLY	5.2
1	F	20	LEU	5.2
1	L	26	ASP	4.8
1	C	21	ASN	4.8
1	K	25(A)	THR	4.8
1	B	23	ASP	4.7
1	I	3	ASP	4.7
1	D	238	SER	4.7
1	H	3	ASP	4.7
1	A	22	GLY	4.5
1	G	64	GLY	4.5
1	K	23	ASP	4.5
1	E	22	GLY	4.5
1	C	23	ASP	4.5
1	F	21	ASN	4.4
1	G	3	ASP	4.3
1	G	23	ASP	4.3
1	D	24	TYR	4.2
1	J	247	ALA	4.2
1	H	135	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	20	LEU	4.1
1	H	26	ASP	4.1
1	K	224	GLY	4.1
1	C	27	GLU	4.0
1	C	224	GLY	4.0
1	H	224	GLY	4.0
1	J	2	THR	4.0
1	L	25	THR	4.0
1	B	3	ASP	4.0
1	K	206	ALA	4.0
1	D	248	LEU	3.9
1	B	22	GLY	3.9
1	G	207	ARG	3.8
1	H	156	GLU	3.8
1	D	224	GLY	3.8
1	H	25	THR	3.8
1	I	27	GLU	3.8
1	H	67	GLU	3.7
1	I	207	ARG	3.7
1	A	4	LEU	3.6
1	J	224	GLY	3.6
1	E	27	GLU	3.6
1	H	27	GLU	3.6
1	D	146	LYS	3.6
1	C	250	HIS	3.6
1	H	207	ARG	3.6
1	K	64	GLY	3.6
1	A	250	HIS	3.6
1	K	207	ARG	3.6
1	C	3	ASP	3.5
1	G	19	THR	3.5
1	L	133	ASN	3.5
1	J	4	LEU	3.5
1	A	214	LYS	3.5
1	F	67	GLU	3.5
1	A	21	ASN	3.5
1	C	207	ARG	3.5
1	G	249	GLY	3.5
1	G	25	THR	3.4
1	B	224	GLY	3.3
1	I	238	SER	3.3
1	G	206	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	27	GLU	3.3
1	L	4	LEU	3.3
1	B	133	ASN	3.3
1	F	23	ASP	3.2
1	A	27	GLU	3.2
1	J	6	ALA	3.2
1	J	67	GLU	3.2
1	A	49	TYR	3.2
1	A	224	GLY	3.2
1	I	224	GLY	3.2
1	K	31	ALA	3.1
1	A	238	SER	3.1
1	L	27	GLU	3.1
1	E	4	LEU	3.1
1	E	156	GLU	3.1
1	G	27	GLU	3.1
1	J	23	ASP	3.1
1	F	224	GLY	3.1
1	F	3	ASP	3.1
1	L	3	ASP	3.1
1	L	29	VAL	3.1
1	G	146	LYS	3.1
1	B	67	GLU	3.1
1	B	248	LEU	3.0
1	H	4	LEU	3.0
1	A	207	ARG	3.0
1	K	27	GLU	3.0
1	G	243	SER	3.0
1	H	146	LYS	3.0
1	J	248	LEU	3.0
1	I	156	GLU	3.0
1	B	27	GLU	3.0
1	D	202	VAL	3.0
1	B	26	ASP	3.0
1	E	206	ALA	3.0
1	A	249	GLY	2.9
1	C	25	THR	2.9
1	H	251	GLY	2.9
1	L	250	HIS	2.9
1	K	19	THR	2.9
1	K	22	GLY	2.9
1	K	180	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	66	PRO	2.9
1	K	3	ASP	2.9
1	D	251	GLY	2.9
1	L	19	THR	2.8
1	J	196	LYS	2.8
1	J	226	ASP	2.8
1	D	196	LYS	2.8
1	G	67	GLU	2.8
1	G	237	ALA	2.8
1	H	19	THR	2.8
1	I	214	LYS	2.8
1	D	26	ASP	2.8
1	J	223	PHE	2.8
1	D	205	GLY	2.8
1	J	246	LYS	2.8
1	G	250	HIS	2.7
1	K	67	GLU	2.7
1	K	4	LEU	2.7
1	L	207	ARG	2.7
1	D	6	ALA	2.7
1	L	67	GLU	2.7
1	C	28	LYS	2.7
1	E	23	ASP	2.7
1	I	26	ASP	2.7
1	I	4	LEU	2.7
1	J	135	LEU	2.7
1	I	19	THR	2.6
1	E	250	HIS	2.6
1	E	224	GLY	2.6
1	D	225	ALA	2.6
1	J	3	ASP	2.6
1	I	25	THR	2.6
1	A	189	ILE	2.6
1	F	214	LYS	2.6
1	B	180	GLU	2.6
1	L	224	GLY	2.6
1	B	246	LYS	2.6
1	L	18	SER	2.6
1	I	146	LYS	2.5
1	J	5	LYS	2.5
1	H	250	HIS	2.5
1	A	25	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	26	ASP	2.5
1	I	248	LEU	2.5
1	J	245	LEU	2.5
1	A	64	GLY	2.5
1	D	206	ALA	2.5
1	E	6	ALA	2.5
1	G	35	GLN	2.5
1	G	26	ASP	2.5
1	A	206	ALA	2.5
1	H	206	ALA	2.5
1	J	206	ALA	2.5
1	G	202	VAL	2.5
1	I	9	LEU	2.4
1	D	19	THR	2.4
1	K	28	LYS	2.4
1	G	29	VAL	2.4
1	E	207	ARG	2.4
1	E	21	ASN	2.4
1	J	222	LEU	2.4
1	L	248	LEU	2.4
1	J	26	ASP	2.4
1	A	65	THR	2.4
1	J	217	ALA	2.4
1	J	225	ALA	2.4
1	I	67	GLU	2.4
1	J	40	VAL	2.4
1	G	222	LEU	2.4
1	H	214	LYS	2.4
1	J	214	LYS	2.4
1	C	19	THR	2.4
1	A	225	ALA	2.4
1	A	67	GLU	2.4
1	A	147	ASP	2.3
1	D	156	GLU	2.3
1	C	206	ALA	2.3
1	G	224	GLY	2.3
1	A	63	GLN	2.3
1	E	20	LEU	2.3
1	J	19	THR	2.3
1	D	247	ALA	2.3
1	E	147	ASP	2.3
1	J	208	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	31	ALA	2.3
1	G	31	ALA	2.3
1	G	242	ALA	2.3
1	I	249	GLY	2.3
1	J	205	GLY	2.3
1	C	67	GLU	2.3
1	F	250	HIS	2.3
1	I	250	HIS	2.3
1	G	60	LEU	2.3
1	L	39	PRO	2.2
1	L	206	ALA	2.2
1	C	7	SER	2.2
1	H	133	ASN	2.2
1	K	146	LYS	2.2
1	D	67	GLU	2.2
1	D	145	LEU	2.2
1	E	67	GLU	2.2
1	J	9	LEU	2.2
1	L	135	LEU	2.2
1	J	250	HIS	2.2
1	A	208	THR	2.2
1	H	247	ALA	2.2
1	G	55	ILE	2.2
1	C	238	SER	2.2
1	D	7	SER	2.2
1	D	9	LEU	2.2
1	G	244	LEU	2.2
1	H	223	PHE	2.1
1	H	227	TRP	2.1
1	C	65	THR	2.1
1	E	208	THR	2.1
1	K	134	VAL	2.1
1	E	7	SER	2.1
1	G	239	GLY	2.1
1	K	249	GLY	2.1
1	H	9	LEU	2.1
1	D	5	LYS	2.1
1	D	250	HIS	2.1
1	C	133	ASN	2.1
1	F	206	ALA	2.1
1	L	237	ALA	2.1
1	H	226	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	226	ASP	2.1
1	D	25	THR	2.1
1	D	207	ARG	2.1
1	H	194	VAL	2.1
1	K	66	PRO	2.1
1	K	237	ALA	2.1
1	J	189	ILE	2.1
1	G	61	LYS	2.1
1	K	65	THR	2.1
1	D	198	VAL	2.1
1	E	133	ASN	2.1
1	A	237	ALA	2.1
1	H	45	ALA	2.1
1	A	23	ASP	2.1
1	A	26	ASP	2.1
1	L	147	ASP	2.1
1	D	246	LYS	2.0
1	L	84	GLU	2.0
1	J	7	SER	2.0
1	J	203	THR	2.0
1	I	251	GLY	2.0
1	L	249	GLY	2.0
1	D	39	PRO	2.0
1	D	222	LEU	2.0
1	F	27	GLU	2.0
1	A	28	LYS	2.0
1	D	189	ILE	2.0
1	D	223	PHE	2.0
1	H	205	GLY	2.0
1	I	133	ASN	2.0
1	D	40	VAL	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

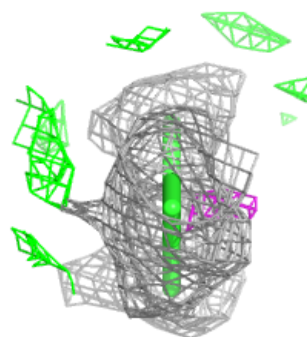
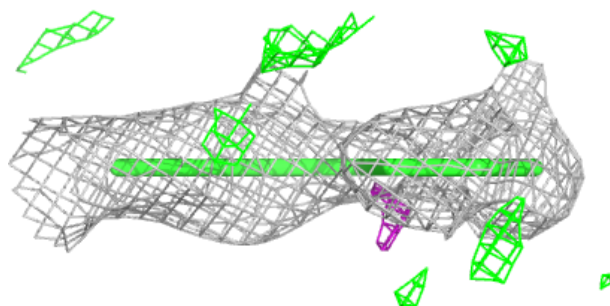
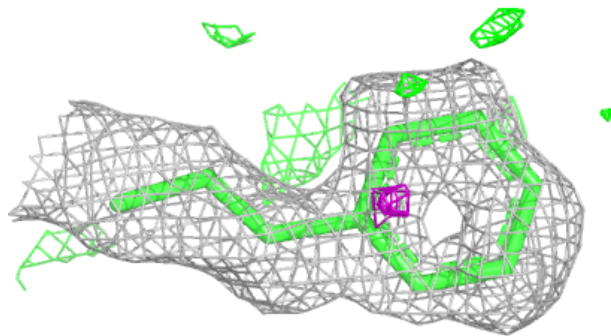
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	I	302	6/6	0.74	0.17	44,45,46,47	0
2	9Y6	K	301	9/10	0.81	0.16	18,22,23,23	0
2	9Y6	L	301	9/10	0.81	0.12	18,21,22,22	0
2	9Y6	J	301	9/10	0.81	0.15	22,22,24,25	0
2	9Y6	G	301	9/10	0.82	0.14	21,28,30,30	0
2	9Y6	H	301	9/10	0.82	0.14	21,22,23,24	0
2	9Y6	D	301	9/10	0.82	0.17	24,27,28,28	0
2	9Y6	A	301	9/10	0.83	0.18	14,24,27,27	0
2	9Y6	E	301	9/10	0.83	0.14	18,22,23,23	0
2	9Y6	B	301	9/10	0.86	0.12	16,17,17,17	0
2	9Y6	I	301	9/10	0.88	0.13	18,23,23,24	0
2	9Y6	C	301	9/10	0.91	0.09	13,19,20,20	0
2	9Y6	F	301	9/10	0.92	0.08	11,18,20,20	0

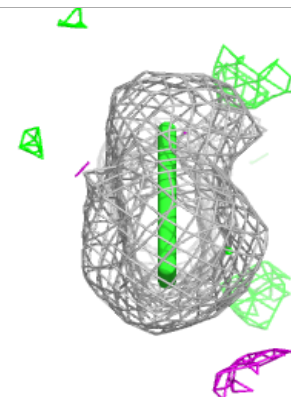
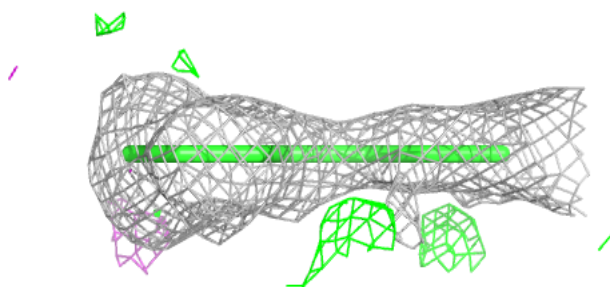
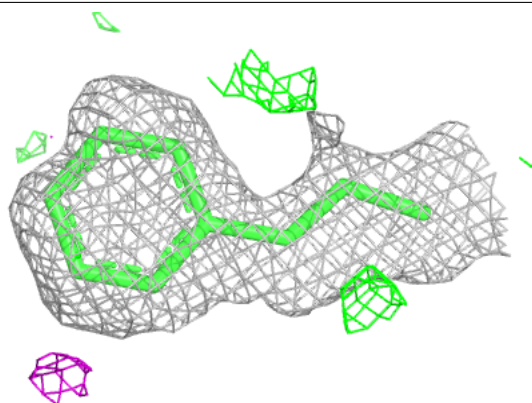
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9Y6 K 301:

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

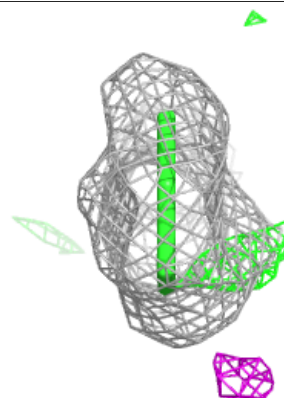
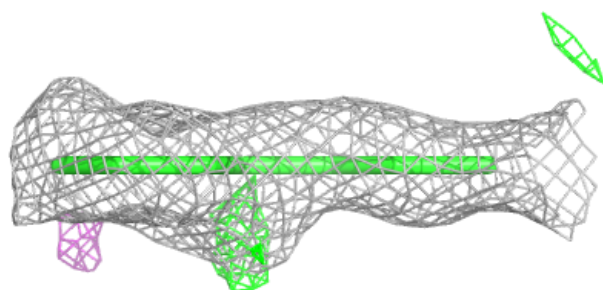
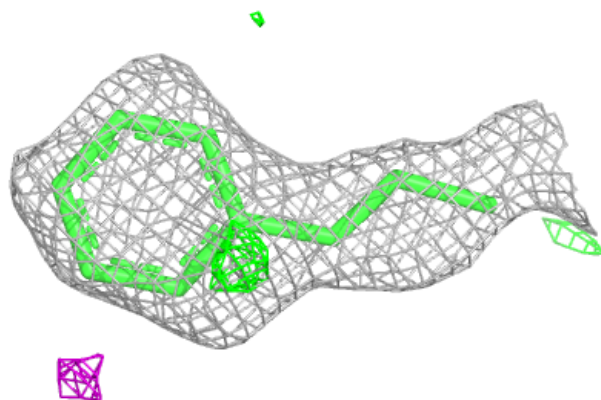
**Electron density around 9Y6 L 301:**

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

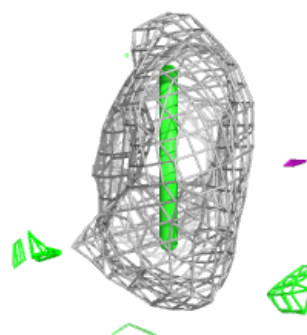
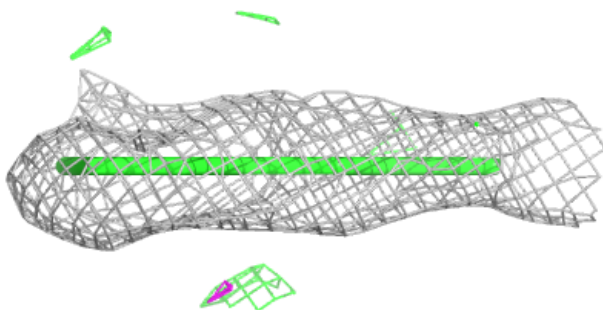
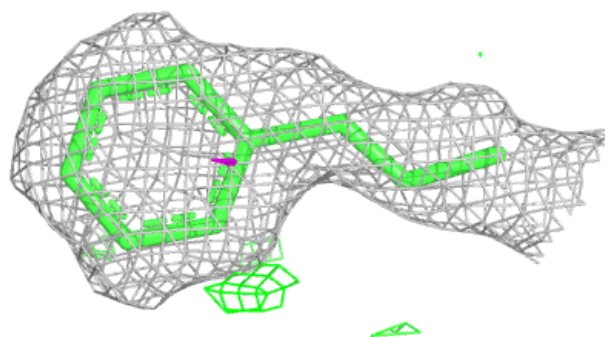


Electron density around 9Y6 J 301:

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

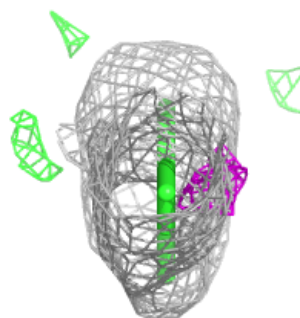
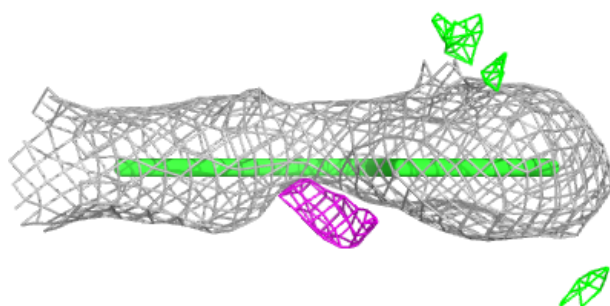
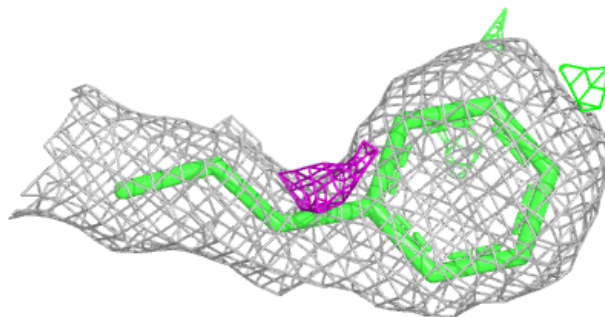
**Electron density around 9Y6 G 301:**

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

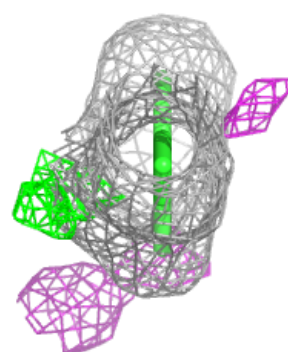
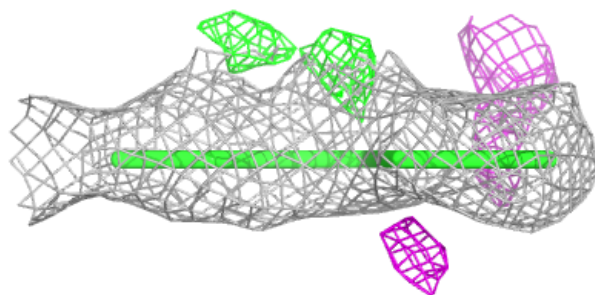
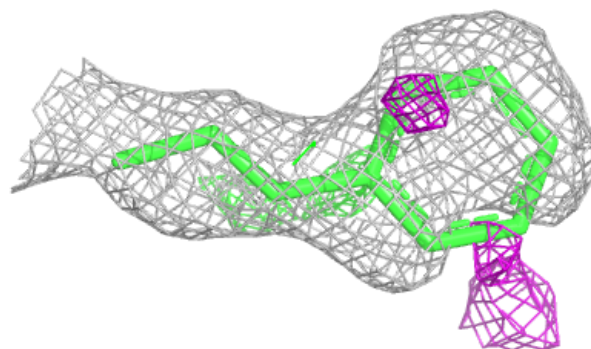


Electron density around 9Y6 H 301:

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

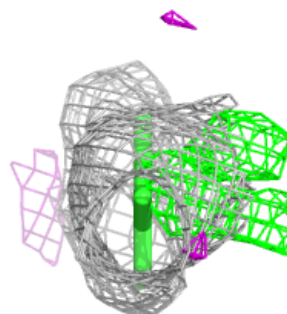
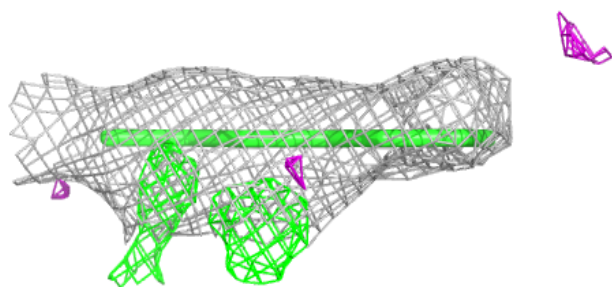
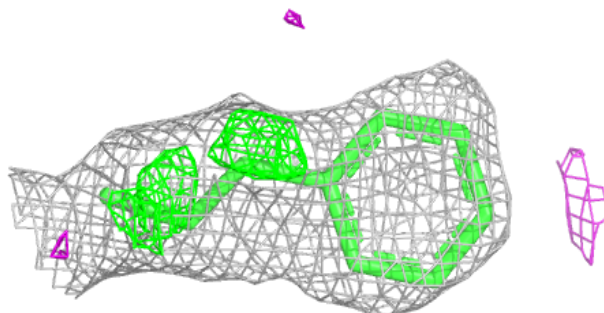
**Electron density around 9Y6 D 301:**

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

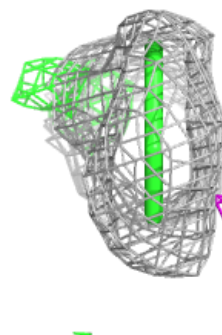
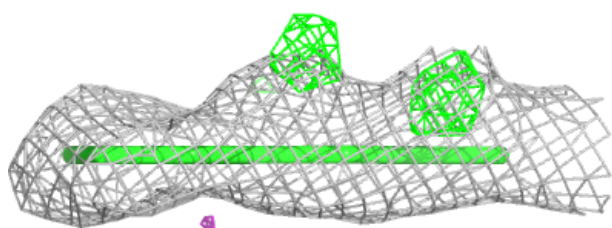
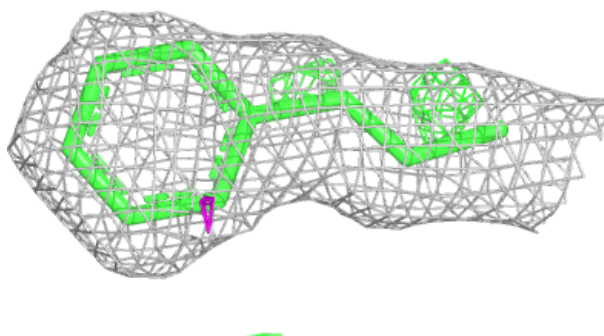


Electron density around 9Y6 A 301:

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

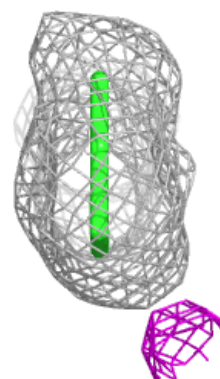
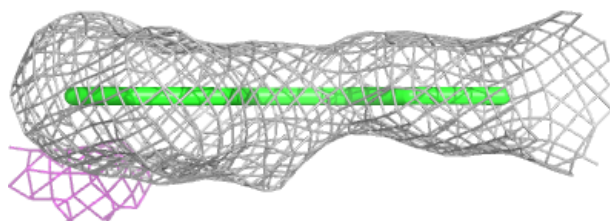
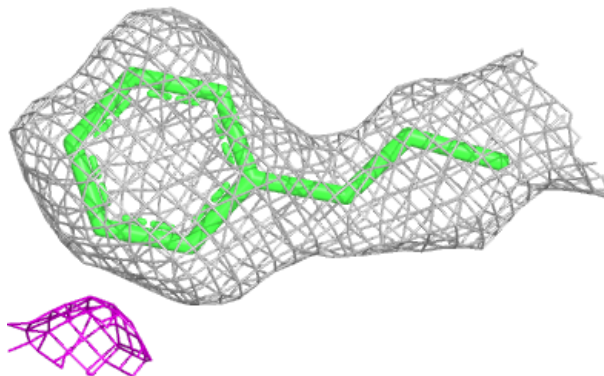
**Electron density around 9Y6 E 301:**

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

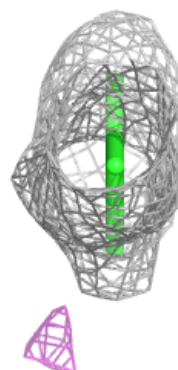
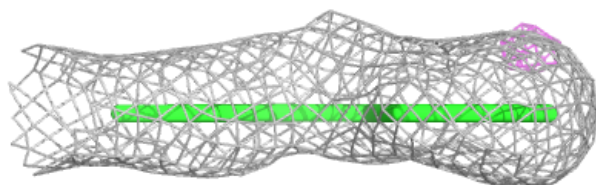
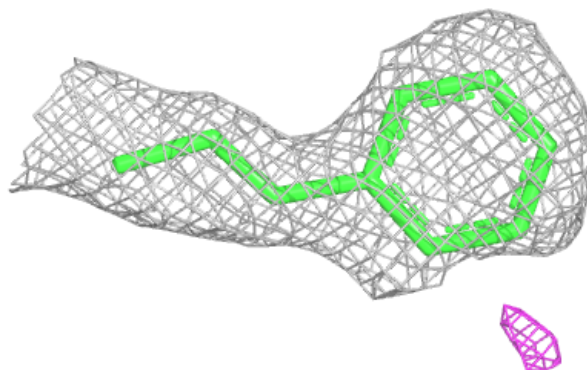


Electron density around 9Y6 B 301:

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

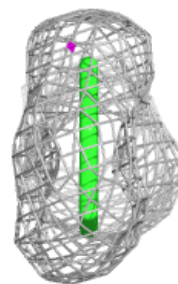
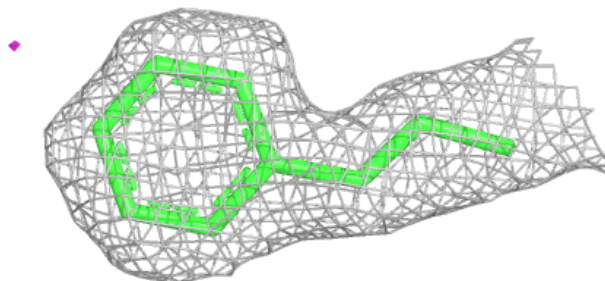
**Electron density around 9Y6 I 301:**

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

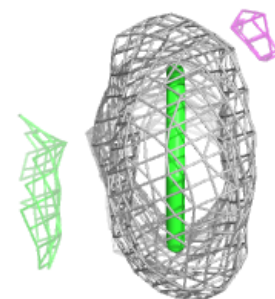
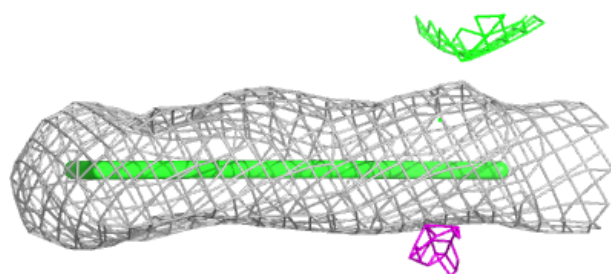
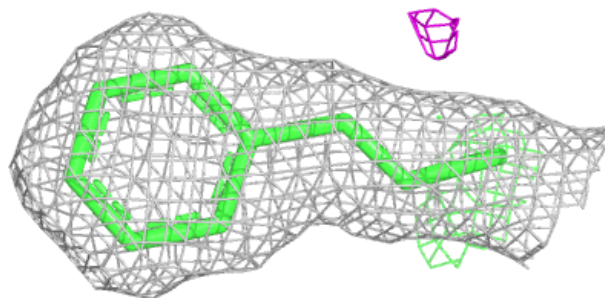


Electron density around 9Y6 C 301:

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

**Electron density around 9Y6 F 301:**

$2mF_o-DF_c$ (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.