



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 PM UTC

PDB ID : 7CJ9 / pdb_00007cj9
Title : Crystal structure of N-terminal His-tagged D-allulose 3-epimerase from *Methylobomonas* sp. with additional C-terminal residues
Authors : Yoshida, H.; Yoshihara, A.; Kamitori, S.
Deposited on : 2020-07-09
Resolution : 1.58 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

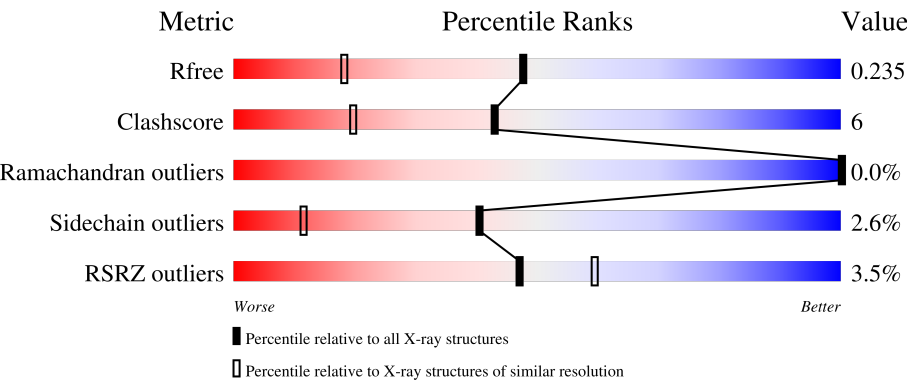
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	316	2% 83% 8% 9%
1	B	316	5% 83% 8% 8%
1	C	316	2% 78% 12% 9%
1	D	316	3% 80% 10% 9%
1	E	316	7% 77% 12% 9%

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Mol	Chain	Length	Quality of chain
1	F	316	83% 7% • 9%
1	G	316	5% 79% 11% 9%
1	H	316	% 81% 9% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20140 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 Epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	2	0
			2207	1399	382	418	8			
1	B	290	Total	C	N	O	S	0	1	0
			2230	1413	387	422	8			
1	C	288	Total	C	N	O	S	0	2	0
			2226	1411	387	420	8			
1	D	289	Total	C	N	O	S	0	1	0
			2224	1410	385	421	8			
1	E	288	Total	C	N	O	S	0	2	0
			2224	1409	387	420	8			
1	F	287	Total	C	N	O	S	0	0	0
			2204	1395	382	419	8			
1	G	286	Total	C	N	O	S	0	0	0
			2198	1392	381	417	8			
1	H	288	Total	C	N	O	S	0	1	0
			2217	1404	384	421	8			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A172U6X0
A	-19	GLY	-	expression tag	UNP A0A172U6X0
A	-18	SER	-	expression tag	UNP A0A172U6X0
A	-17	SER	-	expression tag	UNP A0A172U6X0
A	-16	HIS	-	expression tag	UNP A0A172U6X0
A	-15	HIS	-	expression tag	UNP A0A172U6X0
A	-14	HIS	-	expression tag	UNP A0A172U6X0
A	-13	HIS	-	expression tag	UNP A0A172U6X0
A	-12	HIS	-	expression tag	UNP A0A172U6X0
A	-11	HIS	-	expression tag	UNP A0A172U6X0
A	-10	SER	-	expression tag	UNP A0A172U6X0
A	-9	SER	-	expression tag	UNP A0A172U6X0
A	-8	GLY	-	expression tag	UNP A0A172U6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP A0A172U6X0
A	-6	VAL	-	expression tag	UNP A0A172U6X0
A	-5	PRO	-	expression tag	UNP A0A172U6X0
A	-4	ARG	-	expression tag	UNP A0A172U6X0
A	-3	GLY	-	expression tag	UNP A0A172U6X0
A	-2	SER	-	expression tag	UNP A0A172U6X0
A	-1	HIS	-	expression tag	UNP A0A172U6X0
A	0	SER	-	expression tag	UNP A0A172U6X0
A	9	ILE	TYR	engineered mutation	UNP A0A172U6X0
A	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
A	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
A	287	THR	-	expression tag	UNP A0A172U6X0
A	288	ALA	-	expression tag	UNP A0A172U6X0
A	289	ILE	-	expression tag	UNP A0A172U6X0
A	290	LYS	-	expression tag	UNP A0A172U6X0
A	291	THR	-	expression tag	UNP A0A172U6X0
A	292	ILE	-	expression tag	UNP A0A172U6X0
A	293	GLU	-	expression tag	UNP A0A172U6X0
A	294	LEU	-	expression tag	UNP A0A172U6X0
A	295	HIS	-	expression tag	UNP A0A172U6X0
B	-20	MET	-	initiating methionine	UNP A0A172U6X0
B	-19	GLY	-	expression tag	UNP A0A172U6X0
B	-18	SER	-	expression tag	UNP A0A172U6X0
B	-17	SER	-	expression tag	UNP A0A172U6X0
B	-16	HIS	-	expression tag	UNP A0A172U6X0
B	-15	HIS	-	expression tag	UNP A0A172U6X0
B	-14	HIS	-	expression tag	UNP A0A172U6X0
B	-13	HIS	-	expression tag	UNP A0A172U6X0
B	-12	HIS	-	expression tag	UNP A0A172U6X0
B	-11	HIS	-	expression tag	UNP A0A172U6X0
B	-10	SER	-	expression tag	UNP A0A172U6X0
B	-9	SER	-	expression tag	UNP A0A172U6X0
B	-8	GLY	-	expression tag	UNP A0A172U6X0
B	-7	LEU	-	expression tag	UNP A0A172U6X0
B	-6	VAL	-	expression tag	UNP A0A172U6X0
B	-5	PRO	-	expression tag	UNP A0A172U6X0
B	-4	ARG	-	expression tag	UNP A0A172U6X0
B	-3	GLY	-	expression tag	UNP A0A172U6X0
B	-2	SER	-	expression tag	UNP A0A172U6X0
B	-1	HIS	-	expression tag	UNP A0A172U6X0
B	0	SER	-	expression tag	UNP A0A172U6X0
B	9	ILE	TYR	engineered mutation	UNP A0A172U6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
B	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
B	287	THR	-	expression tag	UNP A0A172U6X0
B	288	ALA	-	expression tag	UNP A0A172U6X0
B	289	ILE	-	expression tag	UNP A0A172U6X0
B	290	LYS	-	expression tag	UNP A0A172U6X0
B	291	THR	-	expression tag	UNP A0A172U6X0
B	292	ILE	-	expression tag	UNP A0A172U6X0
B	293	GLU	-	expression tag	UNP A0A172U6X0
B	294	LEU	-	expression tag	UNP A0A172U6X0
B	295	HIS	-	expression tag	UNP A0A172U6X0
C	-20	MET	-	initiating methionine	UNP A0A172U6X0
C	-19	GLY	-	expression tag	UNP A0A172U6X0
C	-18	SER	-	expression tag	UNP A0A172U6X0
C	-17	SER	-	expression tag	UNP A0A172U6X0
C	-16	HIS	-	expression tag	UNP A0A172U6X0
C	-15	HIS	-	expression tag	UNP A0A172U6X0
C	-14	HIS	-	expression tag	UNP A0A172U6X0
C	-13	HIS	-	expression tag	UNP A0A172U6X0
C	-12	HIS	-	expression tag	UNP A0A172U6X0
C	-11	HIS	-	expression tag	UNP A0A172U6X0
C	-10	SER	-	expression tag	UNP A0A172U6X0
C	-9	SER	-	expression tag	UNP A0A172U6X0
C	-8	GLY	-	expression tag	UNP A0A172U6X0
C	-7	LEU	-	expression tag	UNP A0A172U6X0
C	-6	VAL	-	expression tag	UNP A0A172U6X0
C	-5	PRO	-	expression tag	UNP A0A172U6X0
C	-4	ARG	-	expression tag	UNP A0A172U6X0
C	-3	GLY	-	expression tag	UNP A0A172U6X0
C	-2	SER	-	expression tag	UNP A0A172U6X0
C	-1	HIS	-	expression tag	UNP A0A172U6X0
C	0	SER	-	expression tag	UNP A0A172U6X0
C	9	ILE	TYR	engineered mutation	UNP A0A172U6X0
C	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
C	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
C	287	THR	-	expression tag	UNP A0A172U6X0
C	288	ALA	-	expression tag	UNP A0A172U6X0
C	289	ILE	-	expression tag	UNP A0A172U6X0
C	290	LYS	-	expression tag	UNP A0A172U6X0
C	291	THR	-	expression tag	UNP A0A172U6X0
C	292	ILE	-	expression tag	UNP A0A172U6X0
C	293	GLU	-	expression tag	UNP A0A172U6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	294	LEU	-	expression tag	UNP A0A172U6X0
C	295	HIS	-	expression tag	UNP A0A172U6X0
D	-20	MET	-	initiating methionine	UNP A0A172U6X0
D	-19	GLY	-	expression tag	UNP A0A172U6X0
D	-18	SER	-	expression tag	UNP A0A172U6X0
D	-17	SER	-	expression tag	UNP A0A172U6X0
D	-16	HIS	-	expression tag	UNP A0A172U6X0
D	-15	HIS	-	expression tag	UNP A0A172U6X0
D	-14	HIS	-	expression tag	UNP A0A172U6X0
D	-13	HIS	-	expression tag	UNP A0A172U6X0
D	-12	HIS	-	expression tag	UNP A0A172U6X0
D	-11	HIS	-	expression tag	UNP A0A172U6X0
D	-10	SER	-	expression tag	UNP A0A172U6X0
D	-9	SER	-	expression tag	UNP A0A172U6X0
D	-8	GLY	-	expression tag	UNP A0A172U6X0
D	-7	LEU	-	expression tag	UNP A0A172U6X0
D	-6	VAL	-	expression tag	UNP A0A172U6X0
D	-5	PRO	-	expression tag	UNP A0A172U6X0
D	-4	ARG	-	expression tag	UNP A0A172U6X0
D	-3	GLY	-	expression tag	UNP A0A172U6X0
D	-2	SER	-	expression tag	UNP A0A172U6X0
D	-1	HIS	-	expression tag	UNP A0A172U6X0
D	0	SER	-	expression tag	UNP A0A172U6X0
D	9	ILE	TYR	engineered mutation	UNP A0A172U6X0
D	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
D	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
D	287	THR	-	expression tag	UNP A0A172U6X0
D	288	ALA	-	expression tag	UNP A0A172U6X0
D	289	ILE	-	expression tag	UNP A0A172U6X0
D	290	LYS	-	expression tag	UNP A0A172U6X0
D	291	THR	-	expression tag	UNP A0A172U6X0
D	292	ILE	-	expression tag	UNP A0A172U6X0
D	293	GLU	-	expression tag	UNP A0A172U6X0
D	294	LEU	-	expression tag	UNP A0A172U6X0
D	295	HIS	-	expression tag	UNP A0A172U6X0
E	-20	MET	-	initiating methionine	UNP A0A172U6X0
E	-19	GLY	-	expression tag	UNP A0A172U6X0
E	-18	SER	-	expression tag	UNP A0A172U6X0
E	-17	SER	-	expression tag	UNP A0A172U6X0
E	-16	HIS	-	expression tag	UNP A0A172U6X0
E	-15	HIS	-	expression tag	UNP A0A172U6X0
E	-14	HIS	-	expression tag	UNP A0A172U6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	HIS	-	expression tag	UNP A0A172U6X0
E	-12	HIS	-	expression tag	UNP A0A172U6X0
E	-11	HIS	-	expression tag	UNP A0A172U6X0
E	-10	SER	-	expression tag	UNP A0A172U6X0
E	-9	SER	-	expression tag	UNP A0A172U6X0
E	-8	GLY	-	expression tag	UNP A0A172U6X0
E	-7	LEU	-	expression tag	UNP A0A172U6X0
E	-6	VAL	-	expression tag	UNP A0A172U6X0
E	-5	PRO	-	expression tag	UNP A0A172U6X0
E	-4	ARG	-	expression tag	UNP A0A172U6X0
E	-3	GLY	-	expression tag	UNP A0A172U6X0
E	-2	SER	-	expression tag	UNP A0A172U6X0
E	-1	HIS	-	expression tag	UNP A0A172U6X0
E	0	SER	-	expression tag	UNP A0A172U6X0
E	9	ILE	TYR	engineered mutation	UNP A0A172U6X0
E	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
E	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
E	287	THR	-	expression tag	UNP A0A172U6X0
E	288	ALA	-	expression tag	UNP A0A172U6X0
E	289	ILE	-	expression tag	UNP A0A172U6X0
E	290	LYS	-	expression tag	UNP A0A172U6X0
E	291	THR	-	expression tag	UNP A0A172U6X0
E	292	ILE	-	expression tag	UNP A0A172U6X0
E	293	GLU	-	expression tag	UNP A0A172U6X0
E	294	LEU	-	expression tag	UNP A0A172U6X0
E	295	HIS	-	expression tag	UNP A0A172U6X0
F	-20	MET	-	initiating methionine	UNP A0A172U6X0
F	-19	GLY	-	expression tag	UNP A0A172U6X0
F	-18	SER	-	expression tag	UNP A0A172U6X0
F	-17	SER	-	expression tag	UNP A0A172U6X0
F	-16	HIS	-	expression tag	UNP A0A172U6X0
F	-15	HIS	-	expression tag	UNP A0A172U6X0
F	-14	HIS	-	expression tag	UNP A0A172U6X0
F	-13	HIS	-	expression tag	UNP A0A172U6X0
F	-12	HIS	-	expression tag	UNP A0A172U6X0
F	-11	HIS	-	expression tag	UNP A0A172U6X0
F	-10	SER	-	expression tag	UNP A0A172U6X0
F	-9	SER	-	expression tag	UNP A0A172U6X0
F	-8	GLY	-	expression tag	UNP A0A172U6X0
F	-7	LEU	-	expression tag	UNP A0A172U6X0
F	-6	VAL	-	expression tag	UNP A0A172U6X0
F	-5	PRO	-	expression tag	UNP A0A172U6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ARG	-	expression tag	UNP A0A172U6X0
F	-3	GLY	-	expression tag	UNP A0A172U6X0
F	-2	SER	-	expression tag	UNP A0A172U6X0
F	-1	HIS	-	expression tag	UNP A0A172U6X0
F	0	SER	-	expression tag	UNP A0A172U6X0
F	9	ILE	TYR	engineered mutation	UNP A0A172U6X0
F	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
F	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
F	287	THR	-	expression tag	UNP A0A172U6X0
F	288	ALA	-	expression tag	UNP A0A172U6X0
F	289	ILE	-	expression tag	UNP A0A172U6X0
F	290	LYS	-	expression tag	UNP A0A172U6X0
F	291	THR	-	expression tag	UNP A0A172U6X0
F	292	ILE	-	expression tag	UNP A0A172U6X0
F	293	GLU	-	expression tag	UNP A0A172U6X0
F	294	LEU	-	expression tag	UNP A0A172U6X0
F	295	HIS	-	expression tag	UNP A0A172U6X0
G	-20	MET	-	initiating methionine	UNP A0A172U6X0
G	-19	GLY	-	expression tag	UNP A0A172U6X0
G	-18	SER	-	expression tag	UNP A0A172U6X0
G	-17	SER	-	expression tag	UNP A0A172U6X0
G	-16	HIS	-	expression tag	UNP A0A172U6X0
G	-15	HIS	-	expression tag	UNP A0A172U6X0
G	-14	HIS	-	expression tag	UNP A0A172U6X0
G	-13	HIS	-	expression tag	UNP A0A172U6X0
G	-12	HIS	-	expression tag	UNP A0A172U6X0
G	-11	HIS	-	expression tag	UNP A0A172U6X0
G	-10	SER	-	expression tag	UNP A0A172U6X0
G	-9	SER	-	expression tag	UNP A0A172U6X0
G	-8	GLY	-	expression tag	UNP A0A172U6X0
G	-7	LEU	-	expression tag	UNP A0A172U6X0
G	-6	VAL	-	expression tag	UNP A0A172U6X0
G	-5	PRO	-	expression tag	UNP A0A172U6X0
G	-4	ARG	-	expression tag	UNP A0A172U6X0
G	-3	GLY	-	expression tag	UNP A0A172U6X0
G	-2	SER	-	expression tag	UNP A0A172U6X0
G	-1	HIS	-	expression tag	UNP A0A172U6X0
G	0	SER	-	expression tag	UNP A0A172U6X0
G	9	ILE	TYR	engineered mutation	UNP A0A172U6X0
G	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
G	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
G	287	THR	-	expression tag	UNP A0A172U6X0

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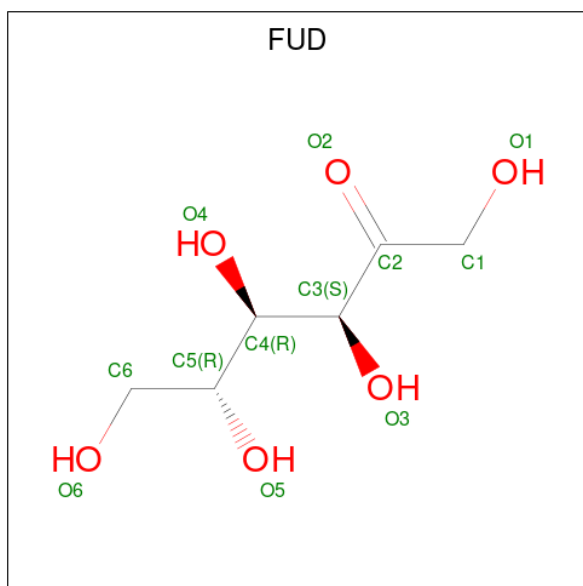
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Chain	Residue	Modelled	Actual	Comment	Reference
G	288	ALA	-	expression tag	UNP A0A172U6X0
G	289	ILE	-	expression tag	UNP A0A172U6X0
G	290	LYS	-	expression tag	UNP A0A172U6X0
G	291	THR	-	expression tag	UNP A0A172U6X0
G	292	ILE	-	expression tag	UNP A0A172U6X0
G	293	GLU	-	expression tag	UNP A0A172U6X0
G	294	LEU	-	expression tag	UNP A0A172U6X0
G	295	HIS	-	expression tag	UNP A0A172U6X0
H	-20	MET	-	initiating methionine	UNP A0A172U6X0
H	-19	GLY	-	expression tag	UNP A0A172U6X0
H	-18	SER	-	expression tag	UNP A0A172U6X0
H	-17	SER	-	expression tag	UNP A0A172U6X0
H	-16	HIS	-	expression tag	UNP A0A172U6X0
H	-15	HIS	-	expression tag	UNP A0A172U6X0
H	-14	HIS	-	expression tag	UNP A0A172U6X0
H	-13	HIS	-	expression tag	UNP A0A172U6X0
H	-12	HIS	-	expression tag	UNP A0A172U6X0
H	-11	HIS	-	expression tag	UNP A0A172U6X0
H	-10	SER	-	expression tag	UNP A0A172U6X0
H	-9	SER	-	expression tag	UNP A0A172U6X0
H	-8	GLY	-	expression tag	UNP A0A172U6X0
H	-7	LEU	-	expression tag	UNP A0A172U6X0
H	-6	VAL	-	expression tag	UNP A0A172U6X0
H	-5	PRO	-	expression tag	UNP A0A172U6X0
H	-4	ARG	-	expression tag	UNP A0A172U6X0
H	-3	GLY	-	expression tag	UNP A0A172U6X0
H	-2	SER	-	expression tag	UNP A0A172U6X0
H	-1	HIS	-	expression tag	UNP A0A172U6X0
H	0	SER	-	expression tag	UNP A0A172U6X0
H	9	ILE	TYR	engineered mutation	UNP A0A172U6X0
H	37	PHE	TYR	engineered mutation	UNP A0A172U6X0
H	286	LEU	TYR	engineered mutation	UNP A0A172U6X0
H	287	THR	-	expression tag	UNP A0A172U6X0
H	288	ALA	-	expression tag	UNP A0A172U6X0
H	289	ILE	-	expression tag	UNP A0A172U6X0
H	290	LYS	-	expression tag	UNP A0A172U6X0
H	291	THR	-	expression tag	UNP A0A172U6X0
H	292	ILE	-	expression tag	UNP A0A172U6X0
H	293	GLU	-	expression tag	UNP A0A172U6X0
H	294	LEU	-	expression tag	UNP A0A172U6X0
H	295	HIS	-	expression tag	UNP A0A172U6X0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0

- Molecule 3 is D-fructose (CCD ID: FUD) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



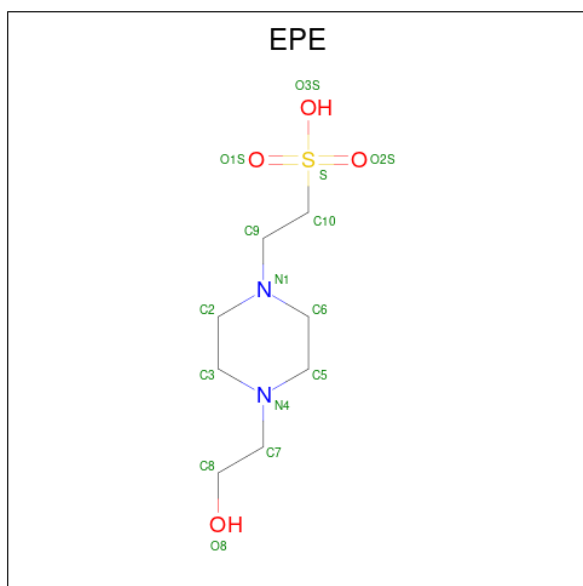
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		
3	G	1	Total	C	O	0	0
			12	6	6		
3	H	1	Total	C	O	0	0
			12	6	6		

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



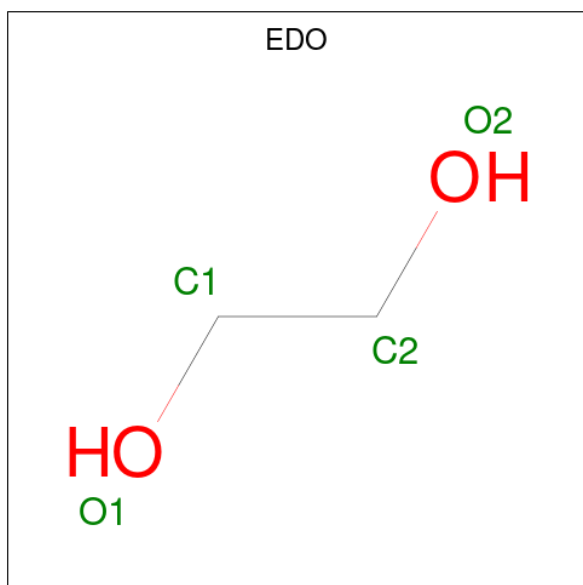
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

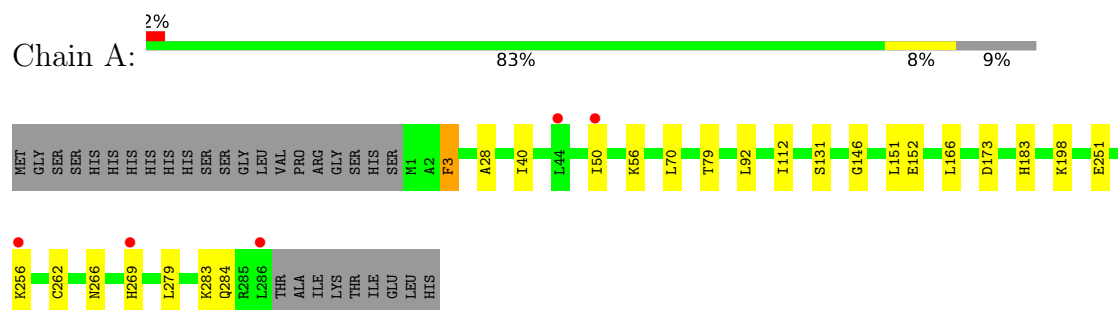
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	281	Total 281	O 281	0	0
6	B	286	Total 286	O 286	0	0
6	C	279	Total 279	O 279	0	0
6	D	277	Total 277	O 277	0	0
6	E	255	Total 255	O 255	0	0
6	F	281	Total 281	O 281	0	0
6	G	227	Total 227	O 227	0	0
6	H	272	Total 272	O 272	0	0

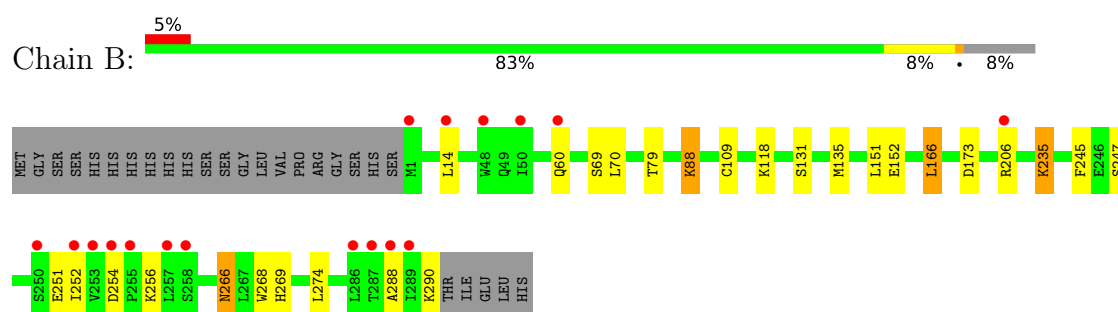
3 Residue-property plots [i](#)

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

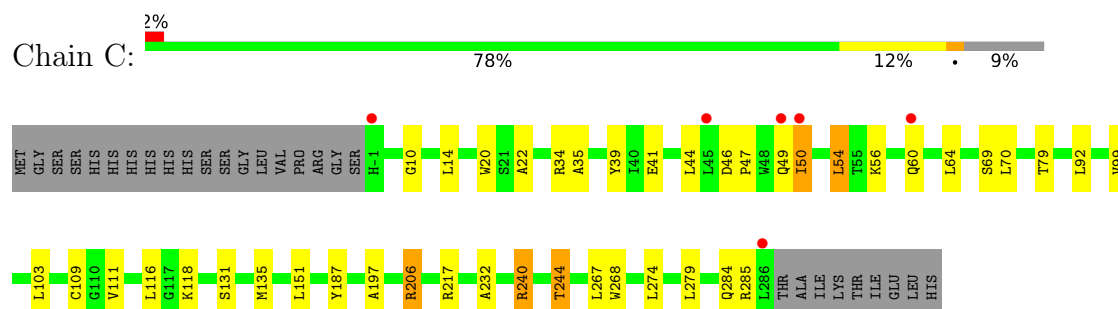
• Molecule 1: Epimerase



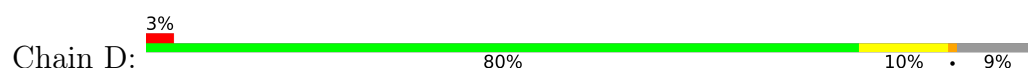
• Molecule 1: Epimerase

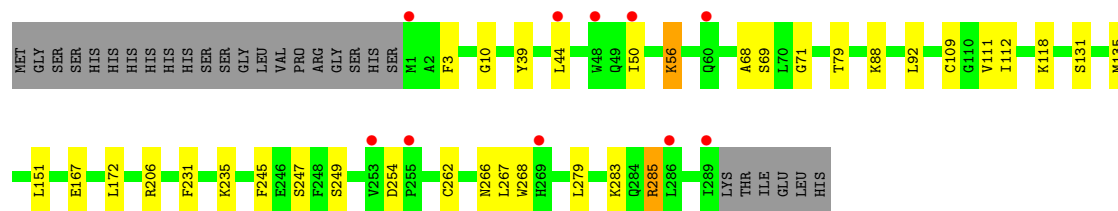


• Molecule 1: Epimerase

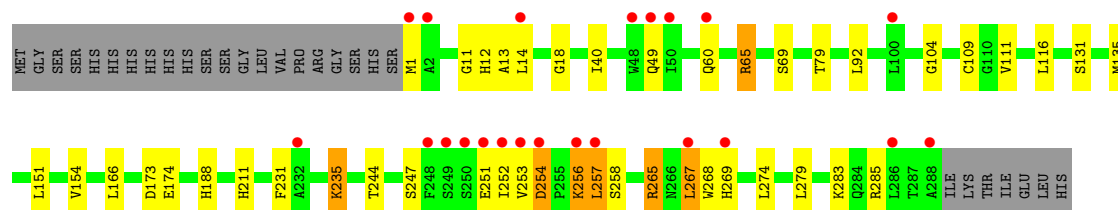
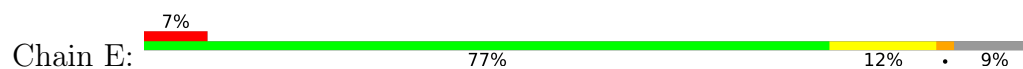


• Molecule 1: Epimerase

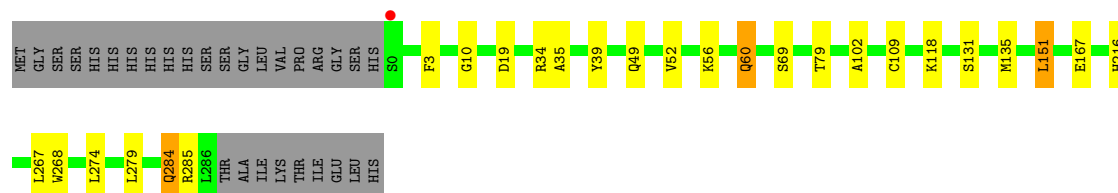
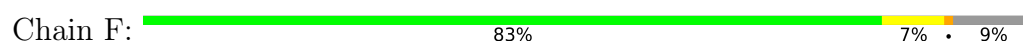




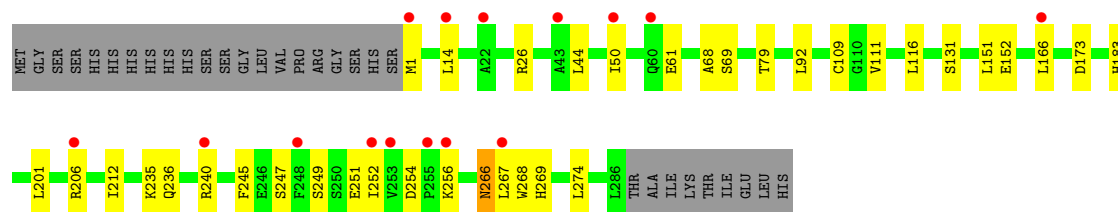
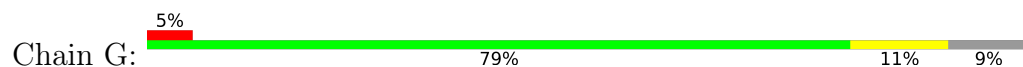
• Molecule 1: Epimerase



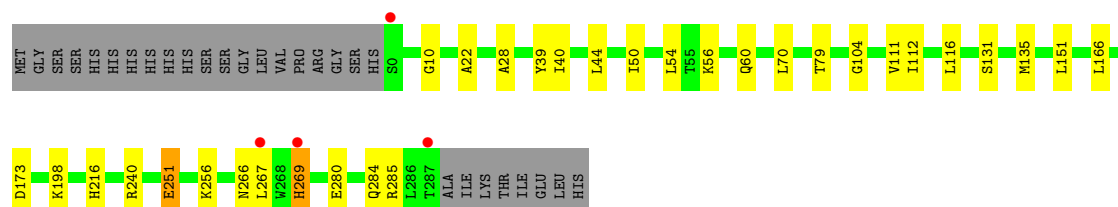
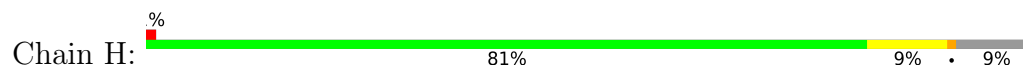
• Molecule 1: Epimerase



• Molecule 1: Epimerase



• Molecule 1: Epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.43Å 92.77Å 93.78Å 87.67° 98.64° 115.60°	Depositor
Resolution (Å)	45.71 – 1.58 45.71 – 1.58	Depositor EDS
% Data completeness (in resolution range)	94.0 (45.71-1.58) 94.0 (45.71-1.58)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.177 , 0.227 0.188 , 0.235	Depositor DCC
R_{free} test set	15718 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20140	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.34% 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: EDO, FUD, EPE, MN

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	0.93	0/2258	1.22	1/3061 (0.0%)
1	B	0.95	0/2278	1.25	1/3088 (0.0%)
1	C	0.92	0/2278	1.24	0/3087
1	D	0.95	0/2272	1.28	2/3081 (0.1%)
1	E	0.95	0/2275	1.28	2/3084 (0.1%)
1	F	0.93	0/2249	1.22	1/3050 (0.0%)
1	G	0.95	0/2243	1.29	3/3042 (0.1%)
1	H	0.93	0/2265	1.22	0/3071
All	All	0.94	0/18118	1.25	10/24564 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	265	ARG	CA-C-N	-6.10	114.39	122.99
1	E	265	ARG	C-N-CA	-6.10	114.39	122.99
1	B	254	ASP	CB-CA-C	5.79	115.90	110.17
1	D	3	PHE	CB-CA-C	5.46	116.96	108.61
1	F	3	PHE	CB-CA-C	5.24	117.00	109.09
1	G	212	ILE	CA-C-N	5.20	125.19	121.65
1	G	212	ILE	C-N-CA	5.20	125.19	121.65
1	D	254	ASP	CB-CA-C	5.18	115.30	110.17
1	G	254	ASP	CB-CA-C	5.13	115.25	110.17
1	A	3	PHE	CB-CA-C	5.11	116.43	108.61

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2207	0	2175	13	0
1	B	2230	0	2197	24	0
1	C	2226	0	2195	39	0
1	D	2224	0	2193	33	0
1	E	2224	0	2195	47	0
1	F	2204	0	2162	20	0
1	G	2198	0	2157	24	0
1	H	2217	0	2182	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	11	0	0
3	B	12	0	11	1	0
3	C	12	0	11	0	0
3	D	12	0	11	1	0
3	E	12	0	11	1	0
3	F	12	0	11	0	0
3	G	12	0	11	0	0
3	H	12	0	11	0	0
4	A	15	0	18	0	0
4	B	15	0	18	0	0
4	C	15	0	18	0	0
4	D	15	0	18	2	0
4	E	15	0	18	0	0
4	F	15	0	18	5	0
4	G	15	0	18	0	0
4	H	15	0	18	0	0
5	C	12	0	18	3	0
5	D	4	0	6	0	0
5	E	4	0	6	0	0
5	F	8	0	12	0	0
6	A	281	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	286	0	0	2	0
6	C	279	0	0	5	0
6	D	277	0	0	9	0
6	E	255	0	0	9	0
6	F	281	0	0	3	0
6	G	227	0	0	0	0
6	H	272	0	0	5	0
All	All	20140	0	17730	220	0

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 6.

All (220) 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:E:65[A]:ARG:HG3	1:E:65[A]:ARG:HH11	0.97	1.12
1:E:267:LEU:HD22	1:E:267:LEU:H	1.17	1.10
1:C:20:TRP:CD1	1:C:50:ILE:HD12	1.99	0.96
1:E:253:VAL:CG2	1:E:258:SER:HB3	1.96	0.96
1:E:12:HIS:HE1	1:E:14:LEU:HD12	1.33	0.92
1:E:65[A]:ARG:HG3	1:E:65[A]:ARG:NH1	1.79	0.91
1:A:173:ASP:OD1	1:C:34:ARG:HD3	1.70	0.91
1:E:65[A]:ARG:HH11	1:E:65[A]:ARG:CG	1.82	0.87
1:C:41:GLU:OE1	1:C:244:THR:HG21	1.73	0.87
1:C:240:ARG:HH11	1:C:240:ARG:HG3	1.39	0.86
1:E:12:HIS:CE1	1:E:14:LEU:HD12	2.12	0.85
1:G:251:GLU:HG2	1:G:269:HIS:HA	1.58	0.83
1:B:166:LEU:HD22	1:B:166:LEU:H	1.44	0.82
1:E:60:GLN:HG3	6:E:524:HOH:O	1.80	0.82
1:E:253:VAL:HG23	1:E:258:SER:HB3	1.62	0.79
1:C:39:TYR:OH	1:C:244:THR:HG22	1.86	0.76
1:H:166:LEU:HD11	1:H:198:LYS:HE3	1.70	0.73
1:G:166:LEU:H	1:G:166:LEU:HD22	1.53	0.72
1:B:60:GLN:HG3	6:B:563:HOH:O	1.89	0.72
1:E:267:LEU:HD22	1:E:267:LEU:N	2.00	0.72
1:H:285:ARG:CZ	6:H:420:HOH:O	2.37	0.72
1:C:56[B]:LYS:HE3	1:C:103:LEU:O	1.90	0.71
1:E:256:LYS:HD2	6:E:462:HOH:O	1.89	0.71
1:D:44:LEU:HD12	1:D:68:ALA:HB1	1.73	0.70
1:H:251:GLU:HG3	1:H:269:HIS:HA	1.74	0.69
1:A:251:GLU:HG2	1:A:269:HIS:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ARG:HG2	6:D:640:HOH:O	1.92	0.68
1:H:251:GLU:HG2	1:H:266:ASN:HD21	1.58	0.67
1:C:47:PRO:O	1:C:50:ILE:HG22	1.95	0.67
1:B:252:ILE:HD12	1:B:268:TRP:CZ3	2.30	0.66
1:C:44:LEU:HA	6:C:493:HOH:O	1.95	0.66
6:A:492:HOH:O	1:B:118[B]:LYS:HD2	1.97	0.65
1:D:167:GLU:CD	4:D:304:EPE:H32	2.22	0.65
1:B:252:ILE:HD12	1:B:268:TRP:CH2	2.31	0.65
1:B:166:LEU:HD22	1:B:166:LEU:N	2.12	0.65
1:F:167:GLU:CD	4:F:305:EPE:H32	2.22	0.64
1:F:34:ARG:HD3	1:H:173:ASP:OD2	1.97	0.63
1:D:167:GLU:OE2	4:D:304:EPE:H32	1.98	0.63
1:G:266:ASN:C	1:G:266:ASN:HD22	2.07	0.62
1:F:49:GLN:NE2	6:F:401:HOH:O	2.33	0.62
1:H:22:ALA:HA	1:H:54:LEU:HD21	1.82	0.61
1:B:251:GLU:HG2	1:B:269:HIS:HA	1.81	0.61
1:E:12:HIS:HE1	1:E:14:LEU:CD1	2.12	0.61
1:F:56:LYS:O	1:F:60:GLN:HG3	2.01	0.61
1:F:167:GLU:OE2	4:F:305:EPE:H32	2.00	0.61
1:H:56:LYS:O	1:H:60:GLN:HG3	2.02	0.60
1:C:118[A]:LYS:HE2	1:D:262:CYS:SG	2.41	0.60
1:H:251:GLU:HG2	1:H:266:ASN:ND2	2.16	0.60
1:H:216:HIS:O	1:H:267:LEU:HD21	2.02	0.60
1:D:151:LEU:N	1:D:151:LEU:HD22	2.16	0.60
6:C:584:HOH:O	1:D:267:LEU:CD1	2.49	0.59
1:D:151:LEU:HD23	1:D:172:LEU:HD21	1.83	0.59
1:A:28:ALA:HB1	1:A:40:ILE:HD11	1.85	0.59
1:G:111:VAL:HG21	1:G:116:LEU:HD13	1.84	0.58
1:C:240:ARG:HH11	1:C:240:ARG:CG	2.13	0.58
1:B:151:LEU:HD22	1:B:151:LEU:N	2.19	0.58
1:H:216:HIS:O	1:H:267:LEU:CD2	2.51	0.58
1:B:135:MET:HA	1:B:135:MET:HE2	1.85	0.58
1:E:279:LEU:HD11	1:E:283:LYS:HE2	1.84	0.58
1:G:166:LEU:HD22	1:G:166:LEU:N	2.19	0.57
1:D:118[B]:LYS:HD2	6:D:424:HOH:O	2.03	0.57
1:E:254:ASP:HB3	6:E:406:HOH:O	2.04	0.57
1:D:44:LEU:HD12	1:D:68:ALA:CB	2.34	0.57
1:C:56[A]:LYS:NZ	6:C:401:HOH:O	2.38	0.57
1:B:266:ASN:C	1:B:266:ASN:HD22	2.14	0.56
1:G:151:LEU:HD22	1:G:151:LEU:N	2.22	0.55
1:H:135:MET:HE2	1:H:135:MET:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:TRP:CD2	1:C:274:LEU:HD22	2.43	0.54
1:E:151:LEU:HD22	1:E:151:LEU:N	2.23	0.54
1:B:70:LEU:HD12	1:B:70:LEU:C	2.33	0.54
1:G:252:ILE:HD12	1:G:268:TRP:CZ3	2.41	0.54
1:A:56:LYS:HD2	6:A:513:HOH:O	2.09	0.53
1:A:79:THR:HG22	1:A:131:SER:HB2	1.91	0.53
1:E:65[A]:ARG:NH1	1:E:65[A]:ARG:CG	2.52	0.53
1:E:254:ASP:OD2	1:E:256:LYS:HB3	2.08	0.53
1:E:14:LEU:HD13	1:E:257:LEU:CD1	2.38	0.53
1:D:279:LEU:HD11	1:D:283:LYS:HE2	1.89	0.53
1:B:235:LYS:HG3	6:B:415:HOH:O	2.08	0.53
1:D:79:THR:HG22	1:D:131:SER:HB2	1.91	0.53
6:C:584:HOH:O	1:D:267:LEU:HD12	2.09	0.53
1:E:267:LEU:N	1:E:267:LEU:HD13	2.24	0.53
1:A:112:ILE:HD11	1:A:151:LEU:HD23	1.92	0.52
1:D:88:LYS:HE3	6:D:608:HOH:O	2.09	0.52
1:E:174:GLU:HA	1:G:26:ARG:HD2	1.91	0.52
1:H:251:GLU:CG	1:H:266:ASN:HD21	2.23	0.52
1:G:173:ASP:OD1	1:G:206:ARG:NH1	2.43	0.52
1:B:166:LEU:H	1:B:166:LEU:CD2	2.17	0.52
1:G:79:THR:HG22	1:G:131:SER:HB2	1.92	0.52
3:D:303:FUD:O3	3:D:303:FUD:O5	2.28	0.51
1:A:279:LEU:HD11	1:A:283:LYS:HE2	1.92	0.51
1:C:197:ALA:HB1	5:C:301:EDO:H21	1.92	0.51
1:H:240:ARG:CZ	6:H:410:HOH:O	2.58	0.51
1:H:44:LEU:CD2	1:H:50:ILE:HG13	2.41	0.51
1:C:70:LEU:C	1:C:70:LEU:HD12	2.35	0.51
1:E:18:GLY:HA3	1:E:252:ILE:O	2.10	0.51
1:C:46:ASP:OD2	1:C:49:GLN:NE2	2.44	0.51
1:H:28:ALA:HB1	1:H:40:ILE:HD11	1.91	0.51
1:C:35:ALA:O	1:C:279:LEU:HD23	2.11	0.50
1:D:44:LEU:CD2	1:D:50:ILE:HG13	2.41	0.50
1:G:44:LEU:HD12	1:G:68:ALA:HB1	1.93	0.49
1:B:173:ASP:OD1	1:B:206:ARG:NH1	2.45	0.49
1:H:280:GLU:HG2	6:H:637:HOH:O	2.12	0.49
1:E:13:ALA:HA	1:E:40:ILE:HD11	1.94	0.49
1:C:50:ILE:HG21	1:C:99:VAL:HG11	1.95	0.49
1:C:267:LEU:N	1:C:267:LEU:HD12	2.27	0.49
1:C:79:THR:HG22	1:C:131:SER:HB2	1.95	0.48
1:G:201:LEU:CD2	1:G:236:GLN:HG2	2.43	0.48
1:C:111:VAL:HG21	1:C:116:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:MET:HA	1:E:135:MET:HE2	1.95	0.48
1:F:69:SER:HA	1:F:109:CYS:O	2.13	0.48
1:E:267:LEU:H	1:E:267:LEU:CD2	1.97	0.48
1:C:22:ALA:HA	1:C:54:LEU:HD11	1.94	0.48
1:E:1:MET:HB2	6:E:409:HOH:O	2.13	0.48
1:D:112:ILE:HD11	1:D:151:LEU:HD13	1.96	0.48
1:C:240:ARG:HG3	1:C:240:ARG:NH1	2.16	0.48
1:F:35:ALA:O	1:F:279:LEU:HD23	2.14	0.48
1:F:79:THR:HG22	1:F:131:SER:HB2	1.96	0.47
1:C:206:ARG:HG3	6:C:600:HOH:O	2.15	0.47
1:F:10:GLY:HA3	1:F:39:TYR:CE1	2.50	0.47
1:D:44:LEU:HD21	1:D:50:ILE:HG13	1.96	0.47
1:D:92:LEU:C	1:D:92:LEU:HD23	2.38	0.47
1:G:92:LEU:C	1:G:92:LEU:HD23	2.39	0.46
1:E:79:THR:HG22	1:E:131:SER:HB2	1.96	0.46
1:G:252:ILE:CD1	1:G:268:TRP:CZ3	2.99	0.46
1:C:135:MET:HA	1:C:135:MET:HE2	1.98	0.46
1:F:151:LEU:N	1:F:151:LEU:HD23	2.31	0.46
1:H:70:LEU:C	1:H:70:LEU:HD12	2.40	0.46
1:H:112:ILE:HD11	1:H:151:LEU:HD23	1.98	0.46
1:D:88:LYS:CE	6:D:608:HOH:O	2.63	0.46
1:B:69:SER:HA	1:B:109:CYS:O	2.15	0.46
1:C:92:LEU:C	1:C:92:LEU:HD23	2.41	0.46
1:C:69:SER:HA	1:C:109:CYS:O	2.16	0.46
1:A:70:LEU:C	1:A:70:LEU:HD12	2.41	0.46
1:E:92:LEU:C	1:E:92:LEU:HD23	2.41	0.46
1:F:10:GLY:HA3	1:F:39:TYR:CZ	2.51	0.46
1:D:71:GLY:HA2	1:D:111:VAL:O	2.16	0.46
1:E:111:VAL:HG21	1:E:116:LEU:HD13	1.98	0.46
1:G:245:PHE:CZ	1:G:247:SER:HB2	2.51	0.45
1:D:135:MET:HE2	1:D:135:MET:HA	1.99	0.45
1:E:14:LEU:HD13	1:E:257:LEU:HD12	1.96	0.45
1:B:79:THR:HG22	1:B:131:SER:HB2	1.99	0.45
1:D:56:LYS:CG	6:D:539:HOH:O	2.65	0.45
1:E:69:SER:HA	1:E:109:CYS:O	2.16	0.45
1:F:135:MET:HA	1:F:135:MET:HE2	1.99	0.45
1:E:265:ARG:HA	6:E:506:HOH:O	2.17	0.45
1:C:10:GLY:HA3	1:C:39:TYR:CE1	2.52	0.45
1:D:56:LYS:HG2	6:D:539:HOH:O	2.16	0.45
1:E:252:ILE:HD12	1:E:268:TRP:CH2	2.52	0.45
1:G:69:SER:HA	1:G:109:CYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ASN:HB2	6:D:402:HOH:O	2.17	0.44
1:C:41:GLU:OE1	1:C:244:THR:CG2	2.56	0.44
1:F:284:GLN:HG2	1:F:285:ARG:NH2	2.33	0.44
1:H:10:GLY:HA3	1:H:39:TYR:CZ	2.53	0.44
1:E:251:GLU:HA	1:E:251:GLU:OE1	2.18	0.44
1:A:166:LEU:HD11	1:A:198:LYS:HD3	2.00	0.44
1:F:19:ASP:OD1	1:F:19:ASP:C	2.60	0.44
1:B:245:PHE:CZ	1:B:247:SER:HB2	2.53	0.44
1:H:79:THR:HG22	1:H:131:SER:HB2	1.99	0.44
1:E:268:TRP:CD2	1:E:274:LEU:HD22	2.53	0.43
1:C:197:ALA:CB	5:C:301:EDO:H21	2.48	0.43
1:D:56:LYS:HG2	6:D:453:HOH:O	2.17	0.43
1:D:118[A]:LYS:HD2	6:D:424:HOH:O	2.17	0.43
1:F:267:LEU:HD12	1:F:267:LEU:N	2.33	0.43
1:D:10:GLY:HA3	1:D:39:TYR:CE2	2.53	0.43
1:E:49:GLN:NE2	6:E:414:HOH:O	2.52	0.43
1:G:166:LEU:H	1:G:166:LEU:CD2	2.25	0.43
1:H:240:ARG:NE	6:H:410:HOH:O	2.51	0.43
1:A:3:PHE:CE1	1:A:146:GLY:HA2	2.53	0.43
1:E:174:GLU:HA	1:G:26:ARG:CD	2.49	0.43
1:F:268:TRP:CD2	1:F:274:LEU:HD22	2.54	0.43
1:G:44:LEU:CD2	1:G:50:ILE:HG13	2.49	0.43
1:H:166:LEU:CD1	1:H:198:LYS:HE3	2.44	0.43
1:C:20:TRP:CD1	1:C:50:ILE:CD1	2.87	0.42
1:A:262:CYS:SG	1:B:118[B]:LYS:HE3	2.59	0.42
1:H:10:GLY:HA3	1:H:39:TYR:CE1	2.54	0.42
1:D:231:PHE:CG	1:D:285:ARG:HB3	2.53	0.42
1:G:268:TRP:CD2	1:G:274:LEU:HD22	2.54	0.42
1:G:268:TRP:CE2	1:G:274:LEU:HD22	2.55	0.42
1:E:211:HIS:CD2	1:E:244:THR:HB	2.54	0.42
1:E:231:PHE:CG	1:E:285:ARG:HB3	2.55	0.42
1:F:52:VAL:HG11	1:F:102:ALA:HB1	2.01	0.42
1:B:135:MET:HE2	1:B:135:MET:CA	2.48	0.42
1:B:268:TRP:CD2	1:B:274:LEU:HD22	2.54	0.42
1:D:69:SER:HA	1:D:109:CYS:O	2.19	0.42
1:A:152:GLU:HA	1:A:183:HIS:HB3	2.00	0.42
1:E:151:LEU:N	1:E:151:LEU:CD2	2.83	0.42
1:F:268:TRP:CE2	1:F:274:LEU:HD22	2.55	0.42
1:G:152:GLU:HA	1:G:183:HIS:HB3	2.02	0.42
1:B:151:LEU:N	1:B:151:LEU:CD2	2.83	0.41
1:C:118[B]:LYS:HZ3	1:D:118[B]:LYS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ALA:HB3	5:C:301:EDO:H12	2.02	0.41
1:D:245:PHE:CZ	1:D:247:SER:HB2	2.54	0.41
1:H:111:VAL:HG21	1:H:116:LEU:HD13	2.01	0.41
1:E:104:GLY:HA2	6:E:402:HOH:O	2.20	0.41
1:C:56[B]:LYS:CE	1:C:103:LEU:O	2.63	0.41
1:E:69:SER:OG	3:E:303:FUD:H61	2.21	0.41
1:E:173:ASP:O	1:G:26:ARG:HD3	2.20	0.41
1:F:118:LYS:HE3	6:F:484:HOH:O	2.20	0.41
4:F:305:EPE:H31	4:F:305:EPE:H82	1.92	0.41
1:B:152:GLU:OE1	3:B:302:FUD:O4	2.35	0.41
1:C:268:TRP:CE2	1:C:274:LEU:HD22	2.55	0.41
1:H:284:GLN:HE21	1:H:284:GLN:HB2	1.67	0.41
1:E:154:VAL:HA	1:E:188:HIS:CG	2.56	0.41
1:A:92:LEU:C	1:A:92:LEU:HD23	2.46	0.41
1:E:235:LYS:HD3	6:E:511:HOH:O	2.21	0.41
1:C:64:LEU:HD12	1:C:64:LEU:HA	1.95	0.41
1:C:118[B]:LYS:NZ	1:D:118[B]:LYS:HB2	2.35	0.41
1:D:249:SER:HB2	1:D:268:TRP:CE2	2.56	0.41
1:F:167:GLU:OE2	4:F:305:EPE:H52	2.21	0.41
1:H:104:GLY:HA2	6:H:503:HOH:O	2.19	0.41
1:E:135:MET:SD	1:E:151:LEU:HD11	2.61	0.41
4:F:305:EPE:H21	6:F:623:HOH:O	2.21	0.41
1:B:88:LYS:HD2	1:B:88:LYS:HA	1.79	0.40
1:E:11:GLY:O	1:E:40:ILE:HD12	2.22	0.40
1:B:266:ASN:C	1:B:266:ASN:ND2	2.79	0.40
1:C:151:LEU:HD12	1:C:151:LEU:N	2.35	0.40
1:E:254:ASP:HB2	6:E:557:HOH:O	2.20	0.40
1:C:187:TYR:CD1	1:C:217:ARG:HG2	2.57	0.40
1:G:249:SER:HB2	1:G:268:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

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	286/316 (90%)	280 (98%)	6 (2%)	0	100	100
1	B	289/316 (92%)	282 (98%)	6 (2%)	1 (0%)	36	20
1	C	288/316 (91%)	285 (99%)	3 (1%)	0	100	100
1	D	288/316 (91%)	282 (98%)	6 (2%)	0	100	100
1	E	288/316 (91%)	283 (98%)	5 (2%)	0	100	100
1	F	285/316 (90%)	281 (99%)	4 (1%)	0	100	100
1	G	284/316 (90%)	279 (98%)	5 (2%)	0	100	100
1	H	287/316 (91%)	282 (98%)	5 (2%)	0	100	100
All	All	2295/2528 (91%)	2254 (98%)	40 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	ALA

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	225/249 (90%)	221 (98%)	4 (2%)	51	23
1	B	226/249 (91%)	219 (97%)	7 (3%)	35	7
1	C	227/249 (91%)	219 (96%)	8 (4%)	32	6
1	D	226/249 (91%)	223 (99%)	3 (1%)	61	37
1	E	226/249 (91%)	216 (96%)	10 (4%)	25	3
1	F	224/249 (90%)	220 (98%)	4 (2%)	51	23
1	G	223/249 (90%)	215 (96%)	8 (4%)	31	5
1	H	226/249 (91%)	223 (99%)	3 (1%)	61	37
All	All	1803/1992 (90%)	1756 (97%)	47 (3%)	40	11

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	256	LYS
1	A	266	ASN
1	A	284	GLN
1	B	14	LEU
1	B	88	LYS
1	B	166	LEU
1	B	235	LYS
1	B	256	LYS
1	B	266	ASN
1	B	290	LYS
1	C	14	LEU
1	C	50	ILE
1	C	54	LEU
1	C	206	ARG
1	C	240	ARG
1	C	244	THR
1	C	284	GLN
1	C	285	ARG
1	D	56	LYS
1	D	235	LYS
1	D	285	ARG
1	E	65[A]	ARG
1	E	65[B]	ARG
1	E	166	LEU
1	E	235	LYS
1	E	247	SER
1	E	254	ASP
1	E	256	LYS
1	E	257	LEU
1	E	267	LEU
1	E	269	HIS
1	F	60	GLN
1	F	151	LEU
1	F	216	HIS
1	F	284	GLN
1	G	1	MET
1	G	14	LEU
1	G	61	GLU
1	G	235	LYS
1	G	240	ARG
1	G	256	LYS
1	G	266	ASN

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Mol	Chain	Res	Type
1	G	267	LEU
1	H	251	GLU
1	H	256	LYS
1	H	269	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	B	49	GLN
1	B	60	GLN
1	B	266	ASN
1	C	60	GLN
1	C	63	ASN
1	C	236	GLN
1	C	269	HIS
1	C	284	GLN
1	D	49	GLN
1	D	269	HIS
1	E	49	GLN
1	E	60	GLN
1	E	194	ASN
1	E	269	HIS
1	F	49	GLN
1	F	60	GLN
1	F	63	ASN
1	F	284	GLN
1	G	49	GLN
1	G	60	GLN
1	G	194	ASN
1	G	266	ASN
1	H	60	GLN
1	H	63	ASN
1	H	266	ASN
1	H	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EPE	H	303	-	15,15,15	1.98	1 (6%)	19,20,20	1.35	3 (15%)
3	FUD	F	304	2	11,11,11	0.60	0	10,14,14	1.27	0
4	EPE	F	305	-	15,15,15	1.93	1 (6%)	19,20,20	1.80	4 (21%)
3	FUD	H	302	2	11,11,11	0.60	0	10,14,14	1.59	2 (20%)
3	FUD	E	303	2	11,11,11	0.36	0	10,14,14	1.77	2 (20%)
5	EDO	C	301	-	3,3,3	0.16	0	2,2,2	0.02	0
4	EPE	E	304	-	15,15,15	1.85	1 (6%)	19,20,20	0.78	0
5	EDO	C	302	-	3,3,3	0.08	0	2,2,2	0.13	0
5	EDO	F	302	-	3,3,3	0.09	0	2,2,2	0.14	0
3	FUD	C	305	2	11,11,11	0.41	0	10,14,14	0.96	0
4	EPE	D	304	-	15,15,15	1.82	1 (6%)	19,20,20	2.34	7 (36%)
5	EDO	D	301	-	3,3,3	0.03	0	2,2,2	0.13	0
4	EPE	B	303	-	15,15,15	1.94	1 (6%)	19,20,20	1.20	2 (10%)
4	EPE	C	306	-	15,15,15	1.95	1 (6%)	19,20,20	1.17	2 (10%)
4	EPE	G	303	-	15,15,15	1.83	1 (6%)	19,20,20	1.00	2 (10%)
5	EDO	F	301	-	3,3,3	0.38	0	2,2,2	0.23	0
3	FUD	D	303	2	11,11,11	0.36	0	10,14,14	0.95	0
5	EDO	C	303	-	3,3,3	0.15	0	2,2,2	0.15	0
5	EDO	E	301	-	3,3,3	0.16	0	2,2,2	0.12	0
3	FUD	A	302	2	11,11,11	0.60	0	10,14,14	1.38	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPE	A	303	-	15,15,15	2.01	1 (6%)	19,20,20	1.14	2 (10%)
3	FUD	B	302	2	11,11,11	0.70	0	10,14,14	1.52	1 (10%)
3	FUD	G	302	2	11,11,11	0.44	0	10,14,14	1.48	1 (10%)

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	EPE	H	303	-	-	1/9/19/19	0/1/1/1
3	FUD	F	304	2	-	3/16/16/16	-
4	EPE	F	305	-	-	7/9/19/19	0/1/1/1
3	FUD	H	302	2	-	11/16/16/16	-
3	FUD	E	303	2	-	8/16/16/16	-
5	EDO	C	301	-	-	0/1/1/1	-
4	EPE	E	304	-	-	0/9/19/19	0/1/1/1
5	EDO	C	302	-	-	1/1/1/1	-
5	EDO	F	302	-	-	0/1/1/1	-
3	FUD	C	305	2	-	2/16/16/16	-
4	EPE	D	304	-	-	6/9/19/19	0/1/1/1
5	EDO	D	301	-	-	0/1/1/1	-
4	EPE	B	303	-	-	2/9/19/19	0/1/1/1
4	EPE	C	306	-	-	4/9/19/19	0/1/1/1
4	EPE	G	303	-	-	3/9/19/19	0/1/1/1
5	EDO	F	301	-	-	0/1/1/1	-
3	FUD	D	303	2	-	2/16/16/16	-
5	EDO	C	303	-	-	0/1/1/1	-
5	EDO	E	301	-	-	0/1/1/1	-
3	FUD	A	302	2	-	12/16/16/16	-
4	EPE	A	303	-	-	3/9/19/19	0/1/1/1
3	FUD	B	302	2	-	5/16/16/16	-
3	FUD	G	302	2	-	6/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	EPE	C10-S	-7.51	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	306	EPE	C10-S	-7.31	1.67	1.77
4	B	303	EPE	C10-S	-7.21	1.67	1.77
4	H	303	EPE	C10-S	-7.17	1.67	1.77
4	F	305	EPE	C10-S	-7.02	1.67	1.77
4	G	303	EPE	C10-S	-6.82	1.68	1.77
4	E	304	EPE	C10-S	-6.78	1.68	1.77
4	D	304	EPE	C10-S	-6.62	1.68	1.77

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	304	EPE	O1S-S-C10	4.40	113.38	106.73
4	D	304	EPE	O3S-S-C10	4.09	114.00	106.00
4	F	305	EPE	O2S-S-C10	3.99	112.76	106.73
4	D	304	EPE	C5-C6-N1	3.85	118.41	110.65
3	E	303	FUD	C5-C4-C3	3.78	118.26	112.05
4	D	304	EPE	C6-N1-C2	3.66	116.73	108.84
3	G	302	FUD	C5-C4-C3	3.66	118.06	112.05
4	B	303	EPE	O2S-S-C10	3.61	112.19	106.73
4	F	305	EPE	C6-N1-C2	3.55	116.50	108.84
3	E	303	FUD	O6-C6-C5	-3.40	104.02	111.16
4	D	304	EPE	C6-C5-N4	3.29	117.29	110.65
4	C	306	EPE	O1S-S-C10	3.15	111.48	106.73
4	H	303	EPE	O1S-S-C10	2.99	111.24	106.73
3	B	302	FUD	O2-C2-C1	2.81	124.93	120.16
3	H	302	FUD	C5-C4-C3	2.78	116.62	112.05
4	D	304	EPE	C7-N4-C3	2.77	118.61	111.24
3	H	302	FUD	O3-C3-C4	2.62	116.06	110.38
4	F	305	EPE	O1S-S-C10	2.56	110.60	106.73
4	H	303	EPE	C9-N1-C2	-2.50	104.58	111.24
4	C	306	EPE	O2S-S-C10	2.49	110.49	106.73
4	D	304	EPE	O2S-S-C10	-2.49	102.97	106.73
3	A	302	FUD	O3-C3-C4	2.47	115.75	110.38
4	H	303	EPE	O3S-S-C10	2.45	110.79	106.00
4	A	303	EPE	O1S-S-C10	2.38	110.33	106.73
3	A	302	FUD	O2-C2-C1	2.34	124.13	120.16
4	G	303	EPE	O1S-S-C10	2.27	110.15	106.73
4	B	303	EPE	O1S-S-C10	2.25	110.13	106.73
4	A	303	EPE	O3S-S-C10	2.19	110.29	106.00
4	F	305	EPE	C5-N4-C3	2.10	113.37	108.84
4	G	303	EPE	O2S-S-C10	2.02	109.78	106.73

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	FUD	C1-C2-C3-C4
3	A	302	FUD	O2-C2-C3-C4
3	A	302	FUD	C3-C4-C5-C6
3	A	302	FUD	O4-C4-C5-C6
3	A	302	FUD	O4-C4-C5-O5
3	B	302	FUD	C3-C4-C5-C6
3	B	302	FUD	C3-C4-C5-O5
3	B	302	FUD	O4-C4-C5-C6
3	B	302	FUD	O4-C4-C5-O5
3	E	303	FUD	C3-C4-C5-C6
3	E	303	FUD	C3-C4-C5-O5
3	E	303	FUD	O4-C4-C5-O5
3	G	302	FUD	O2-C2-C3-C4
3	G	302	FUD	C3-C4-C5-C6
3	G	302	FUD	C3-C4-C5-O5
3	G	302	FUD	O4-C4-C5-O5
3	H	302	FUD	O2-C2-C3-C4
3	H	302	FUD	C3-C4-C5-C6
3	H	302	FUD	C3-C4-C5-O5
3	H	302	FUD	O4-C4-C5-O5
4	D	304	EPE	C9-C10-S-O1S
4	D	304	EPE	C9-C10-S-O2S
4	F	305	EPE	C10-C9-N1-C6
3	A	302	FUD	O5-C5-C6-O6
3	F	304	FUD	O5-C5-C6-O6
4	A	303	EPE	N4-C7-C8-O8
3	E	303	FUD	C4-C5-C6-O6
4	A	303	EPE	C8-C7-N4-C3
4	D	304	EPE	C8-C7-N4-C3
4	F	305	EPE	C8-C7-N4-C3
3	E	303	FUD	O4-C4-C5-C6
3	G	302	FUD	O4-C4-C5-C6
3	H	302	FUD	O4-C4-C5-C6
3	E	303	FUD	O5-C5-C6-O6
3	F	304	FUD	C4-C5-C6-O6
3	A	302	FUD	C3-C4-C5-O5
4	F	305	EPE	C9-C10-S-O3S
3	A	302	FUD	O3-C3-C4-O4
3	A	302	FUD	C4-C5-C6-O6
3	A	302	FUD	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	H	302	FUD	O5-C5-C6-O6
3	H	302	FUD	O3-C3-C4-O4
3	A	302	FUD	C2-C3-C4-O4
3	A	302	FUD	C2-C3-C4-C5
3	H	302	FUD	O3-C3-C4-C5
4	B	303	EPE	C10-C9-N1-C2
4	B	303	EPE	C10-C9-N1-C6
4	C	306	EPE	C10-C9-N1-C2
4	C	306	EPE	C10-C9-N1-C6
4	G	303	EPE	C10-C9-N1-C2
4	G	303	EPE	C10-C9-N1-C6
4	D	304	EPE	C9-C10-S-O3S
4	F	305	EPE	N4-C7-C8-O8
4	A	303	EPE	C8-C7-N4-C5
4	F	305	EPE	C8-C7-N4-C5
4	C	306	EPE	C9-C10-S-O2S
4	F	305	EPE	C9-C10-S-O1S
4	F	305	EPE	C9-C10-S-O2S
3	F	304	FUD	C3-C4-C5-C6
3	D	303	FUD	C1-C2-C3-C4
3	G	302	FUD	C1-C2-C3-C4
3	H	302	FUD	C1-C2-C3-C4
3	C	305	FUD	O2-C2-C3-C4
3	D	303	FUD	O2-C2-C3-C4
3	E	303	FUD	O2-C2-C3-C4
3	B	302	FUD	O1-C1-C2-O2
4	D	304	EPE	N4-C7-C8-O8
4	D	304	EPE	C8-C7-N4-C5
4	H	303	EPE	S-C10-C9-N1
4	G	303	EPE	C9-C10-S-O3S
3	H	302	FUD	C2-C3-C4-C5
3	H	302	FUD	C4-C5-C6-O6
4	C	306	EPE	C9-C10-S-O3S
3	C	305	FUD	C1-C2-C3-C4
3	E	303	FUD	C1-C2-C3-C4
5	C	302	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

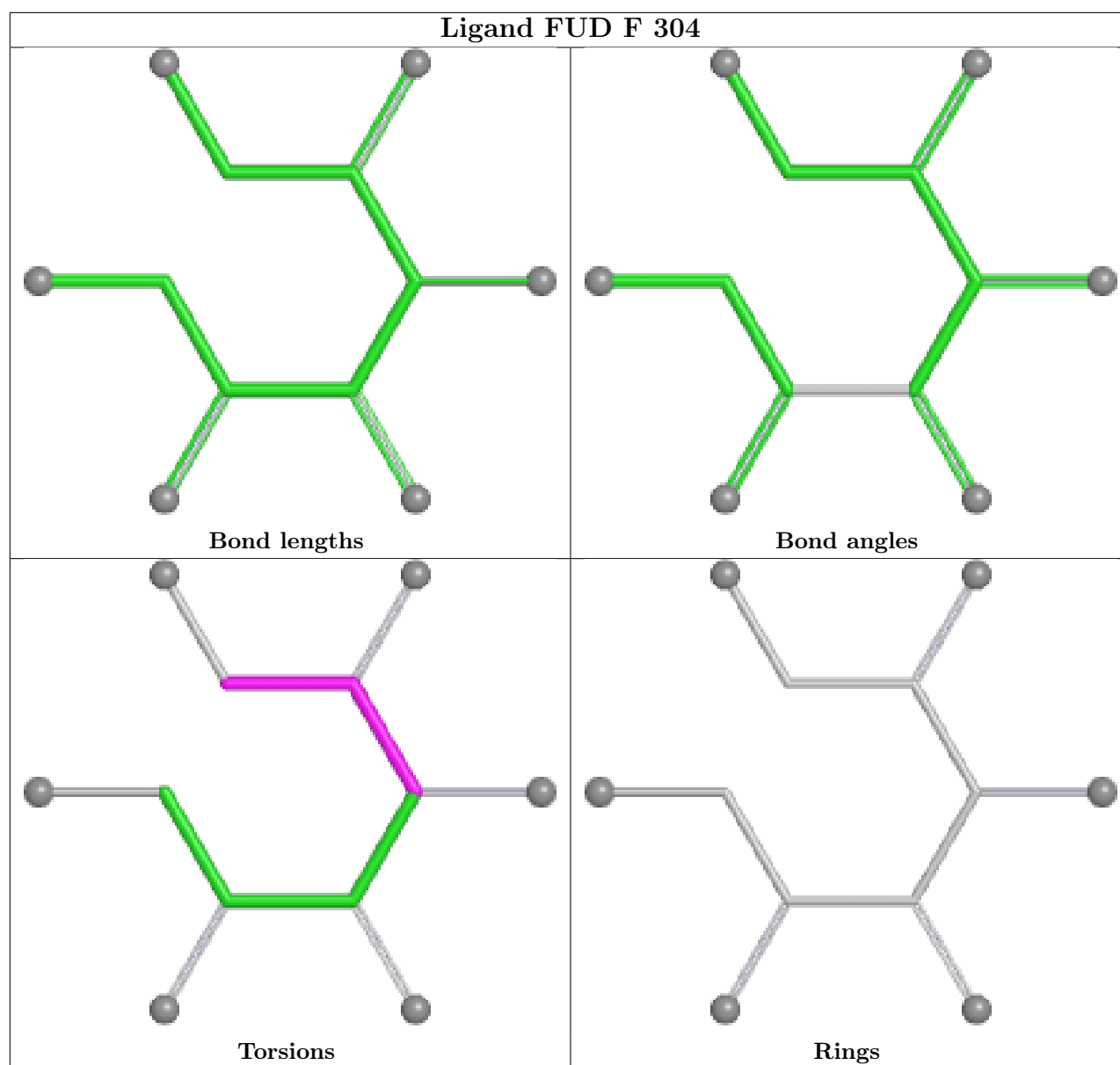
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	305	EPE	5	0

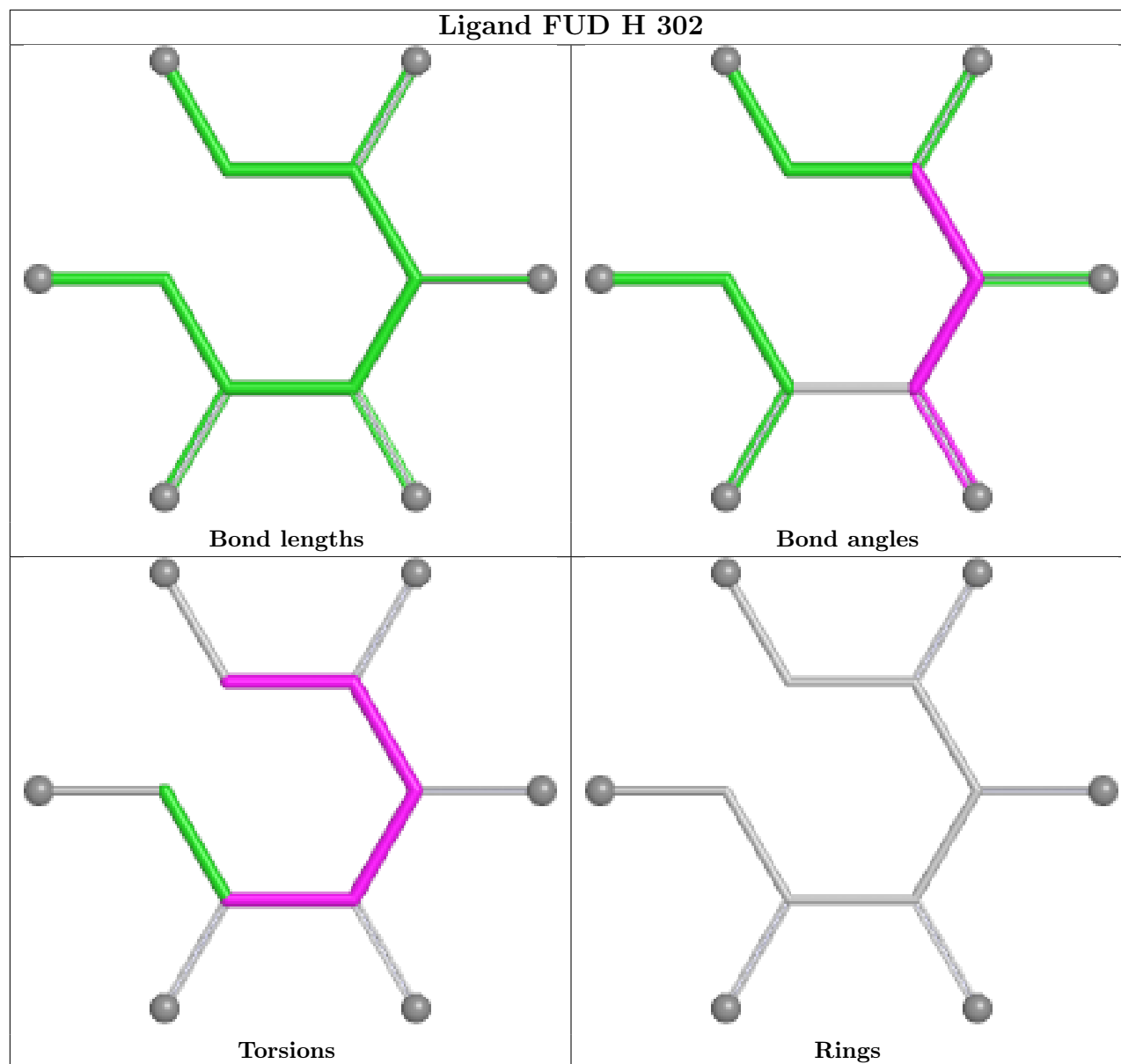
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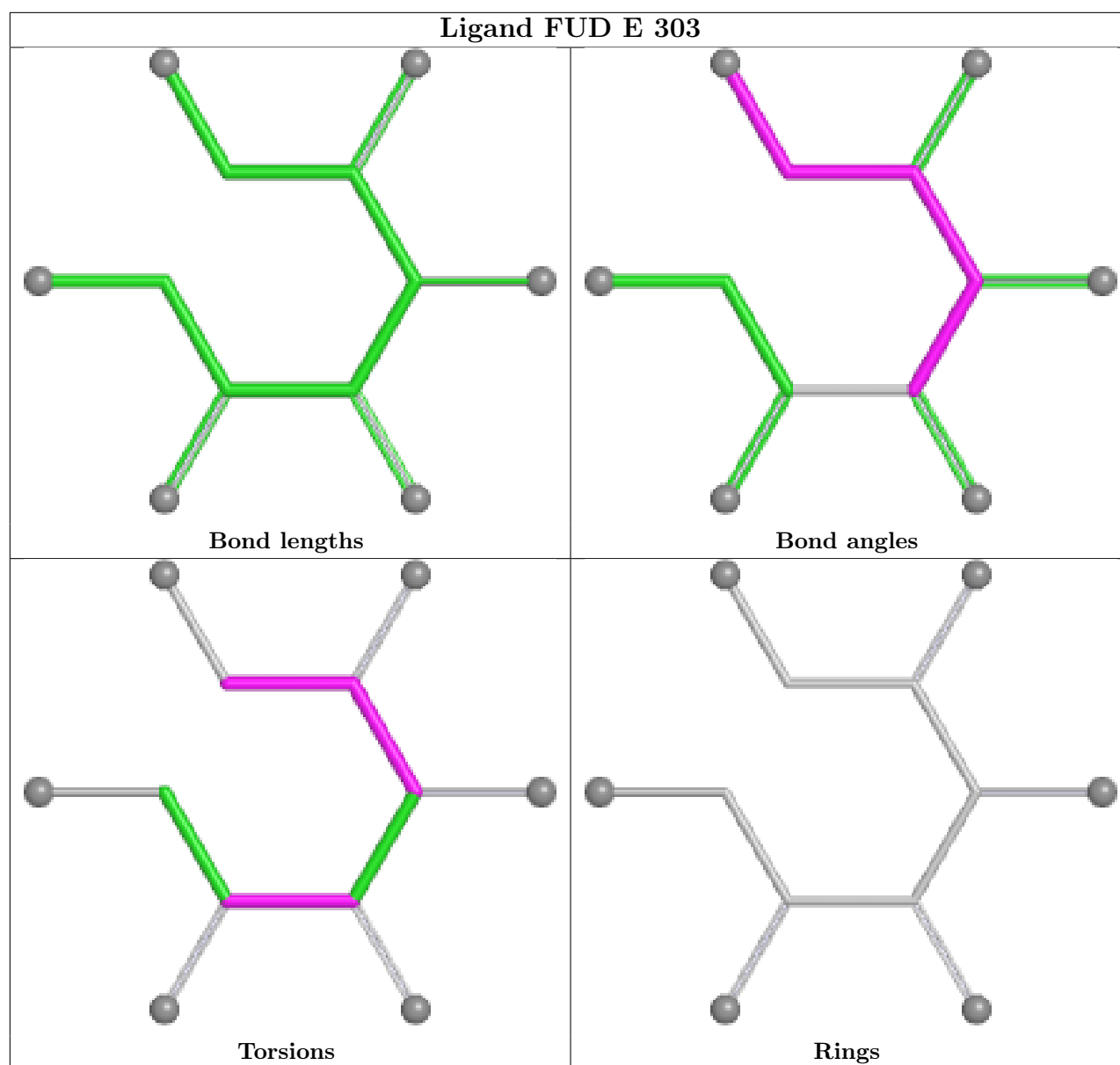
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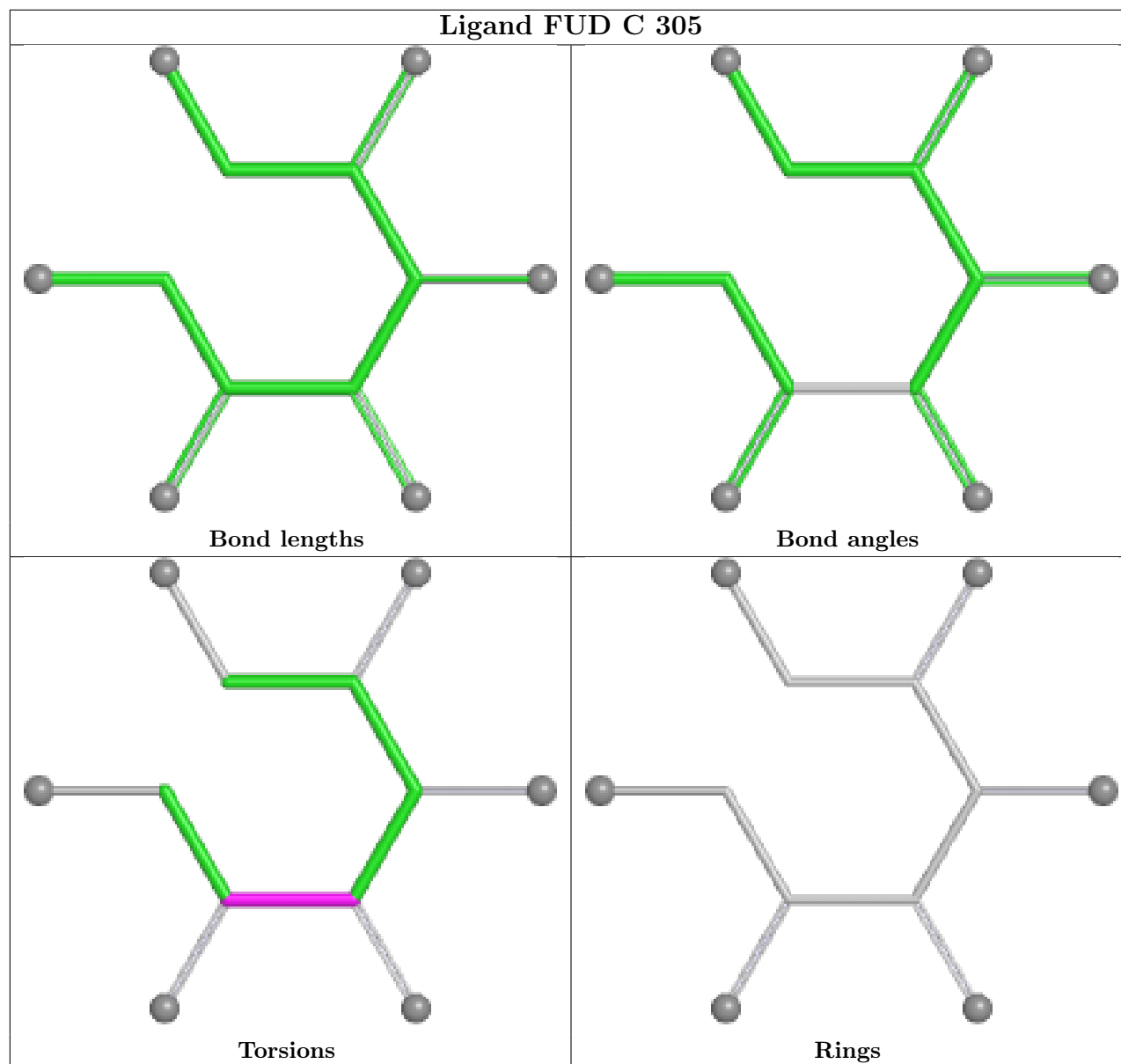
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	303	FUD	1	0
5	C	301	EDO	3	0
4	D	304	EPE	2	0
3	D	303	FUD	1	0
3	B	302	FUD	1	0

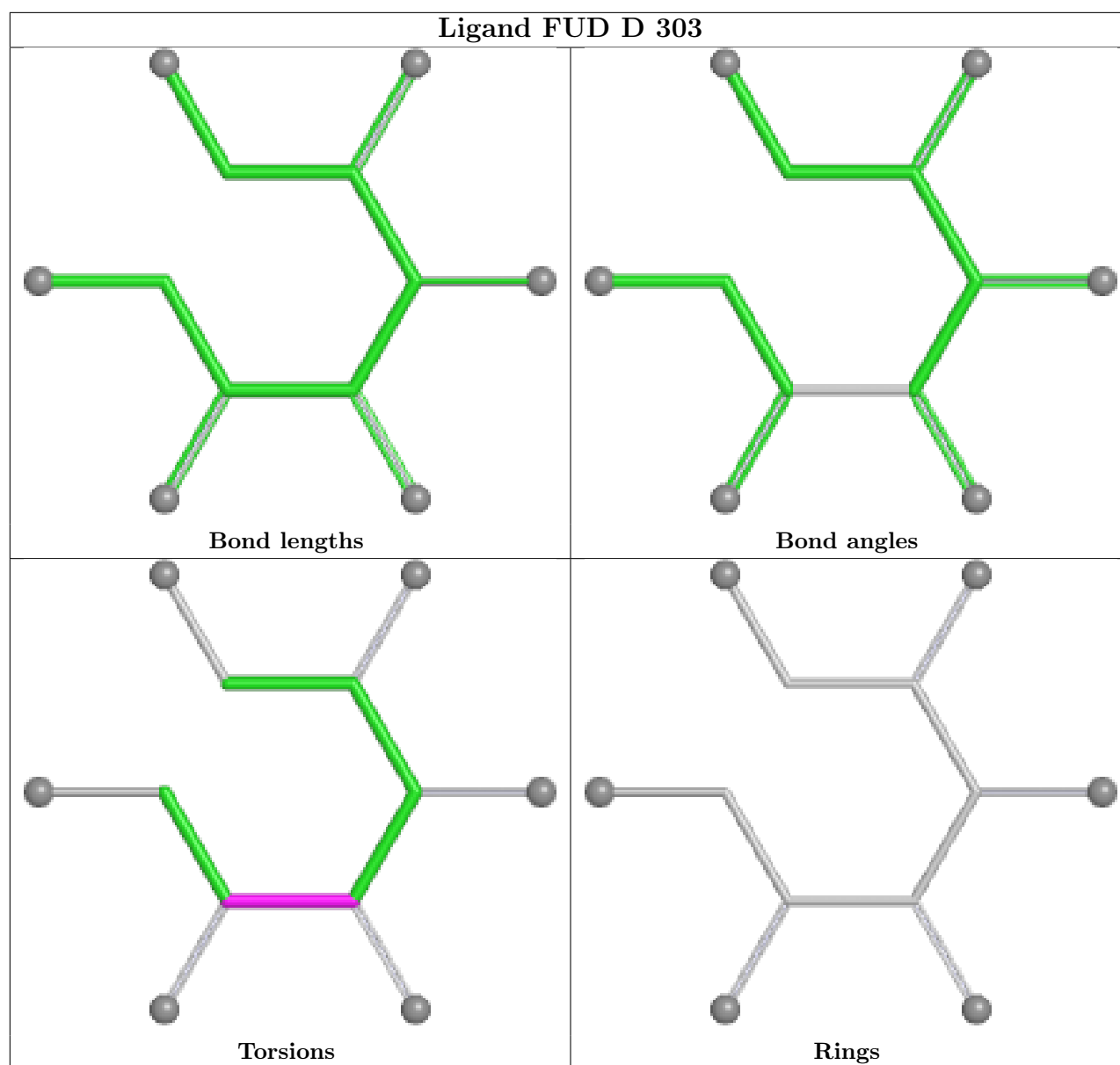
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

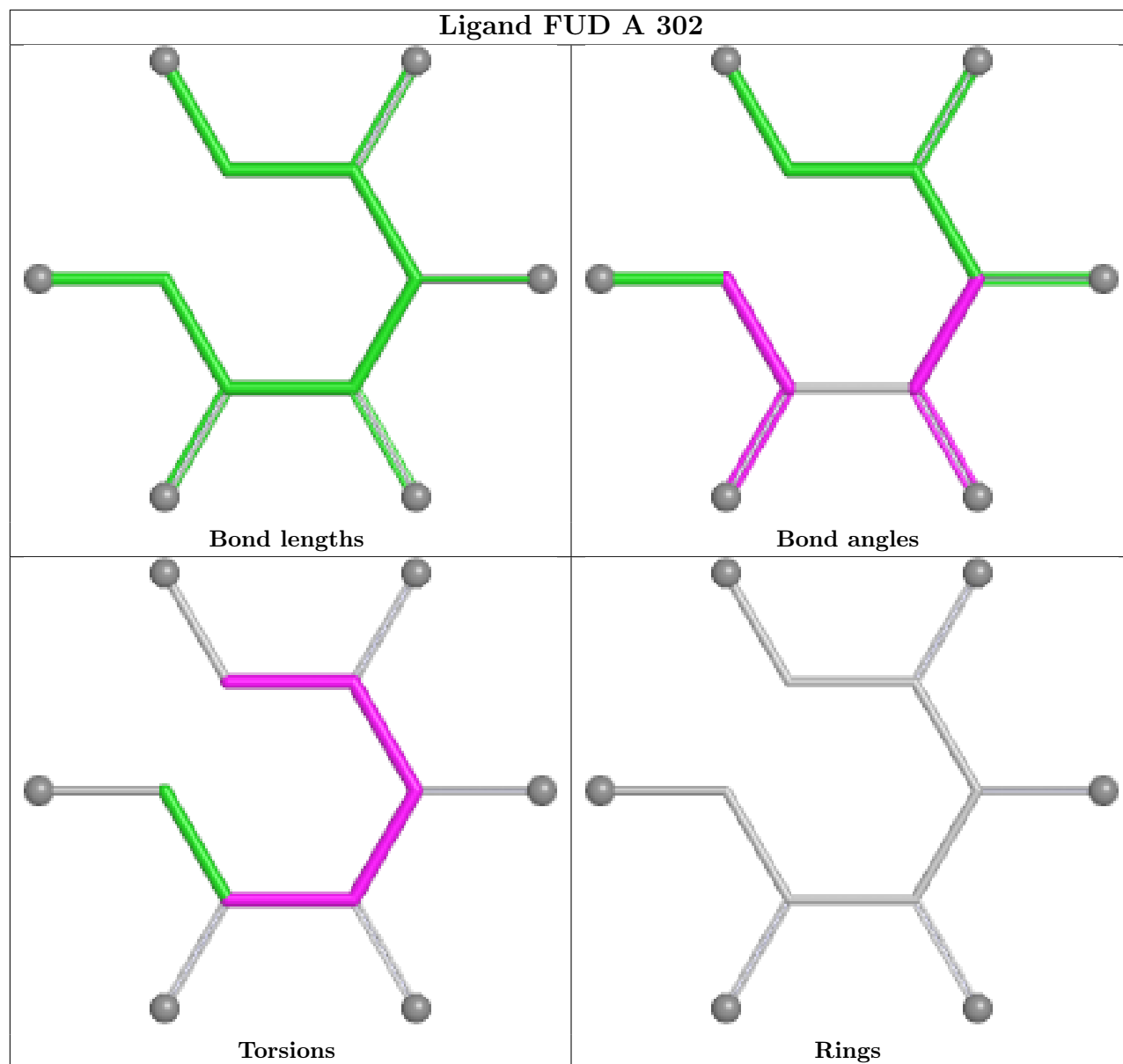


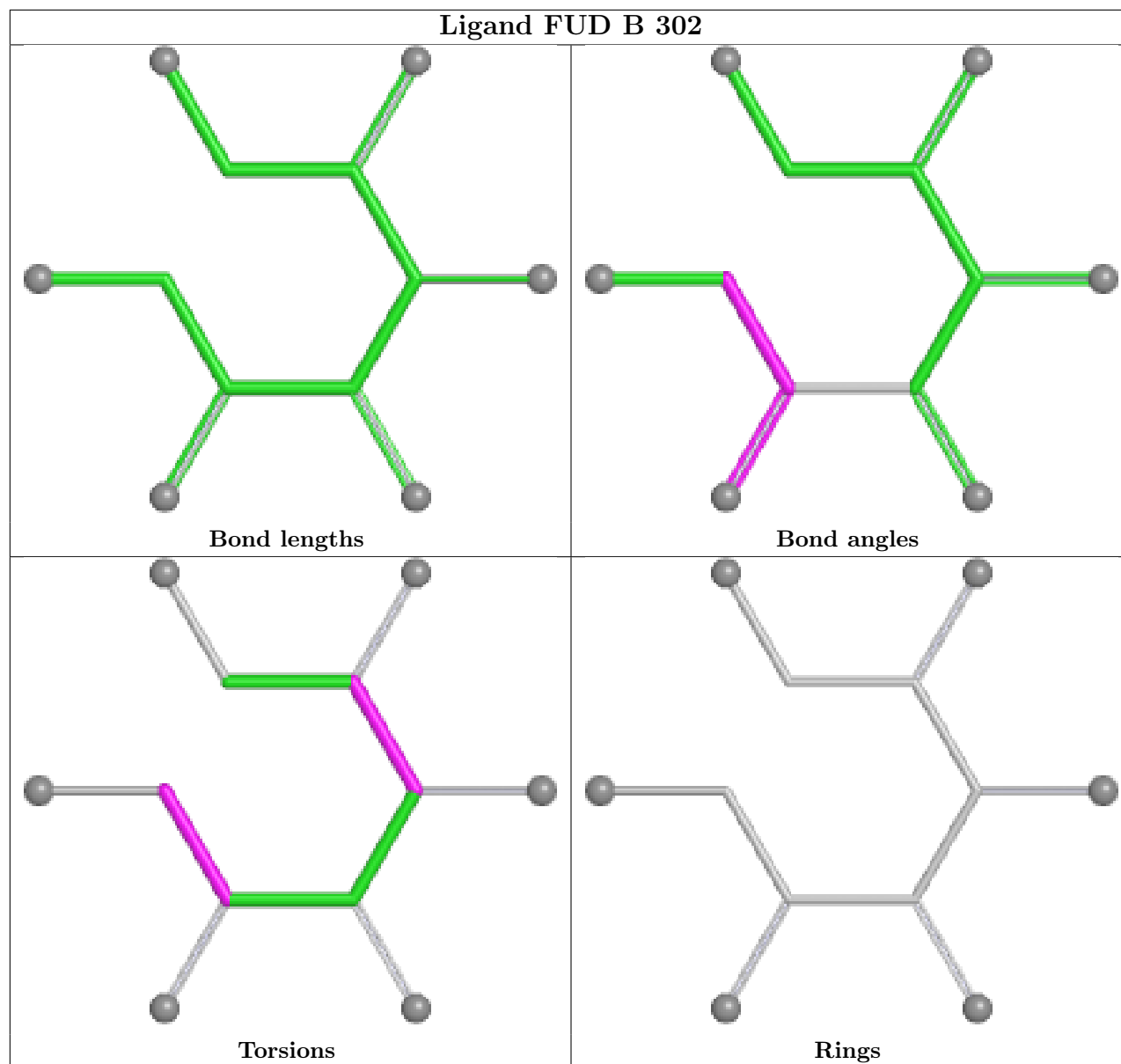


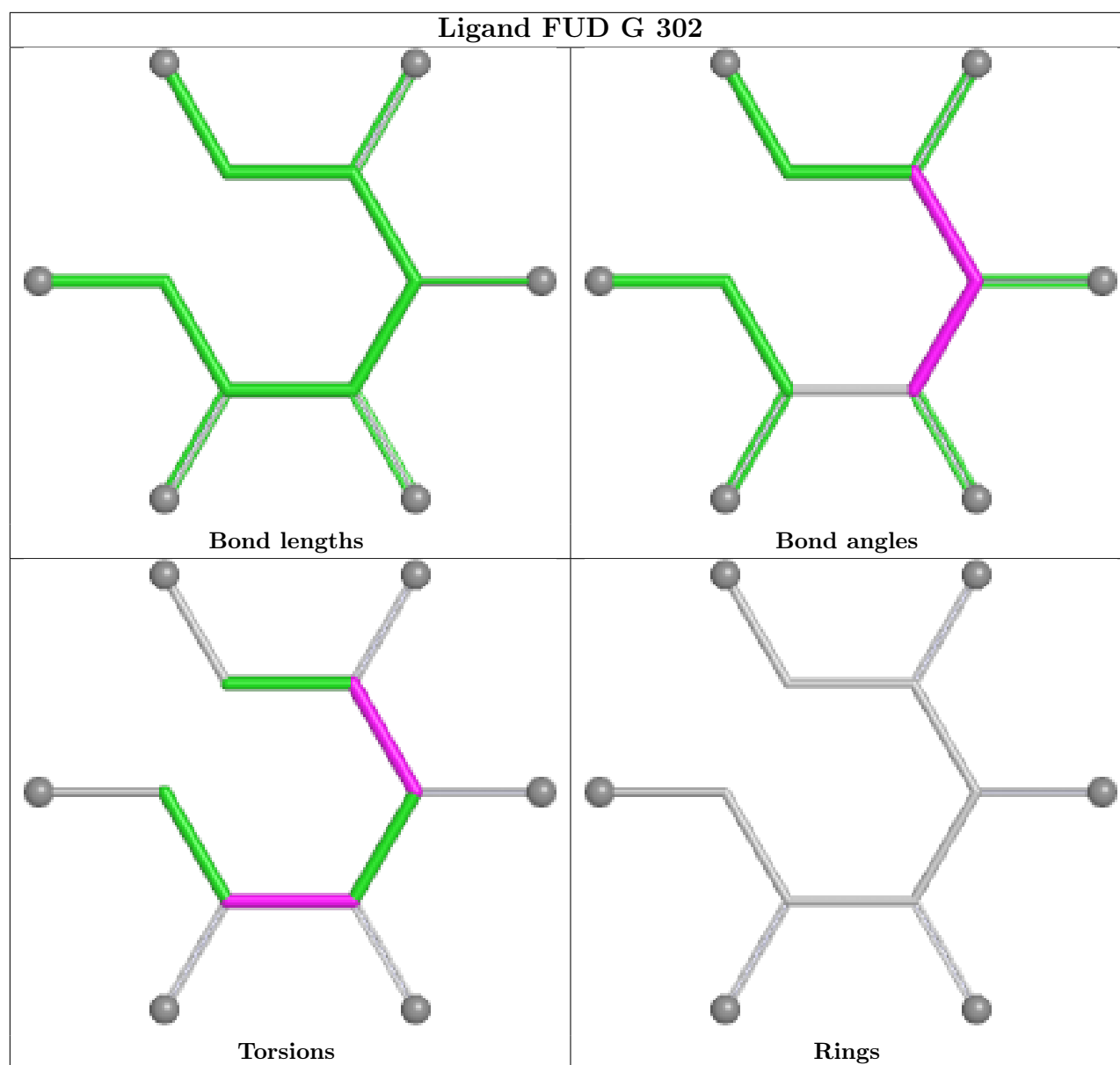












5.7 Other polymers [i](#)

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	286/316 (90%)	0.18	5 (1%) 69 78	12, 18, 31, 41	2 (0%)
1	B	290/316 (91%)	0.39	17 (5%) 28 38	12, 20, 34, 57	1 (0%)
1	C	288/316 (91%)	0.08	6 (2%) 63 73	12, 18, 31, 49	2 (0%)
1	D	289/316 (91%)	0.36	10 (3%) 47 59	13, 21, 33, 64	1 (0%)
1	E	288/316 (91%)	0.55	22 (7%) 20 29	13, 21, 35, 62	2 (0%)
1	F	287/316 (90%)	0.02	1 (0%) 90 91	13, 18, 30, 50	0
1	G	286/316 (90%)	0.51	15 (5%) 33 44	15, 23, 36, 50	0
1	H	288/316 (91%)	0.24	4 (1%) 73 81	13, 19, 32, 63	1 (0%)
All	All	2302/2528 (91%)	0.29	80 (3%) 47 59	12, 20, 33, 64	9 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	289	ILE	5.2
1	E	267	LEU	4.4
1	D	1	MET	4.4
1	H	0	SER	4.3
1	E	288	ALA	3.9
1	E	1	MET	3.8
1	B	289	ILE	3.6
1	G	14	LEU	3.4
1	B	288	ALA	3.4
1	G	255	PRO	3.3
1	G	256	LYS	3.2
1	A	44	LEU	3.2
1	A	50	ILE	3.1
1	B	253	VAL	3.1
1	E	256	LYS	3.1
1	D	255	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	269	HIS	2.9
1	B	287	THR	2.9
1	B	14	LEU	2.9
1	C	50	ILE	2.9
1	D	50	ILE	2.9
1	C	-1	HIS	2.8
1	B	1	MET	2.8
1	E	248	PHE	2.8
1	C	45	LEU	2.8
1	B	60	GLN	2.7
1	G	22	ALA	2.7
1	D	253	VAL	2.7
1	H	269	HIS	2.7
1	E	257	LEU	2.6
1	G	1	MET	2.6
1	G	252	ILE	2.6
1	C	286	LEU	2.5
1	D	269	HIS	2.5
1	E	48	TRP	2.5
1	A	286	LEU	2.5
1	B	252	ILE	2.5
1	E	253	VAL	2.5
1	H	287	THR	2.4
1	A	269	HIS	2.4
1	G	253	VAL	2.4
1	B	255	PRO	2.4
1	H	267	LEU	2.4
1	G	60	GLN	2.3
1	F	0	SER	2.3
1	B	250	SER	2.3
1	G	240	ARG	2.3
1	E	2	ALA	2.3
1	D	286	LEU	2.3
1	E	286	LEU	2.3
1	G	267	LEU	2.3
1	E	60	GLN	2.2
1	E	251	GLU	2.2
1	E	50	ILE	2.2
1	B	257	LEU	2.2
1	E	252	ILE	2.2
1	D	48	TRP	2.2
1	E	49	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	254	ASP	2.2
1	G	43	ALA	2.1
1	B	206	ARG	2.1
1	G	206	ARG	2.1
1	B	50	ILE	2.1
1	E	254	ASP	2.1
1	B	258	SER	2.1
1	E	100	LEU	2.1
1	A	256	LYS	2.1
1	G	50	ILE	2.1
1	C	60	GLN	2.1
1	E	249	SER	2.1
1	G	166	LEU	2.0
1	C	49	GLN	2.0
1	D	60	GLN	2.0
1	E	250	SER	2.0
1	B	48	TRP	2.0
1	E	232	ALA	2.0
1	G	248	PHE	2.0
1	B	286	LEU	2.0
1	D	44	LEU	2.0
1	E	14	LEU	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
5	EDO	C	303	4/4	0.81	0.15	29,31,31,33	0

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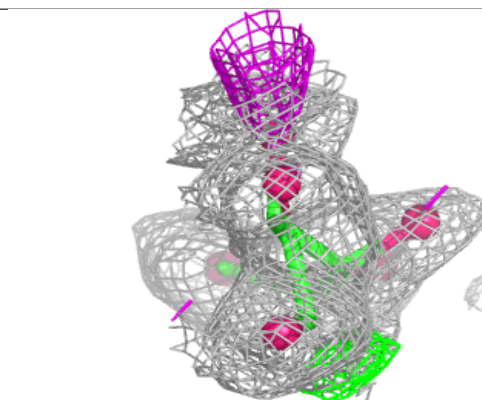
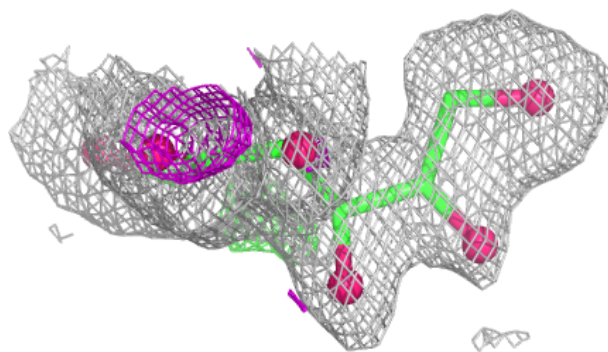
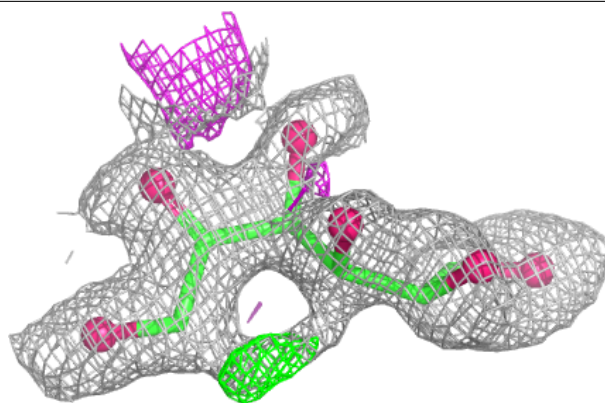
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	E	301	4/4	0.86	0.12	26,26,27,31	0
5	EDO	C	302	4/4	0.87	0.11	26,30,30,33	0
4	EPE	H	303	15/15	0.89	0.12	23,30,59,64	0
5	EDO	D	301	4/4	0.89	0.11	28,28,31,31	0
4	EPE	A	303	15/15	0.89	0.14	22,38,62,62	0
5	EDO	C	301	4/4	0.90	0.17	29,30,33,37	0
4	EPE	F	305	15/15	0.92	0.12	18,30,49,55	0
4	EPE	G	303	15/15	0.92	0.10	23,27,50,52	0
3	FUD	H	302	12/12	0.92	0.13	14,28,35,41	0
3	FUD	G	302	12/12	0.92	0.13	18,29,39,45	0
3	FUD	F	304	12/12	0.93	0.10	14,19,32,36	0
3	FUD	A	302	12/12	0.93	0.13	14,26,39,41	0
3	FUD	B	302	12/12	0.93	0.13	17,26,38,46	0
3	FUD	D	303	12/12	0.93	0.11	17,25,35,45	0
4	EPE	B	303	15/15	0.93	0.10	18,23,45,47	0
4	EPE	C	306	15/15	0.93	0.10	17,22,40,40	0
3	FUD	E	303	12/12	0.93	0.11	16,24,35,41	0
5	EDO	F	301	4/4	0.93	0.11	21,28,30,31	0
5	EDO	F	302	4/4	0.93	0.10	23,23,25,32	0
4	EPE	E	304	15/15	0.94	0.09	21,24,35,37	0
4	EPE	D	304	15/15	0.95	0.09	19,28,40,40	0
3	FUD	C	305	12/12	0.95	0.10	16,20,29,37	0
2	MN	H	301	1/1	0.98	0.10	20,20,20,20	0
2	MN	A	301	1/1	0.99	0.12	20,20,20,20	0
2	MN	B	301	1/1	0.99	0.11	21,21,21,21	0
2	MN	C	304	1/1	0.99	0.09	17,17,17,17	0
2	MN	D	302	1/1	0.99	0.11	21,21,21,21	0
2	MN	E	302	1/1	0.99	0.10	21,21,21,21	0
2	MN	F	303	1/1	0.99	0.10	18,18,18,18	0
2	MN	G	301	1/1	1.00	0.11	23,23,23,23	0

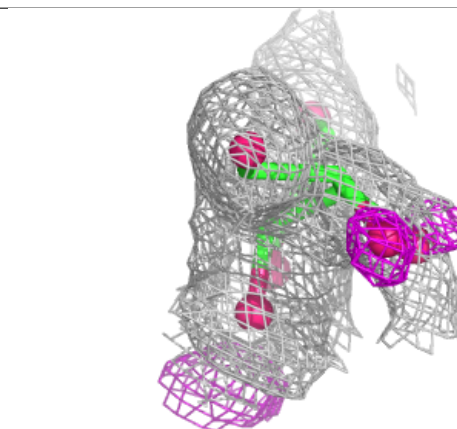
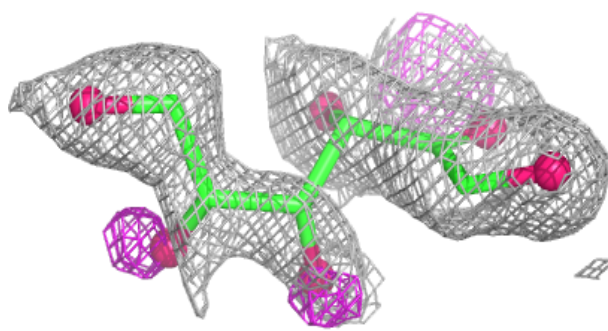
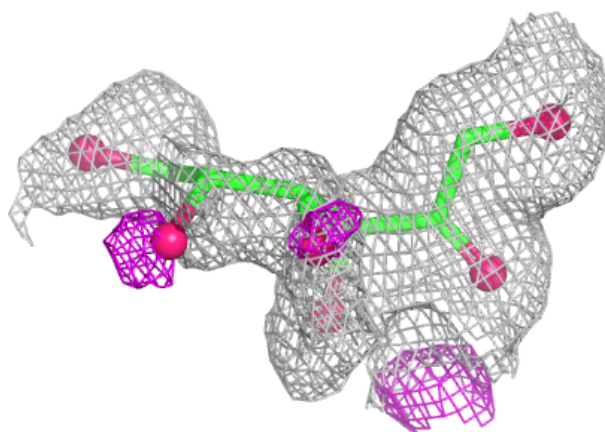
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FUD H 302:

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

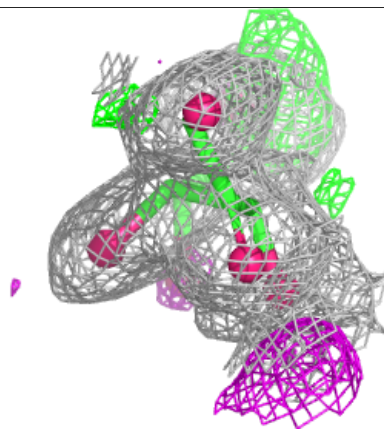
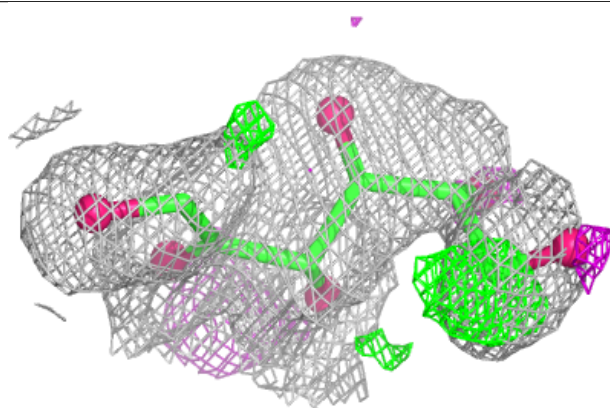
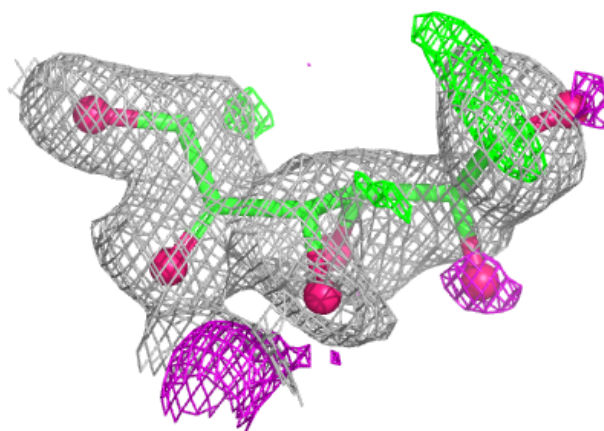
**Electron density around FUD G 302:**

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



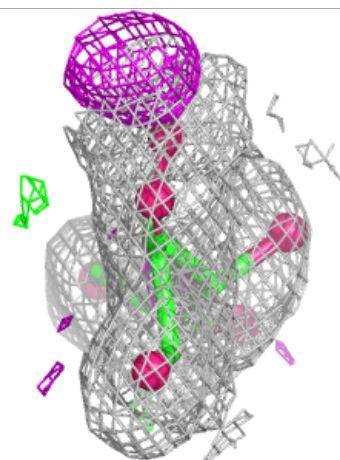
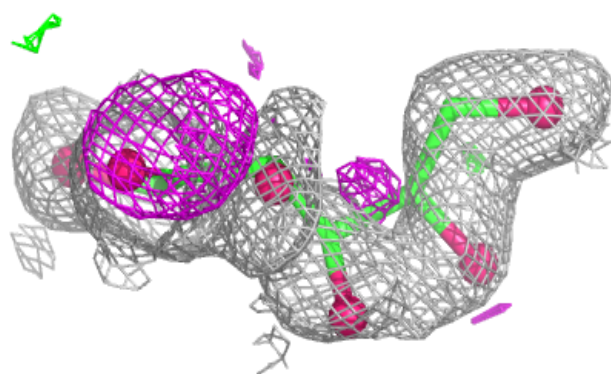
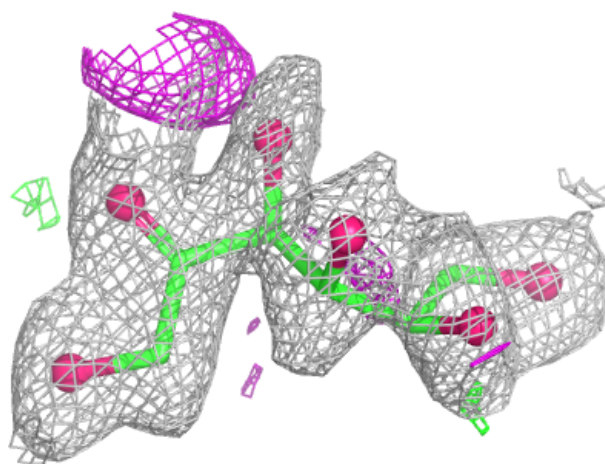
Electron density around FUD F 304:

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



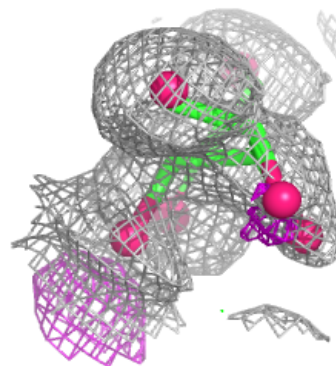
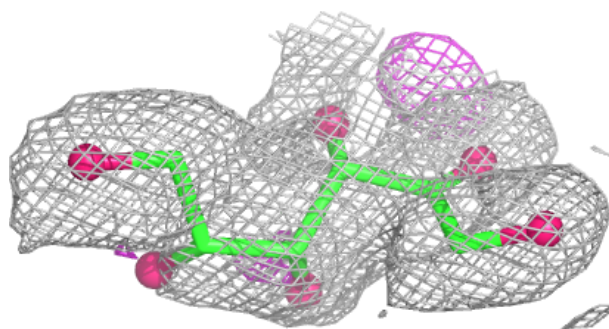
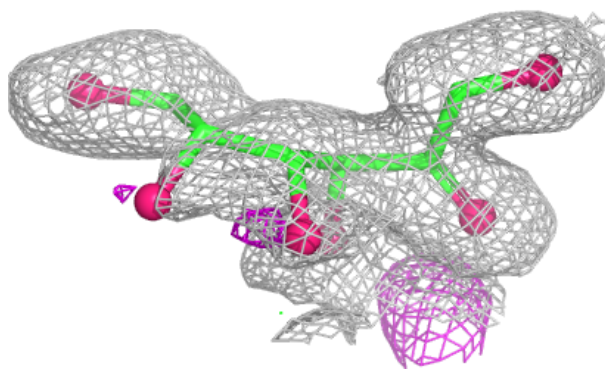
Electron density around FUD A 302:

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

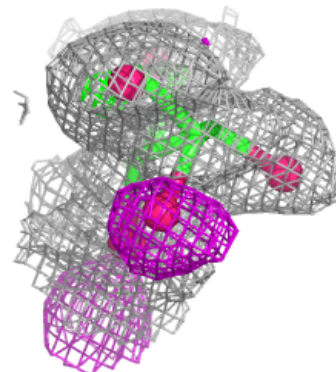
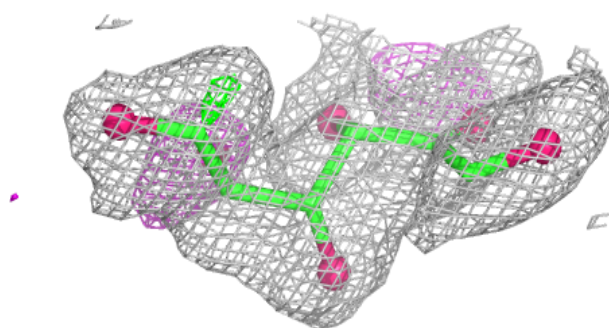
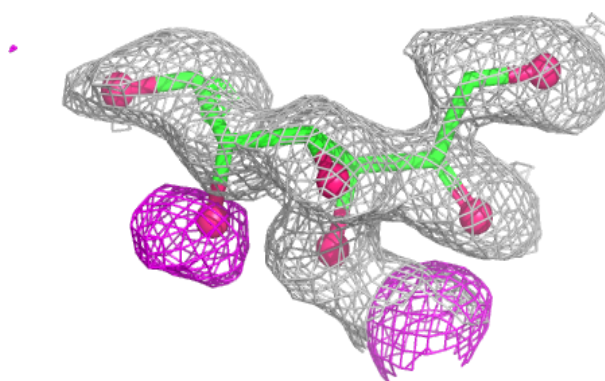


Electron density around FUD B 302:

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

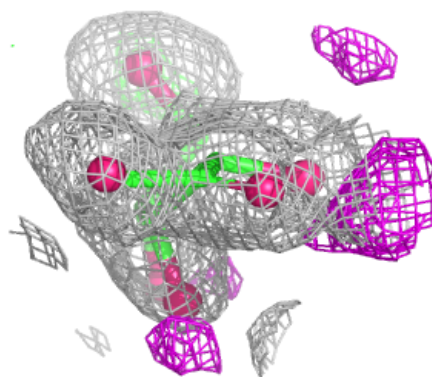
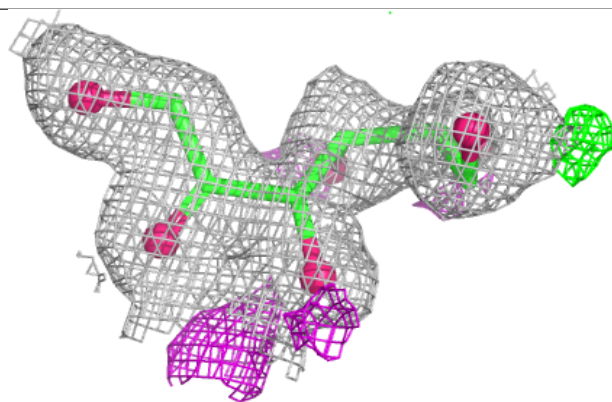
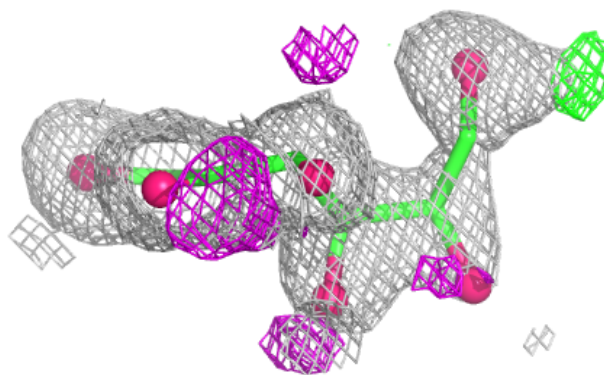
**Electron density around FUD D 303:**

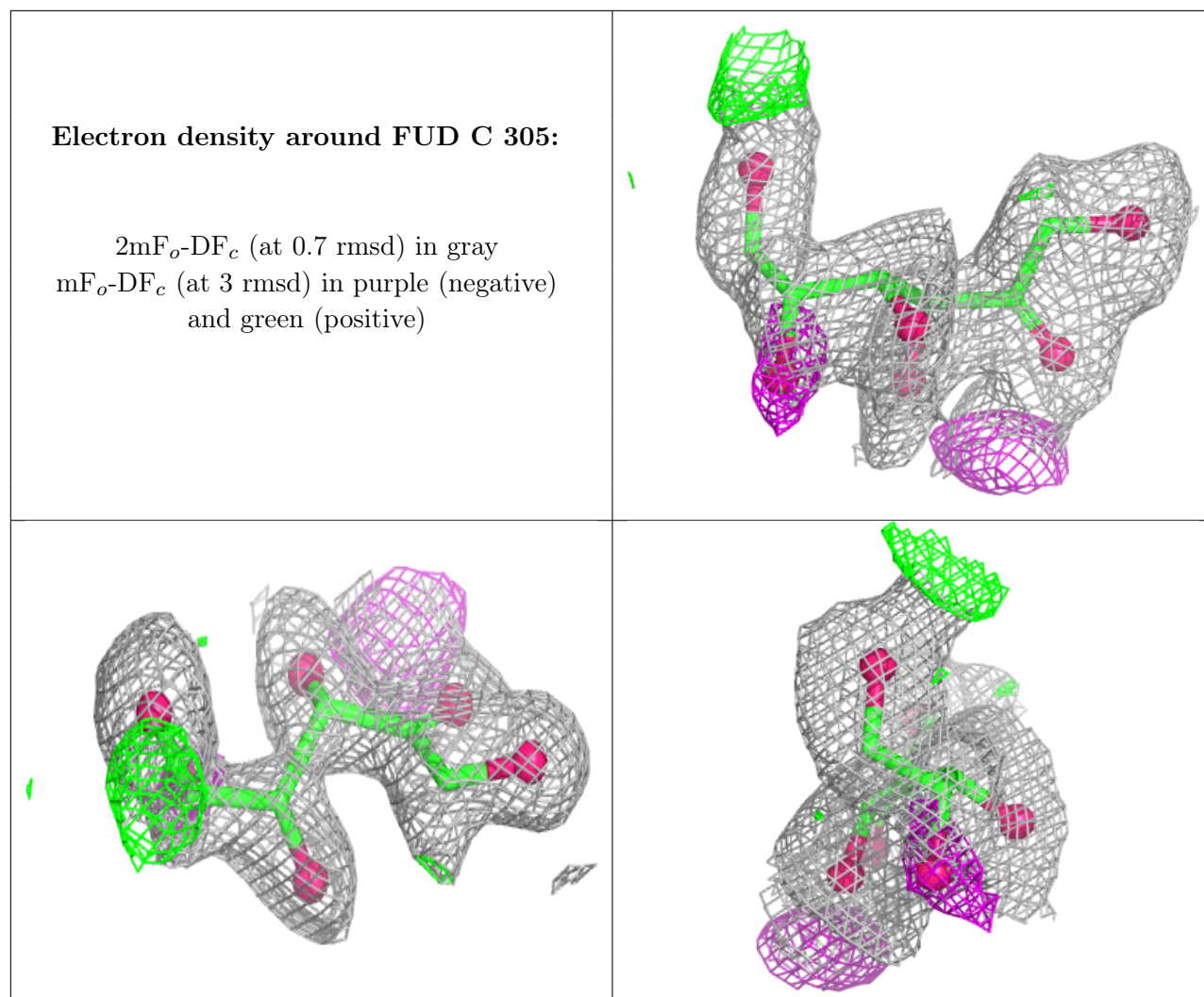
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FUD E 303:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.