



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:19 PM UTC

PDB ID : 7RNL / pdb_00007rnl
EMDB ID : EMD-24579
Title : Yeast CTP Synthase (Ura7) H360R Filament bound to Substrates
Authors : Hansen, J.M.; Lynch, E.M.; Farrell, D.P.; DiMaio, F.; Quispe, J.; Kollman, J.M.
Deposited on : 2021-07-29
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

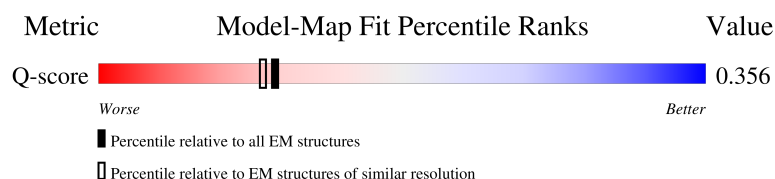
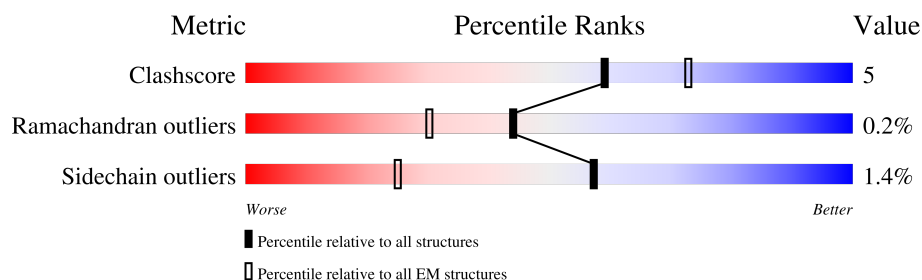
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	
1	B	559	
1	C	559	
1	D	559	

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Mol	Chain	Length	Quality of chain
1	E	559	
1	F	559	
1	G	559	
1	H	559	
1	I	559	
1	J	559	
1	K	559	
1	L	559	
1	M	559	
1	N	559	
1	O	559	
1	P	559	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CTP	A	601	X	-	-	-
2	CTP	A	604	-	-	X	-
2	CTP	B	601	X	-	-	-
2	CTP	C	602	X	-	-	-
2	CTP	D	602	X	-	-	-
2	CTP	E	601	X	-	-	-
2	CTP	E	604	-	-	X	-
2	CTP	F	601	X	-	-	-
2	CTP	F	604	-	-	X	-
2	CTP	G	601	X	-	-	-
2	CTP	G	604	-	-	X	-
2	CTP	H	601	X	-	-	-
2	CTP	I	601	X	-	-	-
2	CTP	J	601	X	-	-	-
2	CTP	K	602	X	-	-	-
2	CTP	L	602	X	-	-	-
2	CTP	M	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CTP	N	602	X	-	-	-
2	CTP	O	602	X	-	-	-
2	CTP	P	602	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 141472 atoms, of which 70352 are hydrogens and 0 are deuteriums.

In the tables below, 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 CTP synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	A	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	C	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	D	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	H	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	E	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	K	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	N	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	I	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	F	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	L	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	O	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	J	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	G	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	M	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		
1	P	559	Total	C	H	N	O	S	0	0
			8766	2775	4381	757	833	20		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP A0A6A5PYW3
B	?	-	MET	deletion	UNP A0A6A5PYW3
B	?	-	PRO	deletion	UNP A0A6A5PYW3
B	?	-	GLU	deletion	UNP A0A6A5PYW3
B	?	-	ILE	deletion	UNP A0A6A5PYW3
B	?	-	ASP	deletion	UNP A0A6A5PYW3
B	?	-	LYS	deletion	UNP A0A6A5PYW3
B	?	-	GLU	deletion	UNP A0A6A5PYW3
B	?	-	HIS	deletion	UNP A0A6A5PYW3
B	?	-	MET	deletion	UNP A0A6A5PYW3
B	?	-	GLY	deletion	UNP A0A6A5PYW3
B	?	-	GLY	deletion	UNP A0A6A5PYW3
A	?	-	TYR	deletion	UNP A0A6A5PYW3
A	?	-	MET	deletion	UNP A0A6A5PYW3
A	?	-	PRO	deletion	UNP A0A6A5PYW3
A	?	-	GLU	deletion	UNP A0A6A5PYW3
A	?	-	ILE	deletion	UNP A0A6A5PYW3
A	?	-	ASP	deletion	UNP A0A6A5PYW3
A	?	-	LYS	deletion	UNP A0A6A5PYW3
A	?	-	GLU	deletion	UNP A0A6A5PYW3
A	?	-	HIS	deletion	UNP A0A6A5PYW3
A	?	-	MET	deletion	UNP A0A6A5PYW3
A	?	-	GLY	deletion	UNP A0A6A5PYW3
A	?	-	GLY	deletion	UNP A0A6A5PYW3
C	?	-	TYR	deletion	UNP A0A6A5PYW3
C	?	-	MET	deletion	UNP A0A6A5PYW3
C	?	-	PRO	deletion	UNP A0A6A5PYW3
C	?	-	GLU	deletion	UNP A0A6A5PYW3
C	?	-	ILE	deletion	UNP A0A6A5PYW3
C	?	-	ASP	deletion	UNP A0A6A5PYW3
C	?	-	LYS	deletion	UNP A0A6A5PYW3
C	?	-	GLU	deletion	UNP A0A6A5PYW3
C	?	-	HIS	deletion	UNP A0A6A5PYW3
C	?	-	MET	deletion	UNP A0A6A5PYW3
C	?	-	GLY	deletion	UNP A0A6A5PYW3
C	?	-	GLY	deletion	UNP A0A6A5PYW3
D	?	-	TYR	deletion	UNP A0A6A5PYW3
D	?	-	MET	deletion	UNP A0A6A5PYW3
D	?	-	PRO	deletion	UNP A0A6A5PYW3
D	?	-	GLU	deletion	UNP A0A6A5PYW3
D	?	-	ILE	deletion	UNP A0A6A5PYW3
D	?	-	ASP	deletion	UNP A0A6A5PYW3
D	?	-	LYS	deletion	UNP A0A6A5PYW3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP A0A6A5PYW3
D	?	-	HIS	deletion	UNP A0A6A5PYW3
D	?	-	MET	deletion	UNP A0A6A5PYW3
D	?	-	GLY	deletion	UNP A0A6A5PYW3
D	?	-	GLY	deletion	UNP A0A6A5PYW3
H	?	-	TYR	deletion	UNP A0A6A5PYW3
H	?	-	MET	deletion	UNP A0A6A5PYW3
H	?	-	PRO	deletion	UNP A0A6A5PYW3
H	?	-	GLU	deletion	UNP A0A6A5PYW3
H	?	-	ILE	deletion	UNP A0A6A5PYW3
H	?	-	ASP	deletion	UNP A0A6A5PYW3
H	?	-	LYS	deletion	UNP A0A6A5PYW3
H	?	-	GLU	deletion	UNP A0A6A5PYW3
H	?	-	HIS	deletion	UNP A0A6A5PYW3
H	?	-	MET	deletion	UNP A0A6A5PYW3
H	?	-	GLY	deletion	UNP A0A6A5PYW3
H	?	-	GLY	deletion	UNP A0A6A5PYW3
E	?	-	TYR	deletion	UNP A0A6A5PYW3
E	?	-	MET	deletion	UNP A0A6A5PYW3
E	?	-	PRO	deletion	UNP A0A6A5PYW3
E	?	-	GLU	deletion	UNP A0A6A5PYW3
E	?	-	ILE	deletion	UNP A0A6A5PYW3
E	?	-	ASP	deletion	UNP A0A6A5PYW3
E	?	-	LYS	deletion	UNP A0A6A5PYW3
E	?	-	GLU	deletion	UNP A0A6A5PYW3
E	?	-	HIS	deletion	UNP A0A6A5PYW3
E	?	-	MET	deletion	UNP A0A6A5PYW3
E	?	-	GLY	deletion	UNP A0A6A5PYW3
E	?	-	GLY	deletion	UNP A0A6A5PYW3
K	?	-	TYR	deletion	UNP A0A6A5PYW3
K	?	-	MET	deletion	UNP A0A6A5PYW3
K	?	-	PRO	deletion	UNP A0A6A5PYW3
K	?	-	GLU	deletion	UNP A0A6A5PYW3
K	?	-	ILE	deletion	UNP A0A6A5PYW3
K	?	-	ASP	deletion	UNP A0A6A5PYW3
K	?	-	LYS	deletion	UNP A0A6A5PYW3
K	?	-	GLU	deletion	UNP A0A6A5PYW3
K	?	-	HIS	deletion	UNP A0A6A5PYW3
K	?	-	MET	deletion	UNP A0A6A5PYW3
K	?	-	GLY	deletion	UNP A0A6A5PYW3
K	?	-	GLY	deletion	UNP A0A6A5PYW3
N	?	-	TYR	deletion	UNP A0A6A5PYW3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	MET	deletion	UNP A0A6A5PYW3
N	?	-	PRO	deletion	UNP A0A6A5PYW3
N	?	-	GLU	deletion	UNP A0A6A5PYW3
N	?	-	ILE	deletion	UNP A0A6A5PYW3
N	?	-	ASP	deletion	UNP A0A6A5PYW3
N	?	-	LYS	deletion	UNP A0A6A5PYW3
N	?	-	GLU	deletion	UNP A0A6A5PYW3
N	?	-	HIS	deletion	UNP A0A6A5PYW3
N	?	-	MET	deletion	UNP A0A6A5PYW3
N	?	-	GLY	deletion	UNP A0A6A5PYW3
N	?	-	GLY	deletion	UNP A0A6A5PYW3
I	?	-	TYR	deletion	UNP A0A6A5PYW3
I	?	-	MET	deletion	UNP A0A6A5PYW3
I	?	-	PRO	deletion	UNP A0A6A5PYW3
I	?	-	GLU	deletion	UNP A0A6A5PYW3
I	?	-	ILE	deletion	UNP A0A6A5PYW3
I	?	-	ASP	deletion	UNP A0A6A5PYW3
I	?	-	LYS	deletion	UNP A0A6A5PYW3
I	?	-	GLU	deletion	UNP A0A6A5PYW3
I	?	-	HIS	deletion	UNP A0A6A5PYW3
I	?	-	MET	deletion	UNP A0A6A5PYW3
I	?	-	GLY	deletion	UNP A0A6A5PYW3
I	?	-	GLY	deletion	UNP A0A6A5PYW3
F	?	-	TYR	deletion	UNP A0A6A5PYW3
F	?	-	MET	deletion	UNP A0A6A5PYW3
F	?	-	PRO	deletion	UNP A0A6A5PYW3
F	?	-	GLU	deletion	UNP A0A6A5PYW3
F	?	-	ILE	deletion	UNP A0A6A5PYW3
F	?	-	ASP	deletion	UNP A0A6A5PYW3
F	?	-	LYS	deletion	UNP A0A6A5PYW3
F	?	-	GLU	deletion	UNP A0A6A5PYW3
F	?	-	HIS	deletion	UNP A0A6A5PYW3
F	?	-	MET	deletion	UNP A0A6A5PYW3
F	?	-	GLY	deletion	UNP A0A6A5PYW3
F	?	-	GLY	deletion	UNP A0A6A5PYW3
L	?	-	TYR	deletion	UNP A0A6A5PYW3
L	?	-	MET	deletion	UNP A0A6A5PYW3
L	?	-	PRO	deletion	UNP A0A6A5PYW3
L	?	-	GLU	deletion	UNP A0A6A5PYW3
L	?	-	ILE	deletion	UNP A0A6A5PYW3
L	?	-	ASP	deletion	UNP A0A6A5PYW3
L	?	-	LYS	deletion	UNP A0A6A5PYW3

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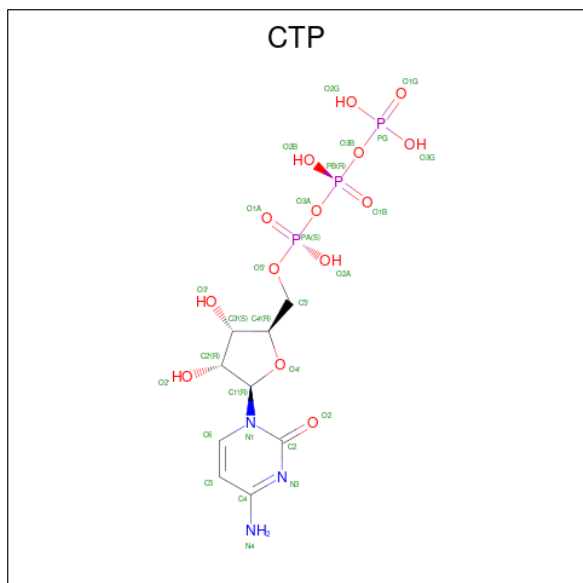
Chain	Residue	Modelled	Actual	Comment	Reference
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L	?	-	HIS	deletion	UNP A0A6A5PYW3
L	?	-	MET	deletion	UNP A0A6A5PYW3
L	?	-	GLY	deletion	UNP A0A6A5PYW3
L	?	-	GLY	deletion	UNP A0A6A5PYW3
O	?	-	TYR	deletion	UNP A0A6A5PYW3
O	?	-	MET	deletion	UNP A0A6A5PYW3
O	?	-	PRO	deletion	UNP A0A6A5PYW3
O	?	-	GLU	deletion	UNP A0A6A5PYW3
O	?	-	ILE	deletion	UNP A0A6A5PYW3
O	?	-	ASP	deletion	UNP A0A6A5PYW3
O	?	-	LYS	deletion	UNP A0A6A5PYW3
O	?	-	GLU	deletion	UNP A0A6A5PYW3
O	?	-	HIS	deletion	UNP A0A6A5PYW3
O	?	-	MET	deletion	UNP A0A6A5PYW3
O	?	-	GLY	deletion	UNP A0A6A5PYW3
O	?	-	GLY	deletion	UNP A0A6A5PYW3
J	?	-	TYR	deletion	UNP A0A6A5PYW3
J	?	-	MET	deletion	UNP A0A6A5PYW3
J	?	-	PRO	deletion	UNP A0A6A5PYW3
J	?	-	GLU	deletion	UNP A0A6A5PYW3
J	?	-	ILE	deletion	UNP A0A6A5PYW3
J	?	-	ASP	deletion	UNP A0A6A5PYW3
J	?	-	LYS	deletion	UNP A0A6A5PYW3
J	?	-	GLU	deletion	UNP A0A6A5PYW3
J	?	-	HIS	deletion	UNP A0A6A5PYW3
J	?	-	MET	deletion	UNP A0A6A5PYW3
J	?	-	GLY	deletion	UNP A0A6A5PYW3
J	?	-	GLY	deletion	UNP A0A6A5PYW3
G	?	-	TYR	deletion	UNP A0A6A5PYW3
G	?	-	MET	deletion	UNP A0A6A5PYW3
G	?	-	PRO	deletion	UNP A0A6A5PYW3
G	?	-	GLU	deletion	UNP A0A6A5PYW3
G	?	-	ILE	deletion	UNP A0A6A5PYW3
G	?	-	ASP	deletion	UNP A0A6A5PYW3
G	?	-	LYS	deletion	UNP A0A6A5PYW3
G	?	-	GLU	deletion	UNP A0A6A5PYW3
G	?	-	HIS	deletion	UNP A0A6A5PYW3
G	?	-	MET	deletion	UNP A0A6A5PYW3
G	?	-	GLY	deletion	UNP A0A6A5PYW3
G	?	-	GLY	deletion	UNP A0A6A5PYW3
M	?	-	TYR	deletion	UNP A0A6A5PYW3

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Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	MET	deletion	UNP A0A6A5PYW3
M	?	-	PRO	deletion	UNP A0A6A5PYW3
M	?	-	GLU	deletion	UNP A0A6A5PYW3
M	?	-	ILE	deletion	UNP A0A6A5PYW3
M	?	-	ASP	deletion	UNP A0A6A5PYW3
M	?	-	LYS	deletion	UNP A0A6A5PYW3
M	?	-	GLU	deletion	UNP A0A6A5PYW3
M	?	-	HIS	deletion	UNP A0A6A5PYW3
M	?	-	MET	deletion	UNP A0A6A5PYW3
M	?	-	GLY	deletion	UNP A0A6A5PYW3
M	?	-	GLY	deletion	UNP A0A6A5PYW3
P	?	-	TYR	deletion	UNP A0A6A5PYW3
P	?	-	MET	deletion	UNP A0A6A5PYW3
P	?	-	PRO	deletion	UNP A0A6A5PYW3
P	?	-	GLU	deletion	UNP A0A6A5PYW3
P	?	-	ILE	deletion	UNP A0A6A5PYW3
P	?	-	ASP	deletion	UNP A0A6A5PYW3
P	?	-	LYS	deletion	UNP A0A6A5PYW3
P	?	-	GLU	deletion	UNP A0A6A5PYW3
P	?	-	HIS	deletion	UNP A0A6A5PYW3
P	?	-	MET	deletion	UNP A0A6A5PYW3
P	?	-	GLY	deletion	UNP A0A6A5PYW3
P	?	-	GLY	deletion	UNP A0A6A5PYW3

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	B	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	A	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	A	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	A	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	C	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	D	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	D	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	H	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	H	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	E	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	E	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	E	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	K	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	N	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	N	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	I	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	I	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	F	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	F	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	F	1	Total 37	C 9	H 8	N 3	O 14	P 3	0
2	L	1	Total 37	C 9	H 8	N 3	O 14	P 3	0

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Mol	Chain	Residues	Atoms						AltConf
2	O	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	O	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	J	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	J	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	G	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	G	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	G	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	M	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	P	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	
2	P	1	Total	C	H	N	O	P	0
			37	9	8	3	14	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	B	2	Total	Mg	0
			2	2	
3	A	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	
3	D	2	Total	Mg	0
			2	2	
3	H	2	Total	Mg	0
			2	2	
3	E	2	Total	Mg	0
			2	2	
3	K	2	Total	Mg	0
			2	2	
3	N	2	Total	Mg	0
			2	2	
3	I	2	Total	Mg	0
			2	2	

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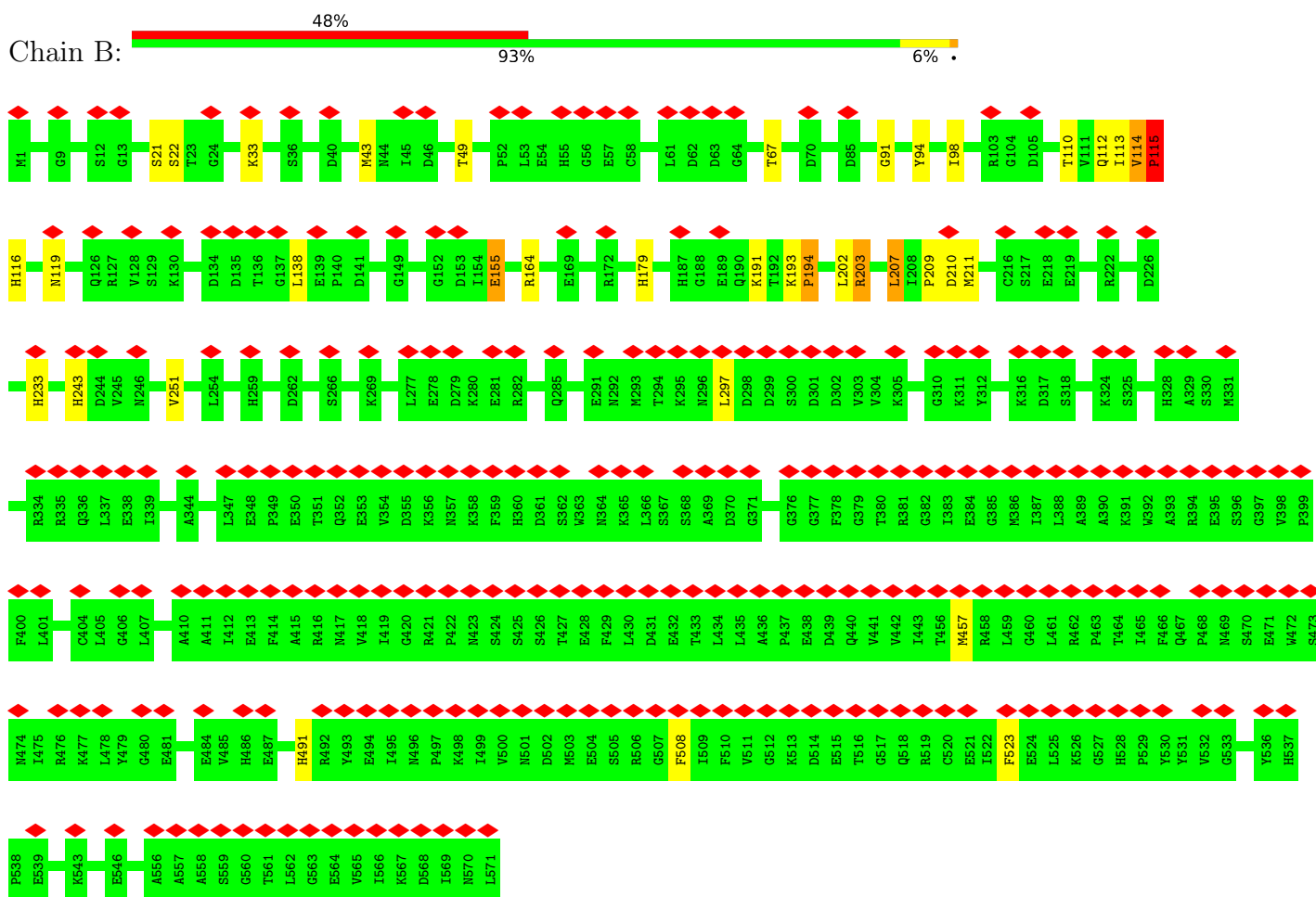
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Mol	Chain	Residues	Atoms		AltConf
3	F	2	Total 2	Mg 2	0
3	L	2	Total 2	Mg 2	0
3	O	2	Total 2	Mg 2	0
3	J	2	Total 2	Mg 2	0
3	G	2	Total 2	Mg 2	0
3	M	2	Total 2	Mg 2	0
3	P	2	Total 2	Mg 2	0

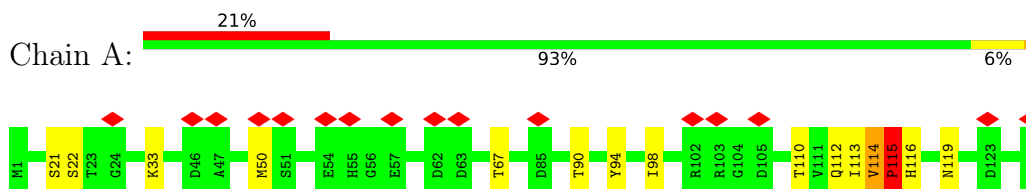
3 Residue-property plots

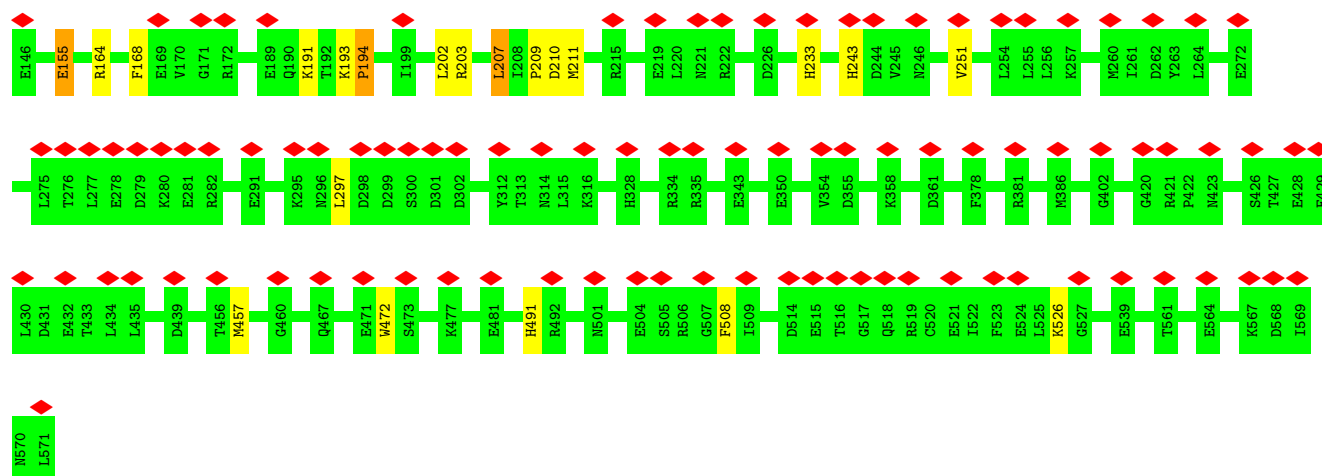
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: CTP synthase

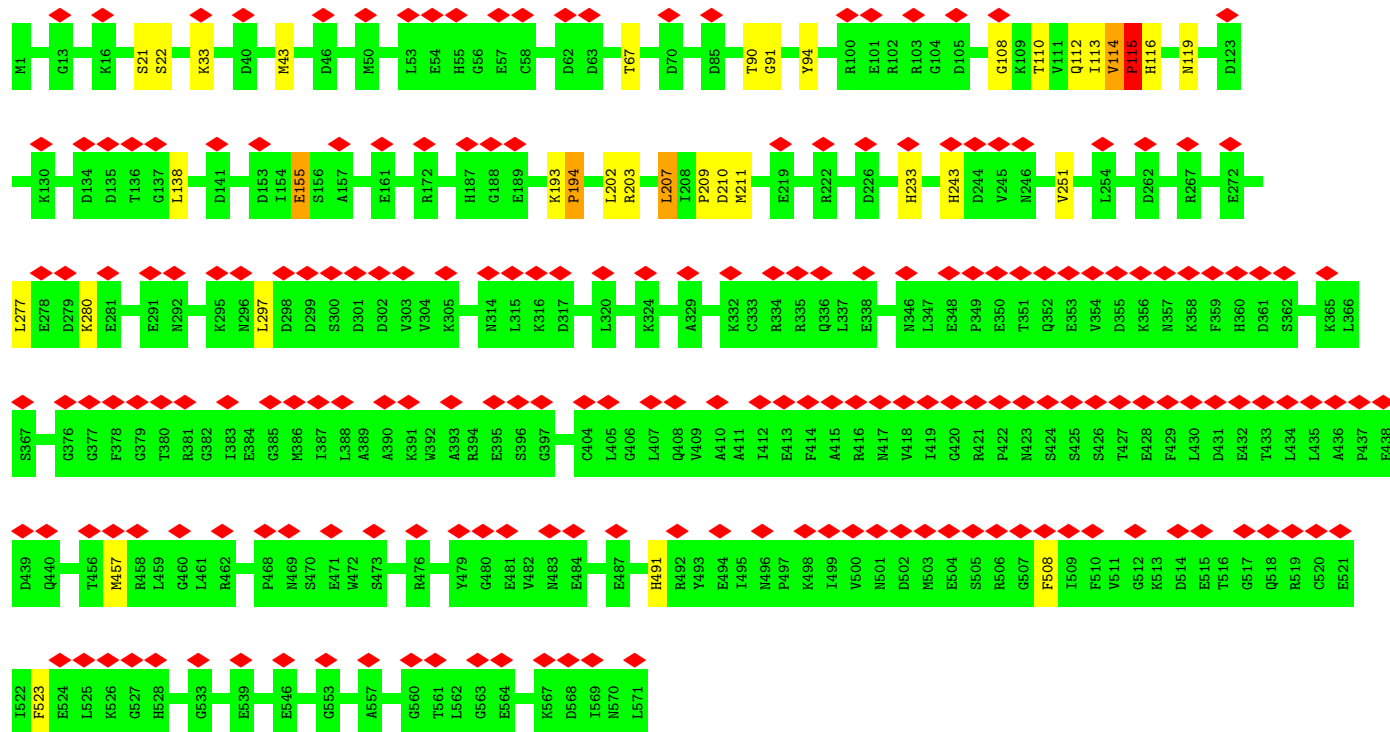


• Molecule 1: CTP synthase

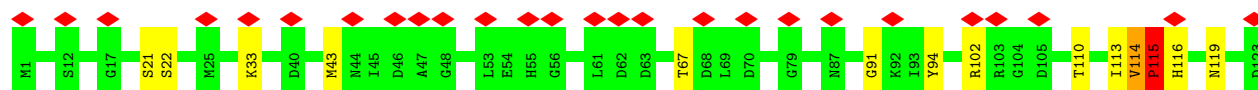


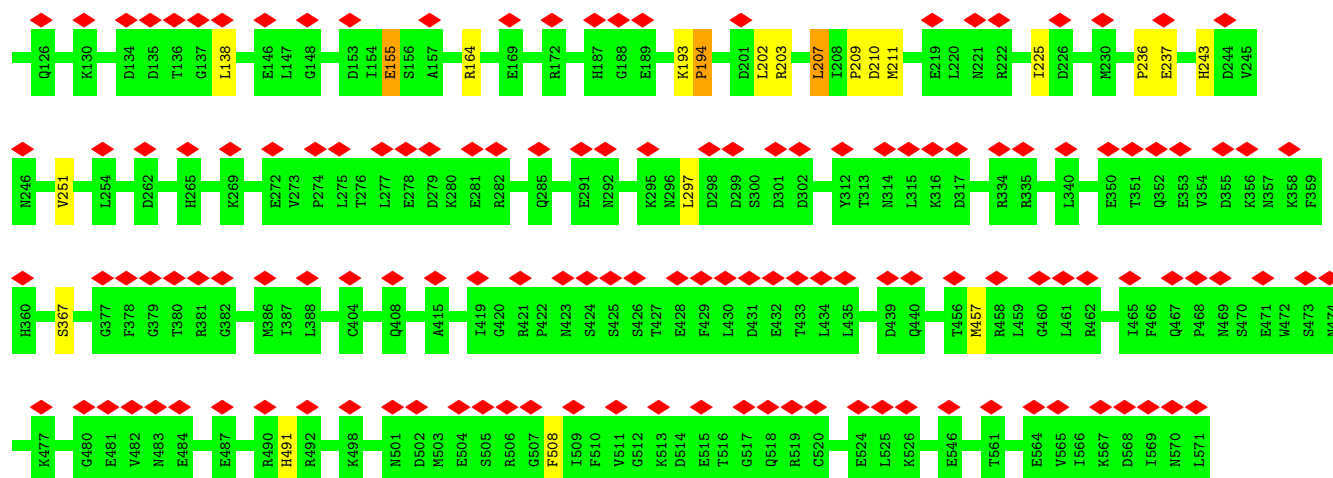


• Molecule 1: CTP synthase

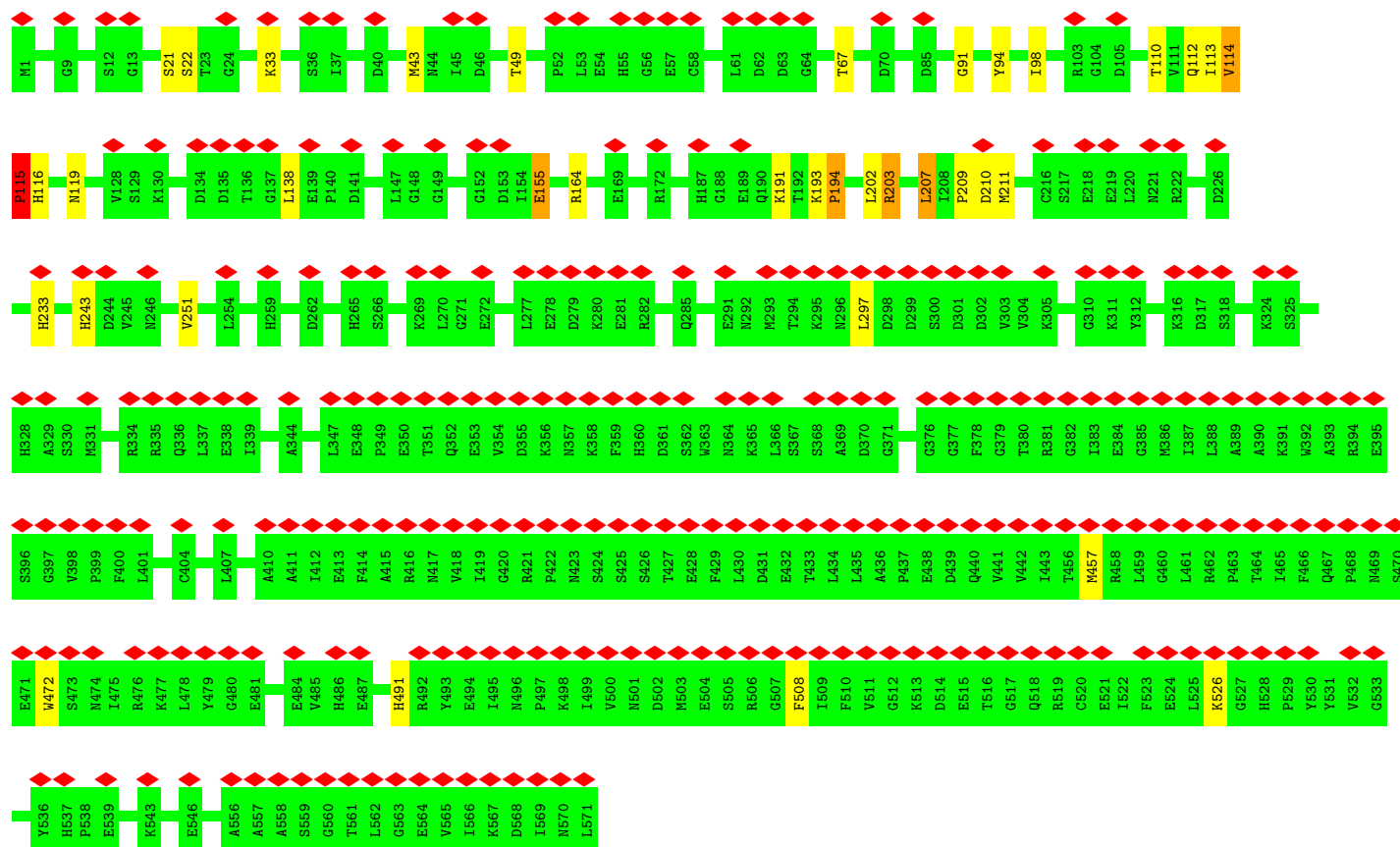
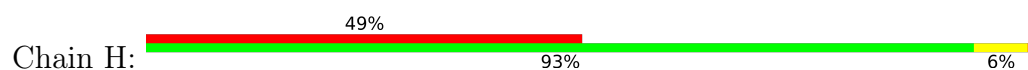


• Molecule 1: CTP synthase



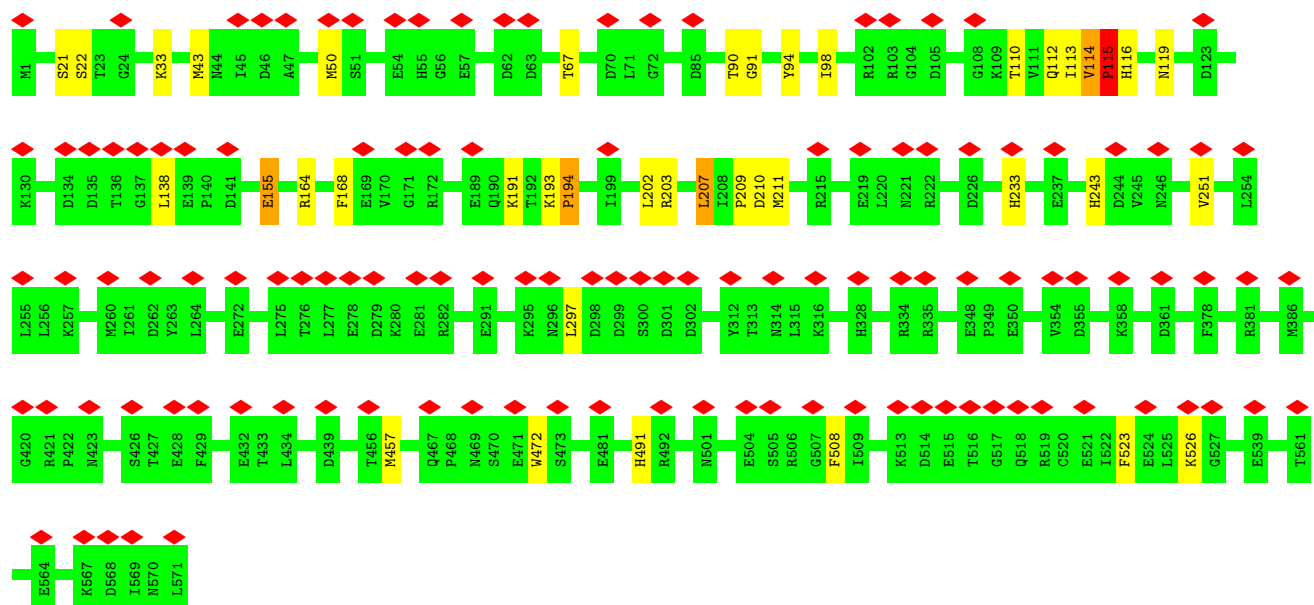


• Molecule 1: CTP synthase



• Molecule 1: CTP synthase





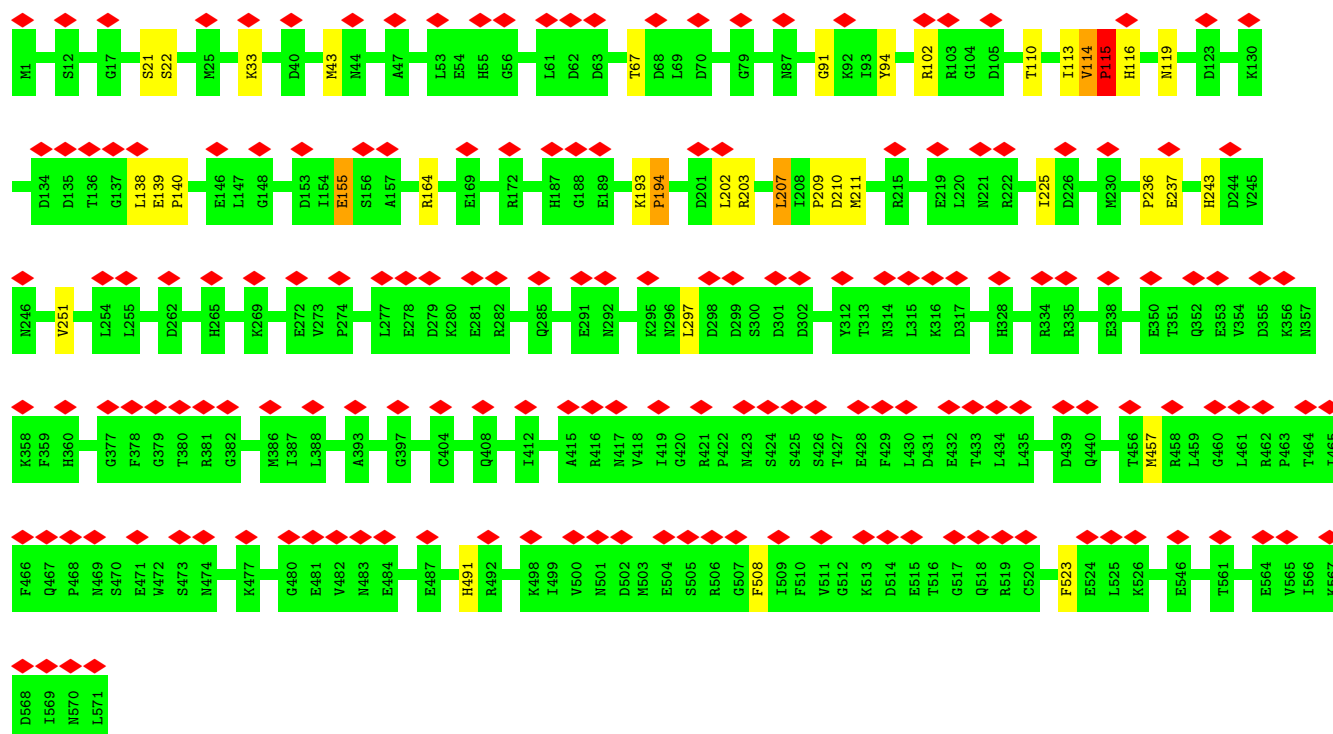
• Molecule 1: CTP synthase

Chain K: 36% 93% 6% •

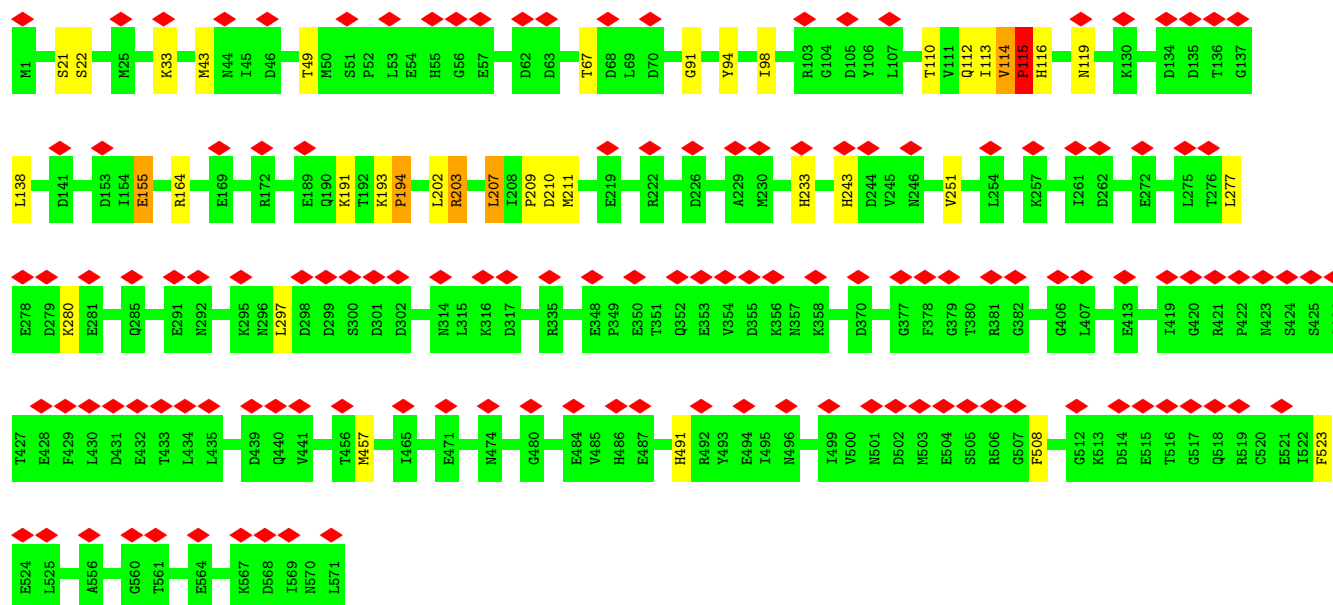
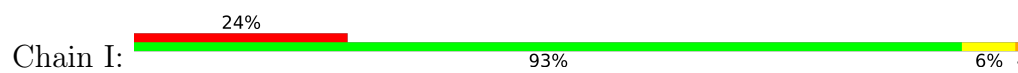


• Molecule 1: CTP synthase

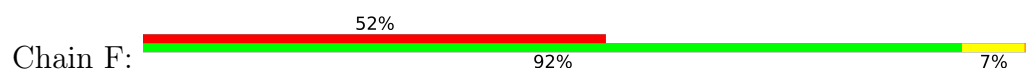
Chain N: 30% 93% 6% •

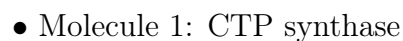


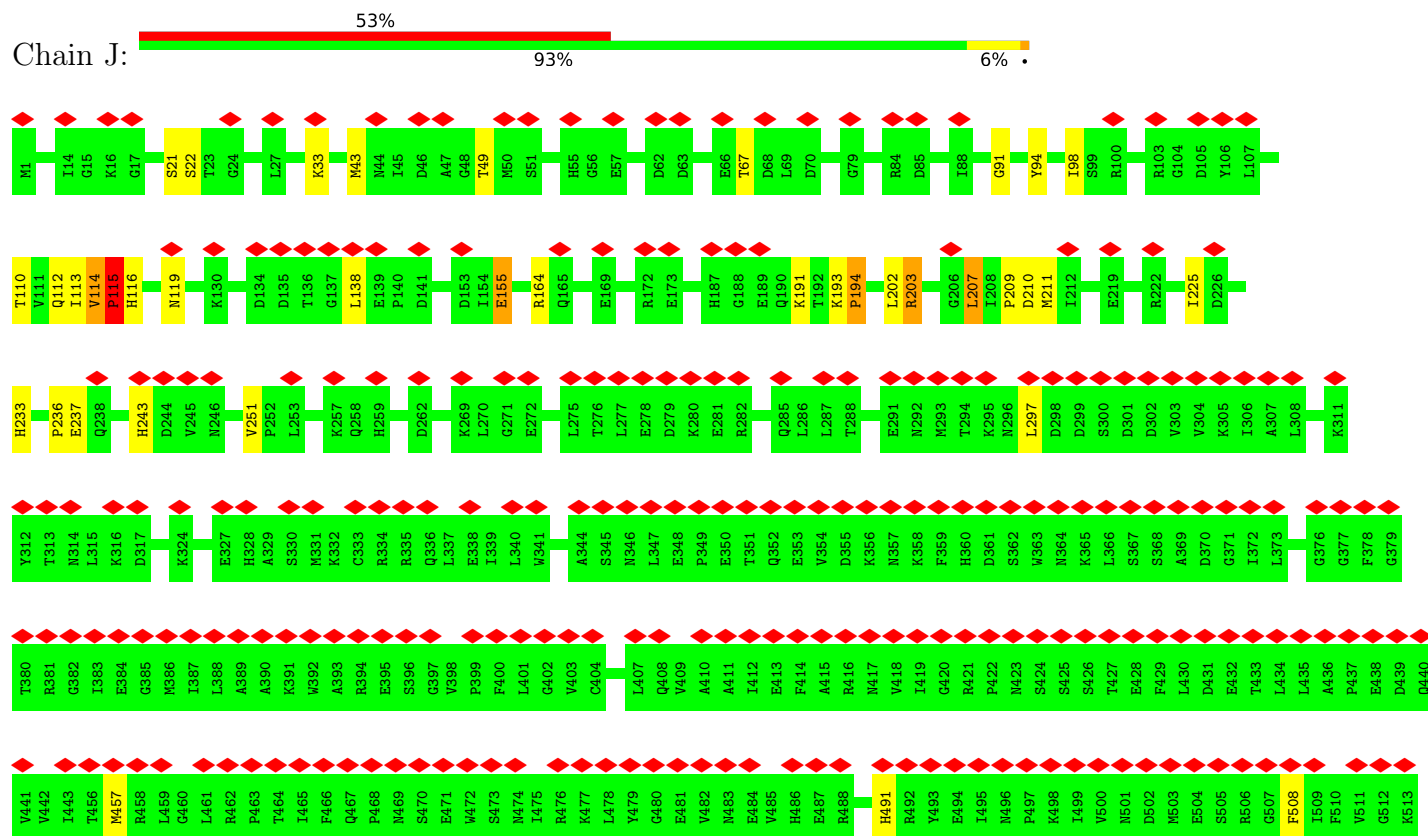
• Molecule 1: CTP synthase

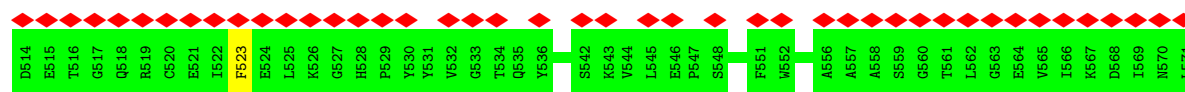


• Molecule 1: CTP synthase

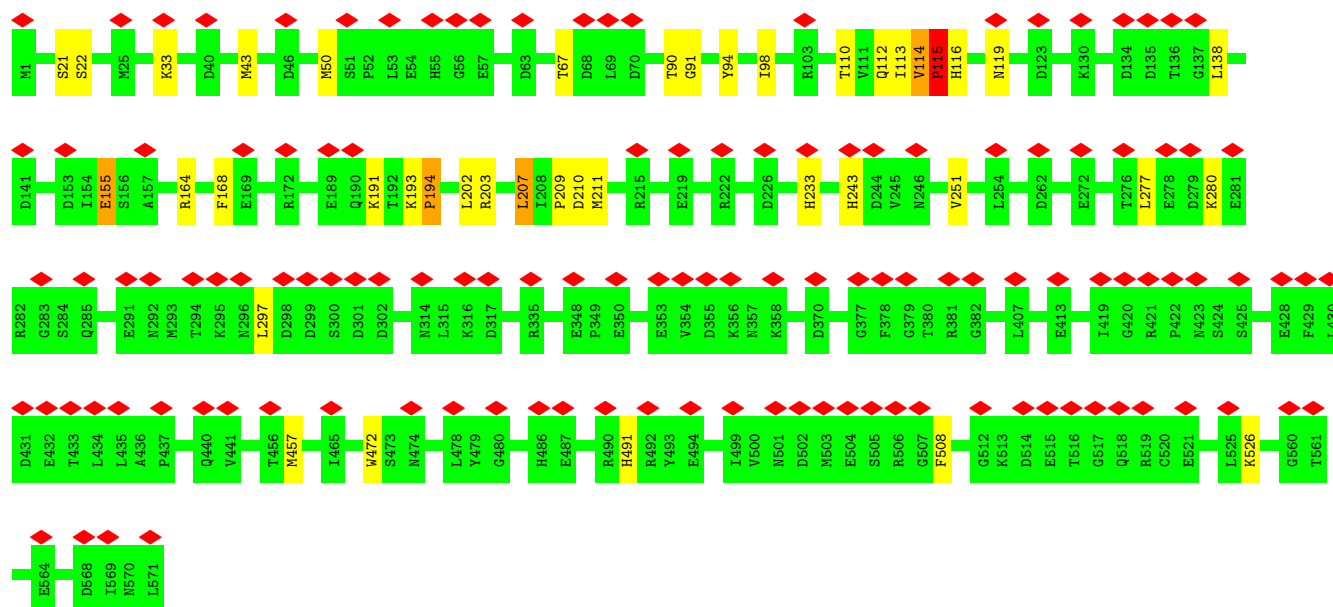
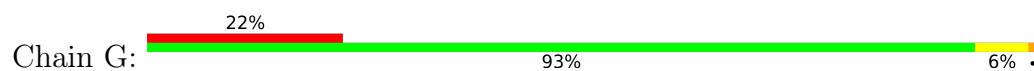




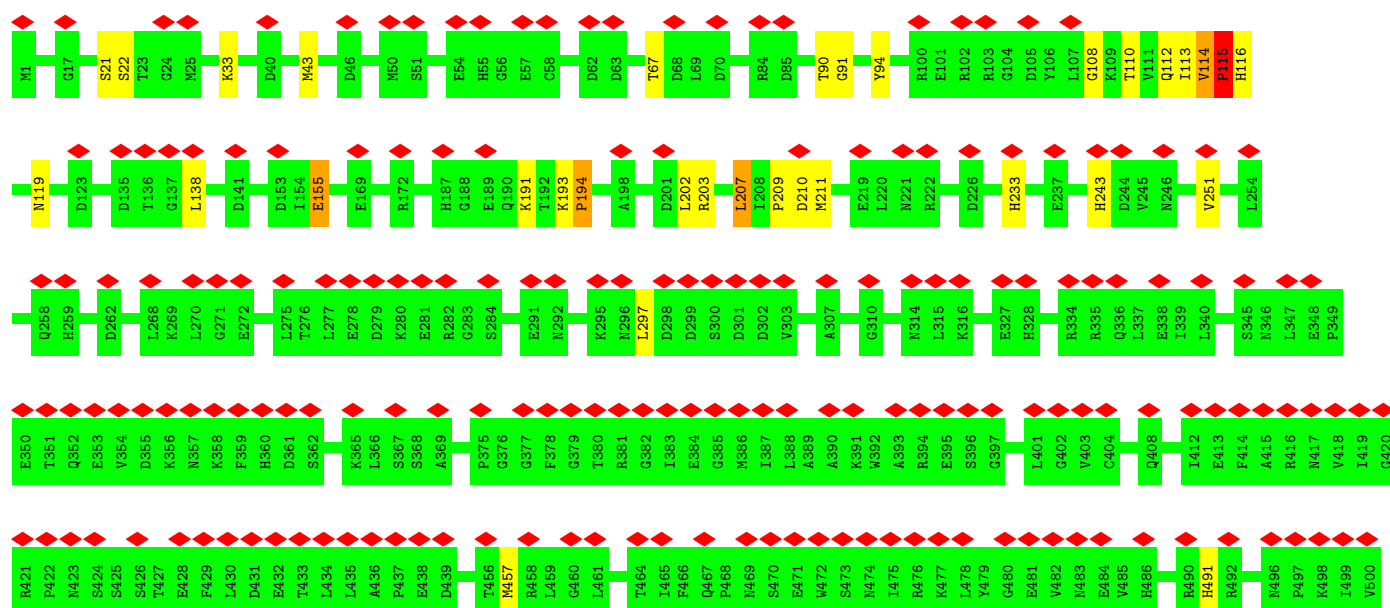
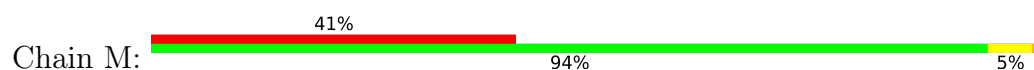


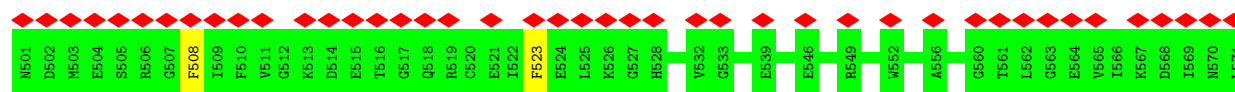


• Molecule 1: CTP synthase

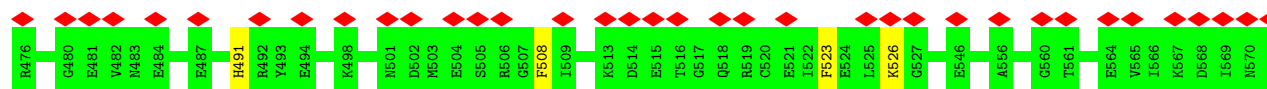
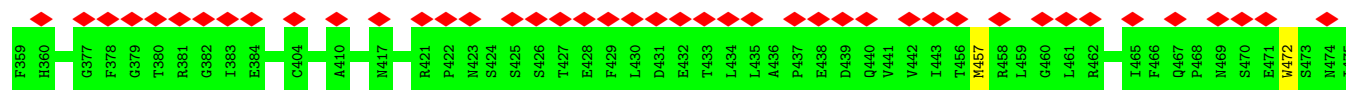
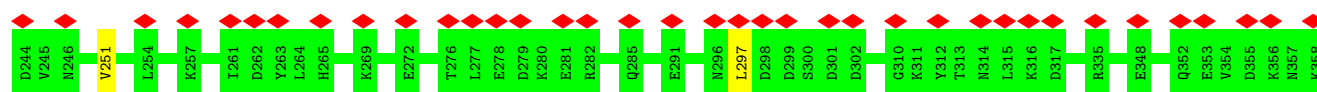
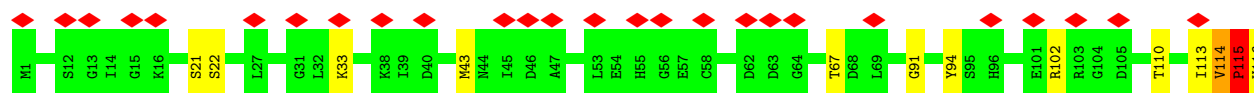
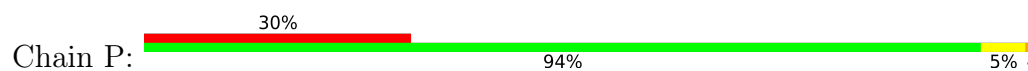


• Molecule 1: CTP synthase





• Molecule 1: CTP synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	53445	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.477	Depositor
Minimum map value	-1.072	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.244	Depositor
Map size ($\text{\AA}$)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTP, MG

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	0.86	4/4471 (0.1%)	1.40	16/6056 (0.3%)
1	B	0.86	4/4471 (0.1%)	1.40	17/6056 (0.3%)
1	C	0.86	4/4471 (0.1%)	1.40	16/6056 (0.3%)
1	D	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	E	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	F	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	G	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	H	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	I	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	J	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	K	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	L	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	M	0.86	4/4471 (0.1%)	1.39	16/6056 (0.3%)
1	N	0.86	4/4471 (0.1%)	1.40	16/6056 (0.3%)
1	O	0.86	4/4471 (0.1%)	1.39	15/6056 (0.2%)
1	P	0.86	4/4471 (0.1%)	1.39	18/6056 (0.3%)
All	All	0.86	64/71536 (0.1%)	1.39	258/96896 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
All	All	0	16

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	115	PRO	C-O	-6.77	1.15	1.24
1	O	115	PRO	C-O	-6.75	1.15	1.24
1	B	115	PRO	C-O	-6.74	1.15	1.24
1	N	115	PRO	C-O	-6.73	1.15	1.24
1	P	115	PRO	C-O	-6.72	1.15	1.24
1	E	115	PRO	C-O	-6.72	1.15	1.24
1	F	115	PRO	C-O	-6.71	1.15	1.24
1	J	115	PRO	C-O	-6.71	1.15	1.24
1	D	115	PRO	C-O	-6.70	1.15	1.24
1	C	115	PRO	C-O	-6.70	1.15	1.24
1	L	115	PRO	C-O	-6.70	1.15	1.24
1	M	115	PRO	C-O	-6.70	1.15	1.24
1	I	115	PRO	C-O	-6.69	1.15	1.24
1	A	115	PRO	C-O	-6.69	1.15	1.24
1	H	115	PRO	C-O	-6.67	1.15	1.24
1	K	115	PRO	C-O	-6.67	1.15	1.24
1	C	203	ARG	CZ-NH2	-5.87	1.25	1.33
1	P	203	ARG	CZ-NH2	-5.84	1.25	1.33
1	A	203	ARG	CZ-NH2	-5.84	1.25	1.33
1	K	203	ARG	CZ-NH2	-5.82	1.25	1.33
1	N	203	ARG	CZ-NH2	-5.82	1.25	1.33
1	F	203	ARG	CZ-NH2	-5.81	1.25	1.33
1	H	203	ARG	CZ-NH2	-5.80	1.25	1.33
1	O	203	ARG	CZ-NH2	-5.80	1.25	1.33
1	J	203	ARG	CZ-NH2	-5.80	1.25	1.33
1	I	203	ARG	CZ-NH2	-5.79	1.25	1.33
1	G	203	ARG	CZ-NH2	-5.79	1.25	1.33
1	B	203	ARG	CZ-NH2	-5.79	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	ARG	CZ-NH2	-5.78	1.25	1.33
1	E	203	ARG	CZ-NH2	-5.77	1.25	1.33
1	M	203	ARG	CZ-NH2	-5.76	1.25	1.33
1	L	203	ARG	CZ-NH2	-5.75	1.25	1.33
1	B	22	SER	CA-CB	-5.47	1.46	1.54
1	M	22	SER	CA-CB	-5.46	1.46	1.54
1	C	22	SER	CA-CB	-5.45	1.46	1.54
1	H	22	SER	CA-CB	-5.45	1.46	1.54
1	J	22	SER	CA-CB	-5.45	1.46	1.54
1	K	22	SER	CA-CB	-5.44	1.46	1.54
1	O	22	SER	CA-CB	-5.44	1.46	1.54
1	F	22	SER	CA-CB	-5.43	1.46	1.54
1	P	22	SER	CA-CB	-5.43	1.46	1.54
1	A	22	SER	CA-CB	-5.42	1.46	1.54
1	I	22	SER	CA-CB	-5.42	1.46	1.54
1	E	22	SER	CA-CB	-5.42	1.46	1.54
1	N	22	SER	CA-CB	-5.40	1.46	1.54
1	D	22	SER	CA-CB	-5.40	1.46	1.54
1	G	22	SER	CA-CB	-5.39	1.46	1.54
1	L	22	SER	CA-CB	-5.39	1.46	1.54
1	M	203	ARG	CZ-NH1	-5.38	1.25	1.32
1	F	203	ARG	CZ-NH1	-5.37	1.25	1.32
1	B	203	ARG	CZ-NH1	-5.36	1.25	1.32
1	K	203	ARG	CZ-NH1	-5.36	1.25	1.32
1	E	203	ARG	CZ-NH1	-5.34	1.25	1.32
1	N	203	ARG	CZ-NH1	-5.32	1.25	1.32
1	J	203	ARG	CZ-NH1	-5.32	1.25	1.32
1	O	203	ARG	CZ-NH1	-5.32	1.25	1.32
1	I	203	ARG	CZ-NH1	-5.32	1.25	1.32
1	A	203	ARG	CZ-NH1	-5.30	1.25	1.32
1	C	203	ARG	CZ-NH1	-5.29	1.25	1.32
1	D	203	ARG	CZ-NH1	-5.29	1.25	1.32
1	L	203	ARG	CZ-NH1	-5.28	1.25	1.32
1	H	203	ARG	CZ-NH1	-5.28	1.25	1.32
1	P	203	ARG	CZ-NH1	-5.27	1.25	1.32
1	G	203	ARG	CZ-NH1	-5.26	1.25	1.32

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	VAL	C-N-CD	-11.10	79.49	125.00
1	N	114	VAL	C-N-CD	-11.10	79.49	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	VAL	C-N-CD	-11.10	79.49	125.00
1	D	114	VAL	C-N-CD	-11.10	79.49	125.00
1	E	114	VAL	C-N-CD	-11.10	79.49	125.00
1	H	114	VAL	C-N-CD	-11.10	79.50	125.00
1	L	114	VAL	C-N-CD	-11.10	79.50	125.00
1	K	114	VAL	C-N-CD	-11.10	79.51	125.00
1	P	114	VAL	C-N-CD	-11.10	79.51	125.00
1	I	114	VAL	C-N-CD	-11.09	79.52	125.00
1	J	114	VAL	C-N-CD	-11.09	79.52	125.00
1	G	114	VAL	C-N-CD	-11.09	79.52	125.00
1	A	114	VAL	C-N-CD	-11.09	79.52	125.00
1	F	114	VAL	C-N-CD	-11.09	79.52	125.00
1	O	114	VAL	C-N-CD	-11.09	79.52	125.00
1	M	114	VAL	C-N-CD	-11.09	79.52	125.00
1	B	115	PRO	CA-N-CD	7.61	122.65	112.00
1	P	115	PRO	CA-N-CD	7.60	122.64	112.00
1	C	115	PRO	CA-N-CD	7.59	122.63	112.00
1	N	115	PRO	CA-N-CD	7.59	122.63	112.00
1	A	115	PRO	CA-N-CD	7.59	122.62	112.00
1	L	115	PRO	CA-N-CD	7.58	122.61	112.00
1	I	115	PRO	CA-N-CD	7.58	122.60	112.00
1	F	115	PRO	CA-N-CD	7.57	122.60	112.00
1	J	115	PRO	CA-N-CD	7.57	122.59	112.00
1	H	115	PRO	CA-N-CD	7.56	122.59	112.00
1	G	115	PRO	CA-N-CD	7.56	122.59	112.00
1	M	115	PRO	CA-N-CD	7.56	122.59	112.00
1	D	115	PRO	CA-N-CD	7.56	122.58	112.00
1	O	115	PRO	CA-N-CD	7.56	122.59	112.00
1	E	115	PRO	CA-N-CD	7.56	122.58	112.00
1	K	115	PRO	CA-N-CD	7.55	122.57	112.00
1	C	115	PRO	N-CA-CB	-7.21	95.68	103.25
1	A	115	PRO	N-CA-CB	-7.21	95.68	103.25
1	L	115	PRO	N-CA-CB	-7.21	95.68	103.25
1	P	115	PRO	N-CA-CB	-7.21	95.68	103.25
1	N	115	PRO	N-CA-CB	-7.20	95.69	103.25
1	J	115	PRO	N-CA-CB	-7.20	95.69	103.25
1	H	115	PRO	N-CA-CB	-7.20	95.69	103.25
1	G	115	PRO	N-CA-CB	-7.20	95.69	103.25
1	M	115	PRO	N-CA-CB	-7.20	95.69	103.25
1	F	115	PRO	N-CA-CB	-7.19	95.70	103.25
1	B	115	PRO	N-CA-CB	-7.18	95.71	103.25
1	I	115	PRO	N-CA-CB	-7.18	95.71	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	115	PRO	N-CA-CB	-7.17	95.72	103.25
1	E	115	PRO	N-CA-CB	-7.17	95.73	103.25
1	K	115	PRO	N-CA-CB	-7.16	95.74	103.25
1	D	115	PRO	N-CA-CB	-7.15	95.74	103.25
1	N	210	ASP	CA-CB-CG	6.11	118.71	112.60
1	M	210	ASP	CA-CB-CG	6.08	118.68	112.60
1	K	210	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	210	ASP	CA-CB-CG	6.04	118.64	112.60
1	E	210	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	210	ASP	CA-CB-CG	6.04	118.64	112.60
1	J	210	ASP	CA-CB-CG	6.04	118.64	112.60
1	I	210	ASP	CA-CB-CG	6.03	118.63	112.60
1	F	210	ASP	CA-CB-CG	6.03	118.63	112.60
1	L	210	ASP	CA-CB-CG	6.03	118.63	112.60
1	P	210	ASP	CA-CB-CG	6.03	118.63	112.60
1	O	210	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	210	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	210	ASP	CA-CB-CG	6.01	118.61	112.60
1	G	210	ASP	CA-CB-CG	6.01	118.61	112.60
1	H	210	ASP	CA-CB-CG	5.99	118.59	112.60
1	P	203	ARG	CD-NE-CZ	5.82	132.54	124.40
1	C	203	ARG	CD-NE-CZ	5.81	132.54	124.40
1	I	203	ARG	CD-NE-CZ	5.81	132.54	124.40
1	H	203	ARG	CD-NE-CZ	5.80	132.52	124.40
1	J	203	ARG	CD-NE-CZ	5.79	132.51	124.40
1	D	203	ARG	CD-NE-CZ	5.79	132.51	124.40
1	K	203	ARG	CD-NE-CZ	5.79	132.50	124.40
1	F	203	ARG	CD-NE-CZ	5.79	132.50	124.40
1	N	203	ARG	CD-NE-CZ	5.78	132.49	124.40
1	G	203	ARG	CD-NE-CZ	5.78	132.49	124.40
1	E	203	ARG	CD-NE-CZ	5.77	132.48	124.40
1	L	203	ARG	CD-NE-CZ	5.77	132.47	124.40
1	B	203	ARG	CD-NE-CZ	5.77	132.47	124.40
1	O	203	ARG	CD-NE-CZ	5.76	132.47	124.40
1	A	203	ARG	CD-NE-CZ	5.76	132.46	124.40
1	H	508	PHE	CA-CB-CG	5.75	119.55	113.80
1	M	203	ARG	CD-NE-CZ	5.75	132.45	124.40
1	K	508	PHE	CA-CB-CG	5.75	119.55	113.80
1	I	508	PHE	CA-CB-CG	5.74	119.54	113.80
1	D	508	PHE	CA-CB-CG	5.72	119.53	113.80
1	E	508	PHE	CA-CB-CG	5.72	119.52	113.80
1	N	508	PHE	CA-CB-CG	5.72	119.52	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	508	PHE	CA-CB-CG	5.72	119.52	113.80
1	A	508	PHE	CA-CB-CG	5.72	119.52	113.80
1	L	508	PHE	CA-CB-CG	5.72	119.52	113.80
1	P	508	PHE	CA-CB-CG	5.72	119.52	113.80
1	F	508	PHE	CA-CB-CG	5.71	119.51	113.80
1	G	508	PHE	CA-CB-CG	5.71	119.51	113.80
1	B	508	PHE	CA-CB-CG	5.70	119.50	113.80
1	O	508	PHE	CA-CB-CG	5.70	119.50	113.80
1	M	508	PHE	CA-CB-CG	5.70	119.50	113.80
1	C	508	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	251	VAL	N-CA-CB	5.46	113.94	110.50
1	D	251	VAL	N-CA-CB	5.44	113.93	110.50
1	H	251	VAL	N-CA-CB	5.44	113.92	110.50
1	L	251	VAL	N-CA-CB	5.44	113.92	110.50
1	C	251	VAL	N-CA-CB	5.43	113.92	110.50
1	M	251	VAL	N-CA-CB	5.43	113.92	110.50
1	J	251	VAL	N-CA-CB	5.41	113.91	110.50
1	O	251	VAL	N-CA-CB	5.41	113.91	110.50
1	N	251	VAL	N-CA-CB	5.40	113.90	110.50
1	G	251	VAL	N-CA-CB	5.39	113.90	110.50
1	A	251	VAL	N-CA-CB	5.39	113.89	110.50
1	I	251	VAL	N-CA-CB	5.39	113.89	110.50
1	F	251	VAL	N-CA-CB	5.38	113.89	110.50
1	P	251	VAL	N-CA-CB	5.37	113.88	110.50
1	K	251	VAL	N-CA-CB	5.37	113.88	110.50
1	E	251	VAL	N-CA-CB	5.35	113.87	110.50
1	D	110	THR	CA-C-O	-5.34	115.74	121.56
1	O	110	THR	CA-C-O	-5.32	115.77	121.56
1	G	110	THR	CA-C-O	-5.32	115.77	121.56
1	M	110	THR	CA-C-O	-5.31	115.77	121.56
1	P	110	THR	CA-C-O	-5.30	115.78	121.56
1	A	110	THR	CA-C-O	-5.29	115.80	121.56
1	B	110	THR	CA-C-O	-5.28	115.80	121.56
1	H	110	THR	CA-C-O	-5.28	115.80	121.56
1	N	110	THR	CA-C-O	-5.28	115.80	121.56
1	J	110	THR	CA-C-O	-5.28	115.80	121.56
1	E	110	THR	CA-C-O	-5.28	115.81	121.56
1	C	110	THR	CA-C-O	-5.27	115.81	121.56
1	C	209	PRO	CA-C-O	-5.27	115.24	121.67
1	I	110	THR	CA-C-O	-5.27	115.82	121.56
1	K	110	THR	CA-C-O	-5.26	115.83	121.56
1	F	110	THR	CA-C-O	-5.25	115.84	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	110	THR	CA-C-O	-5.25	115.84	121.56
1	B	209	PRO	CA-C-O	-5.25	115.27	121.67
1	A	209	PRO	CA-C-O	-5.25	115.27	121.67
1	D	209	PRO	CA-C-O	-5.24	115.27	121.67
1	F	209	PRO	CA-C-O	-5.24	115.28	121.67
1	P	209	PRO	CA-C-O	-5.24	115.28	121.67
1	H	209	PRO	CA-C-O	-5.24	115.28	121.67
1	O	209	PRO	CA-C-O	-5.23	115.28	121.67
1	E	209	PRO	CA-C-O	-5.23	115.29	121.67
1	G	209	PRO	CA-C-O	-5.23	115.29	121.67
1	K	209	PRO	CA-C-O	-5.23	115.29	121.67
1	N	209	PRO	CA-C-O	-5.23	115.29	121.67
1	J	209	PRO	CA-C-O	-5.23	115.29	121.67
1	L	209	PRO	CA-C-O	-5.22	115.30	121.67
1	M	209	PRO	CA-C-O	-5.22	115.31	121.67
1	E	155	GLU	N-CA-C	-5.21	106.78	113.23
1	A	155	GLU	N-CA-C	-5.20	106.79	113.23
1	P	155	GLU	N-CA-C	-5.20	106.79	113.23
1	N	155	GLU	N-CA-C	-5.19	106.79	113.23
1	G	155	GLU	N-CA-C	-5.19	106.80	113.23
1	D	194	PRO	N-CA-C	-5.18	106.06	113.47
1	I	155	GLU	N-CA-C	-5.18	106.81	113.23
1	I	209	PRO	CA-C-O	-5.18	115.35	121.67
1	M	155	GLU	N-CA-C	-5.18	106.81	113.23
1	K	155	GLU	N-CA-C	-5.18	106.81	113.23
1	J	155	GLU	N-CA-C	-5.17	106.81	113.23
1	C	155	GLU	N-CA-C	-5.17	106.82	113.23
1	D	155	GLU	N-CA-C	-5.17	106.82	113.23
1	F	155	GLU	N-CA-C	-5.17	106.82	113.23
1	H	211	MET	CA-C-O	-5.17	115.31	121.56
1	H	155	GLU	N-CA-C	-5.16	106.83	113.23
1	N	211	MET	CA-C-O	-5.16	115.31	121.56
1	I	194	PRO	N-CA-C	-5.16	106.09	113.47
1	O	155	GLU	N-CA-C	-5.16	106.83	113.23
1	B	211	MET	CA-C-O	-5.16	115.32	121.56
1	A	194	PRO	N-CA-C	-5.16	106.09	113.47
1	N	194	PRO	N-CA-C	-5.16	106.09	113.47
1	L	194	PRO	N-CA-C	-5.16	106.09	113.47
1	M	194	PRO	N-CA-C	-5.16	106.09	113.47
1	H	194	PRO	N-CA-C	-5.16	106.10	113.47
1	B	155	GLU	N-CA-C	-5.16	106.84	113.23
1	K	194	PRO	N-CA-C	-5.16	106.10	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	211	MET	CA-C-O	-5.16	115.32	121.56
1	J	194	PRO	N-CA-C	-5.16	106.10	113.47
1	G	194	PRO	N-CA-C	-5.15	106.10	113.47
1	B	194	PRO	N-CA-C	-5.15	106.11	113.47
1	L	155	GLU	N-CA-C	-5.15	106.85	113.23
1	J	211	MET	CA-C-O	-5.15	115.33	121.56
1	C	211	MET	CA-C-O	-5.14	115.33	121.56
1	O	211	MET	CA-C-O	-5.14	115.34	121.56
1	F	194	PRO	N-CA-C	-5.14	106.12	113.47
1	H	21	SER	CA-C-N	5.14	130.54	122.11
1	H	21	SER	C-N-CA	5.14	130.54	122.11
1	I	211	MET	CA-C-O	-5.14	115.34	121.56
1	P	194	PRO	N-CA-C	-5.14	106.12	113.47
1	P	211	MET	CA-C-O	-5.14	115.35	121.56
1	A	211	MET	CA-C-O	-5.13	115.35	121.56
1	D	211	MET	CA-C-O	-5.13	115.35	121.56
1	G	211	MET	CA-C-O	-5.13	115.35	121.56
1	M	211	MET	CA-C-O	-5.13	115.35	121.56
1	K	211	MET	CA-C-O	-5.13	115.36	121.56
1	F	211	MET	CA-C-O	-5.13	115.36	121.56
1	C	194	PRO	N-CA-C	-5.12	106.14	113.47
1	E	194	PRO	N-CA-C	-5.12	106.14	113.47
1	E	211	MET	CA-C-O	-5.12	115.36	121.56
1	F	21	SER	CA-C-N	5.12	130.51	122.11
1	F	21	SER	C-N-CA	5.12	130.51	122.11
1	O	194	PRO	N-CA-C	-5.12	106.15	113.47
1	I	21	SER	CA-C-N	5.12	130.50	122.11
1	I	21	SER	C-N-CA	5.12	130.50	122.11
1	B	21	SER	CA-C-N	5.11	130.50	122.11
1	B	21	SER	C-N-CA	5.11	130.50	122.11
1	N	21	SER	CA-C-N	5.11	130.50	122.11
1	N	21	SER	C-N-CA	5.11	130.50	122.11
1	P	21	SER	CA-C-N	5.11	130.50	122.11
1	P	21	SER	C-N-CA	5.11	130.50	122.11
1	G	21	SER	CA-C-N	5.11	130.49	122.11
1	G	21	SER	C-N-CA	5.11	130.49	122.11
1	D	21	SER	CA-C-N	5.11	130.49	122.11
1	D	21	SER	C-N-CA	5.11	130.49	122.11
1	C	21	SER	CA-C-N	5.11	130.49	122.11
1	C	21	SER	C-N-CA	5.11	130.49	122.11
1	J	21	SER	CA-C-N	5.11	130.48	122.11
1	J	21	SER	C-N-CA	5.11	130.48	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	21	SER	CA-C-N	5.10	130.47	122.11
1	E	21	SER	C-N-CA	5.10	130.47	122.11
1	M	21	SER	CA-C-N	5.10	130.47	122.11
1	M	21	SER	C-N-CA	5.10	130.47	122.11
1	P	115	PRO	N-CD-CG	-5.09	95.56	103.20
1	L	21	SER	CA-C-N	5.09	130.46	122.11
1	L	21	SER	C-N-CA	5.09	130.46	122.11
1	A	21	SER	CA-C-N	5.09	130.45	122.11
1	A	21	SER	C-N-CA	5.09	130.45	122.11
1	O	21	SER	CA-C-N	5.08	130.44	122.11
1	O	21	SER	C-N-CA	5.08	130.44	122.11
1	D	115	PRO	N-CD-CG	-5.08	95.58	103.20
1	K	21	SER	CA-C-N	5.08	130.43	122.11
1	K	21	SER	C-N-CA	5.08	130.43	122.11
1	A	115	PRO	N-CD-CG	-5.07	95.59	103.20
1	C	115	PRO	N-CD-CG	-5.07	95.60	103.20
1	B	115	PRO	N-CD-CG	-5.06	95.61	103.20
1	I	115	PRO	N-CD-CG	-5.06	95.61	103.20
1	L	115	PRO	N-CD-CG	-5.06	95.61	103.20
1	M	115	PRO	N-CD-CG	-5.06	95.61	103.20
1	P	110	THR	N-CA-C	-5.06	103.37	110.50
1	E	115	PRO	N-CD-CG	-5.05	95.62	103.20
1	K	115	PRO	N-CD-CG	-5.05	95.62	103.20
1	J	115	PRO	N-CD-CG	-5.05	95.62	103.20
1	N	115	PRO	N-CD-CG	-5.05	95.63	103.20
1	H	115	PRO	N-CD-CG	-5.05	95.63	103.20
1	F	115	PRO	N-CD-CG	-5.04	95.63	103.20
1	L	110	THR	N-CA-C	-5.04	103.39	110.50
1	B	110	THR	N-CA-C	-5.04	103.40	110.50
1	G	110	THR	N-CA-C	-5.04	103.40	110.50
1	N	110	THR	N-CA-C	-5.03	103.40	110.50
1	H	110	THR	N-CA-C	-5.03	103.41	110.50
1	E	110	THR	N-CA-C	-5.03	103.41	110.50
1	K	110	THR	N-CA-C	-5.03	103.41	110.50
1	O	115	PRO	N-CD-CG	-5.03	95.66	103.20
1	I	110	THR	N-CA-C	-5.03	103.41	110.50
1	F	110	THR	N-CA-C	-5.03	103.41	110.50
1	J	110	THR	N-CA-C	-5.02	103.42	110.50
1	G	115	PRO	N-CD-CG	-5.02	95.67	103.20
1	A	110	THR	N-CA-C	-5.02	103.42	110.50
1	C	110	THR	N-CA-C	-5.01	103.43	110.50
1	M	110	THR	N-CA-C	-5.01	103.43	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	THR	N-CA-C	-5.01	103.44	110.50
1	B	179	HIS	CB-CG-CD2	-5.00	124.70	131.20
1	P	127	ARG	CA-C-N	5.00	126.86	120.56
1	P	127	ARG	C-N-CA	5.00	126.86	120.56

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	TYR	Sidechain
1	B	94	TYR	Sidechain
1	C	94	TYR	Sidechain
1	D	94	TYR	Sidechain
1	E	94	TYR	Sidechain
1	F	94	TYR	Sidechain
1	G	94	TYR	Sidechain
1	H	94	TYR	Sidechain
1	I	94	TYR	Sidechain
1	J	94	TYR	Sidechain
1	K	94	TYR	Sidechain
1	L	94	TYR	Sidechain
1	M	94	TYR	Sidechain
1	N	94	TYR	Sidechain
1	O	94	TYR	Sidechain
1	P	94	TYR	Sidechain

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	4385	4381	4392	58	0
1	B	4385	4381	4392	54	0
1	C	4385	4381	4392	56	0
1	D	4385	4381	4392	57	0
1	E	4385	4381	4392	60	0
1	F	4385	4381	4392	73	0
1	G	4385	4381	4392	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	4385	4381	4392	55	0
1	I	4385	4381	4392	74	0
1	J	4385	4381	4392	71	0
1	K	4385	4381	4392	53	0
1	L	4385	4381	4392	43	0
1	M	4385	4381	4392	42	0
1	N	4385	4381	4392	57	0
1	O	4385	4381	4392	39	0
1	P	4385	4381	4392	39	0
2	A	87	24	35	15	0
2	B	58	16	23	0	0
2	C	29	8	11	0	0
2	D	58	16	23	4	0
2	E	87	24	35	15	0
2	F	87	24	35	15	0
2	G	87	24	35	14	0
2	H	58	16	23	1	0
2	I	58	16	23	0	0
2	J	58	16	23	1	0
2	K	29	8	11	0	0
2	L	29	8	11	0	0
2	M	29	8	11	0	0
2	N	58	16	23	4	0
2	O	58	16	23	4	0
2	P	58	16	23	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
All	All	71120	70352	70640	651	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 5.

All (651) 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:O:114:VAL:HG23	1:O:115:PRO:CD	1.10	1.58
1:K:114:VAL:HG23	1:K:115:PRO:CD	1.10	1.58
1:G:114:VAL:HG23	1:G:115:PRO:CD	1.10	1.58
1:L:114:VAL:HG23	1:L:115:PRO:CD	1.10	1.57
1:E:114:VAL:HG23	1:E:115:PRO:CD	1.10	1.56
1:P:114:VAL:HG23	1:P:115:PRO:CD	1.10	1.56
1:F:114:VAL:HG23	1:F:115:PRO:CD	1.10	1.56
1:A:114:VAL:HG23	1:A:115:PRO:CD	1.10	1.56
1:A:114:VAL:CG2	1:A:115:PRO:HD2	1.37	1.55
1:B:114:VAL:HG23	1:B:115:PRO:CD	1.10	1.55
1:L:114:VAL:CG2	1:L:115:PRO:HD2	1.37	1.55
1:D:114:VAL:HG23	1:D:115:PRO:CD	1.10	1.55
1:G:114:VAL:CG2	1:G:115:PRO:HD2	1.37	1.55
1:D:114:VAL:CG2	1:D:115:PRO:HD2	1.37	1.55
1:I:114:VAL:CG2	1:I:115:PRO:HD2	1.37	1.55
1:M:114:VAL:HG23	1:M:115:PRO:CD	1.10	1.55
1:D:114:VAL:CG2	1:D:115:PRO:CD	1.86	1.54
1:J:114:VAL:HG23	1:J:115:PRO:CD	1.10	1.54
1:C:114:VAL:CG2	1:C:115:PRO:CD	1.86	1.54
1:B:114:VAL:CG2	1:B:115:PRO:CD	1.86	1.54
1:K:114:VAL:CG2	1:K:115:PRO:HD2	1.37	1.54
1:A:114:VAL:CG2	1:A:115:PRO:CD	1.86	1.53
1:N:114:VAL:CG2	1:N:115:PRO:HD2	1.37	1.53
1:I:114:VAL:HG23	1:I:115:PRO:CD	1.10	1.53
1:B:114:VAL:CG2	1:B:115:PRO:HD2	1.37	1.53
1:H:114:VAL:HG23	1:H:115:PRO:CD	1.10	1.52
1:O:114:VAL:CG2	1:O:115:PRO:HD2	1.37	1.52
1:K:114:VAL:CG2	1:K:115:PRO:CD	1.86	1.52
1:N:114:VAL:HG23	1:N:115:PRO:CD	1.10	1.52
1:P:114:VAL:CG2	1:P:115:PRO:HD2	1.37	1.52
1:C:114:VAL:CG2	1:C:115:PRO:HD2	1.37	1.51
1:C:114:VAL:HG23	1:C:115:PRO:CD	1.10	1.51
1:H:114:VAL:CG2	1:H:115:PRO:CD	1.86	1.51
1:J:114:VAL:CG2	1:J:115:PRO:HD2	1.37	1.51
1:F:114:VAL:CG2	1:F:115:PRO:HD2	1.37	1.51
1:E:114:VAL:CG2	1:E:115:PRO:HD2	1.37	1.50
1:N:114:VAL:CG2	1:N:115:PRO:CD	1.86	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:VAL:CG2	1:E:115:PRO:CD	1.86	1.50
1:P:114:VAL:CG2	1:P:115:PRO:CD	1.85	1.49
1:H:114:VAL:CG2	1:H:115:PRO:HD2	1.37	1.49
1:I:114:VAL:CG2	1:I:115:PRO:CD	1.86	1.49
1:L:114:VAL:CG2	1:L:115:PRO:CD	1.86	1.49
1:F:114:VAL:CG2	1:F:115:PRO:CD	1.86	1.49
1:M:114:VAL:CG2	1:M:115:PRO:HD2	1.37	1.49
1:O:114:VAL:CG2	1:O:115:PRO:CD	1.86	1.47
1:J:114:VAL:CG2	1:J:115:PRO:CD	1.86	1.47
1:G:114:VAL:CG2	1:G:115:PRO:CD	1.86	1.47
1:M:114:VAL:CG2	1:M:115:PRO:CD	1.85	1.46
1:B:155:GLU:OE2	1:D:113:ILE:CB	1.73	1.37
1:J:155:GLU:OE2	1:P:113:ILE:CB	1.73	1.34
1:H:155:GLU:OE2	1:N:113:ILE:CB	1.73	1.34
1:I:155:GLU:OE2	1:O:113:ILE:CB	1.73	1.34
1:L:114:VAL:CG2	1:L:115:PRO:HD3	1.69	1.20
1:D:236:PRO:HB2	1:G:277:LEU:HD21	1.20	1.19
1:F:114:VAL:CG2	1:F:115:PRO:HD3	1.69	1.18
1:I:155:GLU:CD	1:O:113:ILE:HB	1.70	1.17
1:B:155:GLU:CD	1:D:113:ILE:HB	1.70	1.17
1:M:114:VAL:CB	1:M:115:PRO:HD3	1.76	1.16
1:K:114:VAL:CB	1:K:115:PRO:HD3	1.76	1.16
1:E:114:VAL:CB	1:E:115:PRO:HD3	1.76	1.15
1:J:155:GLU:CD	1:P:113:ILE:HB	1.70	1.15
1:N:236:PRO:HB2	1:I:277:LEU:HD21	1.21	1.15
1:B:114:VAL:CB	1:B:115:PRO:HD3	1.76	1.15
1:H:155:GLU:CD	1:N:113:ILE:HB	1.70	1.15
1:I:114:VAL:CG2	1:I:115:PRO:HD3	1.69	1.14
1:G:114:VAL:CB	1:G:115:PRO:HD3	1.76	1.14
1:P:114:VAL:CB	1:P:115:PRO:CD	2.22	1.14
1:J:114:VAL:CG2	1:J:115:PRO:HD3	1.69	1.13
1:M:114:VAL:CB	1:M:115:PRO:CD	2.22	1.13
1:P:114:VAL:CG2	1:P:115:PRO:HD3	1.69	1.13
1:A:114:VAL:CG2	1:A:115:PRO:HD3	1.69	1.13
1:C:114:VAL:CB	1:C:115:PRO:HD3	1.76	1.13
1:L:114:VAL:CB	1:L:115:PRO:HD3	1.76	1.13
1:H:114:VAL:CB	1:H:115:PRO:HD3	1.76	1.13
1:P:114:VAL:CB	1:P:115:PRO:HD3	1.76	1.13
1:N:114:VAL:CB	1:N:115:PRO:HD3	1.76	1.12
1:B:114:VAL:CG2	1:B:115:PRO:HD3	1.69	1.11
1:N:225:ILE:CG2	1:I:277:LEU:HD11	1.78	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:114:VAL:CB	1:O:115:PRO:HD3	1.76	1.11
1:J:114:VAL:CB	1:J:115:PRO:HD3	1.76	1.11
1:D:114:VAL:CG2	1:D:115:PRO:HD3	1.69	1.11
1:D:114:VAL:CB	1:D:115:PRO:CD	2.22	1.11
1:F:114:VAL:CB	1:F:115:PRO:CD	2.22	1.11
1:G:114:VAL:CG2	1:G:115:PRO:HD3	1.69	1.11
1:D:114:VAL:CB	1:D:115:PRO:HD3	1.76	1.11
1:G:114:VAL:CB	1:G:115:PRO:CD	2.22	1.11
1:I:114:VAL:CB	1:I:115:PRO:HD3	1.76	1.11
1:A:114:VAL:CB	1:A:115:PRO:CD	2.22	1.10
1:O:114:VAL:CG2	1:O:115:PRO:HD3	1.69	1.10
1:F:114:VAL:CB	1:F:115:PRO:HD3	1.76	1.10
1:D:225:ILE:HG22	1:G:277:LEU:HD11	1.34	1.10
1:N:225:ILE:HG22	1:I:277:LEU:HD11	1.30	1.10
1:M:114:VAL:CG2	1:M:115:PRO:HD3	1.69	1.10
1:H:114:VAL:CG2	1:H:115:PRO:HD3	1.69	1.09
1:I:114:VAL:CB	1:I:115:PRO:CD	2.22	1.09
1:C:114:VAL:CB	1:C:115:PRO:CD	2.22	1.09
1:K:114:VAL:CG2	1:K:115:PRO:HD3	1.69	1.09
1:H:114:VAL:CB	1:H:115:PRO:CD	2.22	1.08
1:A:114:VAL:CB	1:A:115:PRO:HD3	1.76	1.08
1:C:114:VAL:CG2	1:C:115:PRO:HD3	1.69	1.08
1:C:277:LEU:HD21	1:J:236:PRO:HB2	1.32	1.07
1:C:277:LEU:HD11	1:J:225:ILE:CG2	1.84	1.05
1:N:114:VAL:CB	1:N:115:PRO:CD	2.22	1.05
1:E:114:VAL:CG2	1:E:115:PRO:HD3	1.69	1.05
1:I:155:GLU:OE2	1:O:113:ILE:HB	0.87	1.05
1:J:155:GLU:OE2	1:P:113:ILE:HB	0.87	1.05
1:C:277:LEU:HD11	1:J:225:ILE:HG22	1.37	1.04
1:N:114:VAL:CG2	1:N:115:PRO:HD3	1.69	1.04
1:L:114:VAL:CB	1:L:115:PRO:CD	2.22	1.04
1:H:155:GLU:OE2	1:N:113:ILE:HB	0.87	1.03
1:B:155:GLU:OE2	1:D:113:ILE:HB	0.87	1.03
1:E:114:VAL:HG23	1:E:115:PRO:CG	1.89	1.03
1:I:114:VAL:HG23	1:I:115:PRO:CG	1.89	1.03
1:L:114:VAL:HG23	1:L:115:PRO:CG	1.89	1.03
1:E:114:VAL:CB	1:E:115:PRO:CD	2.22	1.02
1:N:114:VAL:HG23	1:N:115:PRO:CG	1.89	1.02
1:M:114:VAL:HG23	1:M:115:PRO:CG	1.89	1.02
1:A:114:VAL:HG23	1:A:115:PRO:CG	1.89	1.02
1:N:236:PRO:HB2	1:I:277:LEU:CD2	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:VAL:CB	1:K:115:PRO:CD	2.22	1.02
1:J:114:VAL:CB	1:J:115:PRO:CD	2.22	1.02
1:G:114:VAL:HG23	1:G:115:PRO:CG	1.89	1.02
1:P:114:VAL:HG23	1:P:115:PRO:CG	1.89	1.02
1:B:114:VAL:HG23	1:B:115:PRO:CG	1.89	1.02
1:C:114:VAL:HG23	1:C:115:PRO:CG	1.89	1.01
1:D:114:VAL:HG23	1:D:115:PRO:CG	1.89	1.01
1:F:114:VAL:HG23	1:F:115:PRO:CG	1.89	1.01
1:J:114:VAL:HG23	1:J:115:PRO:CG	1.89	1.01
1:H:114:VAL:HG23	1:H:115:PRO:CG	1.89	1.01
1:K:114:VAL:HG23	1:K:115:PRO:CG	1.89	1.01
1:O:114:VAL:HG23	1:O:115:PRO:CG	1.89	1.01
1:L:114:VAL:HG23	1:L:115:PRO:HD3	1.32	1.00
1:O:114:VAL:CB	1:O:115:PRO:CD	2.22	1.00
1:B:114:VAL:CB	1:B:115:PRO:CD	2.22	1.00
1:N:114:VAL:HB	1:N:115:PRO:HD3	1.44	1.00
1:G:114:VAL:HB	1:G:115:PRO:HD3	1.44	1.00
1:B:114:VAL:HB	1:B:115:PRO:HD3	1.44	1.00
1:H:114:VAL:HB	1:H:115:PRO:HD3	1.44	1.00
1:L:114:VAL:HB	1:L:115:PRO:HD3	1.44	1.00
1:J:114:VAL:HB	1:J:115:PRO:HD3	1.44	0.99
1:C:114:VAL:HB	1:C:115:PRO:HD3	1.44	0.99
1:I:114:VAL:HB	1:I:115:PRO:HD3	1.44	0.99
1:N:225:ILE:HG22	1:I:277:LEU:CD1	1.92	0.99
1:P:114:VAL:HG23	1:P:115:PRO:HD3	1.32	0.99
1:K:114:VAL:HB	1:K:115:PRO:HD3	1.44	0.98
1:F:114:VAL:HG23	1:F:115:PRO:HD3	1.32	0.98
1:P:114:VAL:HB	1:P:115:PRO:HD3	1.44	0.98
1:A:114:VAL:HG23	1:A:115:PRO:HD3	1.32	0.98
1:D:236:PRO:HB2	1:G:277:LEU:CD2	1.93	0.98
1:D:236:PRO:CB	1:G:277:LEU:HD21	1.94	0.97
1:A:114:VAL:HB	1:A:115:PRO:HD3	1.44	0.96
1:D:114:VAL:HB	1:D:115:PRO:HD3	1.44	0.96
1:O:114:VAL:HB	1:O:115:PRO:HD3	1.44	0.96
1:M:114:VAL:HB	1:M:115:PRO:HD3	1.44	0.96
1:F:114:VAL:HB	1:F:115:PRO:HD3	1.43	0.96
1:E:114:VAL:HB	1:E:115:PRO:HD3	1.44	0.96
1:D:225:ILE:CG2	1:G:277:LEU:HD11	1.95	0.95
1:J:114:VAL:HG23	1:J:115:PRO:HD3	1.32	0.92
1:K:277:LEU:HD11	1:F:225:ILE:CG2	2.00	0.92
1:D:225:ILE:HG22	1:G:277:LEU:CD1	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:114:VAL:HG23	1:N:115:PRO:HD3	1.32	0.90
1:C:277:LEU:CD2	1:J:236:PRO:HB2	2.00	0.90
1:C:277:LEU:CD1	1:J:225:ILE:HG22	2.02	0.89
1:D:114:VAL:HG23	1:D:115:PRO:HD3	1.32	0.88
1:G:114:VAL:HG23	1:G:115:PRO:HD3	1.32	0.88
1:N:236:PRO:CB	1:I:277:LEU:HD21	2.04	0.88
1:K:277:LEU:HD21	1:F:236:PRO:HB2	1.55	0.87
1:C:233:HIS:HE1	1:D:164:ARG:HD2	1.42	0.84
1:H:164:ARG:CG	1:E:233:HIS:HE1	1.91	0.84
1:J:164:ARG:CG	1:G:233:HIS:HE1	1.91	0.83
1:I:164:ARG:CG	1:F:233:HIS:HE1	1.91	0.83
1:K:277:LEU:HD11	1:F:225:ILE:HG22	1.60	0.83
1:B:164:ARG:CG	1:A:233:HIS:HE1	1.91	0.83
1:M:233:HIS:HE1	1:P:164:ARG:HD2	1.42	0.82
1:K:233:HIS:HE1	1:N:164:ARG:HD2	1.43	0.82
1:B:164:ARG:HD2	1:A:233:HIS:CE1	2.15	0.82
1:H:164:ARG:HD2	1:E:233:HIS:CE1	2.15	0.82
1:E:113:ILE:CG1	1:K:155:GLU:OE1	2.26	0.82
1:L:233:HIS:HE1	1:O:164:ARG:HD2	1.43	0.81
1:J:164:ARG:HD2	1:G:233:HIS:CE1	2.15	0.81
1:A:113:ILE:CG1	1:C:155:GLU:OE1	2.26	0.81
1:I:164:ARG:HD2	1:F:233:HIS:CE1	2.15	0.81
1:C:280:LYS:NZ	1:J:237:GLU:OE2	2.15	0.80
1:B:114:VAL:HG23	1:B:115:PRO:HD3	1.32	0.80
1:N:225:ILE:CG2	1:I:277:LEU:CD1	2.54	0.80
1:N:225:ILE:HG21	1:I:277:LEU:HD11	1.63	0.80
1:H:164:ARG:CD	1:E:233:HIS:HE1	1.95	0.79
1:B:164:ARG:CD	1:A:233:HIS:HE1	1.95	0.79
1:I:164:ARG:HD2	1:F:233:HIS:HE1	1.47	0.79
1:F:113:ILE:CG1	1:L:155:GLU:OE1	2.26	0.79
1:E:114:VAL:CG2	2:E:604:CTP:H2'	2.14	0.78
1:J:164:ARG:CD	1:G:233:HIS:HE1	1.95	0.78
1:F:114:VAL:CG2	2:F:604:CTP:H2'	2.14	0.78
1:C:277:LEU:HD11	1:J:225:ILE:HG21	1.66	0.77
1:I:164:ARG:CD	1:F:233:HIS:HE1	1.95	0.77
1:A:114:VAL:CG2	2:A:604:CTP:H2'	2.14	0.77
1:G:113:ILE:CG1	1:M:155:GLU:OE1	2.26	0.77
1:G:114:VAL:CG2	2:G:604:CTP:H2'	2.14	0.77
1:N:237:GLU:OE2	1:I:280:LYS:NZ	2.18	0.77
1:I:155:GLU:OE2	1:O:113:ILE:CG2	2.33	0.76
1:B:155:GLU:OE2	1:D:113:ILE:CG2	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:GLU:OE2	1:P:113:ILE:CG2	2.33	0.76
1:D:236:PRO:CB	1:G:277:LEU:CD2	2.59	0.76
1:H:155:GLU:OE2	1:N:113:ILE:CG2	2.33	0.76
1:N:236:PRO:HB2	1:I:277:LEU:CG	2.15	0.76
1:K:233:HIS:CE1	1:N:164:ARG:HD2	2.21	0.76
1:J:164:ARG:HD2	1:G:233:HIS:HE1	1.48	0.76
1:C:233:HIS:CE1	1:D:164:ARG:HD2	2.21	0.75
1:M:233:HIS:CE1	1:P:164:ARG:HD2	2.21	0.75
1:L:233:HIS:CE1	1:O:164:ARG:HD2	2.21	0.75
1:B:164:ARG:HD2	1:A:233:HIS:HE1	1.48	0.74
1:N:236:PRO:CB	1:I:277:LEU:CD2	2.63	0.74
1:C:277:LEU:CD1	1:J:225:ILE:CG2	2.62	0.74
1:H:164:ARG:HD2	1:E:233:HIS:HE1	1.47	0.74
1:B:164:ARG:CG	1:A:233:HIS:CE1	2.71	0.73
1:H:164:ARG:CG	1:E:233:HIS:CE1	2.71	0.73
1:E:114:VAL:HG22	2:E:604:CTP:H2'	1.71	0.73
1:K:280:LYS:NZ	1:F:237:GLU:OE2	2.22	0.73
1:J:164:ARG:CG	1:G:233:HIS:CE1	2.71	0.73
1:I:164:ARG:CG	1:F:233:HIS:CE1	2.71	0.73
1:A:114:VAL:HG22	2:A:604:CTP:H2'	1.71	0.73
1:H:114:VAL:HG23	1:H:115:PRO:HD2	0.85	0.73
1:F:114:VAL:HG22	2:F:604:CTP:H2'	1.71	0.72
1:O:114:VAL:HG23	1:O:115:PRO:HD3	1.32	0.72
1:F:113:ILE:HG13	1:L:155:GLU:OE1	1.89	0.72
1:G:113:ILE:HG13	1:M:155:GLU:OE1	1.89	0.72
1:G:114:VAL:HG22	2:G:604:CTP:H2'	1.71	0.72
1:N:236:PRO:CB	1:I:277:LEU:HG	2.19	0.72
1:D:236:PRO:CB	1:G:277:LEU:CG	2.68	0.71
1:K:277:LEU:HD11	1:F:225:ILE:HG21	1.71	0.71
1:E:113:ILE:HG13	1:K:155:GLU:OE1	1.89	0.71
1:N:236:PRO:CB	1:I:277:LEU:CG	2.69	0.71
1:K:277:LEU:CD1	1:F:225:ILE:HG22	2.21	0.71
1:K:277:LEU:CD2	1:F:236:PRO:HB2	2.20	0.70
1:A:113:ILE:HG13	1:C:155:GLU:OE1	1.89	0.70
1:C:114:VAL:HG23	1:C:115:PRO:HD2	0.85	0.70
1:M:114:VAL:HG23	1:M:115:PRO:HD3	1.32	0.70
1:D:236:PRO:HB2	1:G:277:LEU:CG	2.22	0.69
1:C:277:LEU:HD21	1:J:236:PRO:CB	2.17	0.68
1:D:236:PRO:CG	1:G:277:LEU:CD2	2.71	0.68
1:J:114:VAL:HG23	1:J:115:PRO:HD2	0.85	0.68
2:F:602:CTP:H2'	1:L:114:VAL:CG2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:HG23	1:C:115:PRO:HD3	1.32	0.68
1:E:155:GLU:OE1	1:K:113:ILE:CG1	2.41	0.67
2:G:602:CTP:H2'	1:M:114:VAL:CG2	2.24	0.67
1:G:114:VAL:HG22	1:G:115:PRO:HD2	1.67	0.67
1:A:114:VAL:HG23	1:A:115:PRO:HD2	0.85	0.67
1:C:277:LEU:CG	1:J:236:PRO:HB2	2.25	0.67
1:L:114:VAL:HG22	1:L:115:PRO:HD2	1.67	0.67
1:F:155:GLU:OE1	1:L:113:ILE:CG1	2.41	0.67
1:B:114:VAL:HG23	1:B:115:PRO:HD2	0.85	0.66
2:A:602:CTP:H2'	1:C:114:VAL:CG2	2.24	0.66
1:I:114:VAL:HG22	1:I:115:PRO:HD2	1.67	0.66
2:E:602:CTP:H2'	1:K:114:VAL:CG2	2.24	0.66
1:O:114:VAL:HG23	1:O:115:PRO:HD2	0.85	0.66
1:P:114:VAL:HG22	1:P:115:PRO:HD2	1.67	0.65
1:L:114:VAL:HG23	1:L:115:PRO:HD2	0.85	0.65
1:L:233:HIS:HE1	1:O:164:ARG:CD	2.09	0.65
1:E:113:ILE:HD12	1:K:155:GLU:OE1	1.97	0.65
1:F:113:ILE:HD12	1:L:155:GLU:OE1	1.97	0.65
1:B:233:HIS:HE1	1:A:164:ARG:CG	2.10	0.65
1:A:114:VAL:HG22	1:A:115:PRO:HD2	1.67	0.64
1:I:233:HIS:HE1	1:F:164:ARG:CG	2.10	0.64
1:D:236:PRO:CB	1:G:277:LEU:HG	2.27	0.64
1:N:114:VAL:HG23	1:N:115:PRO:HD2	0.85	0.64
1:G:155:GLU:OE1	1:M:113:ILE:CG1	2.41	0.64
1:M:233:HIS:HE1	1:P:164:ARG:CD	2.09	0.64
1:N:114:VAL:HG22	1:N:115:PRO:HD2	1.67	0.64
1:G:113:ILE:HD12	1:M:155:GLU:OE1	1.97	0.64
1:A:113:ILE:HD12	1:C:155:GLU:OE1	1.97	0.64
1:C:233:HIS:HE1	1:D:164:ARG:CD	2.09	0.64
1:J:233:HIS:HE1	1:G:164:ARG:CG	2.10	0.64
1:H:233:HIS:HE1	1:E:164:ARG:CG	2.10	0.64
1:K:114:VAL:HG23	1:K:115:PRO:HD2	0.85	0.63
1:D:114:VAL:HG22	1:D:115:PRO:HD2	1.67	0.63
1:C:277:LEU:HG	1:J:236:PRO:CB	2.29	0.63
1:D:225:ILE:CG2	1:G:277:LEU:CD1	2.69	0.63
1:K:233:HIS:HE1	1:N:164:ARG:CD	2.09	0.62
1:A:155:GLU:OE1	1:C:113:ILE:CG1	2.41	0.62
1:D:236:PRO:CG	1:G:277:LEU:HD21	2.30	0.62
1:E:114:VAL:HG22	1:E:115:PRO:HD2	1.67	0.62
1:G:114:VAL:HG23	1:G:115:PRO:HD2	0.85	0.62
1:E:113:ILE:CD1	1:K:155:GLU:OE1	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:277:LEU:CD1	1:F:225:ILE:CG2	2.75	0.62
1:K:114:VAL:HG22	1:K:115:PRO:HD2	1.67	0.62
1:A:113:ILE:CD1	1:C:155:GLU:OE1	2.48	0.61
1:E:112:GLN:HB3	2:E:604:CTP:O2'	2.00	0.61
1:B:114:VAL:HG22	1:B:115:PRO:HD2	1.67	0.61
1:H:112:GLN:CD	2:N:603:CTP:O3'	2.43	0.61
1:M:114:VAL:HG23	1:M:115:PRO:HD2	0.85	0.61
1:B:112:GLN:CD	2:D:603:CTP:O3'	2.43	0.61
1:G:112:GLN:HB3	2:G:604:CTP:O2'	2.01	0.61
1:G:113:ILE:CD1	1:M:155:GLU:OE1	2.48	0.61
1:I:112:GLN:CD	2:O:603:CTP:O3'	2.44	0.61
1:E:114:VAL:HG23	1:E:115:PRO:HD2	0.85	0.61
1:F:112:GLN:HB3	2:F:604:CTP:O2'	2.01	0.61
1:P:114:VAL:HG23	1:P:115:PRO:HD2	0.85	0.61
1:C:277:LEU:CD2	1:J:236:PRO:CB	2.76	0.61
1:F:113:ILE:CD1	1:L:155:GLU:OE1	2.48	0.61
1:A:112:GLN:HB3	2:A:604:CTP:O2'	2.00	0.60
1:J:112:GLN:CD	2:P:603:CTP:O3'	2.44	0.60
1:C:114:VAL:HG22	1:C:115:PRO:HD2	1.67	0.60
1:F:114:VAL:HG23	1:F:115:PRO:HD2	0.85	0.60
1:K:277:LEU:CG	1:F:236:PRO:HB2	2.32	0.60
1:D:114:VAL:HG23	1:D:115:PRO:HD2	0.85	0.59
1:H:114:VAL:HG22	1:H:115:PRO:HD2	1.67	0.59
1:I:114:VAL:HG23	1:I:115:PRO:HD2	0.85	0.59
1:C:277:LEU:CG	1:J:236:PRO:CB	2.81	0.59
1:E:155:GLU:OE1	1:K:113:ILE:HD12	2.03	0.58
1:F:155:GLU:OE1	1:L:113:ILE:HD12	2.03	0.58
1:B:113:ILE:HD12	1:D:155:GLU:OE1	2.03	0.58
1:O:114:VAL:HG22	1:O:115:PRO:HD2	1.67	0.58
1:A:155:GLU:OE1	1:C:113:ILE:HD12	2.03	0.58
1:I:113:ILE:HD12	1:O:155:GLU:OE1	2.03	0.58
1:J:114:VAL:HG22	1:J:115:PRO:HD2	1.67	0.58
1:G:155:GLU:OE1	1:M:113:ILE:HD12	2.03	0.57
1:J:113:ILE:HD12	1:P:155:GLU:OE1	2.03	0.57
1:H:113:ILE:HD12	1:N:155:GLU:OE1	2.03	0.57
1:F:114:VAL:HG22	1:F:115:PRO:HD2	1.67	0.57
1:E:114:VAL:HG21	2:E:604:CTP:H2'	1.88	0.56
1:G:113:ILE:HD11	1:M:90:THR:HG21	1.88	0.56
1:K:277:LEU:HG	1:F:236:PRO:CB	2.36	0.56
1:M:114:VAL:HG22	1:M:115:PRO:HD2	1.67	0.56
1:D:236:PRO:HB2	1:G:277:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG21	1:C:113:ILE:HD11	1.88	0.56
1:E:90:THR:HG21	1:K:113:ILE:HD11	1.88	0.56
1:A:113:ILE:HD11	1:C:90:THR:HG21	1.88	0.55
1:G:90:THR:HG21	1:M:113:ILE:HD11	1.88	0.55
1:A:114:VAL:HG11	2:A:604:CTP:C6	2.42	0.55
1:E:113:ILE:HD11	1:K:90:THR:HG21	1.88	0.55
1:E:114:VAL:HG11	2:E:604:CTP:C6	2.42	0.55
1:N:236:PRO:HB3	1:I:277:LEU:HG	1.88	0.55
1:G:114:VAL:HG11	2:G:604:CTP:C6	2.42	0.55
2:G:602:CTP:H2'	1:M:114:VAL:HG22	1.88	0.55
1:F:114:VAL:HG21	2:F:604:CTP:H2'	1.88	0.55
1:G:114:VAL:HG21	2:G:604:CTP:H2'	1.88	0.55
1:A:114:VAL:HG21	2:A:604:CTP:H2'	1.88	0.55
2:A:602:CTP:H2'	1:C:114:VAL:HG22	1.88	0.55
1:N:225:ILE:HG22	1:I:277:LEU:HD12	1.86	0.54
1:H:164:ARG:HG3	1:E:233:HIS:CE1	2.42	0.54
1:F:113:ILE:HD11	1:L:90:THR:HG21	1.88	0.54
1:F:114:VAL:HG11	2:F:604:CTP:C6	2.42	0.54
1:G:155:GLU:OE1	1:M:113:ILE:HG13	2.08	0.54
1:D:225:ILE:HG21	1:G:277:LEU:HD11	1.87	0.54
1:I:164:ARG:HG3	1:F:233:HIS:CE1	2.42	0.54
1:F:155:GLU:OE1	1:L:113:ILE:HG13	2.08	0.54
1:F:90:THR:HG21	1:L:113:ILE:HD11	1.88	0.54
2:G:602:CTP:H2'	1:M:114:VAL:HG21	1.90	0.54
2:F:602:CTP:H2'	1:L:114:VAL:HG22	1.88	0.54
1:E:155:GLU:OE1	1:K:113:ILE:HG13	2.08	0.54
1:J:164:ARG:HG3	1:G:233:HIS:CE1	2.42	0.53
1:H:113:ILE:CG1	1:N:155:GLU:OE1	2.57	0.53
1:N:236:PRO:CG	1:I:277:LEU:CD2	2.86	0.53
1:J:113:ILE:CG1	1:P:155:GLU:OE1	2.57	0.53
1:A:155:GLU:OE1	1:C:113:ILE:HG13	2.08	0.53
2:F:602:CTP:H2'	1:L:114:VAL:HG21	1.90	0.53
2:A:602:CTP:H2'	1:C:114:VAL:HG21	1.90	0.53
2:E:602:CTP:H2'	1:K:114:VAL:HG22	1.88	0.53
2:E:602:CTP:H2'	1:K:114:VAL:HG21	1.90	0.53
1:B:113:ILE:CG1	1:D:155:GLU:OE1	2.57	0.53
1:B:164:ARG:HG3	1:A:233:HIS:CE1	2.42	0.53
1:I:207:LEU:HD12	1:I:207:LEU:H	1.74	0.53
1:K:207:LEU:HD12	1:K:207:LEU:H	1.74	0.52
1:G:207:LEU:HD12	1:G:207:LEU:H	1.74	0.52
1:A:114:VAL:HG11	2:A:604:CTP:N1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:207:LEU:HD12	1:L:207:LEU:H	1.74	0.52
1:B:207:LEU:HD12	1:B:207:LEU:H	1.74	0.52
1:I:113:ILE:CG1	1:O:155:GLU:OE1	2.57	0.52
1:G:114:VAL:HG11	2:G:604:CTP:N1	2.25	0.52
1:E:114:VAL:HG11	2:E:604:CTP:N1	2.25	0.52
1:P:207:LEU:HD12	1:P:207:LEU:H	1.74	0.52
1:C:207:LEU:HD12	1:C:207:LEU:H	1.74	0.52
1:H:207:LEU:HD12	1:H:207:LEU:H	1.74	0.52
1:F:114:VAL:HG11	2:F:604:CTP:N1	2.25	0.52
1:J:207:LEU:H	1:J:207:LEU:HD12	1.74	0.52
1:I:164:ARG:CD	1:F:233:HIS:CE1	2.80	0.52
1:O:207:LEU:H	1:O:207:LEU:HD12	1.74	0.52
1:H:233:HIS:CE1	1:E:164:ARG:CG	2.93	0.52
1:F:207:LEU:HD12	1:F:207:LEU:H	1.75	0.51
1:E:207:LEU:H	1:E:207:LEU:HD12	1.74	0.51
1:A:207:LEU:HD12	1:A:207:LEU:H	1.74	0.51
1:E:191:LYS:NZ	2:N:603:CTP:O1G	2.40	0.51
1:J:164:ARG:CD	1:G:233:HIS:CE1	2.80	0.51
1:N:207:LEU:HD12	1:N:207:LEU:H	1.74	0.51
1:J:233:HIS:CE1	1:G:164:ARG:CG	2.93	0.50
1:D:207:LEU:HD12	1:D:207:LEU:H	1.75	0.50
1:B:233:HIS:CE1	1:A:164:ARG:CG	2.93	0.50
1:M:207:LEU:HD12	1:M:207:LEU:H	1.74	0.50
1:B:113:ILE:HG13	1:D:155:GLU:OE1	2.12	0.50
1:F:155:GLU:OE1	1:L:113:ILE:CD1	2.60	0.50
1:L:114:VAL:HG23	1:L:115:PRO:HG2	1.90	0.50
1:D:236:PRO:HB2	1:G:277:LEU:CD1	2.41	0.50
1:E:155:GLU:OE1	1:K:113:ILE:CD1	2.60	0.50
1:A:155:GLU:OE1	1:C:113:ILE:CD1	2.60	0.50
1:I:113:ILE:HG13	1:O:155:GLU:OE1	2.12	0.49
1:D:237:GLU:OE2	1:G:280:LYS:NZ	2.42	0.49
1:H:113:ILE:HG13	1:N:155:GLU:OE1	2.12	0.49
1:D:236:PRO:HB3	1:G:277:LEU:HG	1.94	0.49
1:J:233:HIS:CE1	1:G:168:PHE:HE2	2.31	0.49
1:G:155:GLU:OE1	1:M:113:ILE:CD1	2.60	0.49
1:I:233:HIS:CE1	1:F:168:PHE:HE2	2.31	0.49
1:J:164:ARG:HG2	1:G:233:HIS:HE1	1.76	0.48
1:B:114:VAL:O	1:B:116:HIS:N	2.47	0.48
1:G:191:LYS:NZ	2:P:603:CTP:O1G	2.40	0.48
1:K:114:VAL:O	1:K:116:HIS:N	2.47	0.48
1:C:114:VAL:O	1:C:116:HIS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:VAL:O	1:E:116:HIS:N	2.47	0.48
1:N:114:VAL:O	1:N:116:HIS:N	2.47	0.48
1:I:155:GLU:CD	1:O:113:ILE:CB	2.59	0.48
1:I:191:LYS:NZ	2:F:604:CTP:O1G	2.43	0.48
1:I:233:HIS:CG	1:F:168:PHE:CZ	3.02	0.48
1:C:114:VAL:HG23	1:C:115:PRO:HG2	1.90	0.48
1:I:114:VAL:O	1:I:116:HIS:N	2.47	0.48
1:J:113:ILE:HG13	1:P:155:GLU:OE1	2.12	0.48
1:B:113:ILE:CD1	1:D:155:GLU:OE1	2.62	0.48
1:B:233:HIS:CG	1:A:168:PHE:CZ	3.02	0.48
1:I:113:ILE:CD1	1:O:155:GLU:OE1	2.62	0.48
1:M:114:VAL:O	1:M:116:HIS:N	2.47	0.48
1:B:98:ILE:HD11	1:D:43:MET:CE	2.44	0.48
1:H:233:HIS:CG	1:E:168:PHE:CZ	3.01	0.48
1:I:164:ARG:HG2	1:F:233:HIS:HE1	1.76	0.48
1:G:114:VAL:O	1:G:116:HIS:N	2.47	0.48
1:I:233:HIS:CE1	1:F:164:ARG:CG	2.93	0.48
1:F:114:VAL:O	1:F:116:HIS:N	2.47	0.48
1:B:233:HIS:CE1	1:A:168:PHE:HE2	2.31	0.48
1:A:114:VAL:O	1:A:116:HIS:N	2.47	0.48
1:A:193:LYS:N	1:A:194:PRO:CD	2.77	0.48
1:H:233:HIS:CE1	1:E:168:PHE:HE2	2.31	0.48
1:I:193:LYS:N	1:I:194:PRO:CD	2.77	0.48
1:L:114:VAL:O	1:L:116:HIS:N	2.47	0.48
1:J:114:VAL:O	1:J:116:HIS:N	2.47	0.48
1:D:114:VAL:O	1:D:116:HIS:N	2.47	0.47
1:L:193:LYS:N	1:L:194:PRO:CD	2.77	0.47
1:H:114:VAL:O	1:H:116:HIS:N	2.47	0.47
1:H:164:ARG:CD	1:E:233:HIS:CE1	2.80	0.47
1:E:193:LYS:N	1:E:194:PRO:CD	2.77	0.47
1:K:233:HIS:HE1	1:N:164:ARG:CG	2.27	0.47
1:N:193:LYS:N	1:N:194:PRO:CD	2.77	0.47
1:I:114:VAL:HG23	1:I:115:PRO:HG2	1.90	0.47
1:L:233:HIS:HE1	1:O:164:ARG:CG	2.27	0.47
1:J:113:ILE:CD1	1:P:155:GLU:OE1	2.62	0.47
1:I:98:ILE:HD11	1:O:43:MET:CE	2.44	0.47
1:J:233:HIS:CG	1:G:168:PHE:CZ	3.02	0.47
1:G:193:LYS:N	1:G:194:PRO:CD	2.77	0.47
1:B:113:ILE:HD12	1:D:155:GLU:CD	2.40	0.47
1:H:98:ILE:HD11	1:N:43:MET:CE	2.44	0.47
1:H:193:LYS:N	1:H:194:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:ILE:HD12	1:O:155:GLU:CD	2.40	0.47
1:O:193:LYS:N	1:O:194:PRO:CD	2.77	0.47
1:P:114:VAL:O	1:P:116:HIS:N	2.47	0.47
1:K:193:LYS:N	1:K:194:PRO:CD	2.77	0.47
1:O:114:VAL:O	1:O:116:HIS:N	2.47	0.47
1:D:114:VAL:HG23	1:D:115:PRO:HG2	1.90	0.47
1:D:193:LYS:N	1:D:194:PRO:CD	2.77	0.47
1:F:114:VAL:HG23	1:F:115:PRO:HG2	1.90	0.47
1:F:193:LYS:N	1:F:194:PRO:CD	2.77	0.47
1:J:98:ILE:HD11	1:P:43:MET:CE	2.44	0.47
1:M:193:LYS:N	1:M:194:PRO:CD	2.77	0.47
1:A:191:LYS:NZ	2:D:603:CTP:O1G	2.40	0.47
1:C:193:LYS:N	1:C:194:PRO:CD	2.77	0.47
1:J:193:LYS:N	1:J:194:PRO:CD	2.77	0.47
1:B:193:LYS:N	1:B:194:PRO:CD	2.77	0.47
1:H:113:ILE:CD1	1:N:155:GLU:OE1	2.62	0.46
1:H:164:ARG:HG2	1:E:233:HIS:HE1	1.76	0.46
1:K:277:LEU:CG	1:F:236:PRO:CB	2.93	0.46
1:F:191:LYS:NZ	2:O:603:CTP:O3G	2.40	0.46
1:J:155:GLU:CD	1:P:113:ILE:CB	2.59	0.46
1:M:233:HIS:HE1	1:P:164:ARG:CG	2.27	0.46
1:C:233:HIS:HE1	1:D:164:ARG:CG	2.27	0.46
1:J:113:ILE:HD12	1:P:155:GLU:CD	2.40	0.46
1:P:193:LYS:N	1:P:194:PRO:CD	2.77	0.46
1:H:191:LYS:NZ	2:E:604:CTP:O3G	2.43	0.46
1:B:155:GLU:OE1	1:D:113:ILE:HD12	2.16	0.46
1:H:113:ILE:HD12	1:N:155:GLU:CD	2.40	0.45
1:H:155:GLU:OE1	1:N:113:ILE:HD12	2.16	0.45
1:P:33:LYS:HE3	1:P:138:LEU:CD1	2.47	0.45
1:A:33:LYS:HE3	1:A:138:LEU:CD1	2.47	0.45
1:D:33:LYS:HE3	1:D:138:LEU:CD1	2.47	0.45
1:G:33:LYS:HE3	1:G:138:LEU:CD1	2.47	0.45
1:O:33:LYS:HE3	1:O:138:LEU:CD1	2.47	0.45
1:E:114:VAL:HG11	2:E:604:CTP:C2	2.52	0.45
1:I:233:HIS:HE1	1:F:164:ARG:HG2	1.82	0.45
1:G:114:VAL:HG11	2:G:604:CTP:C2	2.52	0.45
1:I:33:LYS:HE3	1:I:138:LEU:CD1	2.47	0.45
1:L:33:LYS:HE3	1:L:138:LEU:CD1	2.47	0.45
1:D:367:SER:O	1:L:360:HIS:ND1	2.45	0.45
1:F:114:VAL:HG11	2:F:604:CTP:C2	2.52	0.45
1:J:155:GLU:OE1	1:P:113:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LYS:HE3	1:C:138:LEU:CD1	2.47	0.45
1:F:33:LYS:HE3	1:F:138:LEU:CD1	2.47	0.45
1:J:33:LYS:HE3	1:J:138:LEU:CD1	2.47	0.45
1:M:33:LYS:HE3	1:M:138:LEU:CD1	2.47	0.45
1:A:114:VAL:HG11	2:A:604:CTP:C2	2.52	0.45
1:H:33:LYS:HE3	1:H:138:LEU:CD1	2.47	0.45
1:E:33:LYS:HE3	1:E:138:LEU:CD1	2.47	0.45
1:N:33:LYS:HE3	1:N:138:LEU:CD1	2.47	0.45
1:I:155:GLU:OE1	1:O:113:ILE:HD12	2.16	0.45
1:J:49:THR:HG23	1:P:102:ARG:NH2	2.32	0.45
1:B:49:THR:HG23	1:D:102:ARG:NH2	2.32	0.44
1:I:164:ARG:HG2	1:F:233:HIS:CE1	2.52	0.44
1:I:203:ARG:HH12	1:F:164:ARG:HD2	1.83	0.44
1:C:277:LEU:HG	1:J:236:PRO:HB3	2.00	0.44
1:H:49:THR:HG23	1:N:102:ARG:NH2	2.33	0.44
1:K:33:LYS:HE3	1:K:138:LEU:CD1	2.47	0.44
1:B:33:LYS:HE3	1:B:138:LEU:CD1	2.47	0.44
1:I:49:THR:HG23	1:O:102:ARG:NH2	2.32	0.44
1:A:114:VAL:HG22	2:A:604:CTP:C2'	2.46	0.44
1:H:233:HIS:ND1	1:E:168:PHE:CE2	2.86	0.44
1:J:33:LYS:HE3	1:J:138:LEU:HD12	2.00	0.44
1:B:203:ARG:HH12	1:A:164:ARG:HD2	1.83	0.44
1:B:233:HIS:ND1	1:A:168:PHE:CE2	2.86	0.44
1:J:112:GLN:HB3	2:P:603:CTP:O2'	2.18	0.44
1:B:112:GLN:HB3	2:D:603:CTP:O2'	2.18	0.43
1:B:164:ARG:HG2	1:A:233:HIS:HE1	1.76	0.43
1:H:114:VAL:HG23	1:H:115:PRO:HG2	1.90	0.43
1:H:203:ARG:HH12	1:E:164:ARG:HD2	1.83	0.43
1:G:50:MET:HA	1:M:108:GLY:O	2.18	0.43
1:P:33:LYS:HE3	1:P:138:LEU:HD12	2.00	0.43
1:E:115:PRO:O	1:E:119:ASN:CG	2.62	0.43
1:J:203:ARG:HH12	1:G:164:ARG:HD2	1.83	0.43
1:J:233:HIS:HE1	1:G:164:ARG:HG2	1.82	0.43
1:A:112:GLN:CD	2:A:604:CTP:O3'	2.62	0.43
1:C:115:PRO:O	1:C:119:ASN:CG	2.62	0.43
1:K:115:PRO:O	1:K:119:ASN:CG	2.62	0.43
1:O:33:LYS:HE3	1:O:138:LEU:HD12	2.00	0.43
1:E:33:LYS:HE3	1:E:138:LEU:HD12	2.00	0.43
1:N:115:PRO:O	1:N:119:ASN:CG	2.62	0.43
1:I:112:GLN:HB3	2:O:603:CTP:O2'	2.18	0.43
1:I:233:HIS:ND1	1:F:168:PHE:CE2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:MET:HA	1:L:108:GLY:O	2.18	0.43
1:F:112:GLN:CD	2:F:604:CTP:O3'	2.62	0.43
1:L:33:LYS:HE3	1:L:138:LEU:HD12	2.00	0.43
1:J:98:ILE:CG1	1:P:43:MET:HE2	2.49	0.43
1:H:155:GLU:CD	1:N:113:ILE:CB	2.59	0.43
1:N:33:LYS:HE3	1:N:138:LEU:HD12	2.00	0.43
1:I:98:ILE:CG1	1:O:43:MET:HE2	2.49	0.43
1:G:33:LYS:HE3	1:G:138:LEU:HD12	2.00	0.43
1:B:233:HIS:CE1	1:A:164:ARG:HD2	2.54	0.43
1:A:115:PRO:O	1:A:119:ASN:CG	2.62	0.43
1:H:115:PRO:O	1:H:119:ASN:CG	2.62	0.43
1:E:50:MET:HA	1:K:108:GLY:O	2.18	0.43
1:N:236:PRO:HB2	1:I:277:LEU:CD1	2.49	0.43
1:I:33:LYS:HE3	1:I:138:LEU:HD12	2.00	0.43
1:L:115:PRO:O	1:L:119:ASN:CG	2.62	0.43
1:J:115:PRO:O	1:J:119:ASN:CG	2.62	0.43
1:B:33:LYS:HE3	1:B:138:LEU:HD12	2.00	0.43
1:B:98:ILE:CG1	1:D:43:MET:HE2	2.49	0.43
1:I:233:HIS:CE1	1:F:164:ARG:HD2	2.54	0.43
1:J:233:HIS:ND1	1:G:168:PHE:CE2	2.86	0.43
1:M:115:PRO:O	1:M:119:ASN:CG	2.62	0.43
1:A:50:MET:HA	1:C:108:GLY:O	2.18	0.42
1:H:112:GLN:HB3	2:N:603:CTP:O2'	2.18	0.42
1:E:112:GLN:CD	2:E:604:CTP:O3'	2.62	0.42
1:I:115:PRO:O	1:I:119:ASN:CG	2.62	0.42
1:O:115:PRO:O	1:O:119:ASN:CG	2.62	0.42
1:J:233:HIS:CE1	1:G:164:ARG:HD2	2.54	0.42
1:B:115:PRO:O	1:B:119:ASN:CG	2.62	0.42
1:C:33:LYS:HE3	1:C:138:LEU:HD12	2.00	0.42
1:H:233:HIS:CE1	1:E:164:ARG:HD2	2.54	0.42
1:I:114:VAL:HG22	2:O:603:CTP:H2'	2.01	0.42
1:O:114:VAL:HG23	1:O:115:PRO:HG2	1.90	0.42
1:B:155:GLU:CD	1:D:113:ILE:CB	2.59	0.42
1:E:114:VAL:HG22	2:E:604:CTP:C2'	2.46	0.42
1:B:233:HIS:CG	1:A:168:PHE:CE2	3.07	0.42
1:D:115:PRO:O	1:D:119:ASN:CG	2.62	0.42
1:K:33:LYS:HE3	1:K:138:LEU:HD12	2.00	0.42
1:B:191:LYS:NZ	2:A:604:CTP:O3G	2.43	0.42
1:I:233:HIS:CG	1:F:168:PHE:CE2	3.07	0.42
1:M:33:LYS:HE3	1:M:138:LEU:HD12	2.00	0.42
1:H:233:HIS:CG	1:E:168:PHE:CE2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:114:VAL:HG23	1:N:115:PRO:HG2	1.90	0.42
1:J:43:MET:O	1:J:91:GLY:HA3	2.20	0.42
1:J:191:LYS:NZ	2:G:604:CTP:O3G	2.43	0.42
1:P:115:PRO:O	1:P:119:ASN:CG	2.62	0.42
1:D:33:LYS:HE3	1:D:138:LEU:HD12	2.00	0.42
2:F:602:CTP:O2'	1:L:112:GLN:HB3	2.20	0.42
1:G:115:PRO:O	1:G:119:ASN:CG	2.62	0.42
1:M:114:VAL:HG23	1:M:115:PRO:HG2	1.90	0.42
1:H:233:HIS:HE1	1:E:164:ARG:HG2	1.82	0.42
1:K:114:VAL:HG23	1:K:115:PRO:HG2	1.90	0.42
1:N:43:MET:O	1:N:91:GLY:HA3	2.20	0.42
1:P:114:VAL:HG23	1:P:115:PRO:HG2	1.90	0.42
2:E:602:CTP:O2'	1:K:112:GLN:HB3	2.20	0.42
1:J:233:HIS:HE1	1:G:164:ARG:CD	2.33	0.42
1:G:43:MET:O	1:G:91:GLY:HA3	2.20	0.42
1:H:33:LYS:HE3	1:H:138:LEU:HD12	2.00	0.42
2:H:602:CTP:O1G	1:K:191:LYS:NZ	2.46	0.42
1:K:43:MET:O	1:K:91:GLY:HA3	2.20	0.42
1:I:233:HIS:HE1	1:F:164:ARG:CD	2.33	0.42
1:F:115:PRO:O	1:F:119:ASN:CG	2.62	0.42
1:A:33:LYS:HE3	1:A:138:LEU:HD12	2.00	0.41
1:H:43:MET:O	1:H:91:GLY:HA3	2.20	0.41
1:E:43:MET:O	1:E:91:GLY:HA3	2.20	0.41
1:F:33:LYS:HE3	1:F:138:LEU:HD12	2.00	0.41
2:J:602:CTP:O1G	1:M:191:LYS:NZ	2.46	0.41
1:B:43:MET:O	1:B:91:GLY:HA3	2.20	0.41
1:H:98:ILE:CG1	1:N:43:MET:HE2	2.49	0.41
1:I:43:MET:O	1:I:91:GLY:HA3	2.20	0.41
1:F:43:MET:O	1:F:91:GLY:HA3	2.20	0.41
1:J:114:VAL:HG23	1:J:115:PRO:HG2	1.90	0.41
1:J:233:HIS:CG	1:G:168:PHE:CE2	3.07	0.41
1:G:112:GLN:CD	2:G:604:CTP:O3'	2.62	0.41
1:M:43:MET:O	1:M:91:GLY:HA3	2.20	0.41
2:A:602:CTP:O2'	1:C:112:GLN:HB3	2.20	0.41
1:C:43:MET:O	1:C:91:GLY:HA3	2.20	0.41
1:H:114:VAL:HG22	2:N:603:CTP:H2'	2.01	0.41
1:E:114:VAL:HG23	1:E:115:PRO:HG2	1.90	0.41
1:F:98:ILE:CG1	1:L:43:MET:HE2	2.51	0.41
1:J:114:VAL:HG22	2:P:603:CTP:H2'	2.01	0.41
1:B:114:VAL:HG22	2:D:603:CTP:H2'	2.01	0.41
1:N:236:PRO:HB2	1:I:277:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:602:CTP:N1	1:C:114:VAL:HG11	2.36	0.41
1:H:164:ARG:HG2	1:E:233:HIS:CE1	2.52	0.41
2:G:602:CTP:N1	1:M:114:VAL:HG11	2.36	0.41
1:D:236:PRO:CB	1:G:277:LEU:HD11	2.51	0.41
1:F:114:VAL:HG22	2:F:604:CTP:C2'	2.46	0.41
1:D:43:MET:O	1:D:91:GLY:HA3	2.20	0.41
1:E:98:ILE:CG1	1:K:43:MET:HE2	2.51	0.41
2:G:602:CTP:O2'	1:M:112:GLN:HB3	2.20	0.41
1:B:233:HIS:HE1	1:A:164:ARG:CD	2.33	0.41
1:C:523:PHE:CD1	1:C:523:PHE:C	2.99	0.41
2:E:602:CTP:N1	1:K:114:VAL:HG11	2.36	0.41
1:K:523:PHE:CD1	1:K:523:PHE:C	2.99	0.41
1:L:43:MET:O	1:L:91:GLY:HA3	2.20	0.41
1:O:43:MET:O	1:O:91:GLY:HA3	2.20	0.41
1:J:523:PHE:CD1	1:J:523:PHE:C	2.99	0.41
1:G:98:ILE:CG1	1:M:43:MET:HE2	2.51	0.41
1:M:523:PHE:CD1	1:M:523:PHE:C	2.99	0.41
1:A:114:VAL:HG23	1:A:115:PRO:HG2	1.90	0.41
1:A:98:ILE:CG1	1:C:43:MET:HE2	2.51	0.40
1:N:523:PHE:CD1	1:N:523:PHE:C	2.99	0.40
1:F:90:THR:HG21	1:L:113:ILE:CD1	2.51	0.40
1:B:523:PHE:CD1	1:B:523:PHE:C	2.99	0.40
1:A:472:TRP:CE2	1:A:526:LYS:HE3	2.57	0.40
1:E:472:TRP:CE2	1:E:526:LYS:HE3	2.57	0.40
1:K:472:TRP:CE2	1:K:526:LYS:HE3	2.57	0.40
1:N:139:GLU:HA	1:N:140:PRO:HD3	1.97	0.40
1:P:472:TRP:CE2	1:P:526:LYS:HE3	2.57	0.40
1:C:277:LEU:HD12	1:J:225:ILE:HG22	1.97	0.40
1:H:472:TRP:CE2	1:H:526:LYS:HE3	2.57	0.40
1:F:472:TRP:CE2	1:F:526:LYS:HE3	2.57	0.40
1:P:43:MET:O	1:P:91:GLY:HA3	2.20	0.40
1:P:523:PHE:CD1	1:P:523:PHE:C	2.99	0.40
1:O:523:PHE:CD1	1:O:523:PHE:C	2.99	0.40
1:G:114:VAL:HG23	1:G:115:PRO:HG2	1.90	0.40
1:B:164:ARG:CD	1:A:233:HIS:CE1	2.80	0.40
1:E:523:PHE:CD1	1:E:523:PHE:C	2.99	0.40
1:I:523:PHE:CD1	1:I:523:PHE:C	2.99	0.40
2:F:602:CTP:N1	1:L:114:VAL:HG11	2.36	0.40
1:L:233:HIS:CE1	1:O:164:ARG:CG	3.05	0.40
1:G:472:TRP:CE2	1:G:526:LYS:HE3	2.57	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 PDB entries followed by that with respect to all EM entries.

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	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	B	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	C	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	D	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	E	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	F	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	G	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	H	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	I	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	J	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	K	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	L	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	M	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	N	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	O	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
1	P	555/559 (99%)	522 (94%)	32 (6%)	1 (0%)	43	72
All	All	8880/8944 (99%)	8352 (94%)	512 (6%)	16 (0%)	44	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	PRO
1	A	115	PRO
1	C	115	PRO
1	D	115	PRO
1	H	115	PRO
1	E	115	PRO

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Mol	Chain	Res	Type
1	K	115	PRO
1	N	115	PRO
1	I	115	PRO
1	F	115	PRO
1	L	115	PRO
1	O	115	PRO
1	J	115	PRO
1	G	115	PRO
1	M	115	PRO
1	P	115	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	B	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	C	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	D	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	E	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	F	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	G	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	H	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	I	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	J	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	K	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	L	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	M	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	N	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	O	488/488 (100%)	481 (99%)	7 (1%)	59	70
1	P	488/488 (100%)	481 (99%)	7 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7808/7808 (100%)	7696 (99%)	112 (1%)	57 70

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	67	THR
1	B	202	LEU
1	B	207	LEU
1	B	243	HIS
1	B	297	LEU
1	B	457	MET
1	B	491	HIS
1	A	67	THR
1	A	202	LEU
1	A	207	LEU
1	A	243	HIS
1	A	297	LEU
1	A	457	MET
1	A	491	HIS
1	C	67	THR
1	C	202	LEU
1	C	207	LEU
1	C	243	HIS
1	C	297	LEU
1	C	457	MET
1	C	491	HIS
1	D	67	THR
1	D	202	LEU
1	D	207	LEU
1	D	243	HIS
1	D	297	LEU
1	D	457	MET
1	D	491	HIS
1	H	67	THR
1	H	202	LEU
1	H	207	LEU
1	H	243	HIS
1	H	297	LEU
1	H	457	MET
1	H	491	HIS
1	E	67	THR
1	E	202	LEU

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Mol	Chain	Res	Type
1	E	207	LEU
1	E	243	HIS
1	E	297	LEU
1	E	457	MET
1	E	491	HIS
1	K	67	THR
1	K	202	LEU
1	K	207	LEU
1	K	243	HIS
1	K	297	LEU
1	K	457	MET
1	K	491	HIS
1	N	67	THR
1	N	202	LEU
1	N	207	LEU
1	N	243	HIS
1	N	297	LEU
1	N	457	MET
1	N	491	HIS
1	I	67	THR
1	I	202	LEU
1	I	207	LEU
1	I	243	HIS
1	I	297	LEU
1	I	457	MET
1	I	491	HIS
1	F	67	THR
1	F	202	LEU
1	F	207	LEU
1	F	243	HIS
1	F	297	LEU
1	F	457	MET
1	F	491	HIS
1	L	67	THR
1	L	202	LEU
1	L	207	LEU
1	L	243	HIS
1	L	297	LEU
1	L	457	MET
1	L	491	HIS
1	O	67	THR
1	O	202	LEU

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Mol	Chain	Res	Type
1	O	207	LEU
1	O	243	HIS
1	O	297	LEU
1	O	457	MET
1	O	491	HIS
1	J	67	THR
1	J	202	LEU
1	J	207	LEU
1	J	243	HIS
1	J	297	LEU
1	J	457	MET
1	J	491	HIS
1	G	67	THR
1	G	202	LEU
1	G	207	LEU
1	G	243	HIS
1	G	297	LEU
1	G	457	MET
1	G	491	HIS
1	M	67	THR
1	M	202	LEU
1	M	207	LEU
1	M	243	HIS
1	M	297	LEU
1	M	457	MET
1	M	491	HIS
1	P	67	THR
1	P	202	LEU
1	P	207	LEU
1	P	243	HIS
1	P	297	LEU
1	P	457	MET
1	P	491	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	ASN
1	B	167	GLN
1	B	196	GLN
1	B	233	HIS
1	B	535	GLN

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Mol	Chain	Res	Type
1	A	44	ASN
1	A	73	ASN
1	A	167	GLN
1	A	196	GLN
1	A	233	HIS
1	A	535	GLN
1	C	44	ASN
1	C	167	GLN
1	C	196	GLN
1	C	233	HIS
1	C	535	GLN
1	D	44	ASN
1	D	196	GLN
1	D	233	HIS
1	D	535	GLN
1	H	44	ASN
1	H	196	GLN
1	H	233	HIS
1	H	535	GLN
1	E	44	ASN
1	E	167	GLN
1	E	196	GLN
1	E	233	HIS
1	E	336	GLN
1	E	535	GLN
1	K	44	ASN
1	K	196	GLN
1	K	233	HIS
1	K	535	GLN
1	N	196	GLN
1	N	233	HIS
1	N	336	GLN
1	N	352	GLN
1	N	535	GLN
1	I	196	GLN
1	I	233	HIS
1	I	469	ASN
1	I	535	GLN
1	F	44	ASN
1	F	196	GLN
1	F	233	HIS
1	F	336	GLN

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Mol	Chain	Res	Type
1	F	535	GLN
1	L	44	ASN
1	L	167	GLN
1	L	196	GLN
1	L	233	HIS
1	L	535	GLN
1	O	44	ASN
1	O	167	GLN
1	O	196	GLN
1	O	233	HIS
1	O	336	GLN
1	O	535	GLN
1	J	196	GLN
1	J	233	HIS
1	J	535	GLN
1	G	44	ASN
1	G	73	ASN
1	G	196	GLN
1	G	233	HIS
1	G	535	GLN
1	M	44	ASN
1	M	167	GLN
1	M	196	GLN
1	M	233	HIS
1	M	535	GLN
1	P	44	ASN
1	P	167	GLN
1	P	196	GLN
1	P	233	HIS
1	P	352	GLN
1	P	535	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 64 ligands modelled in this entry, 32 are monoatomic - leaving 32 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	$\# Z > 2$
2	CTP	A	604	3	29,30,30	0.66	0	43,47,47	0.88	2 (4%)
2	CTP	M	602	3	29,30,30	0.61	0	43,47,47	1.17	5 (11%)
2	CTP	F	602	3	29,30,30	0.68	0	43,47,47	0.86	1 (2%)
2	CTP	B	602	3	29,30,30	0.68	0	43,47,47	0.86	1 (2%)
2	CTP	G	604	3	29,30,30	0.67	0	43,47,47	0.89	2 (4%)
2	CTP	G	602	3	29,30,30	0.66	0	43,47,47	0.88	2 (4%)
2	CTP	P	603	3	29,30,30	0.68	0	43,47,47	0.86	1 (2%)
2	CTP	K	602	3	29,30,30	0.61	0	43,47,47	1.17	5 (11%)
2	CTP	G	601	3	29,30,30	0.60	0	43,47,47	1.17	5 (11%)
2	CTP	E	602	3	29,30,30	0.67	0	43,47,47	0.89	2 (4%)
2	CTP	E	604	3	29,30,30	0.65	0	43,47,47	0.88	2 (4%)
2	CTP	A	602	3	29,30,30	0.67	0	43,47,47	0.89	2 (4%)
2	CTP	O	602	3	29,30,30	0.60	0	43,47,47	1.17	5 (11%)
2	CTP	N	602	3	29,30,30	0.64	0	43,47,47	1.12	4 (9%)
2	CTP	P	602	3	29,30,30	0.65	0	43,47,47	1.19	5 (11%)
2	CTP	H	602	3	29,30,30	0.68	0	43,47,47	0.86	1 (2%)
2	CTP	D	603	3	29,30,30	0.67	0	43,47,47	0.86	1 (2%)
2	CTP	F	601	3	29,30,30	0.64	0	43,47,47	1.12	4 (9%)
2	CTP	J	602	3	29,30,30	0.68	0	43,47,47	0.86	1 (2%)
2	CTP	F	604	3	29,30,30	0.67	0	43,47,47	0.86	1 (2%)
2	CTP	B	601	3	29,30,30	0.65	0	43,47,47	1.19	5 (11%)
2	CTP	O	603	3	29,30,30	0.68	0	43,47,47	0.89	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CTP	C	602	3	29,30,30	0.61	0	43,47,47	1.17	5 (11%)
2	CTP	I	601	3	29,30,30	0.61	0	43,47,47	1.17	5 (11%)
2	CTP	I	602	3	29,30,30	0.66	0	43,47,47	0.88	2 (4%)
2	CTP	D	602	3	29,30,30	0.65	0	43,47,47	1.12	4 (9%)
2	CTP	H	601	3	29,30,30	0.65	0	43,47,47	1.19	5 (11%)
2	CTP	L	602	3	29,30,30	0.65	0	43,47,47	1.19	5 (11%)
2	CTP	J	601	3	29,30,30	0.64	0	43,47,47	1.12	4 (9%)
2	CTP	N	603	3	29,30,30	0.67	0	43,47,47	0.86	1 (2%)
2	CTP	A	601	3	29,30,30	0.61	0	43,47,47	1.17	5 (11%)
2	CTP	E	601	3	29,30,30	0.60	0	43,47,47	1.17	5 (11%)

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	CTP	M	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	F	602	3	-	6/22/38/38	0/2/2/2
2	CTP	B	602	3	-	6/22/38/38	0/2/2/2
2	CTP	G	604	3	-	8/22/38/38	0/2/2/2
2	CTP	G	602	3	-	8/22/38/38	0/2/2/2
2	CTP	P	603	3	-	6/22/38/38	0/2/2/2
2	CTP	K	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	G	601	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	E	602	3	-	8/22/38/38	0/2/2/2
2	CTP	N	603	3	-	6/22/38/38	0/2/2/2
2	CTP	A	602	3	-	8/22/38/38	0/2/2/2
2	CTP	O	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	E	604	3	-	8/22/38/38	0/2/2/2
2	CTP	N	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	P	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	H	602	3	-	6/22/38/38	0/2/2/2
2	CTP	D	603	3	-	6/22/38/38	0/2/2/2
2	CTP	F	601	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	J	602	3	-	6/22/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTP	F	604	3	-	6/22/38/38	0/2/2/2
2	CTP	B	601	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	O	603	3	-	8/22/38/38	0/2/2/2
2	CTP	C	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	I	601	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	A	601	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	D	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	I	602	3	-	8/22/38/38	0/2/2/2
2	CTP	H	601	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	J	601	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	A	604	3	-	8/22/38/38	0/2/2/2
2	CTP	L	602	3	1/1/7/7	7/22/38/38	0/2/2/2
2	CTP	E	601	3	1/1/7/7	7/22/38/38	0/2/2/2

There are no bond length outliers.

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	602	CTP	C5'-C4'-C3'	3.77	128.77	115.21
2	E	601	CTP	C5'-C4'-C3'	3.76	128.76	115.21
2	K	602	CTP	C5'-C4'-C3'	3.76	128.75	115.21
2	A	601	CTP	C5'-C4'-C3'	3.76	128.75	115.21
2	O	602	CTP	C5'-C4'-C3'	3.76	128.74	115.21
2	P	602	CTP	C5'-C4'-C3'	3.76	128.74	115.21
2	N	602	CTP	C5'-C4'-C3'	3.76	128.74	115.21
2	G	601	CTP	C5'-C4'-C3'	3.76	128.73	115.21
2	J	601	CTP	C5'-C4'-C3'	3.76	128.73	115.21
2	I	601	CTP	C5'-C4'-C3'	3.75	128.72	115.21
2	B	601	CTP	C5'-C4'-C3'	3.75	128.71	115.21
2	M	602	CTP	C5'-C4'-C3'	3.75	128.71	115.21
2	D	602	CTP	C5'-C4'-C3'	3.75	128.70	115.21
2	C	602	CTP	C5'-C4'-C3'	3.74	128.69	115.21
2	F	601	CTP	C5'-C4'-C3'	3.74	128.69	115.21
2	H	601	CTP	C5'-C4'-C3'	3.74	128.68	115.21
2	N	603	CTP	O3B-PB-O1B	-3.49	100.20	110.70
2	D	603	CTP	O3B-PB-O1B	-3.49	100.20	110.70
2	F	602	CTP	O3B-PB-O1B	-3.49	100.20	110.70
2	P	603	CTP	O3B-PB-O1B	-3.49	100.21	110.70
2	J	602	CTP	O3B-PB-O1B	-3.49	100.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	CTP	O3B-PB-O1B	-3.48	100.22	110.70
2	F	604	CTP	O3B-PB-O1B	-3.48	100.23	110.70
2	H	602	CTP	O3B-PB-O1B	-3.48	100.24	110.70
2	H	601	CTP	O4'-C4'-C5'	3.06	119.13	109.33
2	M	602	CTP	O4'-C4'-C5'	3.05	119.11	109.33
2	D	602	CTP	O4'-C4'-C5'	3.05	119.11	109.33
2	F	601	CTP	O4'-C4'-C5'	3.05	119.11	109.33
2	L	602	CTP	O4'-C4'-C5'	3.05	119.10	109.33
2	C	602	CTP	O4'-C4'-C5'	3.05	119.10	109.33
2	G	601	CTP	O4'-C4'-C5'	3.04	119.09	109.33
2	P	602	CTP	O4'-C4'-C5'	3.04	119.09	109.33
2	J	601	CTP	O4'-C4'-C5'	3.04	119.08	109.33
2	K	602	CTP	O4'-C4'-C5'	3.04	119.08	109.33
2	A	601	CTP	O4'-C4'-C5'	3.04	119.06	109.33
2	O	602	CTP	O4'-C4'-C5'	3.03	119.05	109.33
2	B	601	CTP	O4'-C4'-C5'	3.03	119.05	109.33
2	N	602	CTP	O4'-C4'-C5'	3.03	119.04	109.33
2	E	601	CTP	O4'-C4'-C5'	3.03	119.04	109.33
2	I	601	CTP	O4'-C4'-C5'	3.03	119.03	109.33
2	B	601	CTP	O4'-C4'-C3'	2.63	110.37	105.15
2	E	602	CTP	O2B-PB-O3B	-2.62	100.19	107.27
2	G	602	CTP	O2B-PB-O3B	-2.62	100.19	107.27
2	I	601	CTP	O4'-C4'-C3'	2.62	110.35	105.15
2	G	604	CTP	O2B-PB-O3B	-2.62	100.20	107.27
2	A	604	CTP	O2B-PB-O3B	-2.62	100.20	107.27
2	C	602	CTP	O4'-C4'-C3'	2.62	110.35	105.15
2	O	603	CTP	O2B-PB-O3B	-2.61	100.21	107.27
2	N	602	CTP	O4'-C4'-C3'	2.61	110.34	105.15
2	F	601	CTP	O4'-C4'-C3'	2.61	110.34	105.15
2	E	604	CTP	O2B-PB-O3B	-2.61	100.22	107.27
2	H	601	CTP	O4'-C4'-C3'	2.61	110.33	105.15
2	O	602	CTP	O4'-C4'-C3'	2.61	110.33	105.15
2	A	602	CTP	O2B-PB-O3B	-2.61	100.23	107.27
2	E	601	CTP	O4'-C4'-C3'	2.60	110.32	105.15
2	K	602	CTP	O4'-C4'-C3'	2.60	110.32	105.15
2	J	601	CTP	O4'-C4'-C3'	2.60	110.31	105.15
2	G	601	CTP	O4'-C4'-C3'	2.60	110.31	105.15
2	A	601	CTP	O4'-C4'-C3'	2.60	110.31	105.15
2	I	602	CTP	O2B-PB-O3B	-2.60	100.25	107.27
2	M	602	CTP	O4'-C4'-C3'	2.60	110.31	105.15
2	D	602	CTP	O4'-C4'-C3'	2.59	110.30	105.15
2	P	602	CTP	O4'-C4'-C3'	2.59	110.30	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	602	CTP	O4'-C4'-C3'	2.57	110.26	105.15
2	H	601	CTP	O2G-PG-O3B	2.55	113.18	104.64
2	L	602	CTP	O2G-PG-O3B	2.54	113.16	104.64
2	M	602	CTP	O2G-PG-O3B	2.53	113.14	104.64
2	K	602	CTP	O2G-PG-O3B	2.53	113.13	104.64
2	O	602	CTP	O2G-PG-O3B	2.53	113.13	104.64
2	C	602	CTP	O2G-PG-O3B	2.53	113.13	104.64
2	A	601	CTP	O2G-PG-O3B	2.53	113.12	104.64
2	I	601	CTP	O2G-PG-O3B	2.53	113.12	104.64
2	E	601	CTP	O2G-PG-O3B	2.53	113.11	104.64
2	G	601	CTP	O2G-PG-O3B	2.53	113.10	104.64
2	P	602	CTP	O2G-PG-O3B	2.52	113.10	104.64
2	B	601	CTP	O2G-PG-O3B	2.52	113.09	104.64
2	I	602	CTP	O2B-PB-O3A	2.44	113.87	107.27
2	O	603	CTP	O2B-PB-O3A	2.44	113.86	107.27
2	G	602	CTP	O2B-PB-O3A	2.44	113.86	107.27
2	E	602	CTP	O2B-PB-O3A	2.44	113.86	107.27
2	E	604	CTP	O2B-PB-O3A	2.43	113.85	107.27
2	G	604	CTP	O2B-PB-O3A	2.43	113.84	107.27
2	A	604	CTP	O2B-PB-O3A	2.41	113.79	107.27
2	A	602	CTP	O2B-PB-O3A	2.41	113.78	107.27
2	D	602	CTP	O3'-C3'-C4'	-2.26	104.58	111.08
2	N	602	CTP	O3'-C3'-C4'	-2.26	104.58	111.08
2	O	602	CTP	O3'-C3'-C4'	-2.26	104.59	111.08
2	B	601	CTP	O3'-C3'-C4'	-2.26	104.59	111.08
2	K	602	CTP	O3'-C3'-C4'	-2.26	104.60	111.08
2	L	602	CTP	O3'-C3'-C4'	-2.26	104.60	111.08
2	J	601	CTP	O3'-C3'-C4'	-2.25	104.61	111.08
2	E	601	CTP	O3'-C3'-C4'	-2.25	104.61	111.08
2	F	601	CTP	O3'-C3'-C4'	-2.25	104.62	111.08
2	M	602	CTP	O3'-C3'-C4'	-2.25	104.62	111.08
2	I	601	CTP	O3'-C3'-C4'	-2.25	104.62	111.08
2	G	601	CTP	O3'-C3'-C4'	-2.25	104.62	111.08
2	P	602	CTP	O3'-C3'-C4'	-2.25	104.62	111.08
2	C	602	CTP	O3'-C3'-C4'	-2.25	104.62	111.08
2	A	601	CTP	O3'-C3'-C4'	-2.25	104.63	111.08
2	H	601	CTP	O3'-C3'-C4'	-2.24	104.64	111.08

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	601	CTP	C4'

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Mol	Chain	Res	Type	Atom
2	A	601	CTP	C4'
2	C	602	CTP	C4'
2	D	602	CTP	C4'
2	H	601	CTP	C4'
2	E	601	CTP	C4'
2	K	602	CTP	C4'
2	N	602	CTP	C4'
2	I	601	CTP	C4'
2	F	601	CTP	C4'
2	L	602	CTP	C4'
2	O	602	CTP	C4'
2	J	601	CTP	C4'
2	G	601	CTP	C4'
2	M	602	CTP	C4'
2	P	602	CTP	C4'

All (224) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	CTP	O4'-C4'-C5'-O5'
2	B	601	CTP	C5'-O5'-PA-O1A
2	B	601	CTP	C5'-O5'-PA-O2A
2	B	601	CTP	C5'-O5'-PA-O3A
2	B	602	CTP	C5'-O5'-PA-O2A
2	B	602	CTP	C5'-O5'-PA-O3A
2	A	601	CTP	O4'-C4'-C5'-O5'
2	A	601	CTP	C5'-O5'-PA-O1A
2	A	601	CTP	C5'-O5'-PA-O2A
2	A	601	CTP	C5'-O5'-PA-O3A
2	A	602	CTP	C5'-O5'-PA-O3A
2	A	604	CTP	C5'-O5'-PA-O3A
2	C	602	CTP	O4'-C4'-C5'-O5'
2	C	602	CTP	C5'-O5'-PA-O1A
2	C	602	CTP	C5'-O5'-PA-O2A
2	C	602	CTP	C5'-O5'-PA-O3A
2	D	602	CTP	O4'-C4'-C5'-O5'
2	D	602	CTP	C5'-O5'-PA-O1A
2	D	602	CTP	C5'-O5'-PA-O2A
2	D	602	CTP	C5'-O5'-PA-O3A
2	D	603	CTP	C5'-O5'-PA-O2A
2	D	603	CTP	C5'-O5'-PA-O3A
2	H	601	CTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	H	601	CTP	C5'-O5'-PA-O1A
2	H	601	CTP	C5'-O5'-PA-O2A
2	H	601	CTP	C5'-O5'-PA-O3A
2	H	602	CTP	C5'-O5'-PA-O2A
2	H	602	CTP	C5'-O5'-PA-O3A
2	E	601	CTP	O4'-C4'-C5'-O5'
2	E	601	CTP	C5'-O5'-PA-O1A
2	E	601	CTP	C5'-O5'-PA-O2A
2	E	601	CTP	C5'-O5'-PA-O3A
2	E	602	CTP	C5'-O5'-PA-O3A
2	E	604	CTP	C5'-O5'-PA-O3A
2	K	602	CTP	O4'-C4'-C5'-O5'
2	K	602	CTP	C5'-O5'-PA-O1A
2	K	602	CTP	C5'-O5'-PA-O2A
2	K	602	CTP	C5'-O5'-PA-O3A
2	N	602	CTP	O4'-C4'-C5'-O5'
2	N	602	CTP	C5'-O5'-PA-O1A
2	N	602	CTP	C5'-O5'-PA-O2A
2	N	602	CTP	C5'-O5'-PA-O3A
2	N	603	CTP	C5'-O5'-PA-O2A
2	N	603	CTP	C5'-O5'-PA-O3A
2	I	601	CTP	O4'-C4'-C5'-O5'
2	I	601	CTP	C5'-O5'-PA-O1A
2	I	601	CTP	C5'-O5'-PA-O2A
2	I	601	CTP	C5'-O5'-PA-O3A
2	I	602	CTP	C5'-O5'-PA-O3A
2	F	601	CTP	O4'-C4'-C5'-O5'
2	F	601	CTP	C5'-O5'-PA-O1A
2	F	601	CTP	C5'-O5'-PA-O2A
2	F	601	CTP	C5'-O5'-PA-O3A
2	F	602	CTP	C5'-O5'-PA-O2A
2	F	602	CTP	C5'-O5'-PA-O3A
2	F	604	CTP	C5'-O5'-PA-O2A
2	F	604	CTP	C5'-O5'-PA-O3A
2	L	602	CTP	O4'-C4'-C5'-O5'
2	L	602	CTP	C5'-O5'-PA-O1A
2	L	602	CTP	C5'-O5'-PA-O2A
2	L	602	CTP	C5'-O5'-PA-O3A
2	O	602	CTP	O4'-C4'-C5'-O5'
2	O	602	CTP	C5'-O5'-PA-O1A
2	O	602	CTP	C5'-O5'-PA-O2A
2	O	602	CTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	O	603	CTP	C5'-O5'-PA-O3A
2	J	601	CTP	O4'-C4'-C5'-O5'
2	J	601	CTP	C5'-O5'-PA-O1A
2	J	601	CTP	C5'-O5'-PA-O2A
2	J	601	CTP	C5'-O5'-PA-O3A
2	J	602	CTP	C5'-O5'-PA-O2A
2	J	602	CTP	C5'-O5'-PA-O3A
2	G	601	CTP	O4'-C4'-C5'-O5'
2	G	601	CTP	C5'-O5'-PA-O1A
2	G	601	CTP	C5'-O5'-PA-O2A
2	G	601	CTP	C5'-O5'-PA-O3A
2	G	602	CTP	C5'-O5'-PA-O3A
2	G	604	CTP	C5'-O5'-PA-O3A
2	M	602	CTP	O4'-C4'-C5'-O5'
2	M	602	CTP	C5'-O5'-PA-O1A
2	M	602	CTP	C5'-O5'-PA-O2A
2	M	602	CTP	C5'-O5'-PA-O3A
2	P	602	CTP	O4'-C4'-C5'-O5'
2	P	602	CTP	C5'-O5'-PA-O1A
2	P	602	CTP	C5'-O5'-PA-O2A
2	P	602	CTP	C5'-O5'-PA-O3A
2	P	603	CTP	C5'-O5'-PA-O2A
2	P	603	CTP	C5'-O5'-PA-O3A
2	B	601	CTP	C4'-C5'-O5'-PA
2	A	601	CTP	C4'-C5'-O5'-PA
2	C	602	CTP	C4'-C5'-O5'-PA
2	D	602	CTP	C4'-C5'-O5'-PA
2	H	601	CTP	C4'-C5'-O5'-PA
2	E	601	CTP	C4'-C5'-O5'-PA
2	K	602	CTP	C4'-C5'-O5'-PA
2	N	602	CTP	C4'-C5'-O5'-PA
2	I	601	CTP	C4'-C5'-O5'-PA
2	F	601	CTP	C4'-C5'-O5'-PA
2	L	602	CTP	C4'-C5'-O5'-PA
2	O	602	CTP	C4'-C5'-O5'-PA
2	J	601	CTP	C4'-C5'-O5'-PA
2	G	601	CTP	C4'-C5'-O5'-PA
2	M	602	CTP	C4'-C5'-O5'-PA
2	P	602	CTP	C4'-C5'-O5'-PA
2	B	601	CTP	PB-O3A-PA-O5'
2	A	601	CTP	PB-O3A-PA-O5'
2	C	602	CTP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
2	D	602	CTP	PB-O3A-PA-O5'
2	H	601	CTP	PB-O3A-PA-O5'
2	E	601	CTP	PB-O3A-PA-O5'
2	K	602	CTP	PB-O3A-PA-O5'
2	N	602	CTP	PB-O3A-PA-O5'
2	I	601	CTP	PB-O3A-PA-O5'
2	F	601	CTP	PB-O3A-PA-O5'
2	L	602	CTP	PB-O3A-PA-O5'
2	O	602	CTP	PB-O3A-PA-O5'
2	J	601	CTP	PB-O3A-PA-O5'
2	G	601	CTP	PB-O3A-PA-O5'
2	M	602	CTP	PB-O3A-PA-O5'
2	P	602	CTP	PB-O3A-PA-O5'
2	A	602	CTP	C5'-O5'-PA-O1A
2	A	604	CTP	C5'-O5'-PA-O1A
2	E	602	CTP	C5'-O5'-PA-O1A
2	E	604	CTP	C5'-O5'-PA-O1A
2	I	602	CTP	C5'-O5'-PA-O1A
2	O	603	CTP	C5'-O5'-PA-O1A
2	G	602	CTP	C5'-O5'-PA-O1A
2	G	604	CTP	C5'-O5'-PA-O1A
2	B	602	CTP	PB-O3A-PA-O2A
2	A	602	CTP	PA-O3A-PB-O1B
2	A	604	CTP	PA-O3A-PB-O1B
2	D	603	CTP	PB-O3A-PA-O2A
2	H	602	CTP	PB-O3A-PA-O2A
2	E	602	CTP	PA-O3A-PB-O1B
2	E	604	CTP	PA-O3A-PB-O1B
2	N	603	CTP	PB-O3A-PA-O2A
2	I	602	CTP	PA-O3A-PB-O1B
2	F	602	CTP	PB-O3A-PA-O2A
2	F	604	CTP	PB-O3A-PA-O2A
2	O	603	CTP	PA-O3A-PB-O1B
2	J	602	CTP	PB-O3A-PA-O2A
2	G	602	CTP	PA-O3A-PB-O1B
2	G	604	CTP	PA-O3A-PB-O1B
2	P	603	CTP	PB-O3A-PA-O2A
2	B	602	CTP	C4'-C5'-O5'-PA
2	A	602	CTP	C4'-C5'-O5'-PA
2	A	604	CTP	C4'-C5'-O5'-PA
2	D	603	CTP	C4'-C5'-O5'-PA
2	H	602	CTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
2	E	602	CTP	C4'-C5'-O5'-PA
2	E	604	CTP	C4'-C5'-O5'-PA
2	N	603	CTP	C4'-C5'-O5'-PA
2	I	602	CTP	C4'-C5'-O5'-PA
2	F	602	CTP	C4'-C5'-O5'-PA
2	F	604	CTP	C4'-C5'-O5'-PA
2	O	603	CTP	C4'-C5'-O5'-PA
2	J	602	CTP	C4'-C5'-O5'-PA
2	G	602	CTP	C4'-C5'-O5'-PA
2	G	604	CTP	C4'-C5'-O5'-PA
2	P	603	CTP	C4'-C5'-O5'-PA
2	A	602	CTP	PB-O3A-PA-O1A
2	A	604	CTP	PB-O3A-PA-O1A
2	E	602	CTP	PB-O3A-PA-O1A
2	E	604	CTP	PB-O3A-PA-O1A
2	I	602	CTP	PB-O3A-PA-O1A
2	O	603	CTP	PB-O3A-PA-O1A
2	G	602	CTP	PB-O3A-PA-O1A
2	G	604	CTP	PB-O3A-PA-O1A
2	B	601	CTP	PB-O3A-PA-O2A
2	B	602	CTP	PB-O3A-PA-O1A
2	A	602	CTP	PG-O3B-PB-O1B
2	A	604	CTP	PG-O3B-PB-O1B
2	D	602	CTP	PB-O3A-PA-O2A
2	D	603	CTP	PB-O3A-PA-O1A
2	H	601	CTP	PB-O3A-PA-O2A
2	H	602	CTP	PB-O3A-PA-O1A
2	E	602	CTP	PG-O3B-PB-O1B
2	E	604	CTP	PG-O3B-PB-O1B
2	N	602	CTP	PB-O3A-PA-O2A
2	N	603	CTP	PB-O3A-PA-O1A
2	I	602	CTP	PG-O3B-PB-O1B
2	F	601	CTP	PB-O3A-PA-O2A
2	F	602	CTP	PB-O3A-PA-O1A
2	F	604	CTP	PB-O3A-PA-O1A
2	L	602	CTP	PB-O3A-PA-O2A
2	O	603	CTP	PG-O3B-PB-O1B
2	J	601	CTP	PB-O3A-PA-O2A
2	J	602	CTP	PB-O3A-PA-O1A
2	G	602	CTP	PG-O3B-PB-O1B
2	G	604	CTP	PG-O3B-PB-O1B
2	P	602	CTP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	P	603	CTP	PB-O3A-PA-O1A
2	B	602	CTP	PG-O3B-PB-O2B
2	A	601	CTP	PB-O3A-PA-O1A
2	A	602	CTP	PB-O3A-PA-O2A
2	A	602	CTP	PG-O3B-PB-O2B
2	A	604	CTP	PB-O3A-PA-O2A
2	A	604	CTP	PG-O3B-PB-O2B
2	C	602	CTP	PB-O3A-PA-O1A
2	D	603	CTP	PG-O3B-PB-O2B
2	H	602	CTP	PG-O3B-PB-O2B
2	E	601	CTP	PB-O3A-PA-O1A
2	E	602	CTP	PB-O3A-PA-O2A
2	E	602	CTP	PG-O3B-PB-O2B
2	E	604	CTP	PB-O3A-PA-O2A
2	E	604	CTP	PG-O3B-PB-O2B
2	K	602	CTP	PB-O3A-PA-O1A
2	N	603	CTP	PG-O3B-PB-O2B
2	I	601	CTP	PB-O3A-PA-O1A
2	I	602	CTP	PB-O3A-PA-O2A
2	I	602	CTP	PG-O3B-PB-O2B
2	F	602	CTP	PG-O3B-PB-O2B
2	F	604	CTP	PG-O3B-PB-O2B
2	O	602	CTP	PB-O3A-PA-O1A
2	O	603	CTP	PB-O3A-PA-O2A
2	O	603	CTP	PG-O3B-PB-O2B
2	J	602	CTP	PG-O3B-PB-O2B
2	G	601	CTP	PB-O3A-PA-O1A
2	G	602	CTP	PB-O3A-PA-O2A
2	G	602	CTP	PG-O3B-PB-O2B
2	G	604	CTP	PB-O3A-PA-O2A
2	G	604	CTP	PG-O3B-PB-O2B
2	M	602	CTP	PB-O3A-PA-O1A
2	P	603	CTP	PG-O3B-PB-O2B

There are no ring outliers.

14 monomers are involved in 77 short contacts:

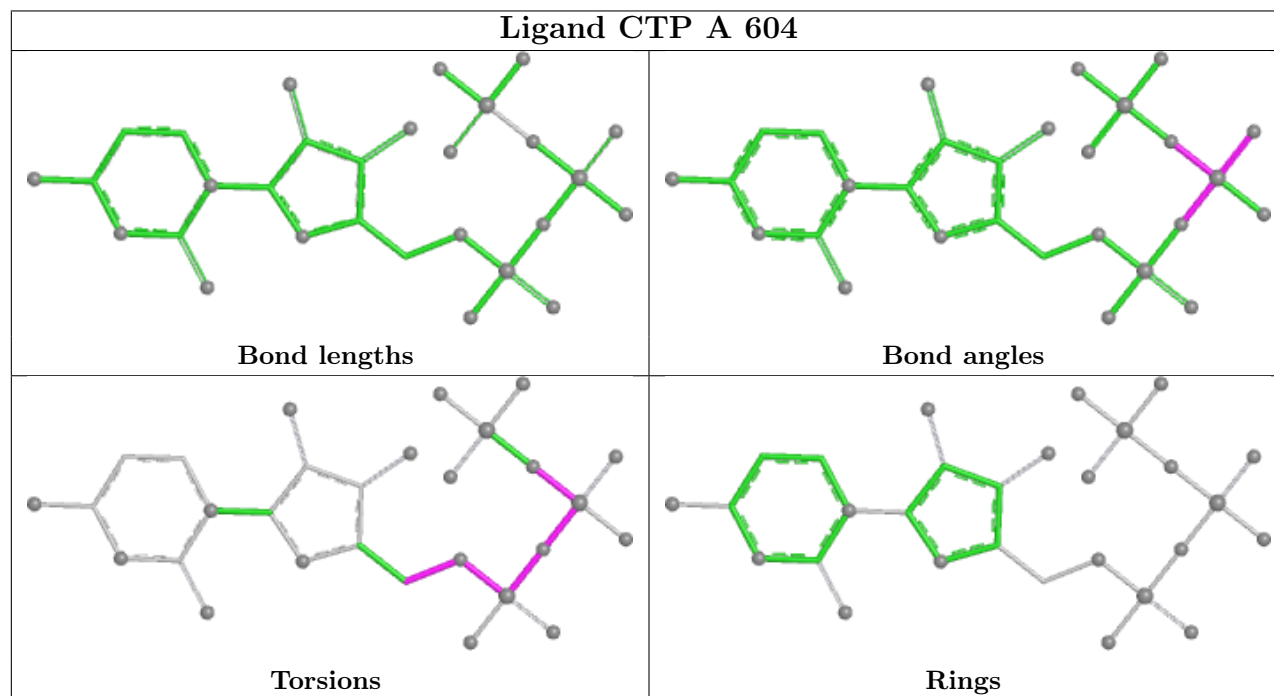
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	CTP	10	0
2	F	602	CTP	5	0
2	G	604	CTP	9	0
2	G	602	CTP	5	0

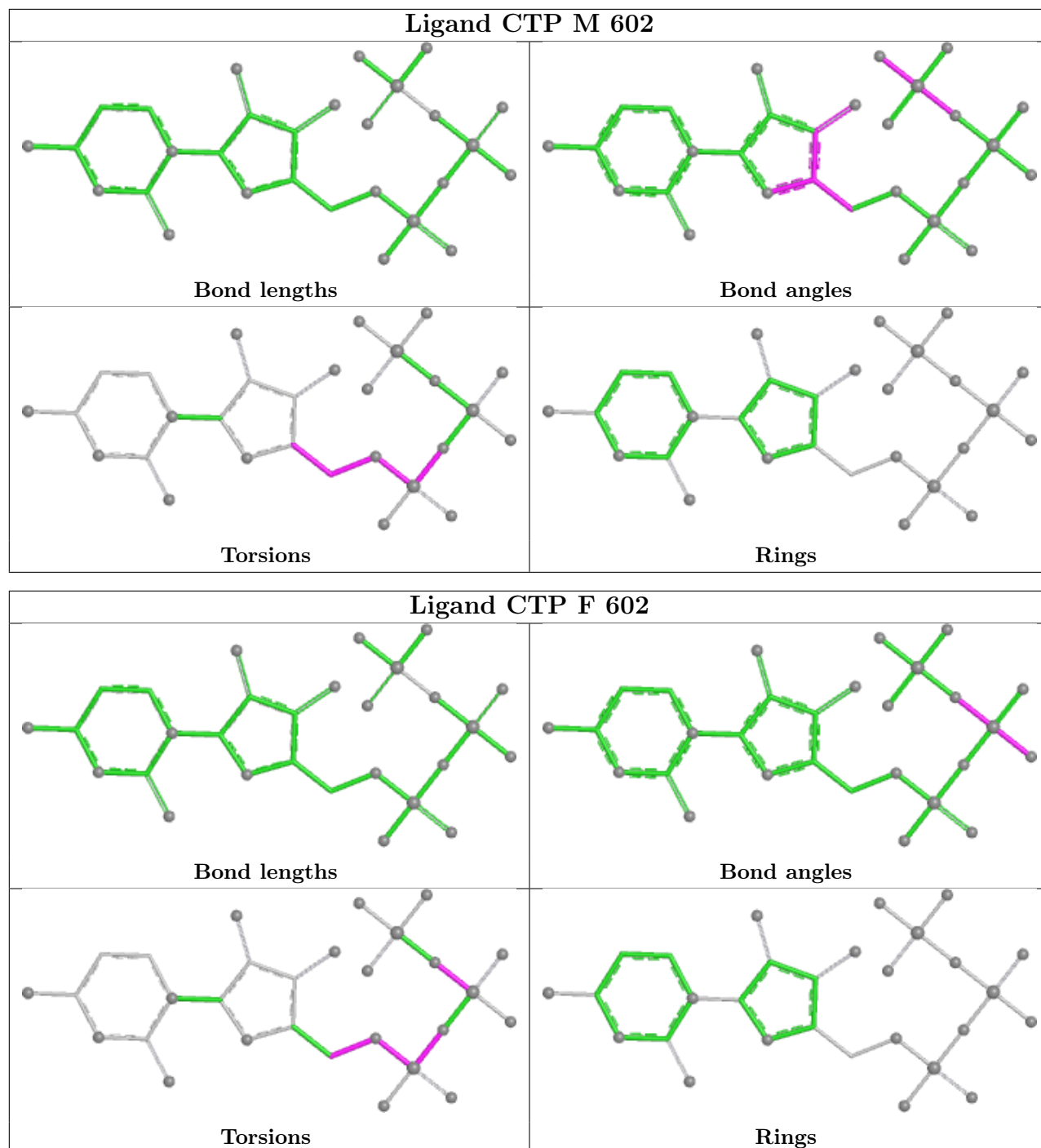
Continued on next page...

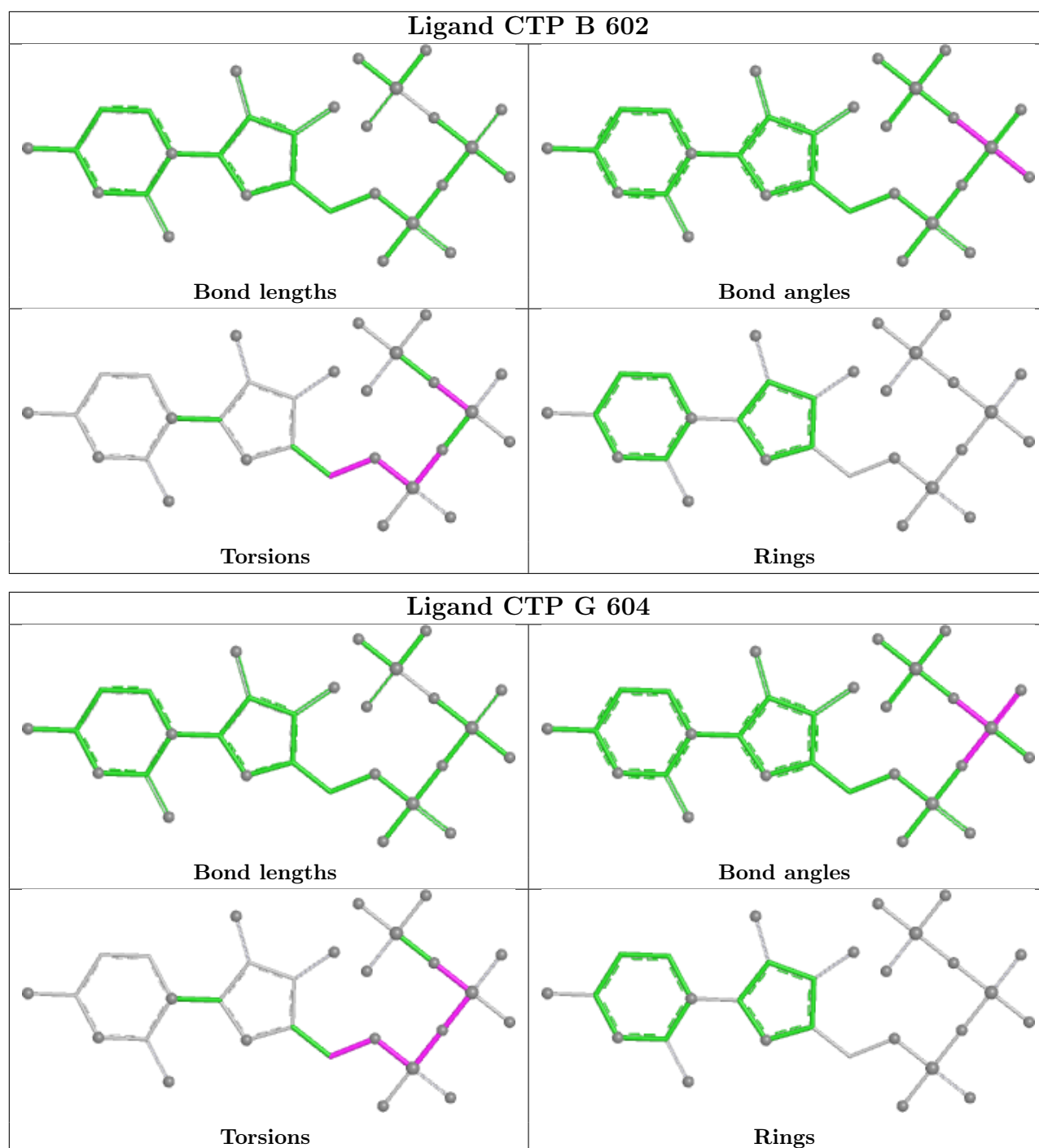
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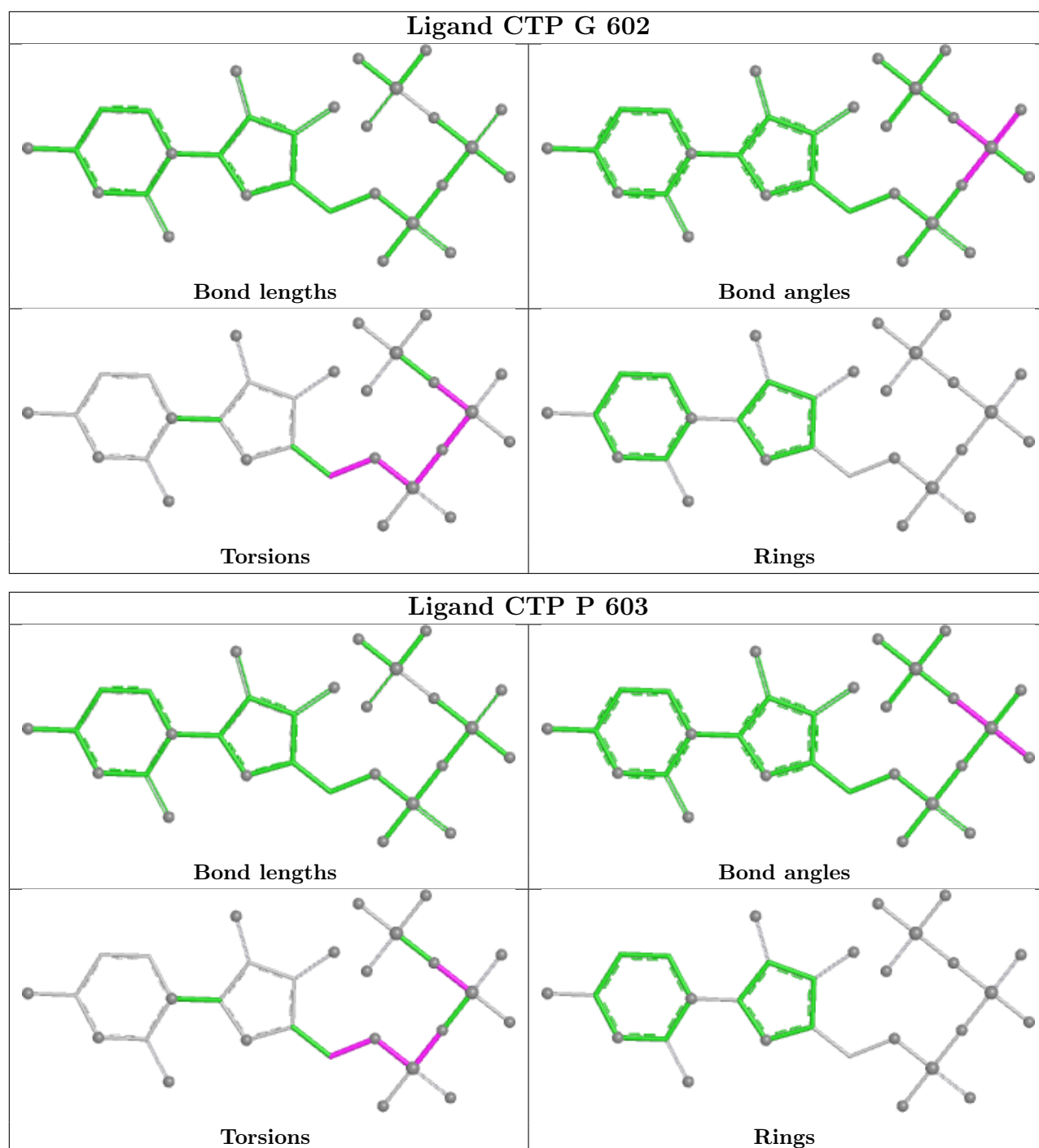
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	603	CTP	4	0
2	E	602	CTP	5	0
2	E	604	CTP	10	0
2	A	602	CTP	5	0
2	H	602	CTP	1	0
2	D	603	CTP	4	0
2	J	602	CTP	1	0
2	F	604	CTP	10	0
2	O	603	CTP	4	0
2	N	603	CTP	4	0

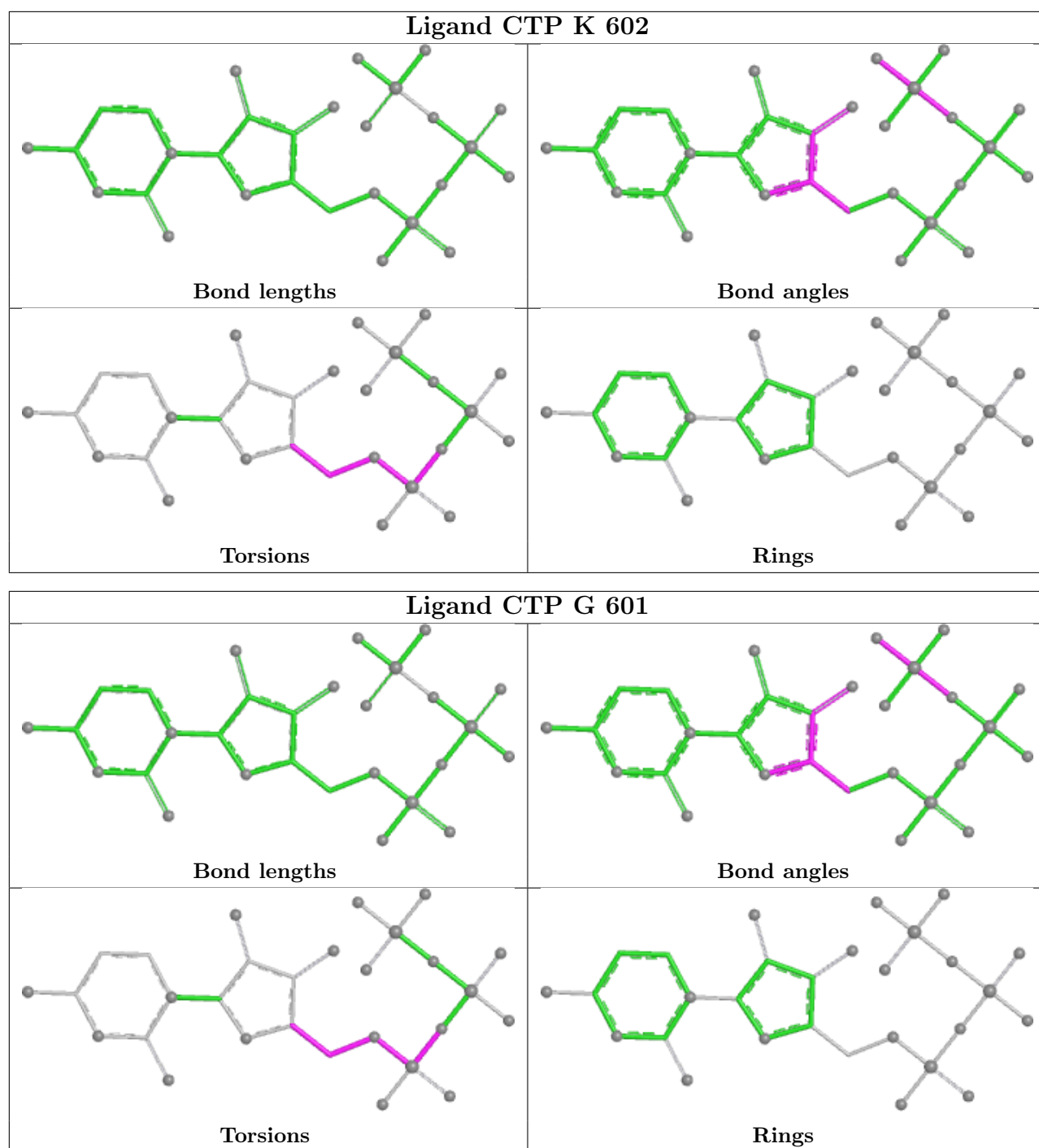
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

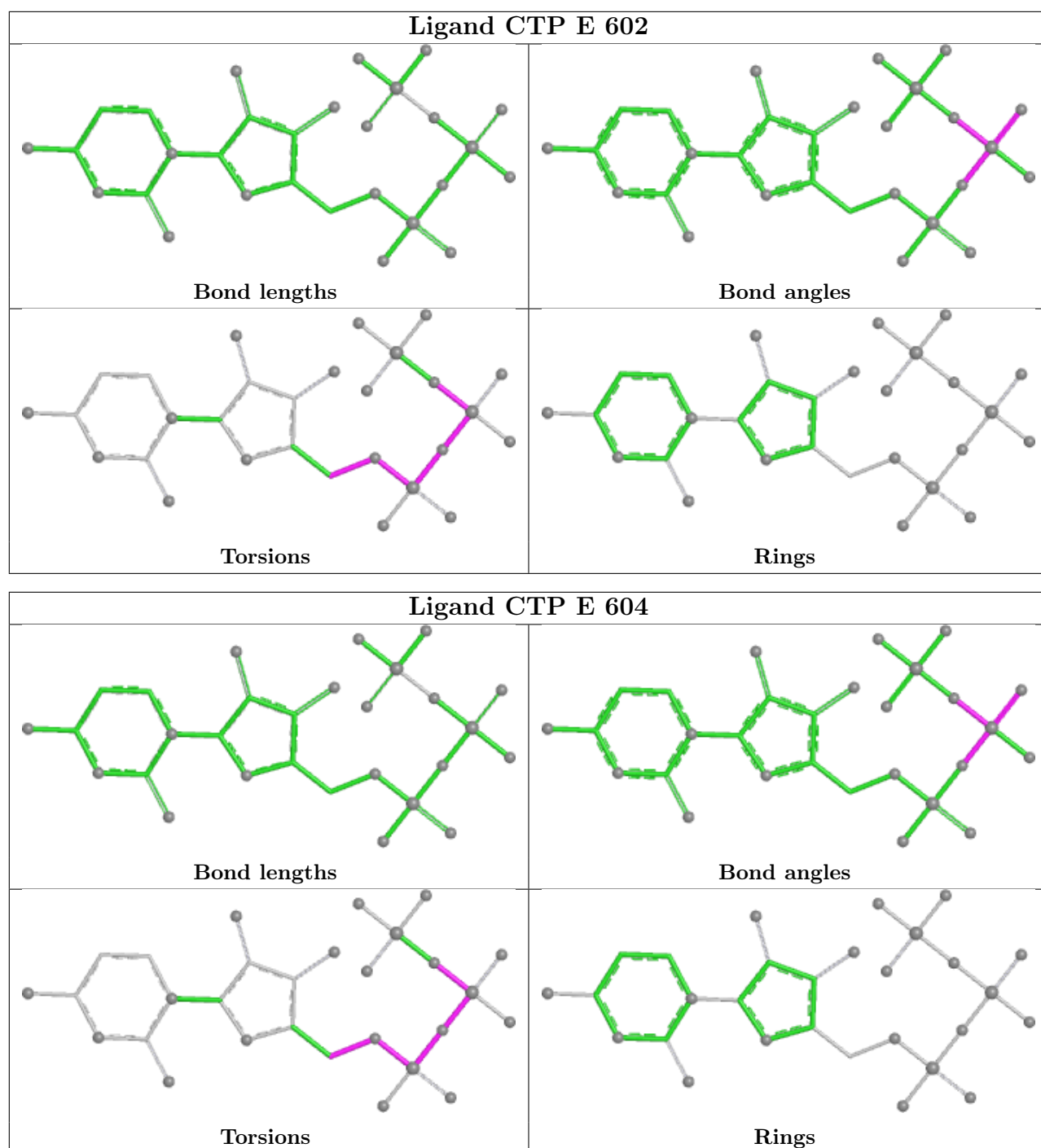


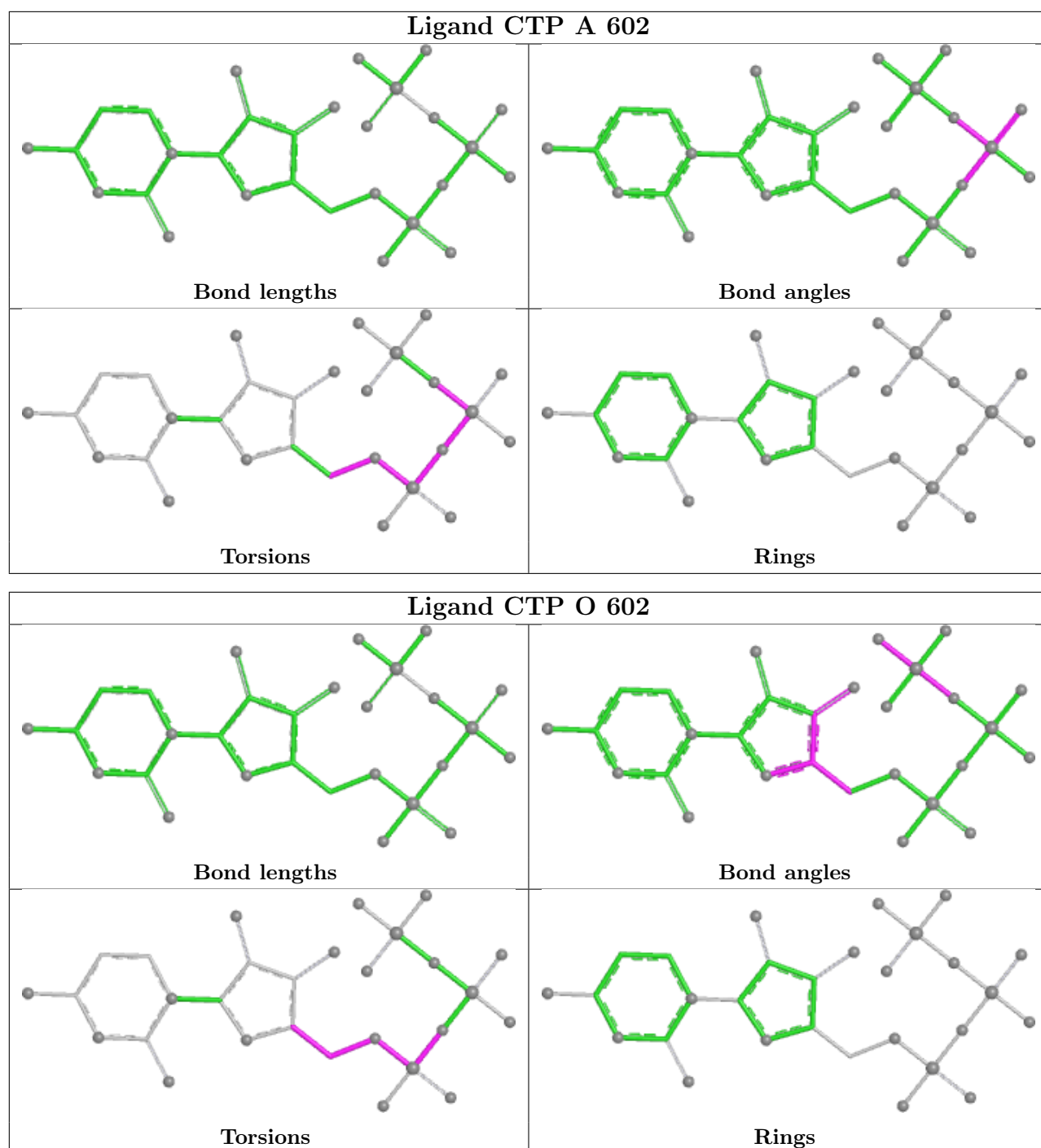


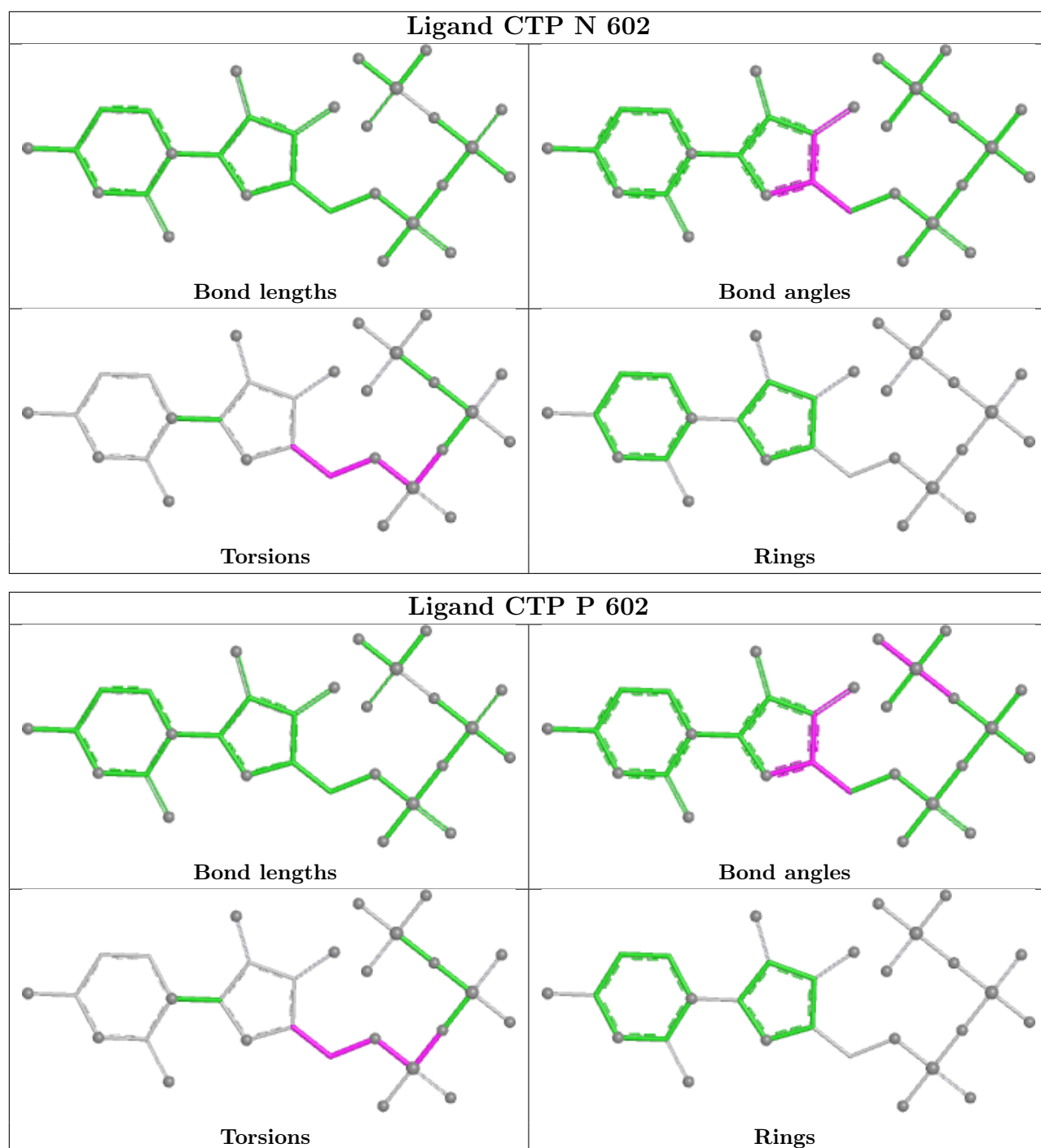


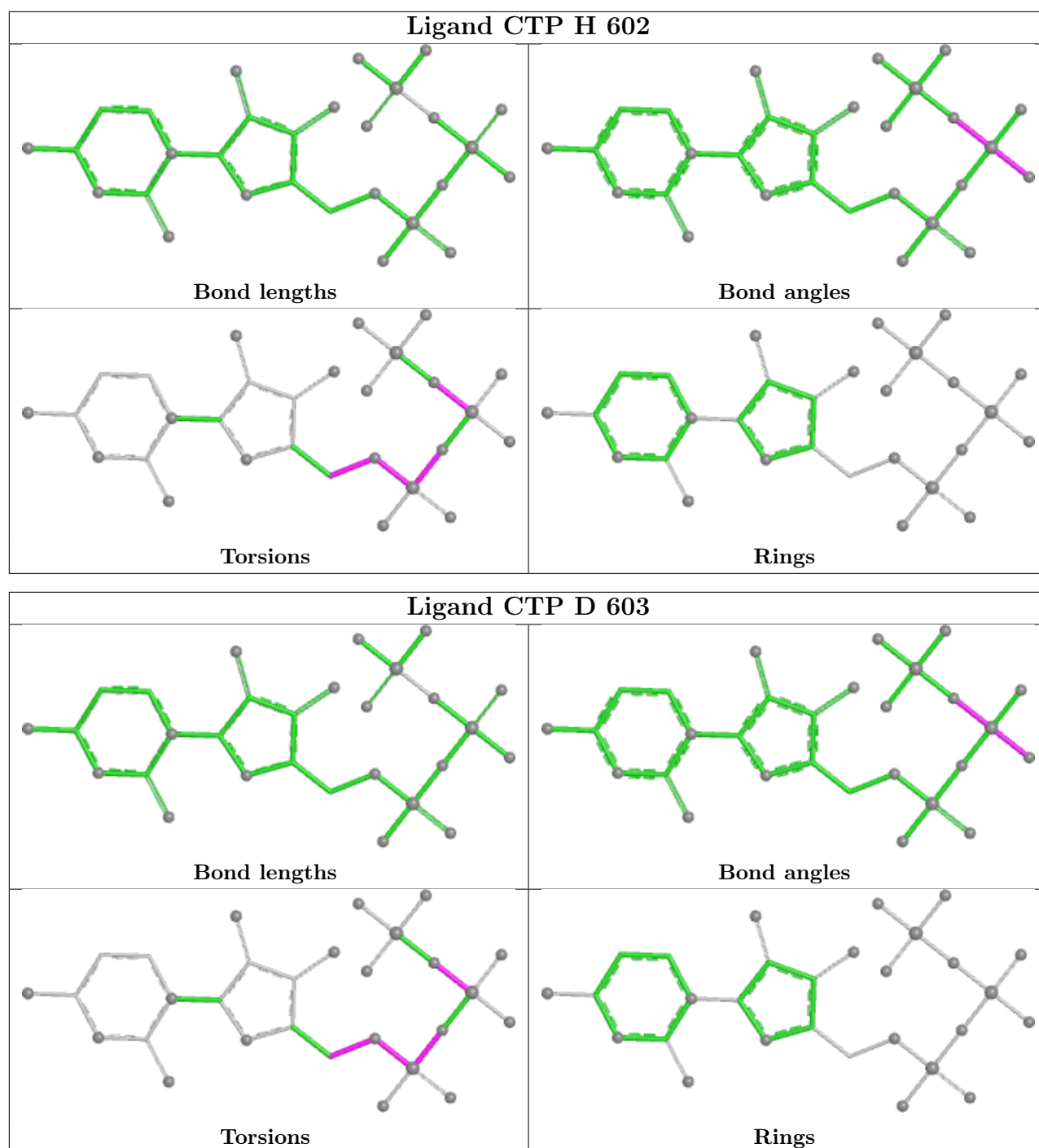


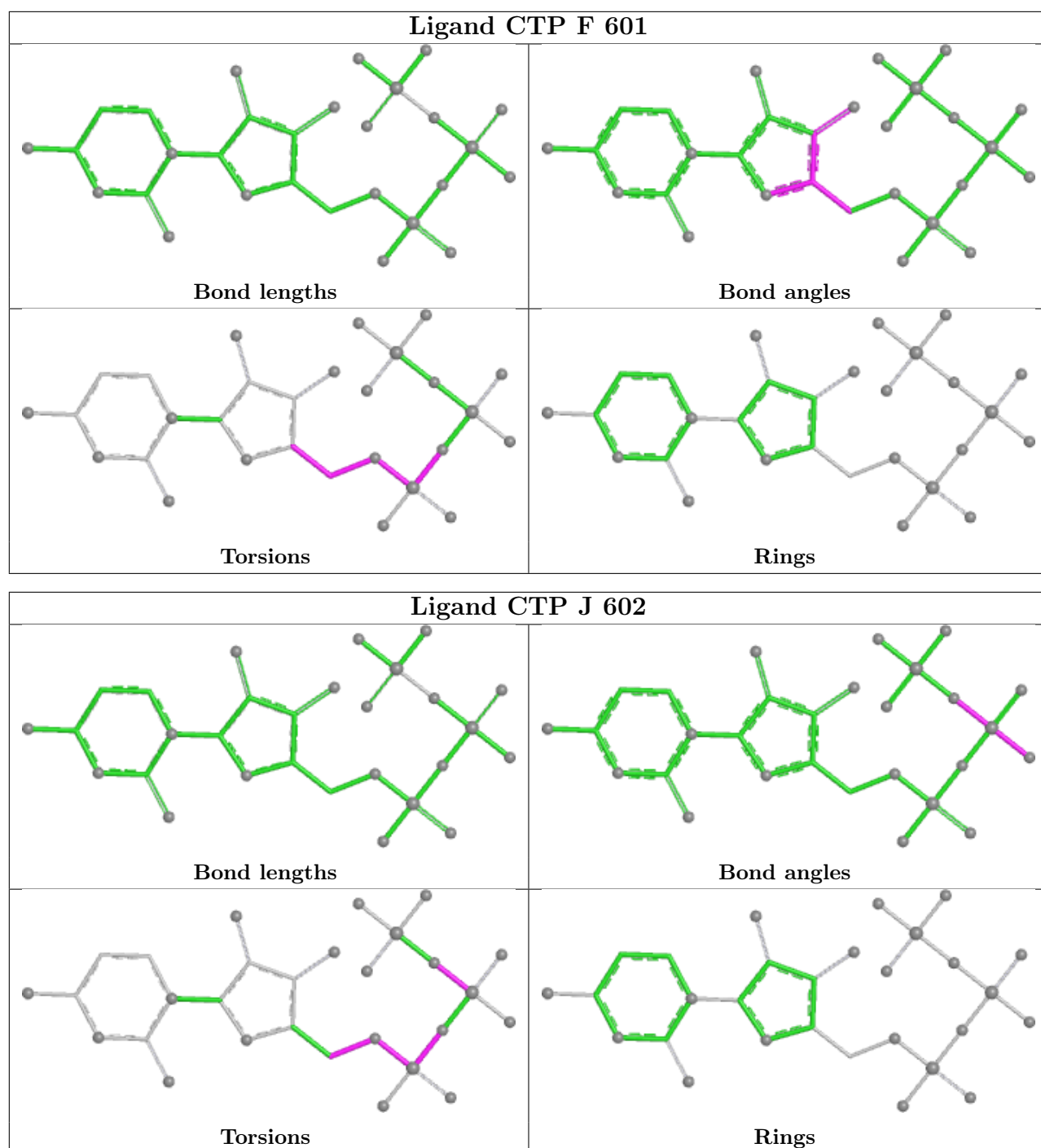


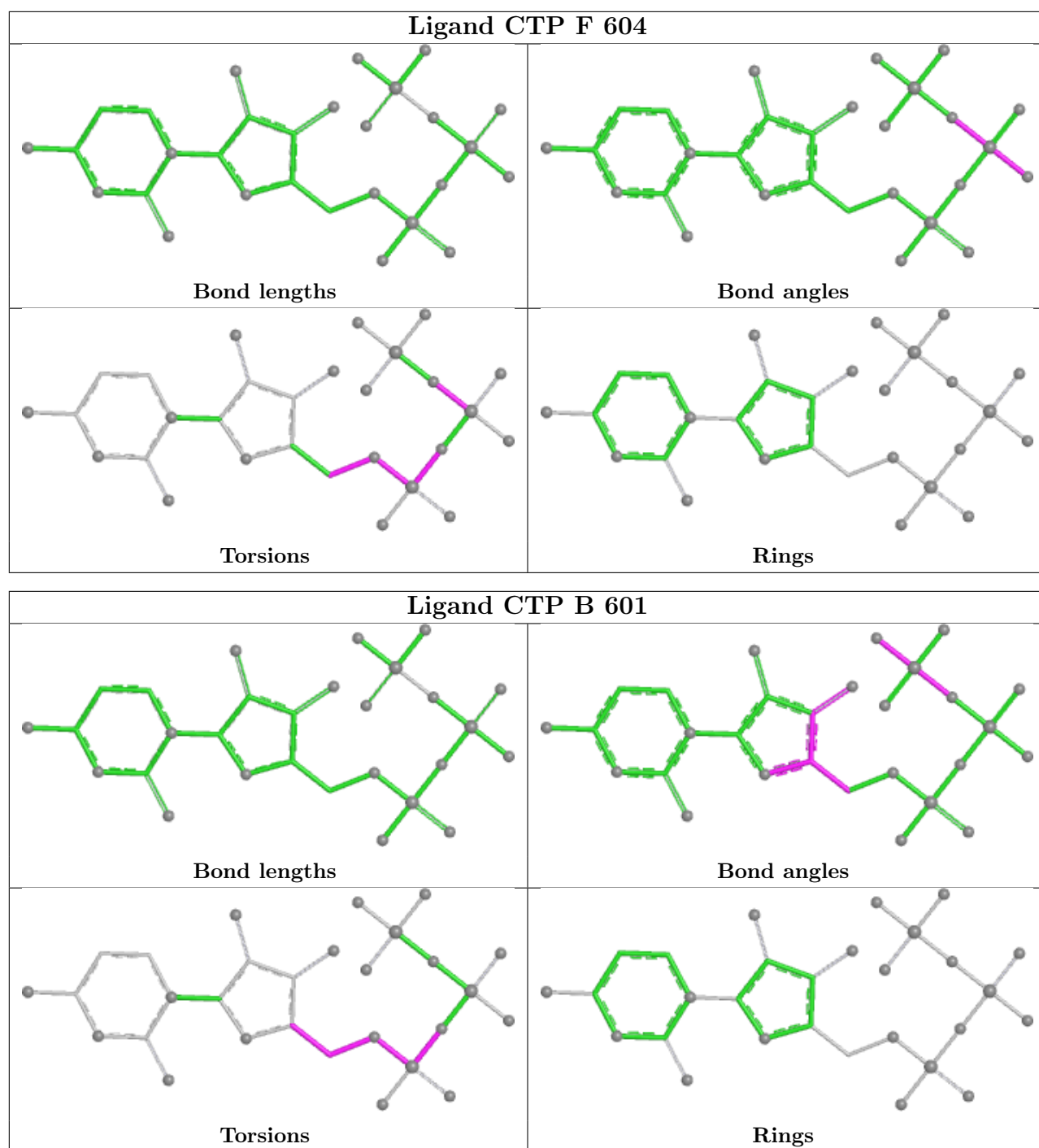


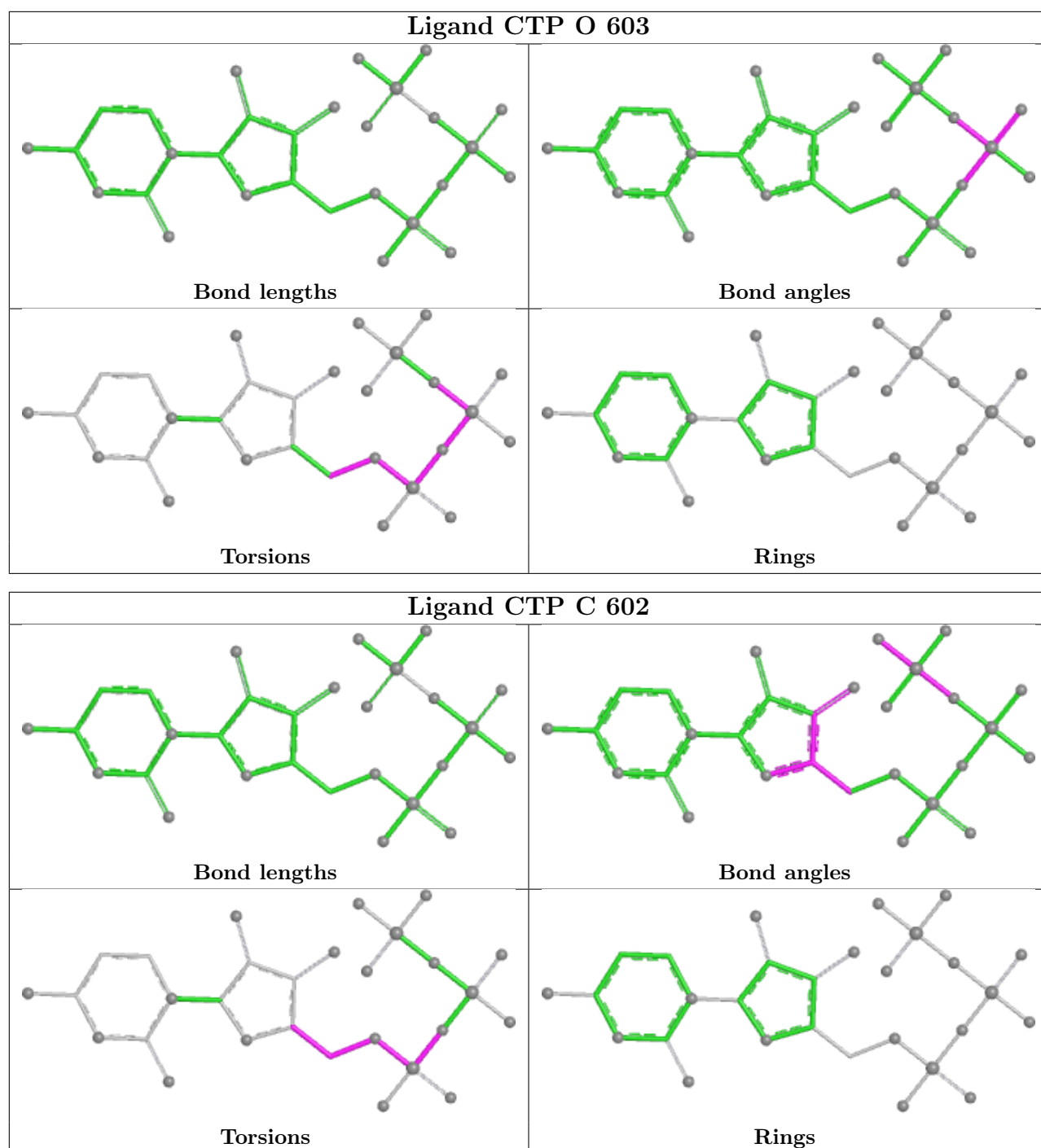


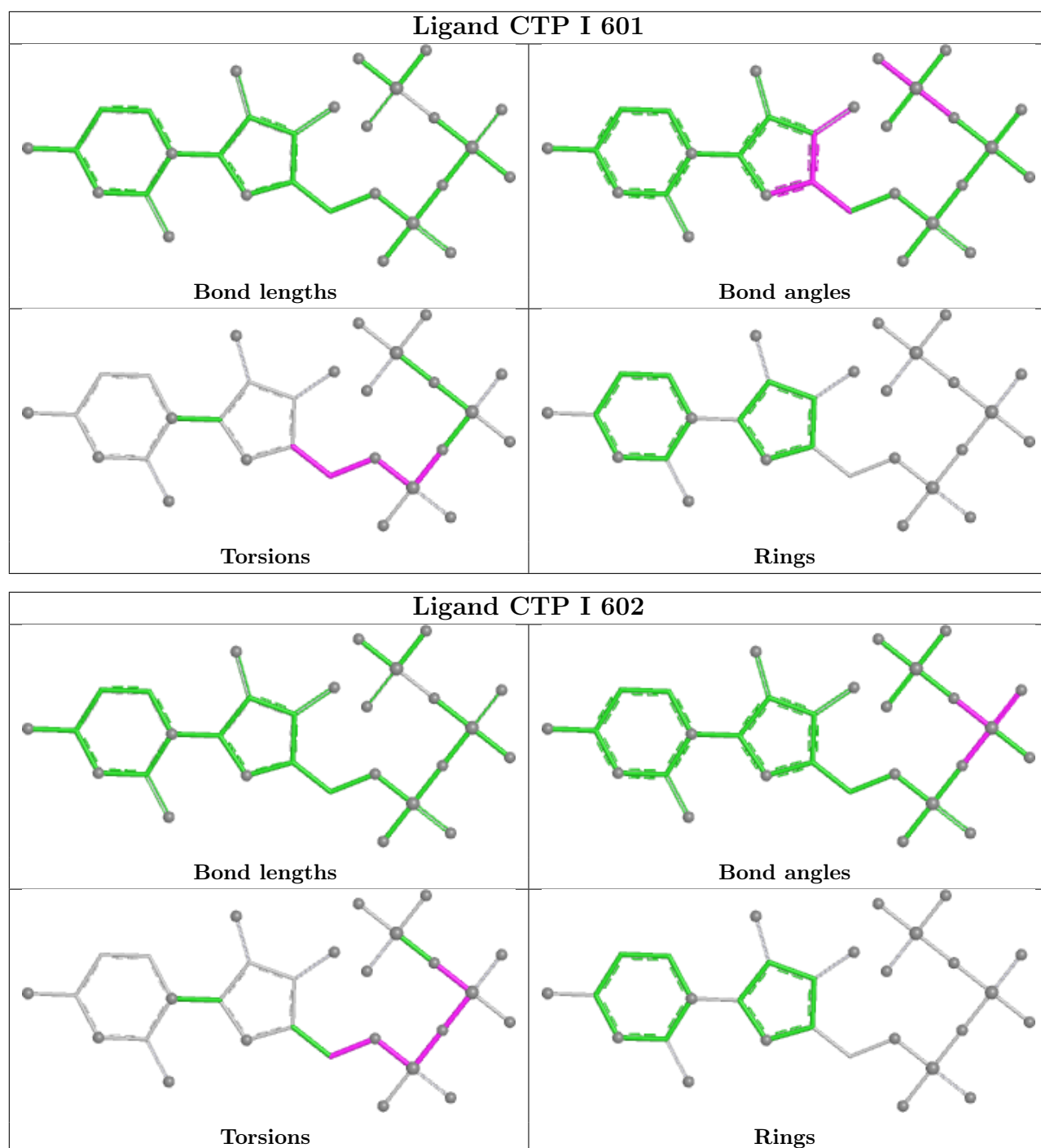


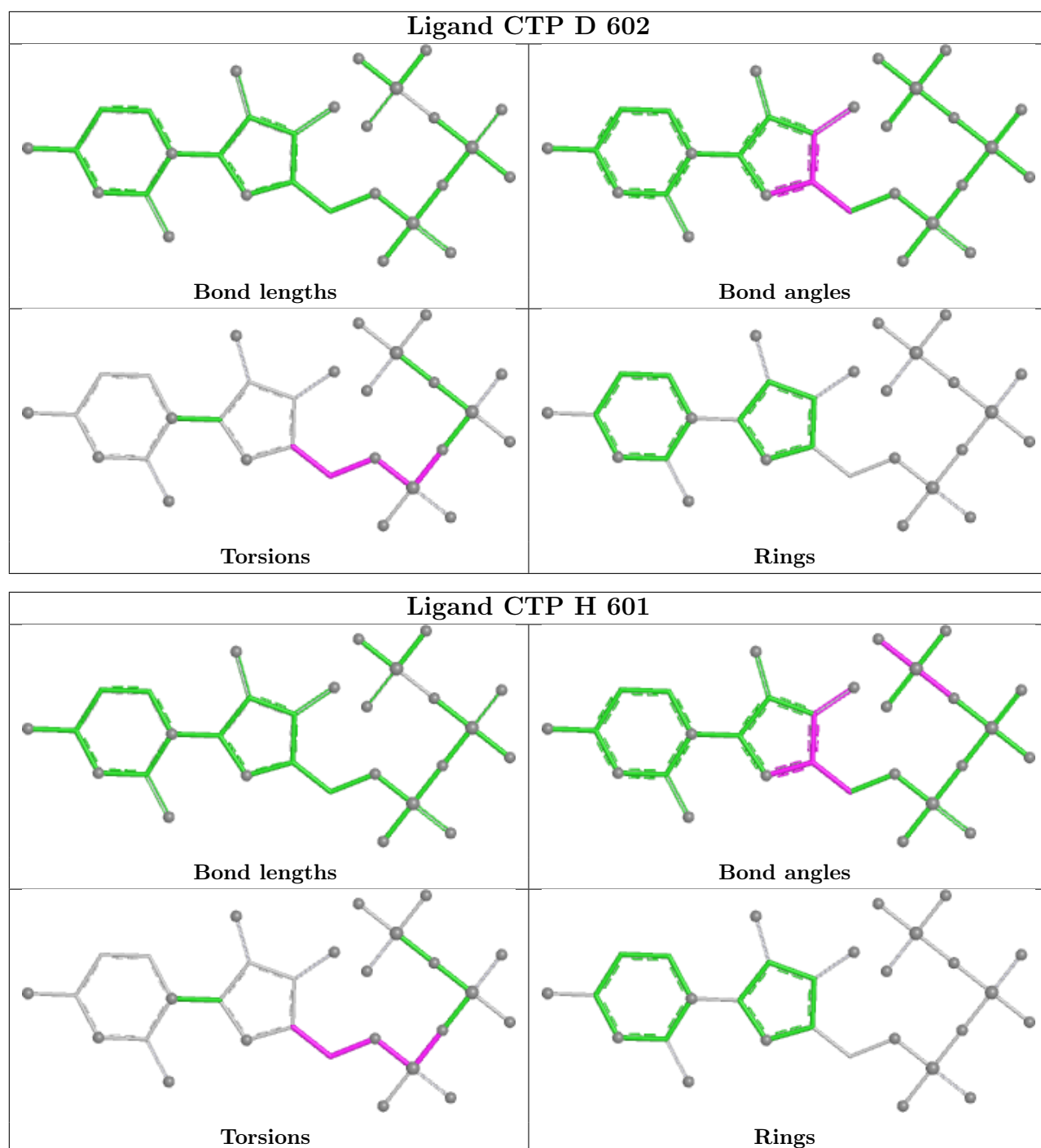


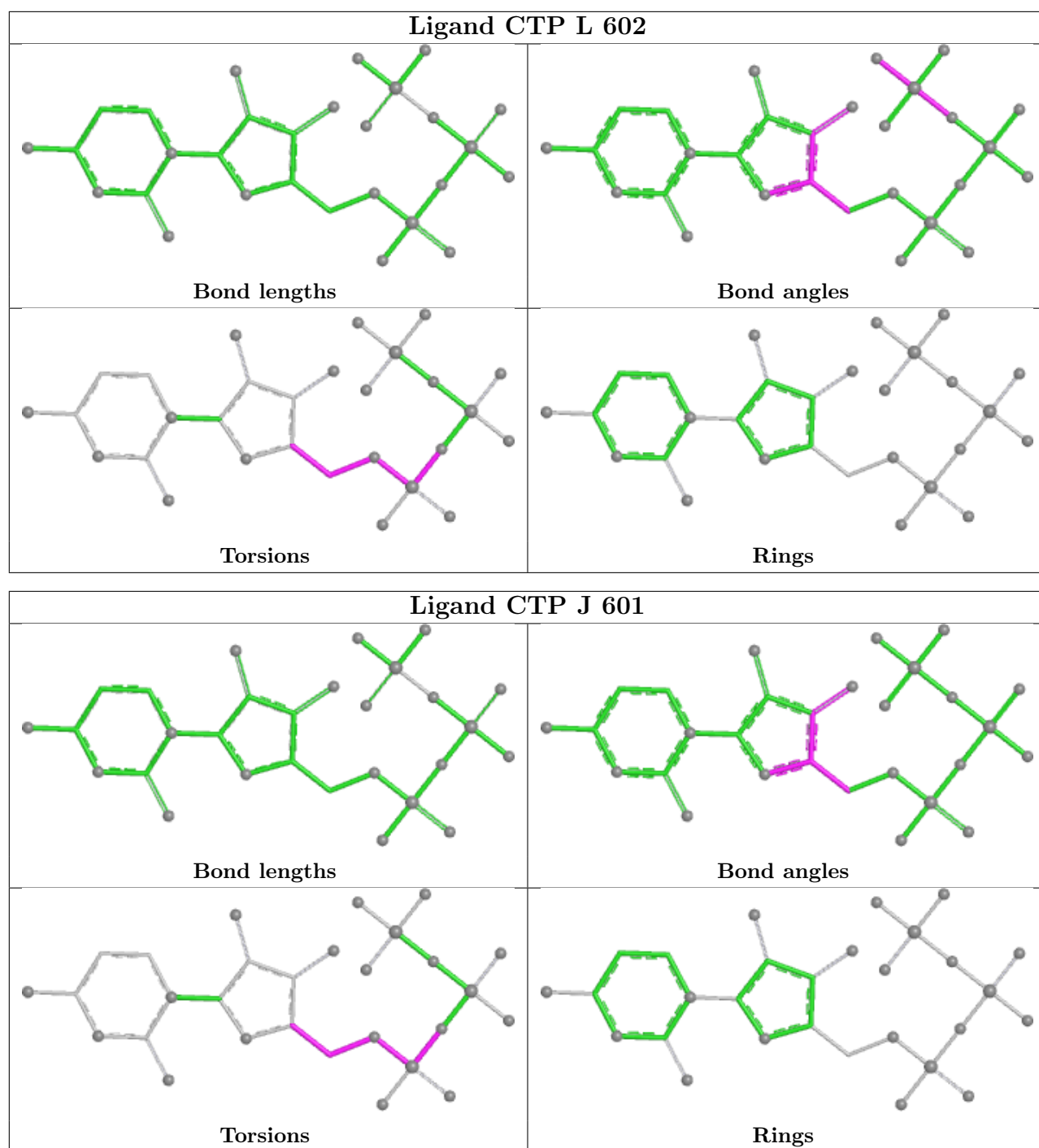


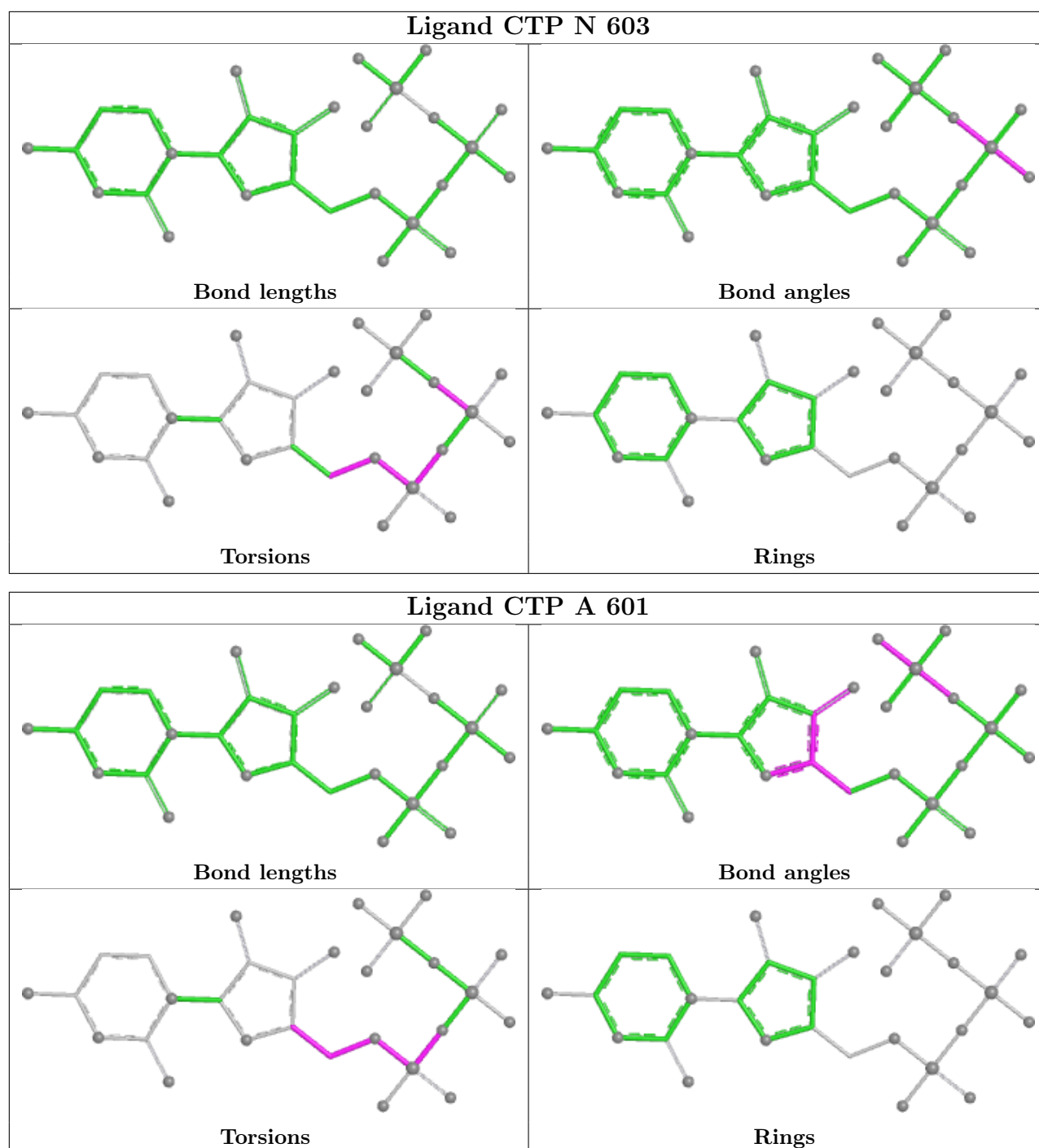


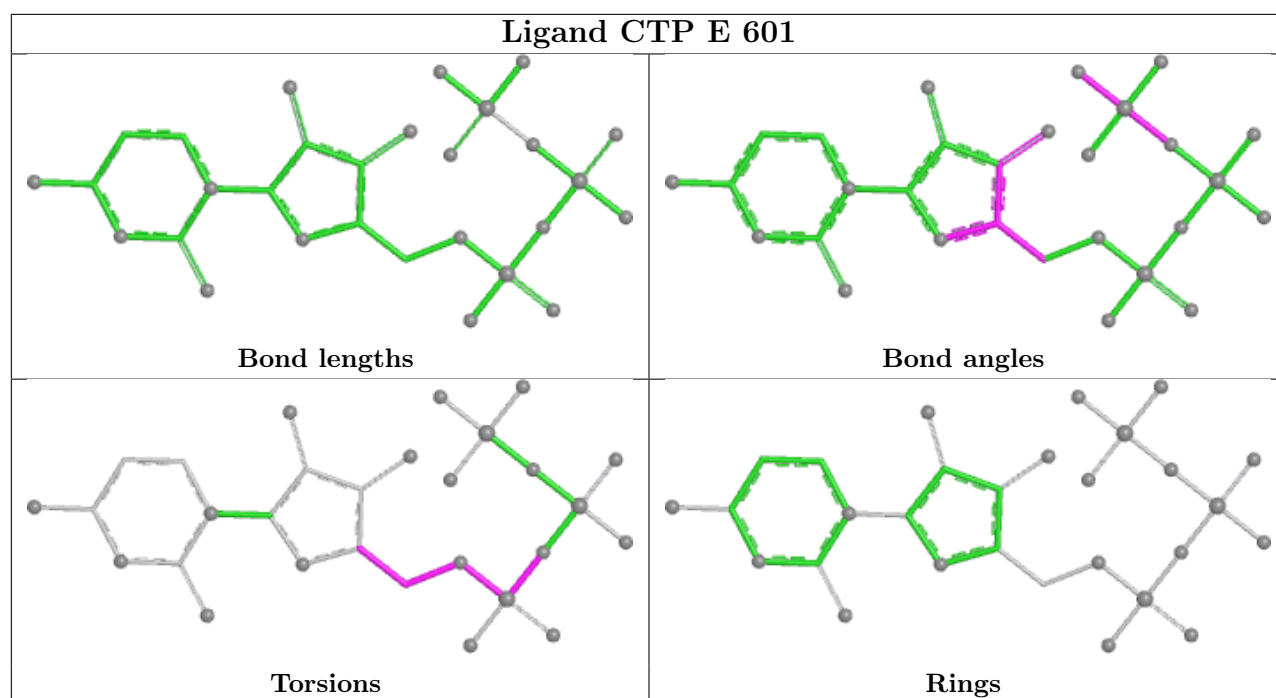












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	C	1
1	D	1
1	H	1
1	E	1
1	K	1
1	N	1
1	I	1
1	F	1
1	L	1
1	O	1
1	J	1
1	G	1
1	M	1
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	443:ILE	C	456:THR	N	3.90
1	A	443:ILE	C	456:THR	N	3.90
1	C	443:ILE	C	456:THR	N	3.90
1	D	443:ILE	C	456:THR	N	3.90
1	H	443:ILE	C	456:THR	N	3.90
1	E	443:ILE	C	456:THR	N	3.90
1	K	443:ILE	C	456:THR	N	3.90
1	N	443:ILE	C	456:THR	N	3.90
1	I	443:ILE	C	456:THR	N	3.90
1	F	443:ILE	C	456:THR	N	3.90
1	L	443:ILE	C	456:THR	N	3.90
1	O	443:ILE	C	456:THR	N	3.90
1	J	443:ILE	C	456:THR	N	3.90
1	G	443:ILE	C	456:THR	N	3.90
1	M	443:ILE	C	456:THR	N	3.90
1	P	443:ILE	C	456:THR	N	3.90

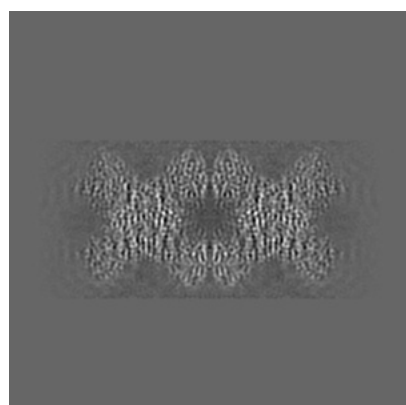
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24579. These allow visual inspection of the internal detail of the map and identification of artifacts.

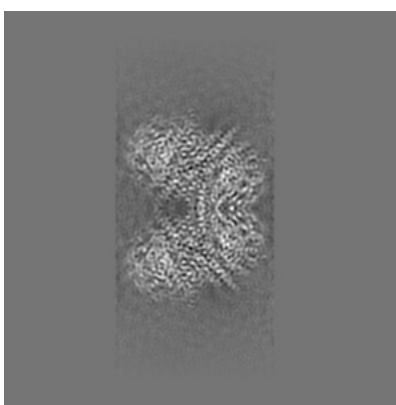
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

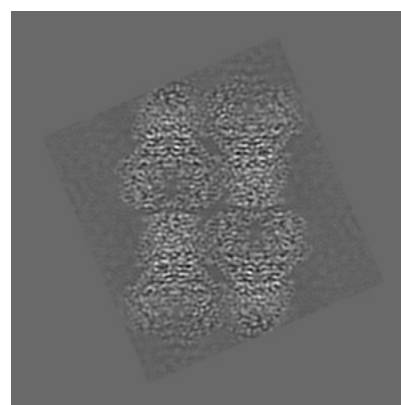
6.1.1 Primary map



X



Y

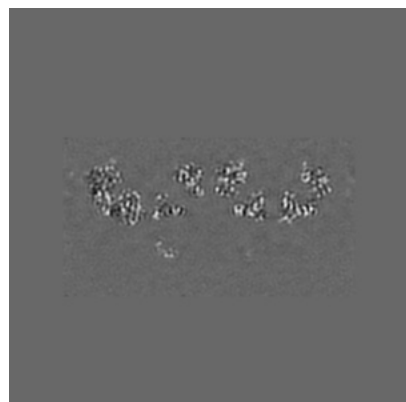


Z

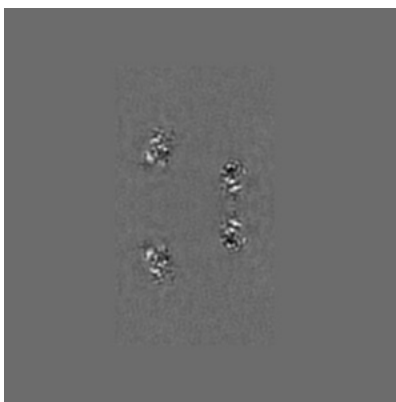
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

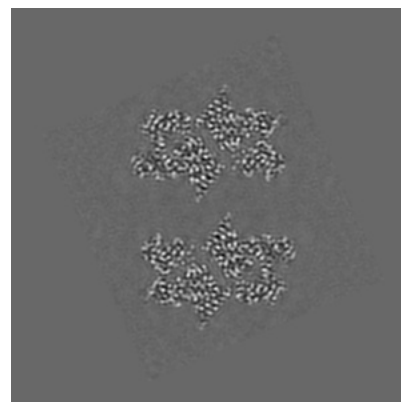
6.2.1 Primary map



X Index: 160



Y Index: 160

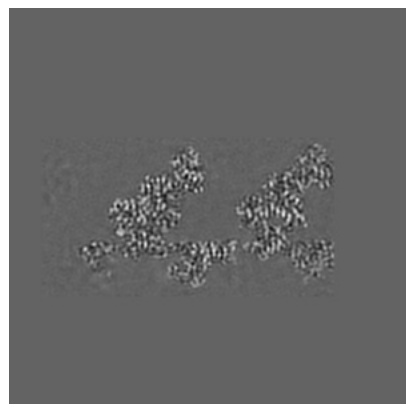


Z Index: 160

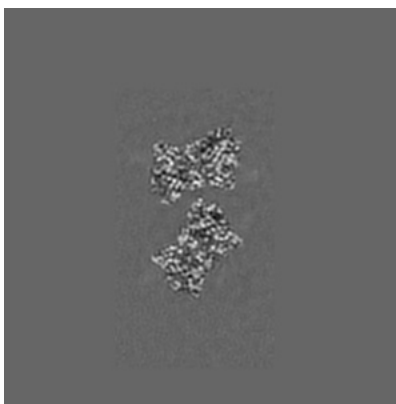
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

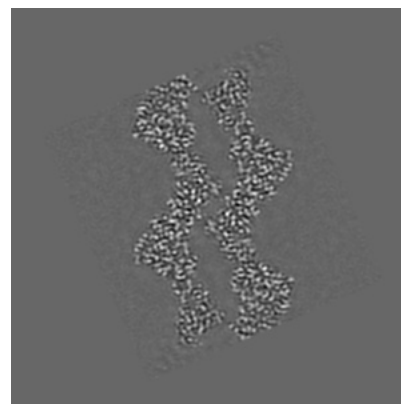
6.3.1 Primary map



X Index: 121



Y Index: 202

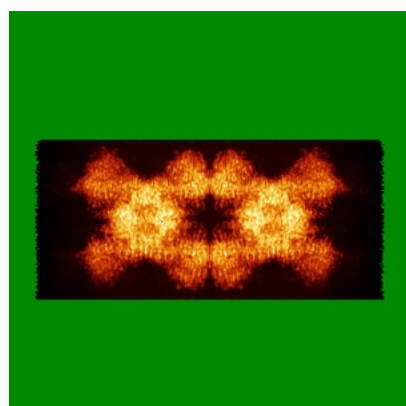


Z Index: 179

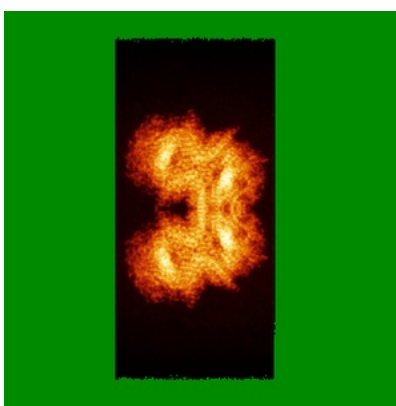
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

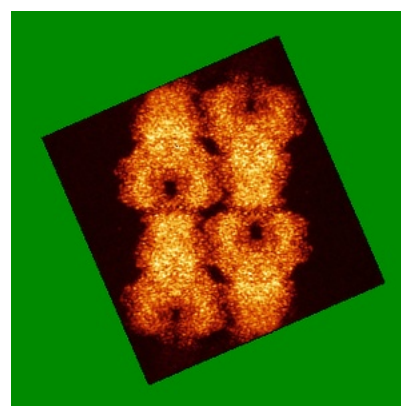
6.4.1 Primary map



X



Y

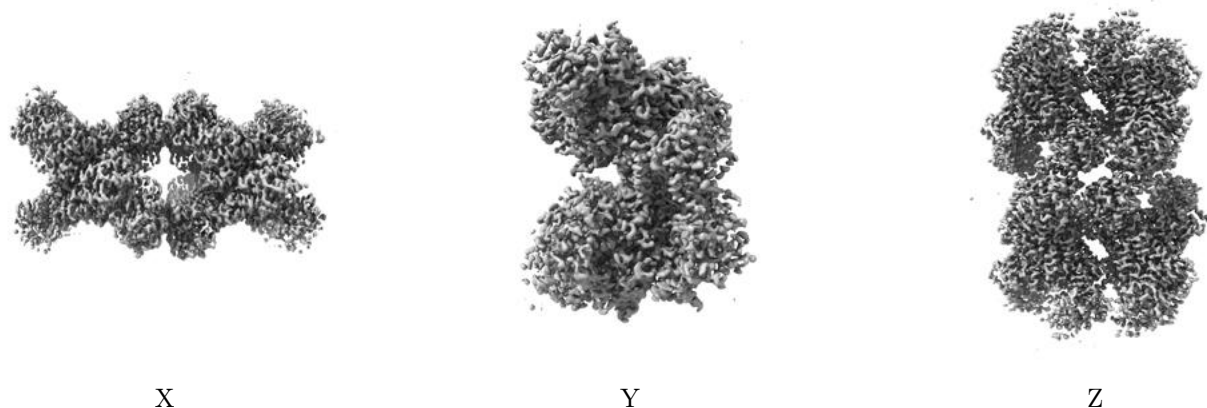


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.244. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

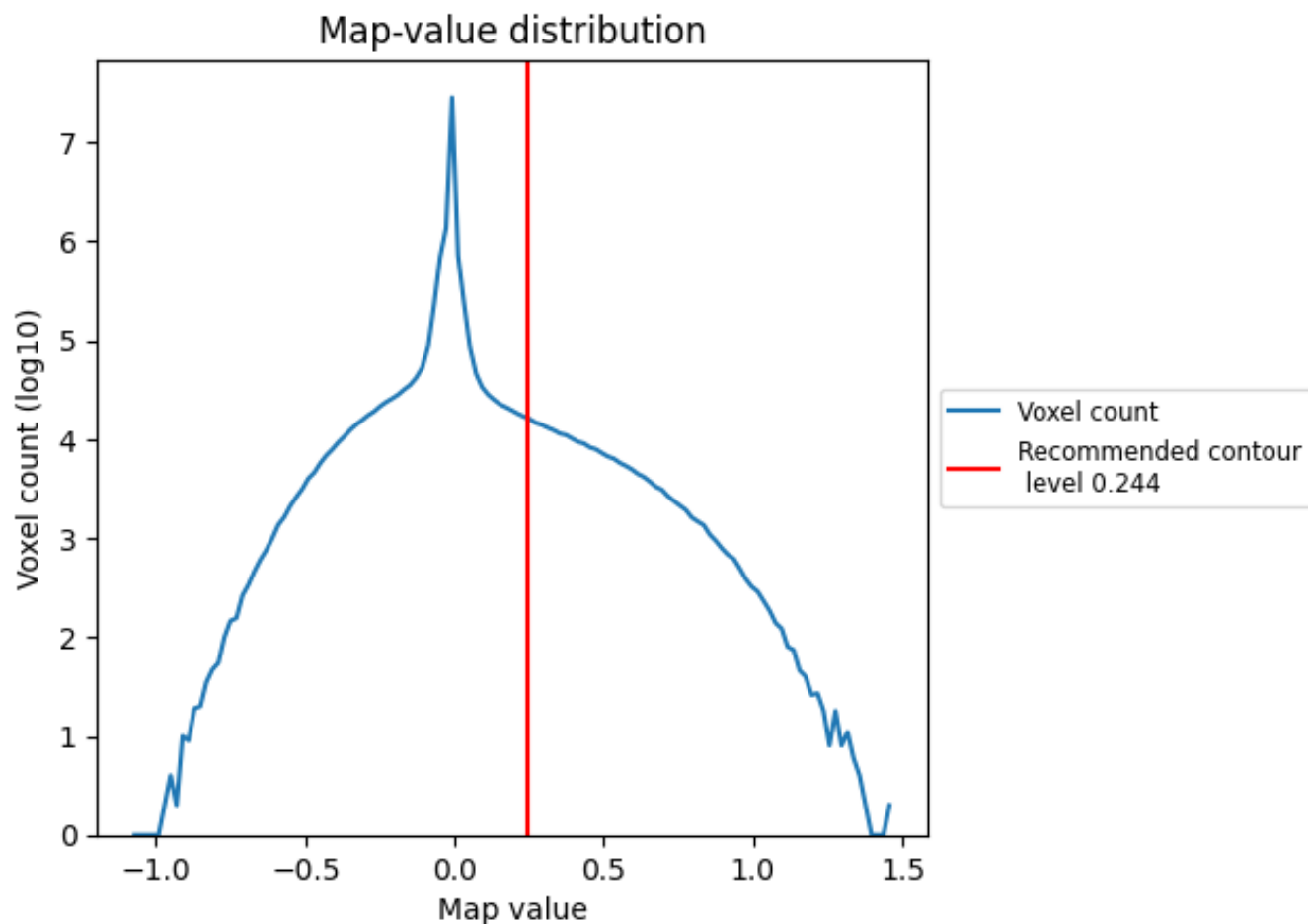
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

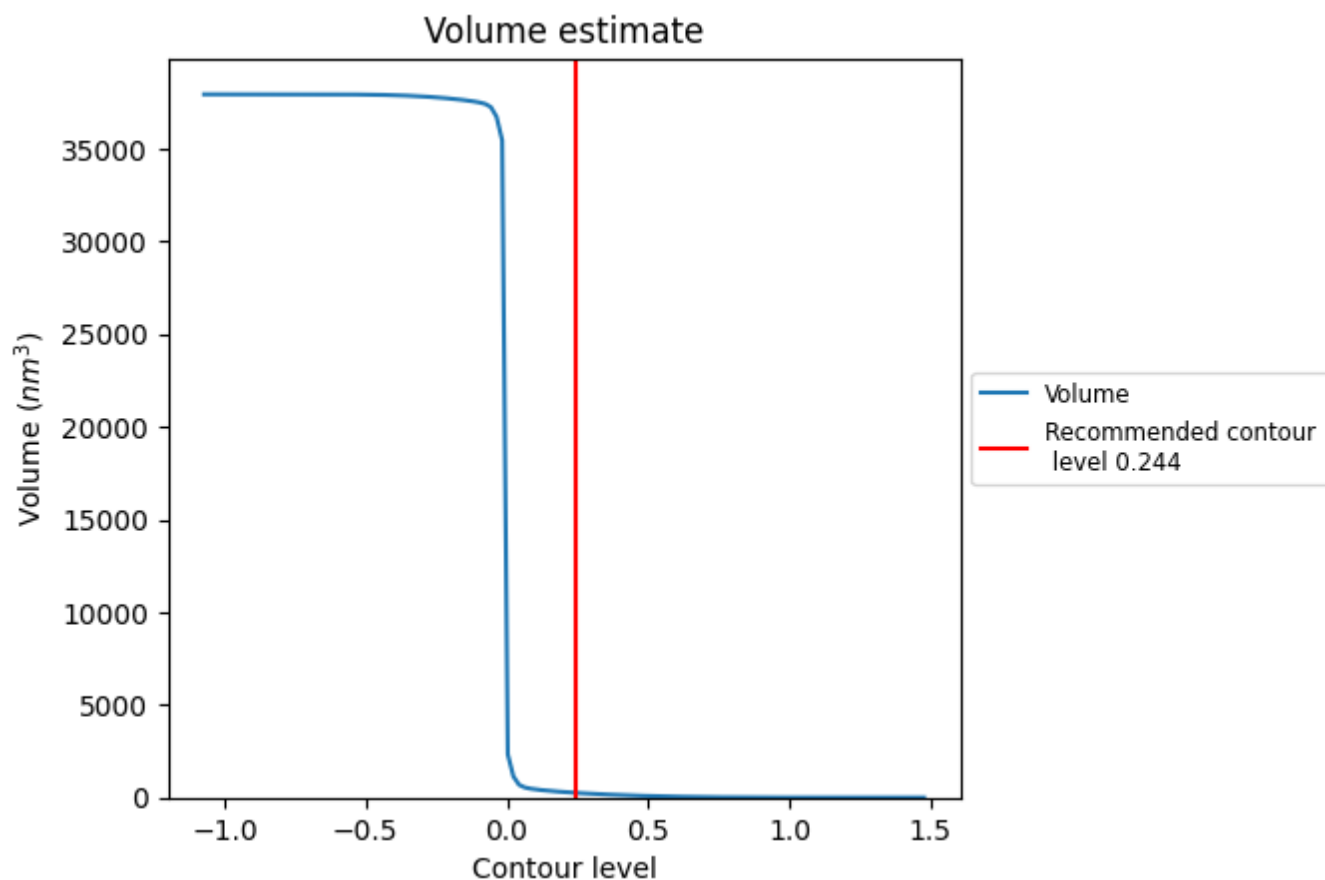
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

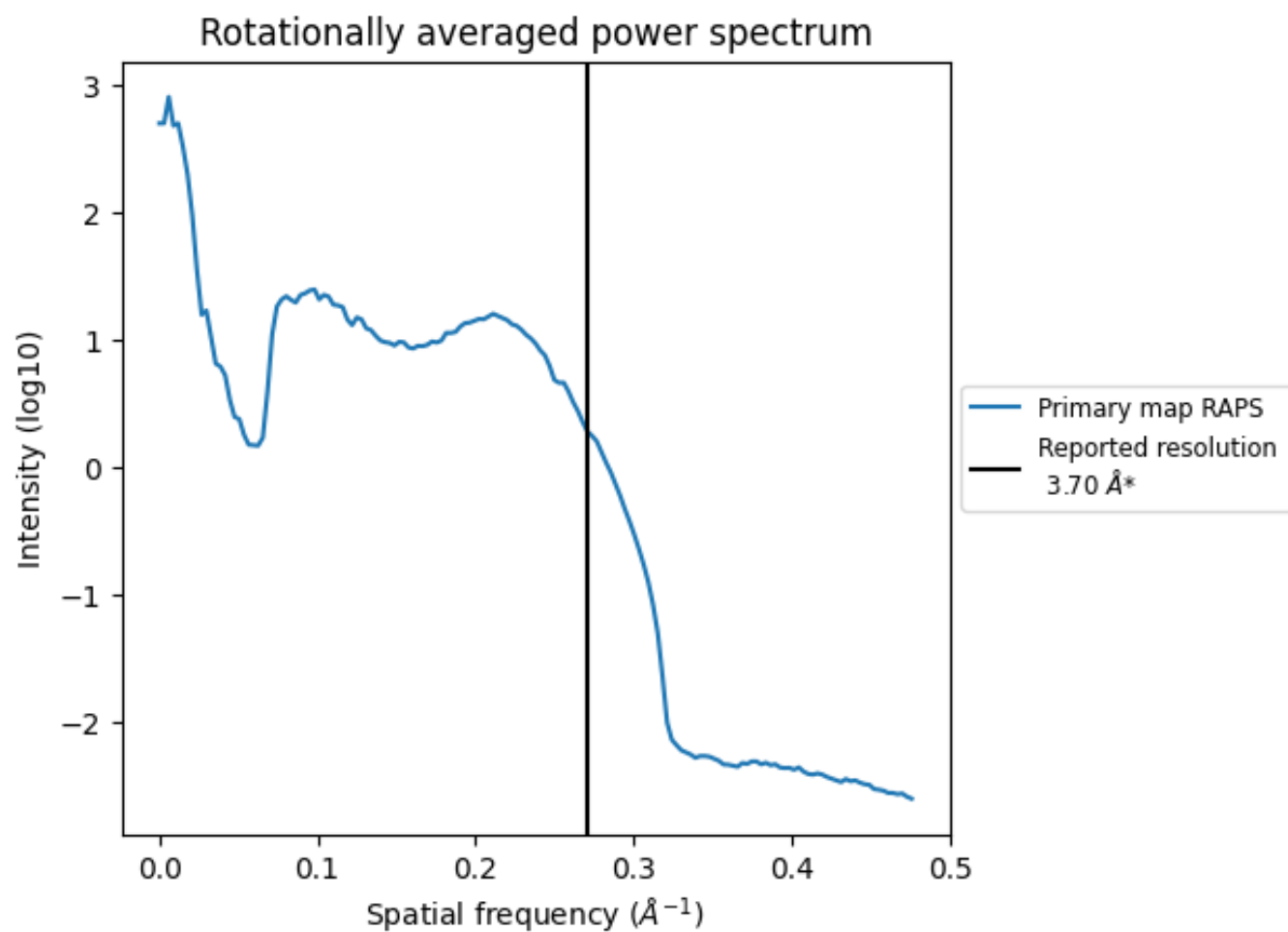
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm³; this corresponds to an approximate mass of 230 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

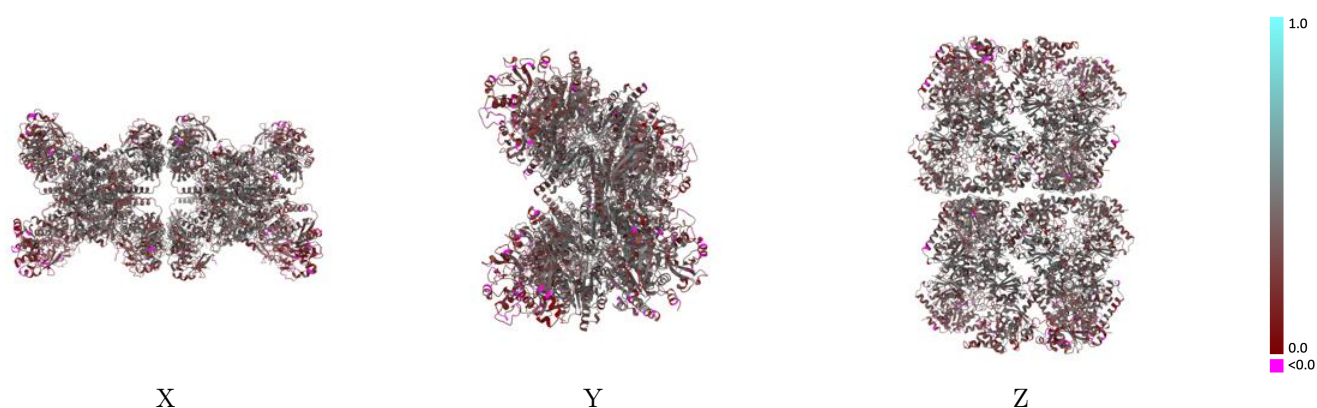
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24579 and PDB model 7RNL. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

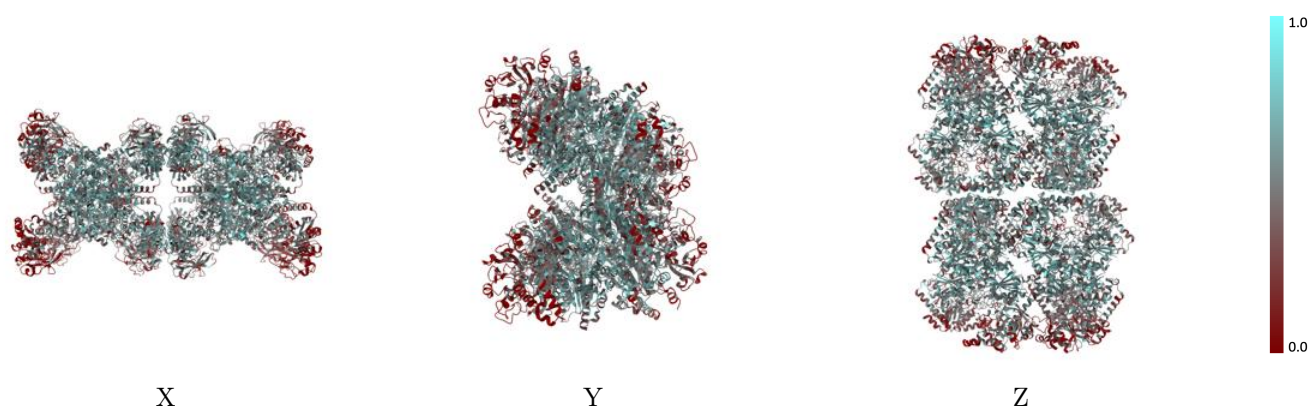
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



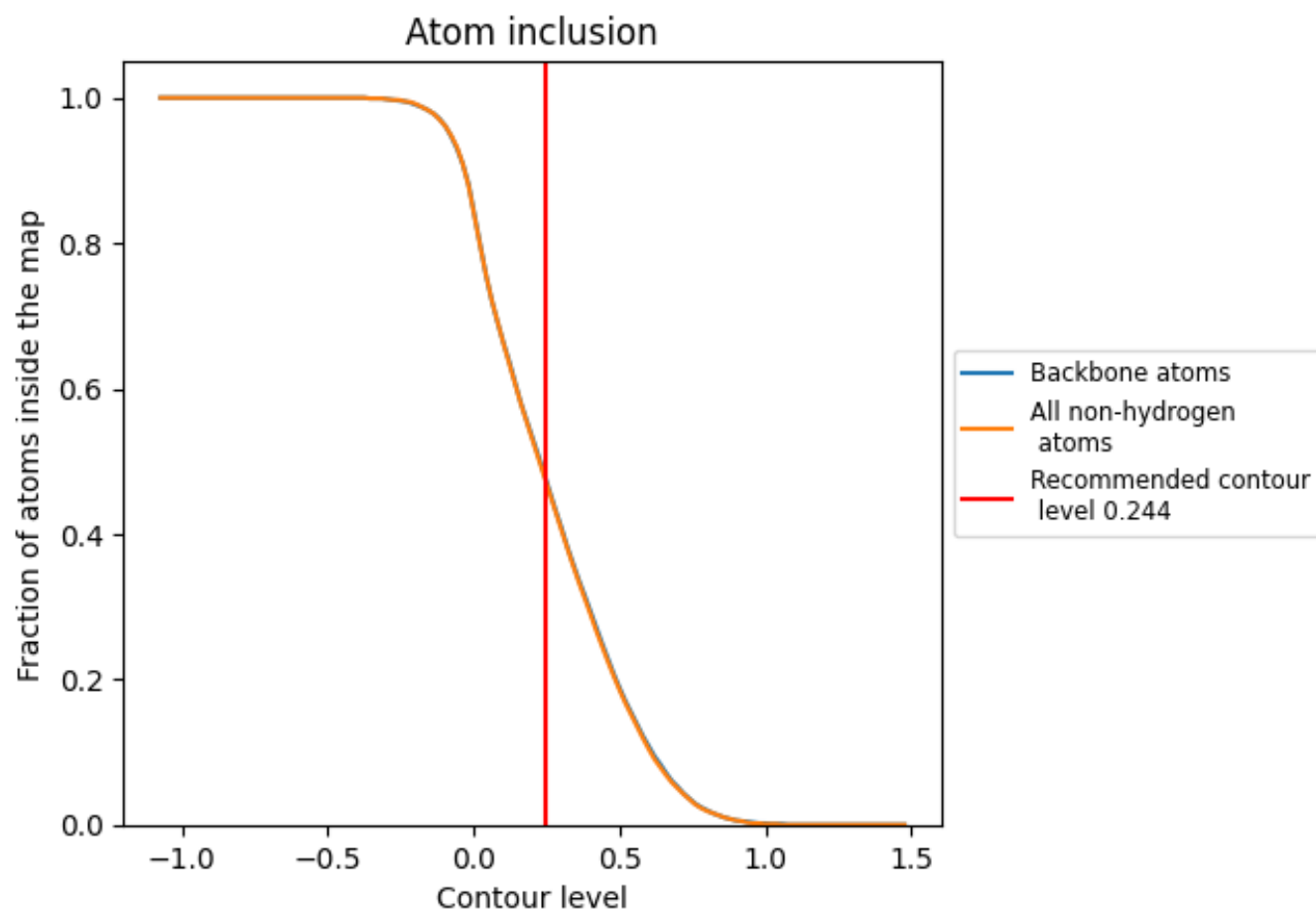
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.244).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.244) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4770	 0.3560
A	 0.5590	 0.3870
B	 0.4050	 0.3190
C	 0.4790	 0.3730
D	 0.5190	 0.3700
E	 0.5550	 0.3870
F	 0.3790	 0.3010
G	 0.5620	 0.3970
H	 0.4010	 0.3160
I	 0.5610	 0.4010
J	 0.3690	 0.3030
K	 0.4780	 0.3710
L	 0.5150	 0.3570
M	 0.4410	 0.3440
N	 0.5160	 0.3720
O	 0.4460	 0.3370
P	 0.5110	 0.3560

