



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:06 AM UTC

PDB ID : 5EUJ / pdb_00005euj
Title : PYRUVATE DECARBOXYLASE FROM ZYMOBACTER PALMAE
Authors : Buddrus, L.; Crennell, S.J.; Leak, D.J.; Danson, M.J.; Andrews, E.S.V.; Arcus, V.L.
Deposited on : 2015-11-18
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

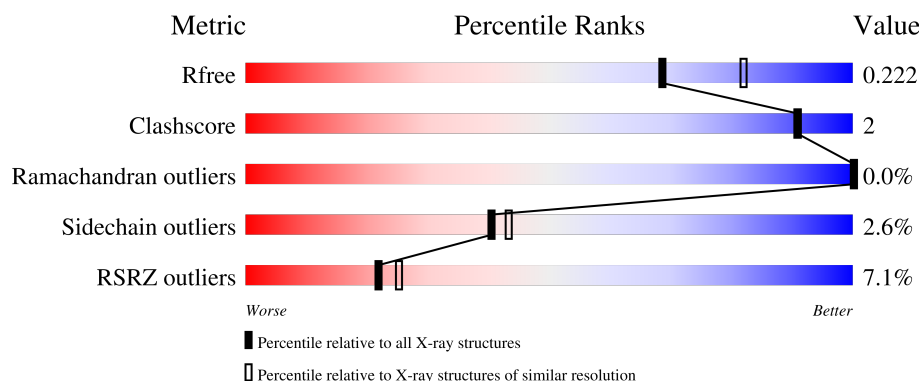
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	573	4% 91% 6% .
1	B	573	4% 92% 5% .
1	C	573	2% 91% 5% .
1	D	573	2% 92% 5% .
1	E	573	2% 91% 6% .

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Mol	Chain	Length	Quality of chain
1	F	573	90% 7% .
1	G	573	91% 6% .
1	H	573	90% 7% .
1	I	573	92% 5% .
1	J	573	92% 5% .
1	K	573	91% 6% .
1	L	573	91% 6% .
1	M	573	91% 6% .
1	N	573	91% 6% .
1	O	573	91% 5% .
1	P	573	92% 5% .
1	Q	573	93% . .
1	R	573	91% 5% .
1	S	573	92% . .
1	T	573	92% 5% .
1	U	573	39% 89% 8% .
1	V	573	26% 91% 6% .
1	W	573	44% 92% 5% .
1	X	573	5% 92% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 107004 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	5	0
			4250	2665	737	823	25			
1	B	555	Total	C	N	O	S	0	4	0
			4237	2658	733	821	25			
1	C	555	Total	C	N	O	S	0	6	0
			4260	2670	742	823	25			
1	D	555	Total	C	N	O	S	0	5	0
			4245	2662	734	824	25			
1	E	556	Total	C	N	O	S	0	4	0
			4244	2662	734	823	25			
1	F	555	Total	C	N	O	S	0	9	0
			4285	2685	745	830	25			
1	G	555	Total	C	N	O	S	0	7	0
			4266	2675	739	827	25			
1	H	555	Total	C	N	O	S	0	6	0
			4252	2666	736	824	26			
1	I	556	Total	C	N	O	S	0	6	0
			4259	2670	737	827	25			
1	J	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	K	555	Total	C	N	O	S	0	7	0
			4266	2673	740	828	25			
1	L	555	Total	C	N	O	S	0	9	0
			4284	2683	745	831	25			
1	M	555	Total	C	N	O	S	0	7	0
			4262	2673	737	827	25			
1	N	555	Total	C	N	O	S	0	7	0
			4265	2672	740	828	25			
1	O	555	Total	C	N	O	S	0	3	0
			4229	2653	732	819	25			
1	P	555	Total	C	N	O	S	0	7	0
			4264	2673	738	828	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	555	Total	C	N	O	S	0	5	0
			4246	2663	734	824	25			
1	R	555	Total	C	N	O	S	0	8	0
			4270	2675	738	832	25			
1	S	555	Total	C	N	O	S	0	2	0
			4221	2649	731	816	25			
1	T	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	U	555	Total	C	N	O	S	0	4	0
			4239	2659	733	822	25			
1	V	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	W	555	Total	C	N	O	S	0	3	0
			4230	2654	732	819	25			
1	X	555	Total	C	N	O	S	0	3	0
			4228	2653	732	818	25			

There are 456 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ALA	ARG	conflict	UNP Q8KTX6
A	245	ALA	GLU	conflict	UNP Q8KTX6
A	557	LEU	-	expression tag	UNP Q8KTX6
A	558	VAL	-	expression tag	UNP Q8KTX6
A	559	PRO	-	expression tag	UNP Q8KTX6
A	560	ARG	-	expression tag	UNP Q8KTX6
A	561	GLY	-	expression tag	UNP Q8KTX6
A	562	SER	-	expression tag	UNP Q8KTX6
A	563	GLY	-	expression tag	UNP Q8KTX6
A	564	GLY	-	expression tag	UNP Q8KTX6
A	565	GLY	-	expression tag	UNP Q8KTX6
A	566	LEU	-	expression tag	UNP Q8KTX6
A	567	GLU	-	expression tag	UNP Q8KTX6
A	568	HIS	-	expression tag	UNP Q8KTX6
A	569	HIS	-	expression tag	UNP Q8KTX6
A	570	HIS	-	expression tag	UNP Q8KTX6
A	571	HIS	-	expression tag	UNP Q8KTX6
A	572	HIS	-	expression tag	UNP Q8KTX6
A	573	HIS	-	expression tag	UNP Q8KTX6
B	134	ALA	ARG	conflict	UNP Q8KTX6
B	245	ALA	GLU	conflict	UNP Q8KTX6
B	557	LEU	-	expression tag	UNP Q8KTX6
B	558	VAL	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	-	expression tag	UNP Q8KTX6
B	560	ARG	-	expression tag	UNP Q8KTX6
B	561	GLY	-	expression tag	UNP Q8KTX6
B	562	SER	-	expression tag	UNP Q8KTX6
B	563	GLY	-	expression tag	UNP Q8KTX6
B	564	GLY	-	expression tag	UNP Q8KTX6
B	565	GLY	-	expression tag	UNP Q8KTX6
B	566	LEU	-	expression tag	UNP Q8KTX6
B	567	GLU	-	expression tag	UNP Q8KTX6
B	568	HIS	-	expression tag	UNP Q8KTX6
B	569	HIS	-	expression tag	UNP Q8KTX6
B	570	HIS	-	expression tag	UNP Q8KTX6
B	571	HIS	-	expression tag	UNP Q8KTX6
B	572	HIS	-	expression tag	UNP Q8KTX6
B	573	HIS	-	expression tag	UNP Q8KTX6
C	134	ALA	ARG	conflict	UNP Q8KTX6
C	245	ALA	GLU	conflict	UNP Q8KTX6
C	557	LEU	-	expression tag	UNP Q8KTX6
C	558	VAL	-	expression tag	UNP Q8KTX6
C	559	PRO	-	expression tag	UNP Q8KTX6
C	560	ARG	-	expression tag	UNP Q8KTX6
C	561	GLY	-	expression tag	UNP Q8KTX6
C	562	SER	-	expression tag	UNP Q8KTX6
C	563	GLY	-	expression tag	UNP Q8KTX6
C	564	GLY	-	expression tag	UNP Q8KTX6
C	565	GLY	-	expression tag	UNP Q8KTX6
C	566	LEU	-	expression tag	UNP Q8KTX6
C	567	GLU	-	expression tag	UNP Q8KTX6
C	568	HIS	-	expression tag	UNP Q8KTX6
C	569	HIS	-	expression tag	UNP Q8KTX6
C	570	HIS	-	expression tag	UNP Q8KTX6
C	571	HIS	-	expression tag	UNP Q8KTX6
C	572	HIS	-	expression tag	UNP Q8KTX6
C	573	HIS	-	expression tag	UNP Q8KTX6
D	134	ALA	ARG	conflict	UNP Q8KTX6
D	245	ALA	GLU	conflict	UNP Q8KTX6
D	557	LEU	-	expression tag	UNP Q8KTX6
D	558	VAL	-	expression tag	UNP Q8KTX6
D	559	PRO	-	expression tag	UNP Q8KTX6
D	560	ARG	-	expression tag	UNP Q8KTX6
D	561	GLY	-	expression tag	UNP Q8KTX6
D	562	SER	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	563	GLY	-	expression tag	UNP Q8KTX6
D	564	GLY	-	expression tag	UNP Q8KTX6
D	565	GLY	-	expression tag	UNP Q8KTX6
D	566	LEU	-	expression tag	UNP Q8KTX6
D	567	GLU	-	expression tag	UNP Q8KTX6
D	568	HIS	-	expression tag	UNP Q8KTX6
D	569	HIS	-	expression tag	UNP Q8KTX6
D	570	HIS	-	expression tag	UNP Q8KTX6
D	571	HIS	-	expression tag	UNP Q8KTX6
D	572	HIS	-	expression tag	UNP Q8KTX6
D	573	HIS	-	expression tag	UNP Q8KTX6
E	134	ALA	ARG	conflict	UNP Q8KTX6
E	245	ALA	GLU	conflict	UNP Q8KTX6
E	557	LEU	-	expression tag	UNP Q8KTX6
E	558	VAL	-	expression tag	UNP Q8KTX6
E	559	PRO	-	expression tag	UNP Q8KTX6
E	560	ARG	-	expression tag	UNP Q8KTX6
E	561	GLY	-	expression tag	UNP Q8KTX6
E	562	SER	-	expression tag	UNP Q8KTX6
E	563	GLY	-	expression tag	UNP Q8KTX6
E	564	GLY	-	expression tag	UNP Q8KTX6
E	565	GLY	-	expression tag	UNP Q8KTX6
E	566	LEU	-	expression tag	UNP Q8KTX6
E	567	GLU	-	expression tag	UNP Q8KTX6
E	568	HIS	-	expression tag	UNP Q8KTX6
E	569	HIS	-	expression tag	UNP Q8KTX6
E	570	HIS	-	expression tag	UNP Q8KTX6
E	571	HIS	-	expression tag	UNP Q8KTX6
E	572	HIS	-	expression tag	UNP Q8KTX6
E	573	HIS	-	expression tag	UNP Q8KTX6
F	134	ALA	ARG	conflict	UNP Q8KTX6
F	245	ALA	GLU	conflict	UNP Q8KTX6
F	557	LEU	-	expression tag	UNP Q8KTX6
F	558	VAL	-	expression tag	UNP Q8KTX6
F	559	PRO	-	expression tag	UNP Q8KTX6
F	560	ARG	-	expression tag	UNP Q8KTX6
F	561	GLY	-	expression tag	UNP Q8KTX6
F	562	SER	-	expression tag	UNP Q8KTX6
F	563	GLY	-	expression tag	UNP Q8KTX6
F	564	GLY	-	expression tag	UNP Q8KTX6
F	565	GLY	-	expression tag	UNP Q8KTX6
F	566	LEU	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	567	GLU	-	expression tag	UNP Q8KTX6
F	568	HIS	-	expression tag	UNP Q8KTX6
F	569	HIS	-	expression tag	UNP Q8KTX6
F	570	HIS	-	expression tag	UNP Q8KTX6
F	571	HIS	-	expression tag	UNP Q8KTX6
F	572	HIS	-	expression tag	UNP Q8KTX6
F	573	HIS	-	expression tag	UNP Q8KTX6
G	134	ALA	ARG	conflict	UNP Q8KTX6
G	245	ALA	GLU	conflict	UNP Q8KTX6
G	557	LEU	-	expression tag	UNP Q8KTX6
G	558	VAL	-	expression tag	UNP Q8KTX6
G	559	PRO	-	expression tag	UNP Q8KTX6
G	560	ARG	-	expression tag	UNP Q8KTX6
G	561	GLY	-	expression tag	UNP Q8KTX6
G	562	SER	-	expression tag	UNP Q8KTX6
G	563	GLY	-	expression tag	UNP Q8KTX6
G	564	GLY	-	expression tag	UNP Q8KTX6
G	565	GLY	-	expression tag	UNP Q8KTX6
G	566	LEU	-	expression tag	UNP Q8KTX6
G	567	GLU	-	expression tag	UNP Q8KTX6
G	568	HIS	-	expression tag	UNP Q8KTX6
G	569	HIS	-	expression tag	UNP Q8KTX6
G	570	HIS	-	expression tag	UNP Q8KTX6
G	571	HIS	-	expression tag	UNP Q8KTX6
G	572	HIS	-	expression tag	UNP Q8KTX6
G	573	HIS	-	expression tag	UNP Q8KTX6
H	134	ALA	ARG	conflict	UNP Q8KTX6
H	245	ALA	GLU	conflict	UNP Q8KTX6
H	557	LEU	-	expression tag	UNP Q8KTX6
H	558	VAL	-	expression tag	UNP Q8KTX6
H	559	PRO	-	expression tag	UNP Q8KTX6
H	560	ARG	-	expression tag	UNP Q8KTX6
H	561	GLY	-	expression tag	UNP Q8KTX6
H	562	SER	-	expression tag	UNP Q8KTX6
H	563	GLY	-	expression tag	UNP Q8KTX6
H	564	GLY	-	expression tag	UNP Q8KTX6
H	565	GLY	-	expression tag	UNP Q8KTX6
H	566	LEU	-	expression tag	UNP Q8KTX6
H	567	GLU	-	expression tag	UNP Q8KTX6
H	568	HIS	-	expression tag	UNP Q8KTX6
H	569	HIS	-	expression tag	UNP Q8KTX6
H	570	HIS	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	571	HIS	-	expression tag	UNP Q8KTX6
H	572	HIS	-	expression tag	UNP Q8KTX6
H	573	HIS	-	expression tag	UNP Q8KTX6
I	134	ALA	ARG	conflict	UNP Q8KTX6
I	245	ALA	GLU	conflict	UNP Q8KTX6
I	557	LEU	-	expression tag	UNP Q8KTX6
I	558	VAL	-	expression tag	UNP Q8KTX6
I	559	PRO	-	expression tag	UNP Q8KTX6
I	560	ARG	-	expression tag	UNP Q8KTX6
I	561	GLY	-	expression tag	UNP Q8KTX6
I	562	SER	-	expression tag	UNP Q8KTX6
I	563	GLY	-	expression tag	UNP Q8KTX6
I	564	GLY	-	expression tag	UNP Q8KTX6
I	565	GLY	-	expression tag	UNP Q8KTX6
I	566	LEU	-	expression tag	UNP Q8KTX6
I	567	GLU	-	expression tag	UNP Q8KTX6
I	568	HIS	-	expression tag	UNP Q8KTX6
I	569	HIS	-	expression tag	UNP Q8KTX6
I	570	HIS	-	expression tag	UNP Q8KTX6
I	571	HIS	-	expression tag	UNP Q8KTX6
I	572	HIS	-	expression tag	UNP Q8KTX6
I	573	HIS	-	expression tag	UNP Q8KTX6
J	134	ALA	ARG	conflict	UNP Q8KTX6
J	245	ALA	GLU	conflict	UNP Q8KTX6
J	557	LEU	-	expression tag	UNP Q8KTX6
J	558	VAL	-	expression tag	UNP Q8KTX6
J	559	PRO	-	expression tag	UNP Q8KTX6
J	560	ARG	-	expression tag	UNP Q8KTX6
J	561	GLY	-	expression tag	UNP Q8KTX6
J	562	SER	-	expression tag	UNP Q8KTX6
J	563	GLY	-	expression tag	UNP Q8KTX6
J	564	GLY	-	expression tag	UNP Q8KTX6
J	565	GLY	-	expression tag	UNP Q8KTX6
J	566	LEU	-	expression tag	UNP Q8KTX6
J	567	GLU	-	expression tag	UNP Q8KTX6
J	568	HIS	-	expression tag	UNP Q8KTX6
J	569	HIS	-	expression tag	UNP Q8KTX6
J	570	HIS	-	expression tag	UNP Q8KTX6
J	571	HIS	-	expression tag	UNP Q8KTX6
J	572	HIS	-	expression tag	UNP Q8KTX6
J	573	HIS	-	expression tag	UNP Q8KTX6
K	134	ALA	ARG	conflict	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	245	ALA	GLU	conflict	UNP Q8KTX6
K	557	LEU	-	expression tag	UNP Q8KTX6
K	558	VAL	-	expression tag	UNP Q8KTX6
K	559	PRO	-	expression tag	UNP Q8KTX6
K	560	ARG	-	expression tag	UNP Q8KTX6
K	561	GLY	-	expression tag	UNP Q8KTX6
K	562	SER	-	expression tag	UNP Q8KTX6
K	563	GLY	-	expression tag	UNP Q8KTX6
K	564	GLY	-	expression tag	UNP Q8KTX6
K	565	GLY	-	expression tag	UNP Q8KTX6
K	566	LEU	-	expression tag	UNP Q8KTX6
K	567	GLU	-	expression tag	UNP Q8KTX6
K	568	HIS	-	expression tag	UNP Q8KTX6
K	569	HIS	-	expression tag	UNP Q8KTX6
K	570	HIS	-	expression tag	UNP Q8KTX6
K	571	HIS	-	expression tag	UNP Q8KTX6
K	572	HIS	-	expression tag	UNP Q8KTX6
K	573	HIS	-	expression tag	UNP Q8KTX6
L	134	ALA	ARG	conflict	UNP Q8KTX6
L	245	ALA	GLU	conflict	UNP Q8KTX6
L	557	LEU	-	expression tag	UNP Q8KTX6
L	558	VAL	-	expression tag	UNP Q8KTX6
L	559	PRO	-	expression tag	UNP Q8KTX6
L	560	ARG	-	expression tag	UNP Q8KTX6
L	561	GLY	-	expression tag	UNP Q8KTX6
L	562	SER	-	expression tag	UNP Q8KTX6
L	563	GLY	-	expression tag	UNP Q8KTX6
L	564	GLY	-	expression tag	UNP Q8KTX6
L	565	GLY	-	expression tag	UNP Q8KTX6
L	566	LEU	-	expression tag	UNP Q8KTX6
L	567	GLU	-	expression tag	UNP Q8KTX6
L	568	HIS	-	expression tag	UNP Q8KTX6
L	569	HIS	-	expression tag	UNP Q8KTX6
L	570	HIS	-	expression tag	UNP Q8KTX6
L	571	HIS	-	expression tag	UNP Q8KTX6
L	572	HIS	-	expression tag	UNP Q8KTX6
L	573	HIS	-	expression tag	UNP Q8KTX6
M	134	ALA	ARG	conflict	UNP Q8KTX6
M	245	ALA	GLU	conflict	UNP Q8KTX6
M	557	LEU	-	expression tag	UNP Q8KTX6
M	558	VAL	-	expression tag	UNP Q8KTX6
M	559	PRO	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	560	ARG	-	expression tag	UNP Q8KTX6
M	561	GLY	-	expression tag	UNP Q8KTX6
M	562	SER	-	expression tag	UNP Q8KTX6
M	563	GLY	-	expression tag	UNP Q8KTX6
M	564	GLY	-	expression tag	UNP Q8KTX6
M	565	GLY	-	expression tag	UNP Q8KTX6
M	566	LEU	-	expression tag	UNP Q8KTX6
M	567	GLU	-	expression tag	UNP Q8KTX6
M	568	HIS	-	expression tag	UNP Q8KTX6
M	569	HIS	-	expression tag	UNP Q8KTX6
M	570	HIS	-	expression tag	UNP Q8KTX6
M	571	HIS	-	expression tag	UNP Q8KTX6
M	572	HIS	-	expression tag	UNP Q8KTX6
M	573	HIS	-	expression tag	UNP Q8KTX6
N	134	ALA	ARG	conflict	UNP Q8KTX6
N	245	ALA	GLU	conflict	UNP Q8KTX6
N	557	LEU	-	expression tag	UNP Q8KTX6
N	558	VAL	-	expression tag	UNP Q8KTX6
N	559	PRO	-	expression tag	UNP Q8KTX6
N	560	ARG	-	expression tag	UNP Q8KTX6
N	561	GLY	-	expression tag	UNP Q8KTX6
N	562	SER	-	expression tag	UNP Q8KTX6
N	563	GLY	-	expression tag	UNP Q8KTX6
N	564	GLY	-	expression tag	UNP Q8KTX6
N	565	GLY	-	expression tag	UNP Q8KTX6
N	566	LEU	-	expression tag	UNP Q8KTX6
N	567	GLU	-	expression tag	UNP Q8KTX6
N	568	HIS	-	expression tag	UNP Q8KTX6
N	569	HIS	-	expression tag	UNP Q8KTX6
N	570	HIS	-	expression tag	UNP Q8KTX6
N	571	HIS	-	expression tag	UNP Q8KTX6
N	572	HIS	-	expression tag	UNP Q8KTX6
N	573	HIS	-	expression tag	UNP Q8KTX6
O	134	ALA	ARG	conflict	UNP Q8KTX6
O	245	ALA	GLU	conflict	UNP Q8KTX6
O	557	LEU	-	expression tag	UNP Q8KTX6
O	558	VAL	-	expression tag	UNP Q8KTX6
O	559	PRO	-	expression tag	UNP Q8KTX6
O	560	ARG	-	expression tag	UNP Q8KTX6
O	561	GLY	-	expression tag	UNP Q8KTX6
O	562	SER	-	expression tag	UNP Q8KTX6
O	563	GLY	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	564	GLY	-	expression tag	UNP Q8KTX6
O	565	GLY	-	expression tag	UNP Q8KTX6
O	566	LEU	-	expression tag	UNP Q8KTX6
O	567	GLU	-	expression tag	UNP Q8KTX6
O	568	HIS	-	expression tag	UNP Q8KTX6
O	569	HIS	-	expression tag	UNP Q8KTX6
O	570	HIS	-	expression tag	UNP Q8KTX6
O	571	HIS	-	expression tag	UNP Q8KTX6
O	572	HIS	-	expression tag	UNP Q8KTX6
O	573	HIS	-	expression tag	UNP Q8KTX6
P	134	ALA	ARG	conflict	UNP Q8KTX6
P	245	ALA	GLU	conflict	UNP Q8KTX6
P	557	LEU	-	expression tag	UNP Q8KTX6
P	558	VAL	-	expression tag	UNP Q8KTX6
P	559	PRO	-	expression tag	UNP Q8KTX6
P	560	ARG	-	expression tag	UNP Q8KTX6
P	561	GLY	-	expression tag	UNP Q8KTX6
P	562	SER	-	expression tag	UNP Q8KTX6
P	563	GLY	-	expression tag	UNP Q8KTX6
P	564	GLY	-	expression tag	UNP Q8KTX6
P	565	GLY	-	expression tag	UNP Q8KTX6
P	566	LEU	-	expression tag	UNP Q8KTX6
P	567	GLU	-	expression tag	UNP Q8KTX6
P	568	HIS	-	expression tag	UNP Q8KTX6
P	569	HIS	-	expression tag	UNP Q8KTX6
P	570	HIS	-	expression tag	UNP Q8KTX6
P	571	HIS	-	expression tag	UNP Q8KTX6
P	572	HIS	-	expression tag	UNP Q8KTX6
P	573	HIS	-	expression tag	UNP Q8KTX6
Q	134	ALA	ARG	conflict	UNP Q8KTX6
Q	245	ALA	GLU	conflict	UNP Q8KTX6
Q	557	LEU	-	expression tag	UNP Q8KTX6
Q	558	VAL	-	expression tag	UNP Q8KTX6
Q	559	PRO	-	expression tag	UNP Q8KTX6
Q	560	ARG	-	expression tag	UNP Q8KTX6
Q	561	GLY	-	expression tag	UNP Q8KTX6
Q	562	SER	-	expression tag	UNP Q8KTX6
Q	563	GLY	-	expression tag	UNP Q8KTX6
Q	564	GLY	-	expression tag	UNP Q8KTX6
Q	565	GLY	-	expression tag	UNP Q8KTX6
Q	566	LEU	-	expression tag	UNP Q8KTX6
Q	567	GLU	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	568	HIS	-	expression tag	UNP Q8KTX6
Q	569	HIS	-	expression tag	UNP Q8KTX6
Q	570	HIS	-	expression tag	UNP Q8KTX6
Q	571	HIS	-	expression tag	UNP Q8KTX6
Q	572	HIS	-	expression tag	UNP Q8KTX6
Q	573	HIS	-	expression tag	UNP Q8KTX6
R	134	ALA	ARG	conflict	UNP Q8KTX6
R	245	ALA	GLU	conflict	UNP Q8KTX6
R	557	LEU	-	expression tag	UNP Q8KTX6
R	558	VAL	-	expression tag	UNP Q8KTX6
R	559	PRO	-	expression tag	UNP Q8KTX6
R	560	ARG	-	expression tag	UNP Q8KTX6
R	561	GLY	-	expression tag	UNP Q8KTX6
R	562	SER	-	expression tag	UNP Q8KTX6
R	563	GLY	-	expression tag	UNP Q8KTX6
R	564	GLY	-	expression tag	UNP Q8KTX6
R	565	GLY	-	expression tag	UNP Q8KTX6
R	566	LEU	-	expression tag	UNP Q8KTX6
R	567	GLU	-	expression tag	UNP Q8KTX6
R	568	HIS	-	expression tag	UNP Q8KTX6
R	569	HIS	-	expression tag	UNP Q8KTX6
R	570	HIS	-	expression tag	UNP Q8KTX6
R	571	HIS	-	expression tag	UNP Q8KTX6
R	572	HIS	-	expression tag	UNP Q8KTX6
R	573	HIS	-	expression tag	UNP Q8KTX6
S	134	ALA	ARG	conflict	UNP Q8KTX6
S	245	ALA	GLU	conflict	UNP Q8KTX6
S	557	LEU	-	expression tag	UNP Q8KTX6
S	558	VAL	-	expression tag	UNP Q8KTX6
S	559	PRO	-	expression tag	UNP Q8KTX6
S	560	ARG	-	expression tag	UNP Q8KTX6
S	561	GLY	-	expression tag	UNP Q8KTX6
S	562	SER	-	expression tag	UNP Q8KTX6
S	563	GLY	-	expression tag	UNP Q8KTX6
S	564	GLY	-	expression tag	UNP Q8KTX6
S	565	GLY	-	expression tag	UNP Q8KTX6
S	566	LEU	-	expression tag	UNP Q8KTX6
S	567	GLU	-	expression tag	UNP Q8KTX6
S	568	HIS	-	expression tag	UNP Q8KTX6
S	569	HIS	-	expression tag	UNP Q8KTX6
S	570	HIS	-	expression tag	UNP Q8KTX6
S	571	HIS	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	572	HIS	-	expression tag	UNP Q8KTX6
S	573	HIS	-	expression tag	UNP Q8KTX6
T	134	ALA	ARG	conflict	UNP Q8KTX6
T	245	ALA	GLU	conflict	UNP Q8KTX6
T	557	LEU	-	expression tag	UNP Q8KTX6
T	558	VAL	-	expression tag	UNP Q8KTX6
T	559	PRO	-	expression tag	UNP Q8KTX6
T	560	ARG	-	expression tag	UNP Q8KTX6
T	561	GLY	-	expression tag	UNP Q8KTX6
T	562	SER	-	expression tag	UNP Q8KTX6
T	563	GLY	-	expression tag	UNP Q8KTX6
T	564	GLY	-	expression tag	UNP Q8KTX6
T	565	GLY	-	expression tag	UNP Q8KTX6
T	566	LEU	-	expression tag	UNP Q8KTX6
T	567	GLU	-	expression tag	UNP Q8KTX6
T	568	HIS	-	expression tag	UNP Q8KTX6
T	569	HIS	-	expression tag	UNP Q8KTX6
T	570	HIS	-	expression tag	UNP Q8KTX6
T	571	HIS	-	expression tag	UNP Q8KTX6
T	572	HIS	-	expression tag	UNP Q8KTX6
T	573	HIS	-	expression tag	UNP Q8KTX6
U	134	ALA	ARG	conflict	UNP Q8KTX6
U	245	ALA	GLU	conflict	UNP Q8KTX6
U	557	LEU	-	expression tag	UNP Q8KTX6
U	558	VAL	-	expression tag	UNP Q8KTX6
U	559	PRO	-	expression tag	UNP Q8KTX6
U	560	ARG	-	expression tag	UNP Q8KTX6
U	561	GLY	-	expression tag	UNP Q8KTX6
U	562	SER	-	expression tag	UNP Q8KTX6
U	563	GLY	-	expression tag	UNP Q8KTX6
U	564	GLY	-	expression tag	UNP Q8KTX6
U	565	GLY	-	expression tag	UNP Q8KTX6
U	566	LEU	-	expression tag	UNP Q8KTX6
U	567	GLU	-	expression tag	UNP Q8KTX6
U	568	HIS	-	expression tag	UNP Q8KTX6
U	569	HIS	-	expression tag	UNP Q8KTX6
U	570	HIS	-	expression tag	UNP Q8KTX6
U	571	HIS	-	expression tag	UNP Q8KTX6
U	572	HIS	-	expression tag	UNP Q8KTX6
U	573	HIS	-	expression tag	UNP Q8KTX6
V	134	ALA	ARG	conflict	UNP Q8KTX6
V	245	ALA	GLU	conflict	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
V	557	LEU	-	expression tag	UNP Q8KTX6
V	558	VAL	-	expression tag	UNP Q8KTX6
V	559	PRO	-	expression tag	UNP Q8KTX6
V	560	ARG	-	expression tag	UNP Q8KTX6
V	561	GLY	-	expression tag	UNP Q8KTX6
V	562	SER	-	expression tag	UNP Q8KTX6
V	563	GLY	-	expression tag	UNP Q8KTX6
V	564	GLY	-	expression tag	UNP Q8KTX6
V	565	GLY	-	expression tag	UNP Q8KTX6
V	566	LEU	-	expression tag	UNP Q8KTX6
V	567	GLU	-	expression tag	UNP Q8KTX6
V	568	HIS	-	expression tag	UNP Q8KTX6
V	569	HIS	-	expression tag	UNP Q8KTX6
V	570	HIS	-	expression tag	UNP Q8KTX6
V	571	HIS	-	expression tag	UNP Q8KTX6
V	572	HIS	-	expression tag	UNP Q8KTX6
V	573	HIS	-	expression tag	UNP Q8KTX6
W	134	ALA	ARG	conflict	UNP Q8KTX6
W	245	ALA	GLU	conflict	UNP Q8KTX6
W	557	LEU	-	expression tag	UNP Q8KTX6
W	558	VAL	-	expression tag	UNP Q8KTX6
W	559	PRO	-	expression tag	UNP Q8KTX6
W	560	ARG	-	expression tag	UNP Q8KTX6
W	561	GLY	-	expression tag	UNP Q8KTX6
W	562	SER	-	expression tag	UNP Q8KTX6
W	563	GLY	-	expression tag	UNP Q8KTX6
W	564	GLY	-	expression tag	UNP Q8KTX6
W	565	GLY	-	expression tag	UNP Q8KTX6
W	566	LEU	-	expression tag	UNP Q8KTX6
W	567	GLU	-	expression tag	UNP Q8KTX6
W	568	HIS	-	expression tag	UNP Q8KTX6
W	569	HIS	-	expression tag	UNP Q8KTX6
W	570	HIS	-	expression tag	UNP Q8KTX6
W	571	HIS	-	expression tag	UNP Q8KTX6
W	572	HIS	-	expression tag	UNP Q8KTX6
W	573	HIS	-	expression tag	UNP Q8KTX6
X	134	ALA	ARG	conflict	UNP Q8KTX6
X	245	ALA	GLU	conflict	UNP Q8KTX6
X	557	LEU	-	expression tag	UNP Q8KTX6
X	558	VAL	-	expression tag	UNP Q8KTX6
X	559	PRO	-	expression tag	UNP Q8KTX6
X	560	ARG	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
X	561	GLY	-	expression tag	UNP Q8KTX6
X	562	SER	-	expression tag	UNP Q8KTX6
X	563	GLY	-	expression tag	UNP Q8KTX6
X	564	GLY	-	expression tag	UNP Q8KTX6
X	565	GLY	-	expression tag	UNP Q8KTX6
X	566	LEU	-	expression tag	UNP Q8KTX6
X	567	GLU	-	expression tag	UNP Q8KTX6
X	568	HIS	-	expression tag	UNP Q8KTX6
X	569	HIS	-	expression tag	UNP Q8KTX6
X	570	HIS	-	expression tag	UNP Q8KTX6
X	571	HIS	-	expression tag	UNP Q8KTX6
X	572	HIS	-	expression tag	UNP Q8KTX6
X	573	HIS	-	expression tag	UNP Q8KTX6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

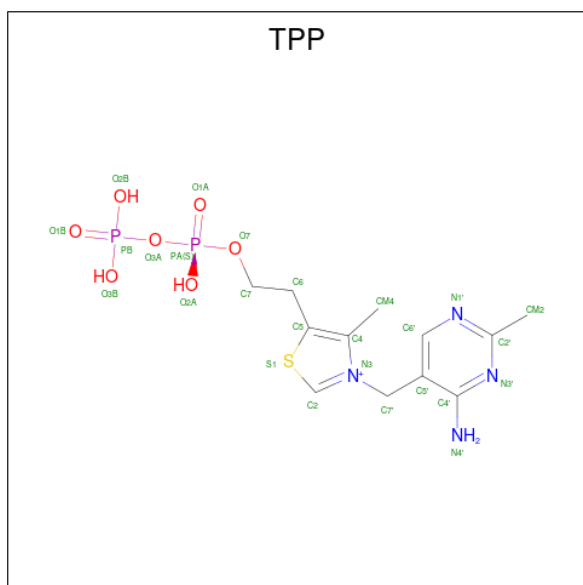
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	L	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	1	Total Mg 1 1	0	0
2	O	1	Total Mg 1 1	0	0
2	P	1	Total Mg 1 1	0	0
2	Q	1	Total Mg 1 1	0	0
2	R	1	Total Mg 1 1	0	0
2	S	1	Total Mg 1 1	0	0
2	T	1	Total Mg 1 1	0	0
2	U	1	Total Mg 1 1	0	0
2	V	1	Total Mg 1 1	0	0
2	W	1	Total Mg 1 1	0	0
2	X	1	Total Mg 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $\text{C}_{12}\text{H}_{19}\text{N}_4\text{O}_7\text{P}_2\text{S}$).



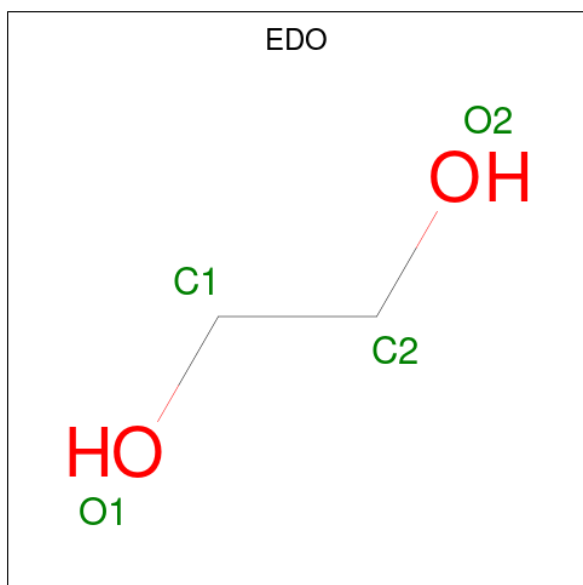
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	G	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	H	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	I	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	J	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	K	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	L	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	M	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	N	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	O	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	P	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	Q	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	R	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	S	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	T	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	U	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	V	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	W	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	X	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	N	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		
4	R	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	157	Total 157	O 157	0	0
5	C	246	Total 246	O 246	0	0
5	D	199	Total 199	O 199	0	0
5	E	221	Total 221	O 221	0	0
5	F	275	Total 275	O 275	0	0
5	G	192	Total 192	O 192	0	0
5	H	150	Total 150	O 150	0	0
5	I	176	Total 176	O 176	0	0
5	J	217	Total 217	O 217	0	0
5	K	206	Total 206	O 206	0	0
5	L	200	Total 200	O 200	0	0
5	M	288	Total 288	O 288	0	0
5	N	269	Total 269	O 269	0	0
5	O	185	Total 185	O 185	0	0
5	P	212	Total 212	O 212	0	0
5	Q	149	Total 149	O 149	0	0
5	R	151	Total 151	O 151	0	0
5	S	184	Total 184	O 184	0	0
5	T	184	Total 184	O 184	0	0
5	U	81	Total 81	O 81	0	0
5	V	66	Total 66	O 66	0	0

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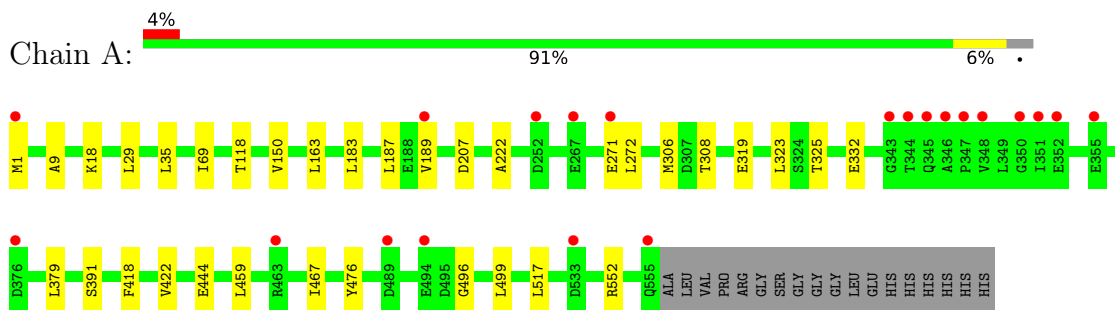
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	W	55	Total 55	O 55	0	0
5	X	114	Total 114	O 114	0	0

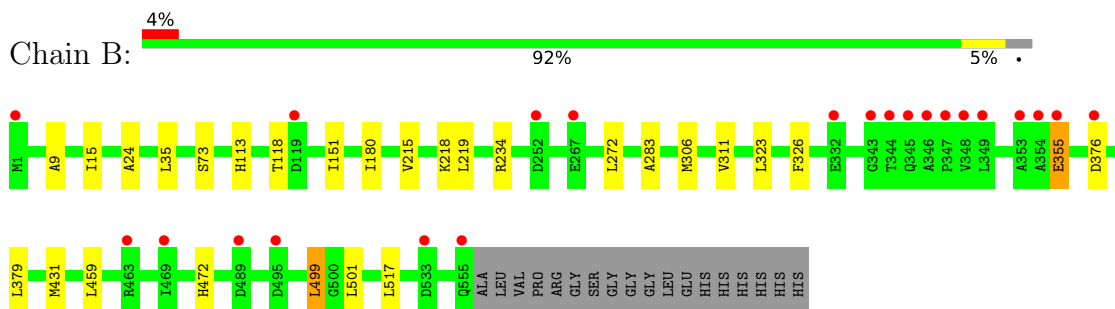
3 Residue-property plots

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

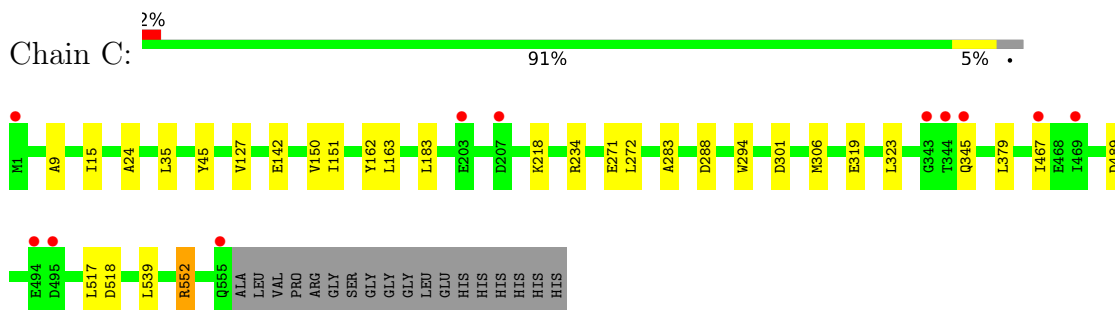
- Molecule 1: Pyruvate decarboxylase



- Molecule 1: Pyruvate decarboxylase

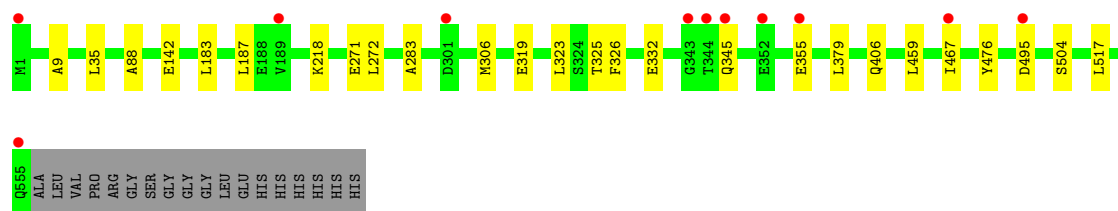


- Molecule 1: Pyruvate decarboxylase

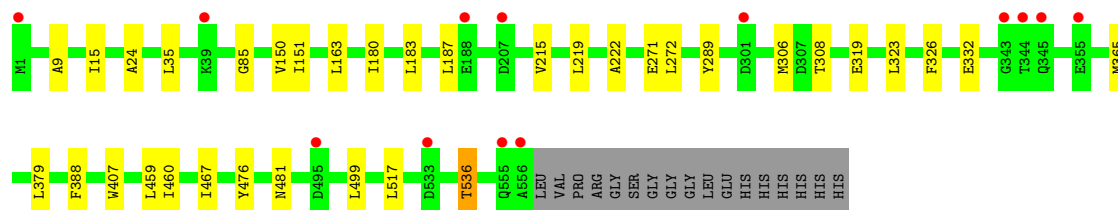
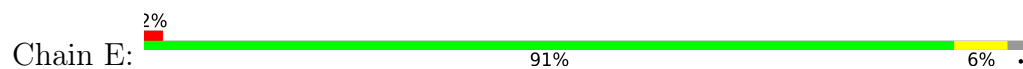


- Molecule 1: Pyruvate decarboxylase

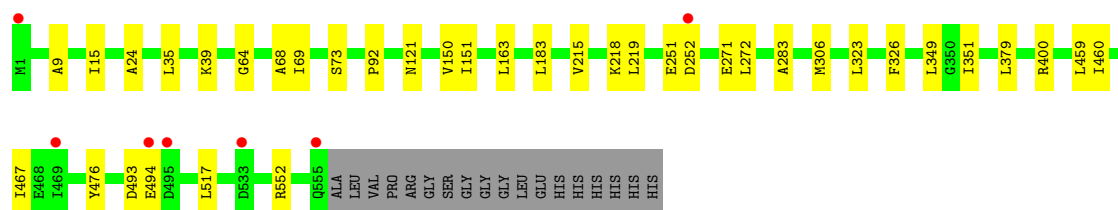
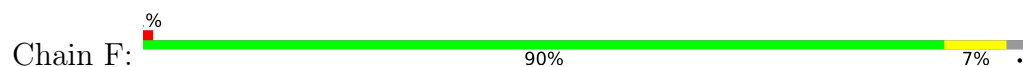




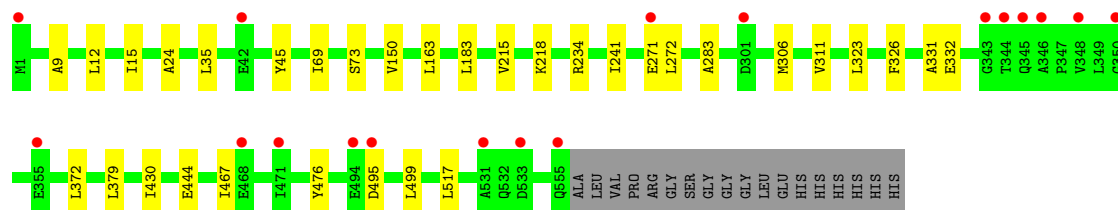
• Molecule 1: Pyruvate decarboxylase



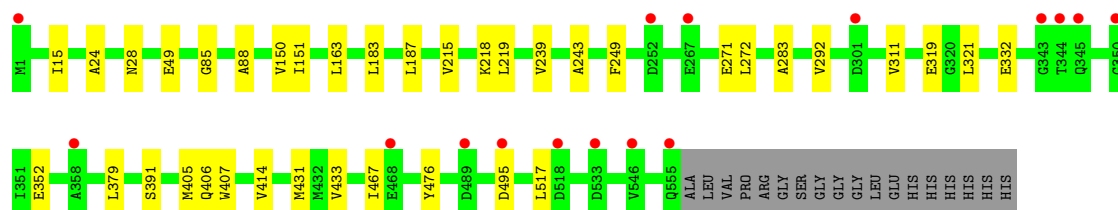
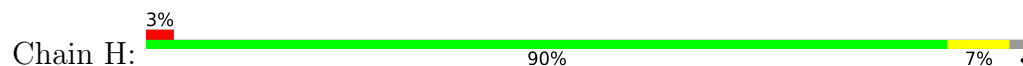
• Molecule 1: Pyruvate decarboxylase



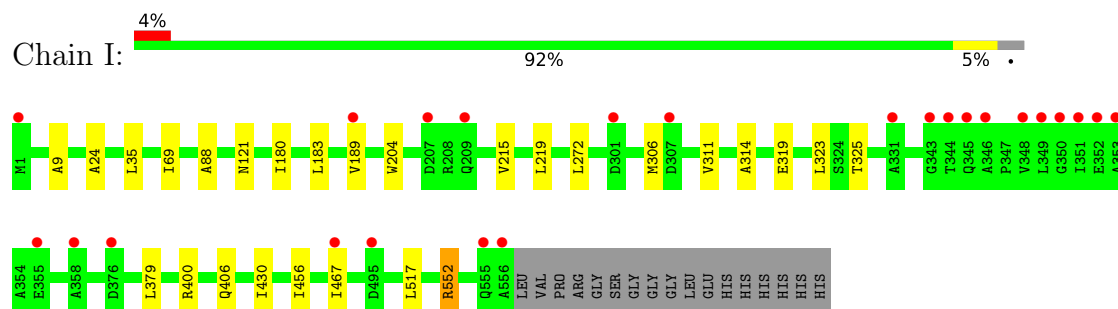
• Molecule 1: Pyruvate decarboxylase



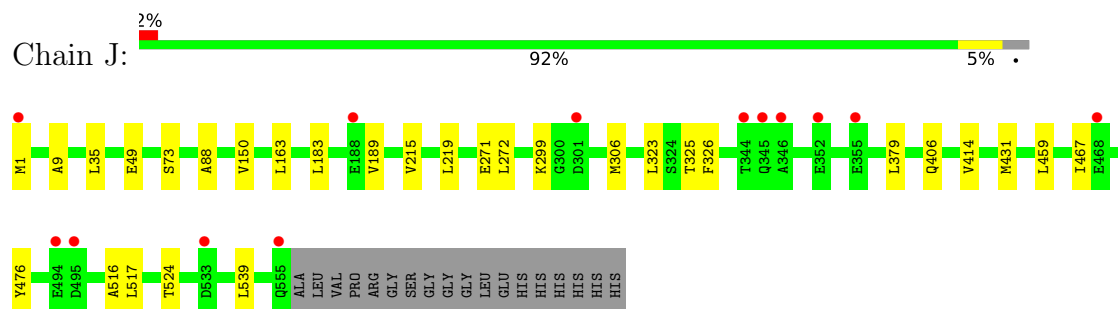
• Molecule 1: Pyruvate decarboxylase



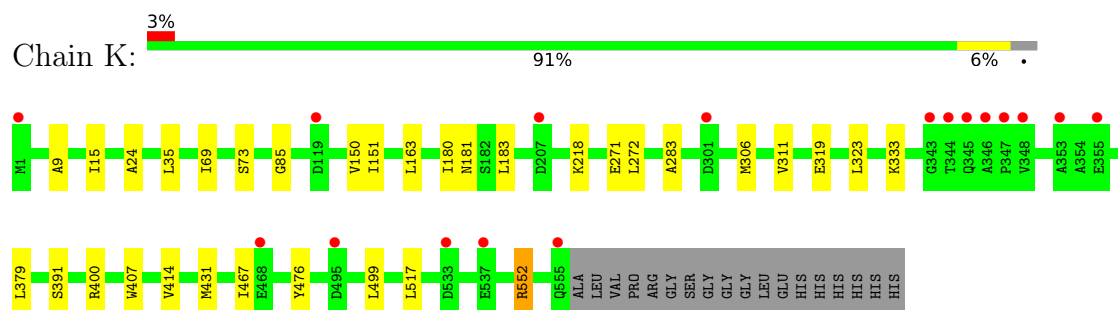
- Molecule 1: Pyruvate decarboxylase



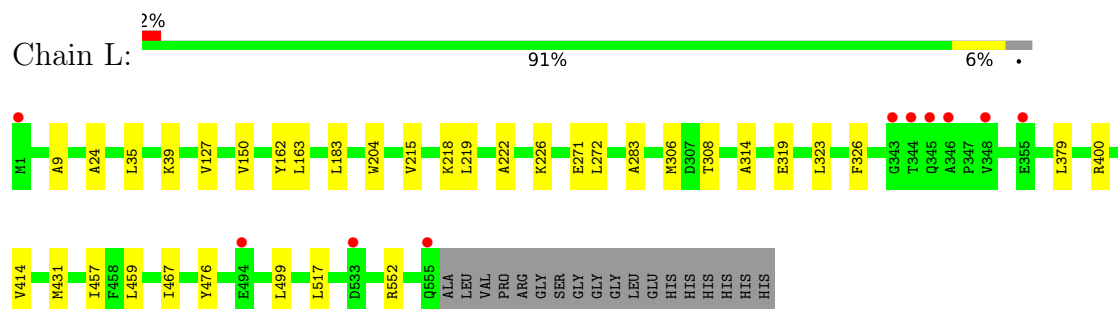
- Molecule 1: Pyruvate decarboxylase



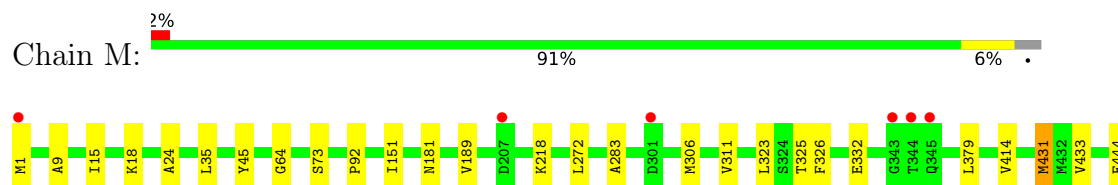
- Molecule 1: Pyruvate decarboxylase

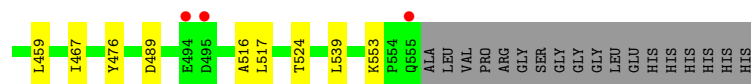


- Molecule 1: Pyruvate decarboxylase

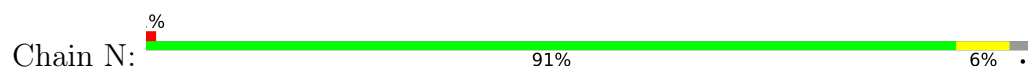


- Molecule 1: Pyruvate decarboxylase

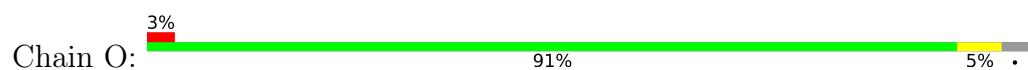




- Molecule 1: Pyruvate decarboxylase



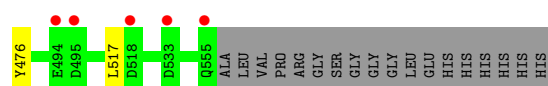
- Molecule 1: Pyruvate decarboxylase



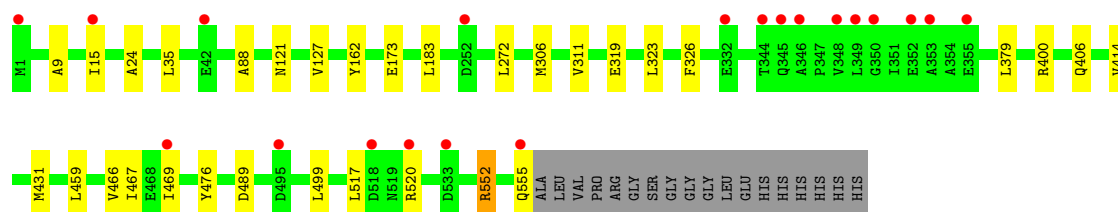
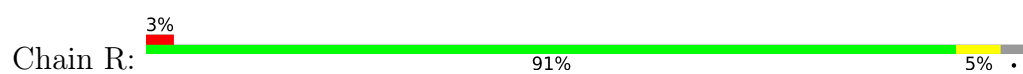
- Molecule 1: Pyruvate decarboxylase



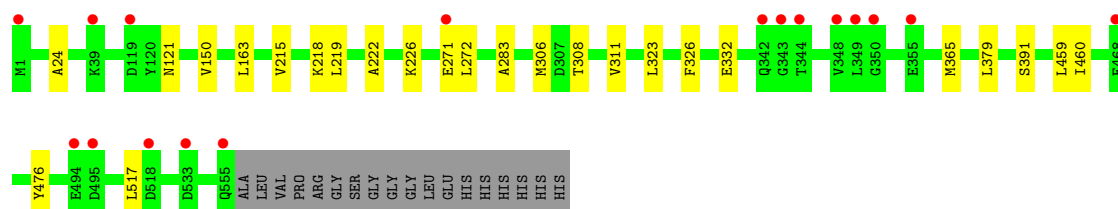
- Molecule 1: Pyruvate decarboxylase



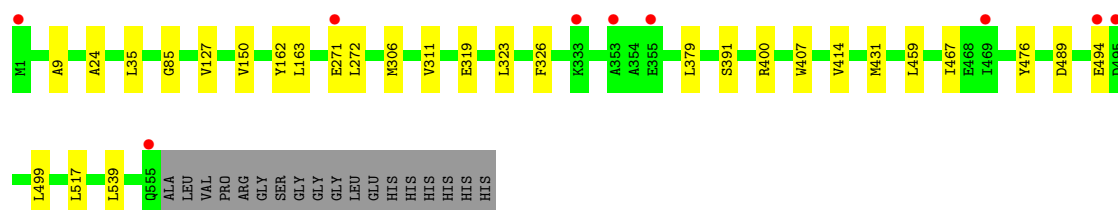
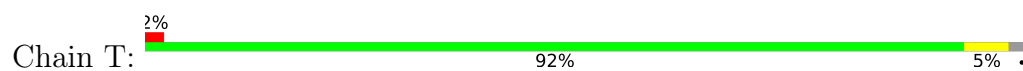
- Molecule 1: Pyruvate decarboxylase



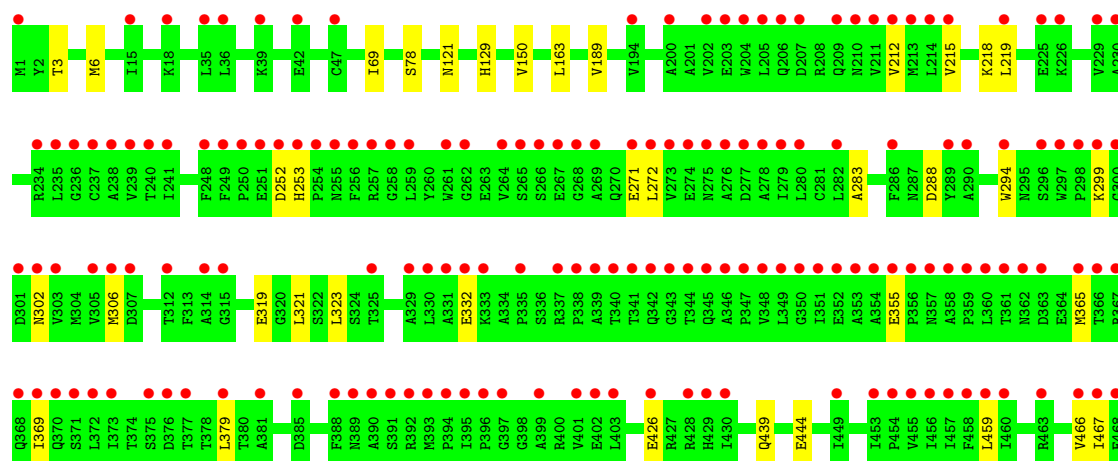
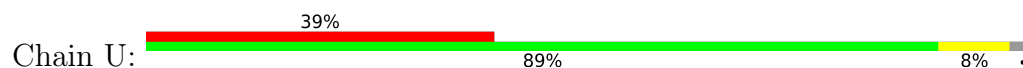
• Molecule 1: Pyruvate decarboxylase

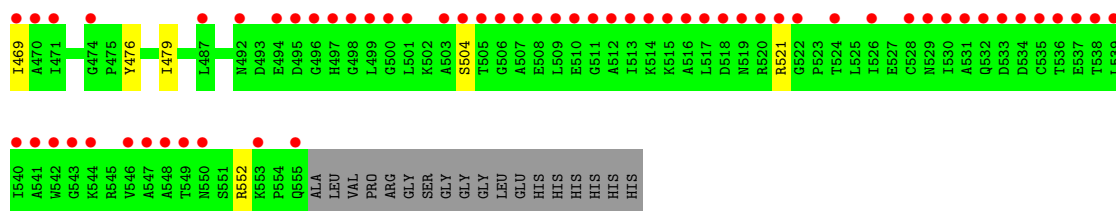


• Molecule 1: Pyruvate decarboxylase

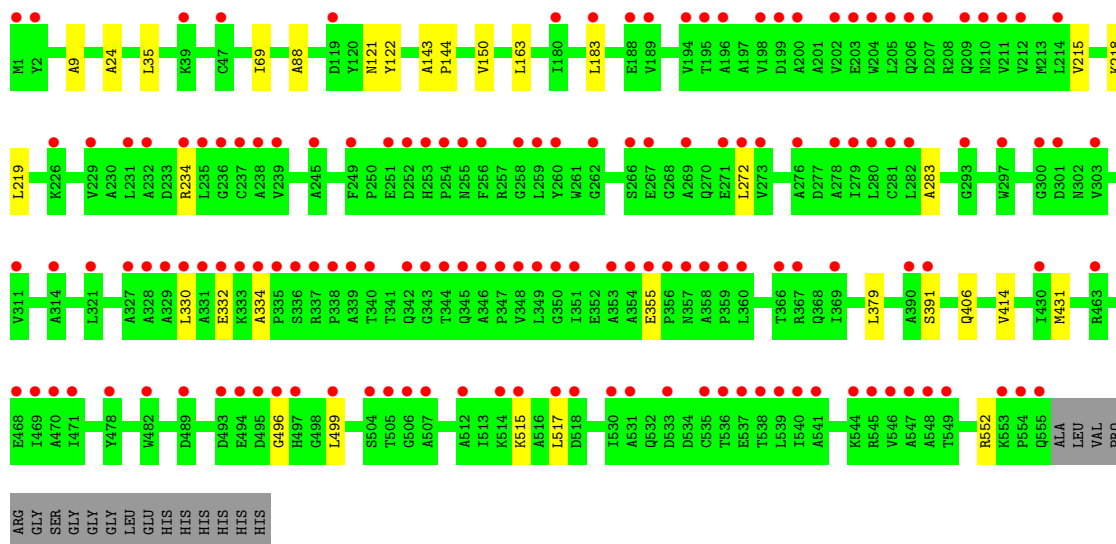
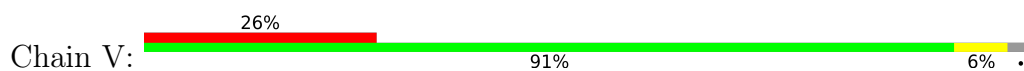


• Molecule 1: Pyruvate decarboxylase

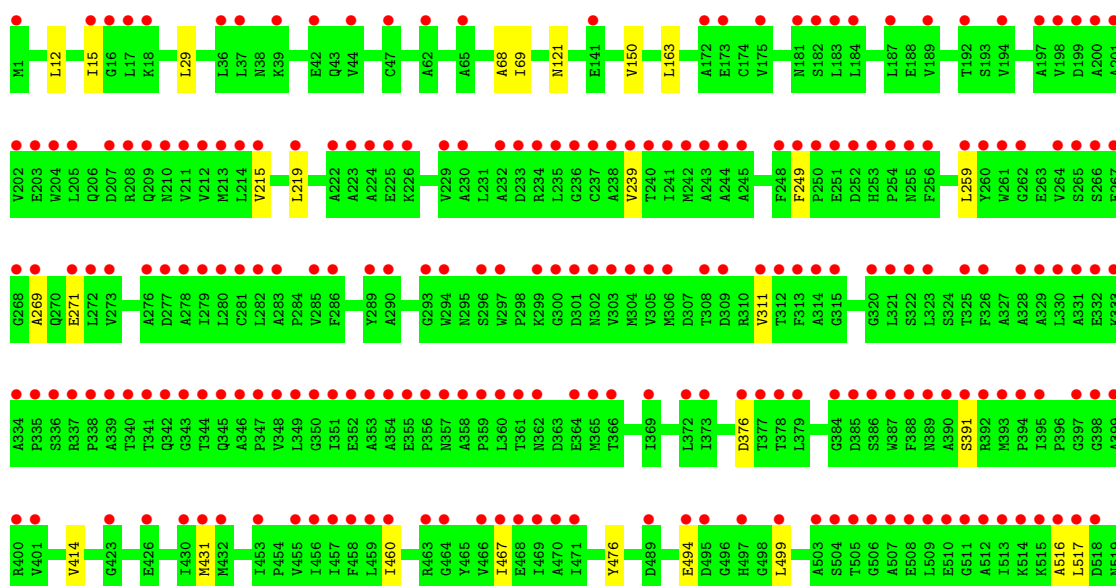


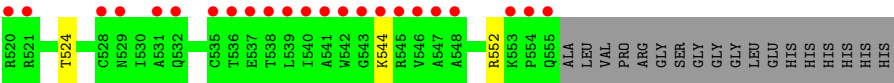


● Molecule 1: Pyruvate decarboxylase

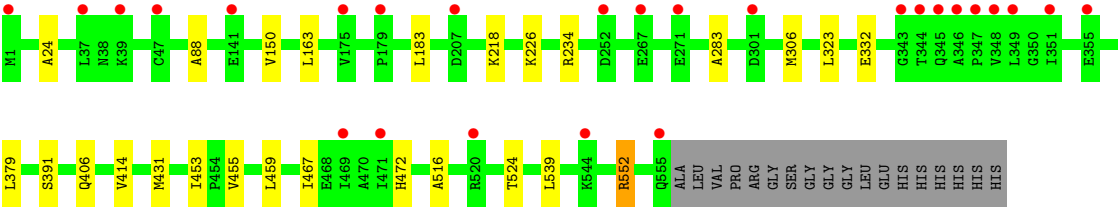
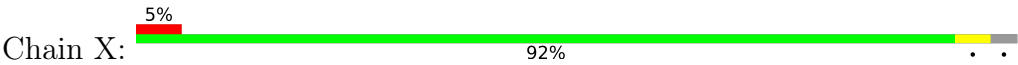


● Molecule 1: Pyruvate decarboxylase





● Molecule 1: Pyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	204.56Å 177.39Å 244.55Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	75.40 – 2.15 75.40 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (75.40-2.15) 98.8 (75.40-2.15)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.186 , 0.220 0.192 , 0.222	Depositor DCC
R_{free} test set	42940 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	107004	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.62	0/4334	0.84	1/5898 (0.0%)
1	B	0.63	0/4321	0.83	0/5882
1	C	0.63	0/4344	0.82	0/5911
1	D	0.63	0/4329	0.82	0/5893
1	E	0.64	0/4327	0.84	0/5888
1	F	0.64	0/4369	0.83	3/5945 (0.1%)
1	G	0.62	0/4350	0.82	0/5921
1	H	0.63	0/4336	0.83	0/5901
1	I	0.62	0/4342	0.84	1/5908 (0.0%)
1	J	0.62	0/4322	0.83	0/5883
1	K	0.63	0/4350	0.81	0/5920
1	L	0.63	0/4368	0.82	0/5945
1	M	0.63	0/4346	0.82	0/5916
1	N	0.64	0/4349	0.83	0/5919
1	O	0.62	0/4313	0.83	0/5870
1	P	0.63	0/4348	0.83	0/5917
1	Q	0.62	0/4330	0.84	0/5894
1	R	0.60	0/4354	0.82	0/5927
1	S	0.61	0/4305	0.83	0/5860
1	T	0.62	0/4322	0.81	0/5883
1	U	0.62	0/4323	0.83	0/5884
1	V	0.60	0/4322	0.84	1/5883 (0.0%)
1	W	0.63	0/4314	0.84	1/5872 (0.0%)
1	X	0.59	0/4312	0.82	0/5870
All	All	0.62	0/104030	0.83	7/141590 (0.0%)

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	T	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	GLY	N-CA-C	6.09	119.03	112.33
1	V	496	GLY	N-CA-C	5.76	118.67	112.33
1	F	252	ASP	N-CA-C	5.33	118.58	111.75
1	F	251	GLU	CA-C-N	5.29	128.10	120.38
1	F	251	GLU	C-N-CA	5.29	128.10	120.38
1	W	269	ALA	N-CA-C	5.25	118.47	111.75
1	I	552	ARG	NE-CZ-NH2	5.17	123.86	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	494	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4250	0	4149	12	0
1	B	4237	0	4138	16	0
1	C	4260	0	4161	18	0
1	D	4245	0	4141	16	0
1	E	4244	0	4141	21	0
1	F	4285	0	4179	16	0
1	G	4266	0	4163	17	0
1	H	4252	0	4148	20	0
1	I	4259	0	4151	12	0
1	J	4238	0	4135	16	0
1	K	4266	0	4157	16	0
1	L	4284	0	4176	16	0
1	M	4262	0	4158	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4265	0	4155	16	0
1	O	4229	0	4129	14	0
1	P	4264	0	4157	15	0
1	Q	4246	0	4143	12	0
1	R	4270	0	4154	14	0
1	S	4221	0	4127	12	0
1	T	4238	0	4135	12	0
1	U	4239	0	4137	16	0
1	V	4238	0	4135	14	0
1	W	4230	0	4132	12	0
1	X	4228	0	4133	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	0	0
3	C	26	0	16	2	0
3	D	26	0	16	2	0
3	E	26	0	16	4	0
3	F	26	0	16	1	0
3	G	26	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	26	0	16	2	0
3	I	26	0	16	2	0
3	J	26	0	16	2	0
3	K	26	0	16	2	0
3	L	26	0	16	2	0
3	M	26	0	16	2	0
3	N	26	0	16	2	0
3	O	26	0	16	2	0
3	P	26	0	16	2	0
3	Q	26	0	16	2	0
3	R	26	0	16	2	0
3	S	26	0	16	0	0
3	T	26	0	16	1	0
3	U	26	0	16	1	0
3	V	26	0	16	0	0
3	W	26	0	16	1	0
3	X	26	0	16	2	0
4	A	4	0	6	0	0
4	F	4	0	6	2	0
4	I	4	0	6	0	0
4	N	4	0	6	0	0
4	Q	4	0	6	0	0
4	R	4	0	6	0	0
5	A	139	0	0	0	0
5	B	157	0	0	0	0
5	C	246	0	0	2	0
5	D	199	0	0	1	0
5	E	221	0	0	0	0
5	F	275	0	0	0	0
5	G	192	0	0	0	0
5	H	150	0	0	1	0
5	I	176	0	0	0	0
5	J	217	0	0	0	0
5	K	206	0	0	1	0
5	L	200	0	0	0	0
5	M	288	0	0	0	0
5	N	269	0	0	0	0
5	O	185	0	0	0	0
5	P	212	0	0	0	0
5	Q	149	0	0	1	0
5	R	151	0	0	1	0
5	S	184	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	184	0	0	0	0
5	U	81	0	0	0	0
5	V	66	0	0	1	0
5	W	55	0	0	0	0
5	X	114	0	0	1	0
All	All	107004	0	99954	338	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 2.

All (338) 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:R:414:VAL:HG22	1:R:431:MET:HE1	1.66	0.78
1:T:414:VAL:HG22	1:T:431:MET:HE1	1.65	0.77
1:W:414:VAL:HG22	1:W:431:MET:HE1	1.66	0.77
1:J:414:VAL:HG22	1:J:431:MET:HE1	1.68	0.74
1:A:9:ALA:HB2	1:A:35:LEU:HD23	1.70	0.73
1:K:414:VAL:HG22	1:K:431:MET:HE1	1.71	0.73
1:O:414:VAL:HG22	1:O:431:MET:HE1	1.69	0.72
1:X:414:VAL:HG22	1:X:431:MET:HE1	1.70	0.72
1:C:9:ALA:HB2	1:C:35:LEU:HD23	1.72	0.70
1:H:414:VAL:HG22	1:H:431:MET:HE1	1.71	0.70
1:V:414:VAL:HG22	1:V:431:MET:HE1	1.72	0.70
1:J:306:MET:HE2	1:J:323:LEU:CD1	2.24	0.68
1:F:9:ALA:HB2	1:F:35:LEU:HD23	1.77	0.67
1:M:414:VAL:HG22	1:M:431:MET:HE1	1.77	0.65
1:N:306:MET:HE2	1:N:323:LEU:CD1	2.26	0.64
1:B:306:MET:HE2	1:B:323:LEU:CD1	2.27	0.64
1:W:215:VAL:HG13	1:W:219:LEU:HD22	1.80	0.64
1:M:306:MET:HE2	1:M:323:LEU:CD1	2.28	0.63
1:K:467:ILE:HG21	3:K:602:TPP:S1	2.39	0.62
1:U:215:VAL:HG13	1:U:219:LEU:HD22	1.80	0.62
1:H:150:VAL:HG21	1:H:163:LEU:HG	1.82	0.62
1:D:306:MET:HE2	1:D:323:LEU:CD1	2.30	0.61
1:I:306:MET:HE2	1:I:323:LEU:CD1	2.30	0.61
1:P:306:MET:HE2	1:P:323:LEU:CD1	2.30	0.61
1:E:306:MET:HE2	1:E:323:LEU:CD1	2.29	0.61
1:S:306:MET:HE2	1:S:323:LEU:CD1	2.31	0.61
3:E:602:TPP:H2	4:F:601:EDO:O2	2.00	0.61
1:J:150:VAL:HG21	1:J:163:LEU:HG	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:552:ARG:NH1	5:R:701:HOH:O	2.33	0.61
1:V:150:VAL:HG21	1:V:163:LEU:HG	1.83	0.61
1:B:9:ALA:HB2	1:B:35:LEU:HD23	1.82	0.61
1:G:306:MET:HE2	1:G:323:LEU:CD1	2.32	0.60
1:M:189:VAL:HG11	1:M:325[A]:THR:HG21	1.84	0.59
1:K:150:VAL:HG21	1:K:163:LEU:HG	1.85	0.59
1:C:306:MET:HE2	1:C:323:LEU:CD1	2.33	0.58
1:E:187:LEU:HD23	1:H:187:LEU:HD23	1.84	0.58
1:X:306:MET:HE2	1:X:323:LEU:CD1	2.33	0.58
1:T:150:VAL:HG21	1:T:163:LEU:HG	1.85	0.58
1:M:9:ALA:HB2	1:M:35:LEU:HD23	1.84	0.58
1:C:234[B]:ARG:NH2	5:C:702:HOH:O	2.35	0.58
1:N:467:ILE:HG21	3:N:602:TPP:S1	2.44	0.58
1:L:306:MET:HE2	1:L:323:LEU:CD1	2.34	0.58
1:X:306:MET:HE2	1:X:323:LEU:HD11	1.86	0.58
1:N:150:VAL:HG21	1:N:163:LEU:HG	1.85	0.57
1:S:215:VAL:HG13	1:S:219:LEU:HD22	1.87	0.57
1:R:9:ALA:HB2	1:R:35:LEU:HD23	1.88	0.56
1:T:306:MET:HE2	1:T:323:LEU:CD1	2.35	0.56
1:J:467:ILE:CG2	3:J:602:TPP:S1	2.94	0.56
1:L:9:ALA:HB2	1:L:35:LEU:HD23	1.87	0.56
1:C:552:ARG:NH1	5:C:701:HOH:O	2.29	0.56
1:P:467:ILE:HG21	3:P:602:TPP:S1	2.46	0.56
1:V:215:VAL:HG13	1:V:219:LEU:HD22	1.87	0.56
1:K:9:ALA:HB2	1:K:35:LEU:HD23	1.87	0.56
1:O:150:VAL:HG21	1:O:163:LEU:HG	1.88	0.56
1:C:518:ASP:O	1:M:18:LYS:NZ	2.39	0.55
1:V:234:ARG:NH1	5:V:701:HOH:O	2.25	0.55
1:H:243:ALA:HB3	1:H:405[A]:MET:HE1	1.88	0.55
1:S:150:VAL:HG21	1:S:163:LEU:HG	1.89	0.55
1:N:9:ALA:HB2	1:N:35:LEU:HD23	1.89	0.54
1:D:306:MET:HE3	1:D:326:PHE:CD2	2.41	0.54
1:E:306:MET:HE3	1:E:326:PHE:CD2	2.43	0.54
1:I:9:ALA:HB2	1:I:35:LEU:HD23	1.90	0.54
1:S:24:ALA:HB2	1:T:476:TYR:HB2	1.89	0.54
1:R:306:MET:HE2	1:R:323:LEU:CD1	2.38	0.54
1:J:9:ALA:HB2	1:J:35:LEU:HD23	1.90	0.54
1:K:467:ILE:CG2	3:K:602:TPP:S1	2.96	0.54
1:N:467:ILE:CG2	3:N:602:TPP:S1	2.96	0.54
1:F:150:VAL:HG21	1:F:163:LEU:HG	1.91	0.53
1:Q:215:VAL:HG13	1:Q:219:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:150:VAL:HG21	1:U:163:LEU:HG	1.89	0.53
1:V:355[A]:GLU:OE1	1:V:355[A]:GLU:N	2.26	0.53
1:A:150:VAL:HG21	1:A:163:LEU:HG	1.91	0.53
1:C:467:ILE:HG21	3:C:602:TPP:S1	2.49	0.53
1:E:9:ALA:HB2	1:E:35:LEU:HD23	1.90	0.53
1:F:306:MET:HE2	1:F:323:LEU:CD1	2.38	0.53
1:W:150:VAL:HG21	1:W:163:LEU:HG	1.91	0.53
1:H:215:VAL:HG13	1:H:219:LEU:HD22	1.90	0.53
1:C:150:VAL:HG21	1:C:163:LEU:HG	1.89	0.53
1:E:388:PHE:HB3	1:E:536:THR:HG21	1.91	0.53
1:K:552[A]:ARG:NH1	5:K:701:HOH:O	2.42	0.53
1:H:467:ILE:HG21	3:H:602:TPP:S1	2.49	0.52
1:U:439:GLN:NE2	1:U:479:ILE:HD12	2.23	0.52
1:O:306:MET:HE2	1:O:323:LEU:CD1	2.40	0.52
1:R:467:ILE:HG21	3:R:602:TPP:S1	2.50	0.52
1:F:15:ILE:HD11	1:F:151:ILE:HG23	1.91	0.52
1:O:365:MET:HE1	1:O:460:ILE:HG12	1.92	0.52
1:K:306:MET:HE2	1:K:323:LEU:CD1	2.40	0.51
1:Q:306:MET:HE2	1:Q:323:LEU:CD1	2.40	0.51
1:U:218:LYS:HB2	1:U:283:ALA:HB1	1.92	0.51
1:X:552:ARG:NH1	5:X:702:HOH:O	2.44	0.51
1:N:218:LYS:HB2	1:N:283:ALA:HB1	1.92	0.51
1:J:306:MET:HE2	1:J:323:LEU:HD11	1.93	0.51
1:D:355[A]:GLU:CD	1:D:355[A]:GLU:H	2.17	0.51
1:U:306:MET:HE2	1:U:323:LEU:HD11	1.93	0.51
1:M:467:ILE:HG21	3:M:602:TPP:S1	2.50	0.51
1:E:467:ILE:HG21	3:E:602:TPP:S1	2.51	0.50
1:G:218:LYS:HB2	1:G:283:ALA:HB1	1.93	0.50
1:R:467:ILE:CG2	3:R:602:TPP:S1	3.00	0.50
1:T:306:MET:HE2	1:T:323:LEU:HD11	1.93	0.50
1:L:306:MET:HB3	1:L:323:LEU:HD13	1.93	0.50
1:F:218:LYS:HB2	1:F:283:ALA:HB1	1.93	0.50
1:M:467:ILE:CG2	3:M:602:TPP:S1	2.99	0.50
1:E:24:ALA:HB2	1:F:476:TYR:HB2	1.93	0.50
1:E:306:MET:HE3	1:E:326:PHE:HD2	1.75	0.50
1:P:467:ILE:CG2	3:P:602:TPP:S1	2.99	0.50
1:V:88:ALA:HB1	1:V:406:GLN:HG3	1.92	0.50
1:B:15:ILE:HD11	1:B:151:ILE:HG23	1.94	0.50
1:P:215:VAL:HG13	1:P:219:LEU:HD22	1.93	0.50
1:U:69:ILE:N	1:U:69:ILE:HD12	2.26	0.49
1:E:15:ILE:HD11	1:E:151:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:LYS:HB2	1:H:283:ALA:HB1	1.94	0.49
1:S:476:TYR:HB2	1:T:24:ALA:HB2	1.95	0.49
1:X:516:ALA:HB2	1:X:524:THR:HG21	1.94	0.49
1:M:306:MET:HE3	1:M:326:PHE:CD2	2.48	0.49
1:P:15:ILE:HD11	1:P:151:ILE:HG23	1.93	0.49
1:S:306:MET:HE3	1:S:326:PHE:CD2	2.47	0.49
1:J:467:ILE:HG21	3:J:602:TPP:S1	2.53	0.49
1:B:499:LEU:HD22	1:B:501:LEU:HD21	1.95	0.49
1:A:69:ILE:HD12	1:A:69:ILE:N	2.27	0.49
1:R:489[B]:ASP:OD1	1:R:489[B]:ASP:N	2.45	0.49
1:A:306:MET:HE2	1:A:323:LEU:CD1	2.42	0.49
1:M:15:ILE:HD11	1:M:151:ILE:HG23	1.95	0.49
1:O:467:ILE:CG2	3:O:602:TPP:S1	3.01	0.49
1:L:431:MET:HE2	1:L:457:ILE:HG23	1.95	0.48
1:Q:141[A]:GLU:CD	1:Q:141[A]:GLU:H	2.21	0.48
1:S:218:LYS:HB2	1:S:283:ALA:HB1	1.94	0.48
1:C:24:ALA:HB2	1:D:476:TYR:HB2	1.96	0.48
1:D:306:MET:HE2	1:D:323:LEU:HD11	1.95	0.48
1:E:289:TYR:OH	4:F:601:EDO:H22	2.14	0.48
1:J:189:VAL:HG11	1:J:325:THR:HG21	1.96	0.48
1:V:218:LYS:HB2	1:V:283:ALA:HB1	1.95	0.48
1:D:467:ILE:HG21	3:D:602:TPP:S1	2.54	0.48
1:I:215:VAL:HG13	1:I:219:LEU:HD22	1.94	0.47
1:L:215:VAL:HG13	1:L:219:LEU:HD22	1.94	0.47
1:C:467:ILE:CG2	3:C:602:TPP:S1	3.02	0.47
1:V:355[A]:GLU:H	1:V:355[A]:GLU:CD	2.11	0.47
1:G:69:ILE:N	1:G:69:ILE:HD12	2.30	0.47
1:H:467:ILE:CG2	3:H:602:TPP:S1	3.02	0.47
1:I:24:ALA:HB2	1:J:476:TYR:HB2	1.95	0.47
1:N:516:ALA:HB2	1:N:524:THR:HG21	1.96	0.47
1:K:218:LYS:HB2	1:K:283:ALA:HB1	1.96	0.47
1:E:222:ALA:HB2	1:E:308:THR:HG22	1.96	0.47
1:T:9:ALA:HB2	1:T:35:LEU:HD23	1.97	0.47
1:L:306:MET:HE3	1:L:326:PHE:CD2	2.49	0.47
1:L:218:LYS:HB2	1:L:283:ALA:HB1	1.97	0.46
1:N:306:MET:HE3	1:N:326:PHE:HD2	1.80	0.46
1:S:306:MET:HE3	1:S:326:PHE:HD2	1.80	0.46
1:V:69:ILE:N	1:V:69:ILE:HD12	2.31	0.46
1:B:306:MET:HB3	1:B:323:LEU:HD13	1.97	0.46
1:E:215:VAL:HG13	1:E:219:LEU:HD22	1.98	0.46
1:H:85:GLY:HA2	1:H:407:TRP:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:141[A]:GLU:CD	1:Q:141[A]:GLU:N	2.73	0.46
1:G:150:VAL:HG21	1:G:163:LEU:HG	1.98	0.46
1:H:15:ILE:HD11	1:H:151:ILE:HG23	1.96	0.46
1:J:306:MET:HE3	1:J:326:PHE:CD2	2.50	0.46
1:F:64:GLY:O	1:F:92:PRO:HG2	2.16	0.46
1:C:218:LYS:HB2	1:C:283:ALA:HB1	1.98	0.46
1:G:45:TYR:CE1	1:H:476:TYR:HB3	2.50	0.46
1:G:372:LEU:HB3	1:G:430[B]:ILE:HD11	1.97	0.46
1:N:306:MET:HE3	1:N:326:PHE:CD2	2.51	0.46
1:W:516:ALA:HB2	1:W:524:THR:HG21	1.98	0.46
1:A:222:ALA:HB2	1:A:308:THR:HG22	1.98	0.46
1:B:306:MET:HE2	1:B:323:LEU:HD11	1.97	0.46
1:E:388:PHE:CB	1:E:536:THR:HG21	2.45	0.46
1:F:349:LEU:HD11	1:F:351:ILE:HD12	1.98	0.46
1:E:467:ILE:CG2	3:E:602:TPP:S1	3.05	0.45
1:G:24:ALA:HB2	1:H:476:TYR:HB2	1.97	0.45
1:L:467:ILE:CG2	3:L:602:TPP:S1	3.04	0.45
1:R:127:VAL:HG11	1:R:162:TYR:CG	2.51	0.45
1:U:426[B]:GLU:CD	1:U:426[B]:GLU:H	2.23	0.45
1:X:218:LYS:HB2	1:X:283:ALA:HB1	1.97	0.45
1:J:215:VAL:HG13	1:J:219:LEU:HD22	1.99	0.45
1:K:15:ILE:HD11	1:K:151:ILE:HG23	1.98	0.45
1:S:306:MET:HB3	1:S:323:LEU:HD13	1.99	0.45
1:W:69:ILE:HD12	1:W:69:ILE:N	2.31	0.45
1:D:467:ILE:CG2	3:D:602:TPP:S1	3.05	0.45
1:M:431:MET:HE2	1:M:433:VAL:HB	1.99	0.45
1:U:466:VAL:HA	1:U:469:ILE:HD12	1.98	0.45
1:V:9:ALA:HB2	1:V:35:LEU:HD23	1.99	0.45
1:B:306:MET:HE3	1:B:326:PHE:HD2	1.82	0.45
1:G:306:MET:HB3	1:G:323:LEU:HD13	1.99	0.45
1:J:306:MET:HB3	1:J:323:LEU:HD13	1.99	0.45
1:D:306:MET:HE3	1:D:326:PHE:HD2	1.80	0.44
1:L:150:VAL:HG21	1:L:163:LEU:HG	2.00	0.44
1:O:467:ILE:HG21	3:O:602:TPP:S1	2.57	0.44
1:P:306:MET:HE3	1:P:326:PHE:CD2	2.51	0.44
1:V:143:ALA:HB3	1:V:144:PRO:HD3	1.99	0.44
1:X:467:ILE:HG21	3:X:602:TPP:S1	2.57	0.44
1:G:467:ILE:HG21	3:G:602:TPP:S1	2.58	0.44
1:M:476:TYR:HB2	1:N:24:ALA:HB2	1.99	0.44
1:V:330:LEU:O	1:V:334:ALA:HB2	2.18	0.44
1:W:29:LEU:HD13	1:X:472:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ALA:C	1:F:69:ILE:HD12	2.42	0.44
1:G:467:ILE:CG2	3:G:602:TPP:S1	3.05	0.44
1:C:15:ILE:O	1:C:15:ILE:HG22	2.17	0.44
1:F:306:MET:HE3	1:F:326:PHE:CD2	2.52	0.44
1:H:88:ALA:HB1	1:H:406:GLN:HG3	2.00	0.44
1:M:306:MET:HB3	1:M:323:LEU:HD13	2.00	0.44
1:U:467:ILE:HG21	3:U:602:TPP:S1	2.57	0.44
1:O:306:MET:HE3	1:O:326:PHE:CD2	2.53	0.44
1:Q:467:ILE:HG21	3:Q:602:TPP:S1	2.58	0.44
1:R:88:ALA:HB1	1:R:406:GLN:HG3	1.98	0.44
1:X:306:MET:HB3	1:X:323:LEU:HD13	1.98	0.44
1:M:24:ALA:HB2	1:N:476:TYR:HB2	1.99	0.44
1:E:85:GLY:HA2	1:E:407:TRP:CG	2.53	0.44
1:Q:476:TYR:HB2	1:R:24:ALA:HB2	1.98	0.44
1:U:288:ASP:HB3	1:U:294:TRP:CZ2	2.53	0.44
1:M:306:MET:HE3	1:M:326:PHE:HD2	1.82	0.43
1:O:476:TYR:HB2	1:P:24:ALA:HB2	2.00	0.43
1:T:467:ILE:CG2	3:T:602:TPP:S1	3.07	0.43
1:W:12:LEU:HA	1:W:15:ILE:HD12	2.00	0.43
1:W:476:TYR:HB2	1:X:24:ALA:HB2	2.00	0.43
1:E:180:ILE:HD12	1:E:180:ILE:O	2.18	0.43
1:D:325[A]:THR:HG23	5:D:806:HOH:O	2.18	0.43
1:K:69:ILE:HD12	1:K:69:ILE:N	2.33	0.43
1:U:189:VAL:HG13	1:U:321:LEU:HA	2.01	0.43
1:W:239:VAL:HG11	1:W:249:PHE:CE2	2.54	0.43
1:C:467:ILE:HG13	1:C:539:LEU:HD11	1.99	0.43
1:A:418:PHE:O	1:A:422:VAL:HG23	2.19	0.43
1:D:306:MET:HB3	1:D:323:LEU:HD13	2.01	0.43
1:X:453:ILE:HG22	1:X:455:VAL:HG23	2.00	0.43
1:A:476:TYR:HB2	1:B:24:ALA:HB2	2.01	0.43
1:B:73:SER:HB2	1:B:113:HIS:O	2.19	0.43
1:B:215:VAL:HG13	1:B:219:LEU:HD22	2.00	0.43
1:B:218:LYS:HB2	1:B:283:ALA:HB1	2.01	0.43
1:I:430:ILE:CD1	1:I:456:ILE:HD12	2.49	0.43
1:N:251:GLU:HG3	1:N:256:PHE:CE2	2.54	0.43
1:S:222:ALA:HB2	1:S:308:THR:HG22	1.99	0.43
1:T:127:VAL:HG11	1:T:162:TYR:CG	2.54	0.43
1:A:189:VAL:HG11	1:A:325:THR:HG21	2.01	0.43
1:B:180:ILE:HD12	1:B:180:ILE:O	2.19	0.43
1:G:306:MET:HE3	1:G:326:PHE:CD2	2.54	0.43
1:G:476:TYR:HB2	1:H:24:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:306:MET:HB3	1:P:323:LEU:HD13	2.00	0.43
1:F:215:VAL:HG13	1:F:219:LEU:HD22	2.01	0.42
1:L:222:ALA:HB2	1:L:308:THR:HG22	2.01	0.42
1:D:9:ALA:HB2	1:D:35:LEU:HD23	2.01	0.42
1:D:88:ALA:HB1	1:D:406:GLN:HG3	2.00	0.42
1:G:9:ALA:HB2	1:G:35:LEU:HD23	2.01	0.42
1:K:476:TYR:HB2	1:L:24:ALA:HB2	2.00	0.42
1:M:64:GLY:O	1:M:92:PRO:HG2	2.19	0.42
1:M:218:LYS:HB2	1:M:283:ALA:HB1	2.00	0.42
1:P:516:ALA:HB2	1:P:524:THR:HG21	2.01	0.42
1:C:288:ASP:HB3	1:C:294:TRP:CZ2	2.55	0.42
1:H:431:MET:HE2	1:H:433:VAL:CG1	2.49	0.42
1:A:29:LEU:HD13	1:B:472:HIS:HB3	2.00	0.42
1:L:467:ILE:HG21	3:L:602:TPP:S1	2.60	0.42
1:F:15:ILE:HD11	1:F:151:ILE:CG2	2.49	0.42
1:I:189:VAL:HG11	1:I:325[A]:THR:HG21	2.02	0.42
1:K:24:ALA:HB2	1:L:476:TYR:HB2	2.01	0.42
1:S:365:MET:HE1	1:S:460:ILE:HG12	2.01	0.42
1:N:99:SER:HB2	1:N:100:PRO:CD	2.50	0.42
1:Q:467:ILE:CG2	3:Q:602:TPP:S1	3.07	0.42
1:W:68:ALA:C	1:W:69:ILE:HD12	2.45	0.42
1:I:69:ILE:N	1:I:69:ILE:HD12	2.34	0.42
1:O:9:ALA:HB2	1:O:35:LEU:HD23	2.02	0.42
1:Q:306:MET:HE2	1:Q:323:LEU:HD11	2.00	0.42
1:W:467:ILE:HG21	3:W:602:TPP:S1	2.59	0.42
1:X:467:ILE:CG2	3:X:602:TPP:S1	3.08	0.42
1:C:15:ILE:HD11	1:C:151:ILE:HG23	2.02	0.42
1:N:85:GLY:HA2	1:N:407:TRP:CG	2.55	0.42
1:P:88:ALA:HB1	1:P:406:GLN:HG3	2.02	0.42
1:X:467:ILE:HG13	1:X:539:LEU:HD11	2.01	0.42
3:I:602:TPP:N1'	1:J:49:GLU:OE2	2.53	0.42
1:K:306:MET:HE2	1:K:323:LEU:HD11	2.02	0.42
1:O:29:LEU:HD13	1:P:472:HIS:HB3	2.02	0.42
1:R:15:ILE:O	1:R:15:ILE:HG22	2.19	0.42
1:W:460:ILE:N	1:W:460:ILE:HD12	2.35	0.42
1:E:467:ILE:HG22	3:E:602:TPP:O3B	2.20	0.41
1:E:481:ASN:ND2	1:F:493:ASP:OD2	2.51	0.41
1:N:64:GLY:O	1:N:92:PRO:HG2	2.20	0.41
1:E:476:TYR:HB2	1:F:24:ALA:HB2	2.01	0.41
1:X:88:ALA:HB1	1:X:406:GLN:HG3	2.02	0.41
3:G:602:TPP:N1'	1:H:49:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:239:VAL:HG11	1:H:249:PHE:CE1	2.56	0.41
1:I:180:ILE:HD12	1:I:180:ILE:O	2.20	0.41
1:K:15:ILE:HG22	1:K:15:ILE:O	2.18	0.41
1:D:218:LYS:HB2	1:D:283:ALA:HB1	2.03	0.41
1:M:15:ILE:HD11	1:M:151:ILE:CG2	2.51	0.41
1:M:306:MET:HE2	1:M:323:LEU:HD11	1.98	0.41
1:Q:45:TYR:CE1	1:R:476:TYR:HB3	2.56	0.41
1:S:306:MET:HE2	1:S:323:LEU:HD11	2.03	0.41
1:U:476:TYR:HB2	1:V:24:ALA:HB2	2.03	0.41
1:B:118:THR:HG21	1:D:142:GLU:OE1	2.20	0.41
1:F:467:ILE:CG2	3:F:603:TPP:S1	3.09	0.41
1:G:306:MET:HE2	1:G:323:LEU:HD11	2.01	0.41
1:M:516:ALA:HB2	1:M:524:THR:HG21	2.02	0.41
1:P:222:ALA:HB2	1:P:308:THR:HG22	2.02	0.41
1:T:306:MET:HE3	1:T:326:PHE:CD2	2.56	0.41
1:H:405[A]:MET:CE	5:H:839:HOH:O	2.69	0.41
1:Q:306:MET:HE3	1:Q:326:PHE:HD2	1.86	0.41
1:U:3:THR:HG23	1:U:6:MET:HE3	2.02	0.41
1:B:355[A]:GLU:CD	1:B:355[A]:GLU:H	2.29	0.41
1:I:306:MET:HB3	1:I:323:LEU:HD13	2.03	0.41
1:M:467:ILE:HG13	1:M:539:LEU:HD11	2.01	0.41
1:R:466:VAL:HA	1:R:469:ILE:HD12	2.03	0.41
1:C:306:MET:HE2	1:C:323:LEU:HD11	2.03	0.41
1:E:150:VAL:HG21	1:E:163:LEU:HG	2.02	0.41
1:E:365:MET:HE1	1:E:460:ILE:HG12	2.01	0.41
1:I:204:TRP:CD1	1:I:314:ALA:HB2	2.55	0.41
1:O:69:ILE:HD12	1:O:69:ILE:N	2.35	0.41
1:P:306:MET:HE3	1:P:326:PHE:HD2	1.86	0.41
1:A:187:LEU:HD23	1:D:187:LEU:HD23	2.02	0.41
1:G:234:ARG:HG2	1:G:331:ALA:O	2.21	0.41
1:I:467:ILE:HG21	3:I:602:TPP:S1	2.61	0.41
1:L:127:VAL:HG11	1:L:162:TYR:CG	2.56	0.41
1:L:204:TRP:CD1	1:L:314:ALA:HB2	2.55	0.41
1:L:414:VAL:HG22	1:L:431:MET:HE1	2.03	0.41
1:O:24:ALA:HB2	1:P:476:TYR:HB2	2.02	0.41
1:O:306:MET:HE3	1:O:326:PHE:HD2	1.85	0.41
1:P:306:MET:HE2	1:P:323:LEU:HD11	2.01	0.41
1:U:129:HIS:HB3	1:V:122:TYR:HB2	2.02	0.41
1:A:467:ILE:CG2	3:A:602:TPP:S1	3.09	0.41
1:G:215:VAL:HB	1:G:241:ILE:HG22	2.03	0.41
1:J:88:ALA:HB1	1:J:406:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG21	1:C:142:GLU:OE1	2.21	0.40
1:T:467:ILE:HG13	1:T:539:LEU:HD11	2.02	0.40
1:B:306:MET:HE3	1:B:326:PHE:CD2	2.56	0.40
1:C:45:TYR:CE1	1:D:476:TYR:HB3	2.56	0.40
1:F:460:ILE:HD12	1:F:460:ILE:N	2.37	0.40
1:G:12:LEU:HA	1:G:15:ILE:HD12	2.03	0.40
1:H:15:ILE:HD11	1:H:151:ILE:CG2	2.51	0.40
1:K:180:ILE:C	1:K:180:ILE:HD12	2.46	0.40
1:O:218:LYS:HB2	1:O:283:ALA:HB1	2.03	0.40
1:R:306:MET:HE3	1:R:326:PHE:CD2	2.56	0.40
1:U:426[A]:GLU:OE1	1:U:426[A]:GLU:HA	2.20	0.40
1:C:127:VAL:HG11	1:C:162:TYR:CG	2.56	0.40
1:J:516:ALA:HB2	1:J:524:THR:HG21	2.04	0.40
1:Q:332:GLU:CD	5:Q:786:HOH:O	2.64	0.40
1:T:85:GLY:HA2	1:T:407:TRP:CG	2.56	0.40
1:U:252:ASP:O	1:U:253:HIS:C	2.64	0.40
1:I:88:ALA:HB1	1:I:406:GLN:HG3	2.04	0.40
1:H:28:ASN:OD1	1:H:28:ASN:C	2.65	0.40
1:J:467:ILE:HG13	1:J:539:LEU:HD11	2.04	0.40
1:K:85:GLY:HA2	1:K:407:TRP:CG	2.56	0.40
1:M:45:TYR:CE1	1:N:476:TYR:HB3	2.56	0.40
1:Q:69:ILE:N	1:Q:69:ILE:HD12	2.36	0.40
1:X:150:VAL:HG21	1:X:163:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	558/573 (97%)	551 (99%)	7 (1%)	0	100	100
1	B	557/573 (97%)	547 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	D	558/573 (97%)	548 (98%)	10 (2%)	0	100	100
1	E	557/573 (97%)	550 (99%)	7 (1%)	0	100	100
1	F	562/573 (98%)	552 (98%)	10 (2%)	0	100	100
1	G	560/573 (98%)	552 (99%)	7 (1%)	1 (0%)	43	44
1	H	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	I	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	J	557/573 (97%)	546 (98%)	10 (2%)	1 (0%)	43	44
1	K	560/573 (98%)	554 (99%)	5 (1%)	1 (0%)	43	44
1	L	562/573 (98%)	550 (98%)	12 (2%)	0	100	100
1	M	560/573 (98%)	548 (98%)	11 (2%)	1 (0%)	43	44
1	N	560/573 (98%)	554 (99%)	6 (1%)	0	100	100
1	O	556/573 (97%)	546 (98%)	9 (2%)	1 (0%)	43	44
1	P	560/573 (98%)	549 (98%)	11 (2%)	0	100	100
1	Q	558/573 (97%)	547 (98%)	11 (2%)	0	100	100
1	R	561/573 (98%)	553 (99%)	8 (1%)	0	100	100
1	S	555/573 (97%)	545 (98%)	10 (2%)	0	100	100
1	T	557/573 (97%)	548 (98%)	9 (2%)	0	100	100
1	U	557/573 (97%)	536 (96%)	21 (4%)	0	100	100
1	V	557/573 (97%)	536 (96%)	21 (4%)	0	100	100
1	W	556/573 (97%)	537 (97%)	19 (3%)	0	100	100
1	X	556/573 (97%)	545 (98%)	11 (2%)	0	100	100
All	All	13401/13752 (97%)	13141 (98%)	255 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	73	SER
1	K	73	SER
1	O	73	SER
1	M	73	SER
1	G	73	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/448 (98%)	423 (96%)	17 (4%)	28	28
1	B	439/448 (98%)	428 (98%)	11 (2%)	42	45
1	C	441/448 (98%)	431 (98%)	10 (2%)	44	49
1	D	440/448 (98%)	429 (98%)	11 (2%)	42	45
1	E	439/448 (98%)	429 (98%)	10 (2%)	44	49
1	F	444/448 (99%)	431 (97%)	13 (3%)	37	39
1	G	442/448 (99%)	432 (98%)	10 (2%)	44	49
1	H	441/448 (98%)	426 (97%)	15 (3%)	32	33
1	I	441/448 (98%)	431 (98%)	10 (2%)	44	49
1	J	439/448 (98%)	431 (98%)	8 (2%)	51	58
1	K	442/448 (99%)	427 (97%)	15 (3%)	32	33
1	L	444/448 (99%)	431 (97%)	13 (3%)	37	39
1	M	442/448 (99%)	430 (97%)	12 (3%)	39	41
1	N	442/448 (99%)	431 (98%)	11 (2%)	42	45
1	O	438/448 (98%)	426 (97%)	12 (3%)	39	41
1	P	442/448 (99%)	429 (97%)	13 (3%)	37	39
1	Q	440/448 (98%)	428 (97%)	12 (3%)	39	41
1	R	443/448 (99%)	428 (97%)	15 (3%)	32	33
1	S	437/448 (98%)	426 (98%)	11 (2%)	42	45
1	T	439/448 (98%)	427 (97%)	12 (3%)	39	41
1	U	439/448 (98%)	420 (96%)	19 (4%)	26	24
1	V	439/448 (98%)	428 (98%)	11 (2%)	42	45
1	W	438/448 (98%)	426 (97%)	12 (3%)	39	41
1	X	438/448 (98%)	429 (98%)	9 (2%)	47	52
All	All	10569/10752 (98%)	10277 (97%)	292 (3%)	40	40

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	LYS
1	A	183	LEU
1	A	207	ASP
1	A	271	GLU
1	A	272	LEU
1	A	319	GLU
1	A	332	GLU
1	A	379	LEU
1	A	391[A]	SER
1	A	391[B]	SER
1	A	444	GLU
1	A	459	LEU
1	A	499	LEU
1	A	517	LEU
1	A	552[A]	ARG
1	A	552[B]	ARG
1	B	234	ARG
1	B	272	LEU
1	B	311	VAL
1	B	355[A]	GLU
1	B	355[B]	GLU
1	B	376	ASP
1	B	379	LEU
1	B	431	MET
1	B	459	LEU
1	B	499	LEU
1	B	517	LEU
1	C	183	LEU
1	C	271	GLU
1	C	272	LEU
1	C	301	ASP
1	C	319	GLU
1	C	345	GLN
1	C	379	LEU
1	C	489	ASP
1	C	517	LEU
1	C	552	ARG
1	D	183	LEU
1	D	271	GLU
1	D	272	LEU
1	D	319	GLU
1	D	332	GLU

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Mol	Chain	Res	Type
1	D	345	GLN
1	D	379	LEU
1	D	459	LEU
1	D	495	ASP
1	D	504	SER
1	D	517	LEU
1	E	183	LEU
1	E	271	GLU
1	E	272	LEU
1	E	319	GLU
1	E	332	GLU
1	E	379	LEU
1	E	459	LEU
1	E	499	LEU
1	E	517	LEU
1	E	536	THR
1	F	39	LYS
1	F	73	SER
1	F	121	ASN
1	F	183	LEU
1	F	271	GLU
1	F	272	LEU
1	F	379	LEU
1	F	400	ARG
1	F	459	LEU
1	F	494	GLU
1	F	517	LEU
1	F	552[A]	ARG
1	F	552[B]	ARG
1	G	183	LEU
1	G	271	GLU
1	G	272	LEU
1	G	311	VAL
1	G	332	GLU
1	G	379	LEU
1	G	444	GLU
1	G	495	ASP
1	G	499	LEU
1	G	517	LEU
1	H	183	LEU
1	H	271	GLU
1	H	272	LEU

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Mol	Chain	Res	Type
1	H	292	VAL
1	H	311	VAL
1	H	319	GLU
1	H	321	LEU
1	H	332	GLU
1	H	352	GLU
1	H	379	LEU
1	H	391[A]	SER
1	H	391[B]	SER
1	H	495[A]	ASP
1	H	495[B]	ASP
1	H	517	LEU
1	I	121[A]	ASN
1	I	121[B]	ASN
1	I	183	LEU
1	I	272	LEU
1	I	311	VAL
1	I	319	GLU
1	I	379	LEU
1	I	400	ARG
1	I	517	LEU
1	I	552	ARG
1	J	1	MET
1	J	183	LEU
1	J	271	GLU
1	J	272	LEU
1	J	299	LYS
1	J	379	LEU
1	J	459	LEU
1	J	517	LEU
1	K	181	ASN
1	K	183	LEU
1	K	271	GLU
1	K	272	LEU
1	K	311	VAL
1	K	319	GLU
1	K	333	LYS
1	K	379	LEU
1	K	391[A]	SER
1	K	391[B]	SER
1	K	400	ARG
1	K	499	LEU

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Mol	Chain	Res	Type
1	K	517	LEU
1	K	552[A]	ARG
1	K	552[B]	ARG
1	L	39	LYS
1	L	183	LEU
1	L	226	LYS
1	L	271	GLU
1	L	272	LEU
1	L	319	GLU
1	L	379	LEU
1	L	400	ARG
1	L	459	LEU
1	L	499	LEU
1	L	517	LEU
1	L	552[A]	ARG
1	L	552[B]	ARG
1	M	1	MET
1	M	181	ASN
1	M	272	LEU
1	M	311	VAL
1	M	332	GLU
1	M	379	LEU
1	M	431	MET
1	M	444	GLU
1	M	459	LEU
1	M	489	ASP
1	M	517	LEU
1	M	553	LYS
1	N	39	LYS
1	N	183	LEU
1	N	271	GLU
1	N	272	LEU
1	N	311	VAL
1	N	319	GLU
1	N	332	GLU
1	N	379	LEU
1	N	444	GLU
1	N	499	LEU
1	N	517	LEU
1	O	17	LEU
1	O	18	LYS
1	O	173	GLU

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Mol	Chain	Res	Type
1	O	183	LEU
1	O	271	GLU
1	O	272	LEU
1	O	311	VAL
1	O	319	GLU
1	O	379	LEU
1	O	400	ARG
1	O	459	LEU
1	O	517	LEU
1	P	183	LEU
1	P	272	LEU
1	P	319	GLU
1	P	345	GLN
1	P	379	LEU
1	P	391[A]	SER
1	P	391[B]	SER
1	P	431	MET
1	P	444	GLU
1	P	459	LEU
1	P	499	LEU
1	P	517	LEU
1	P	537	GLU
1	Q	18	LYS
1	Q	42[A]	GLU
1	Q	42[B]	GLU
1	Q	73	SER
1	Q	163	LEU
1	Q	183	LEU
1	Q	319	GLU
1	Q	332	GLU
1	Q	379	LEU
1	Q	400	ARG
1	Q	431	MET
1	Q	517	LEU
1	R	121[A]	ASN
1	R	121[B]	ASN
1	R	173	GLU
1	R	183	LEU
1	R	272	LEU
1	R	311	VAL
1	R	319	GLU
1	R	379	LEU

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Mol	Chain	Res	Type
1	R	400	ARG
1	R	459	LEU
1	R	499	LEU
1	R	517	LEU
1	R	520	ARG
1	R	552	ARG
1	R	555	GLN
1	S	121	ASN
1	S	226	LYS
1	S	271	GLU
1	S	272	LEU
1	S	311	VAL
1	S	332	GLU
1	S	379	LEU
1	S	391[A]	SER
1	S	391[B]	SER
1	S	459	LEU
1	S	517	LEU
1	T	271	GLU
1	T	272	LEU
1	T	311	VAL
1	T	319	GLU
1	T	379	LEU
1	T	391[A]	SER
1	T	391[B]	SER
1	T	400	ARG
1	T	459	LEU
1	T	489	ASP
1	T	499	LEU
1	T	517	LEU
1	U	78	SER
1	U	121	ASN
1	U	212	VAL
1	U	271	GLU
1	U	272	LEU
1	U	299	LYS
1	U	302	ASN
1	U	319	GLU
1	U	332	GLU
1	U	355[A]	GLU
1	U	355[B]	GLU
1	U	365	MET

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Mol	Chain	Res	Type
1	U	369	ILE
1	U	379	LEU
1	U	444	GLU
1	U	459	LEU
1	U	504	SER
1	U	521	ARG
1	U	552	ARG
1	V	121	ASN
1	V	183	LEU
1	V	272	LEU
1	V	332	GLU
1	V	379	LEU
1	V	391[A]	SER
1	V	391[B]	SER
1	V	499	LEU
1	V	515	LYS
1	V	517	LEU
1	V	552	ARG
1	W	121	ASN
1	W	259	LEU
1	W	271	GLU
1	W	311	VAL
1	W	376	ASP
1	W	391[A]	SER
1	W	391[B]	SER
1	W	494	GLU
1	W	499	LEU
1	W	517	LEU
1	W	544	LYS
1	W	552	ARG
1	X	183	LEU
1	X	226	LYS
1	X	234	ARG
1	X	332	GLU
1	X	379	LEU
1	X	391[A]	SER
1	X	391[B]	SER
1	X	459	LEU
1	X	552	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	B	34	GLN
1	B	38	ASN
1	B	81	ASN
1	B	103	ASN
1	B	270	GLN
1	B	532	GLN
1	C	34	GLN
1	C	103	ASN
1	C	270	GLN
1	C	461	ASN
1	C	481	ASN
1	C	555	GLN
1	D	43	GLN
1	D	121	ASN
1	D	461	ASN
1	D	481	ASN
1	D	532	GLN
1	E	43	GLN
1	E	121	ASN
1	E	461	ASN
1	E	481	ASN
1	F	81	ASN
1	F	121	ASN
1	F	461	ASN
1	F	481	ASN
1	G	20	HIS
1	G	43	GLN
1	G	532	GLN
1	H	497	HIS
1	H	532	GLN
1	I	34	GLN
1	I	461	ASN
1	I	481	ASN
1	I	532	GLN
1	J	181	ASN
1	J	295	ASN
1	J	461	ASN
1	J	481	ASN
1	K	43	GLN
1	K	81	ASN
1	K	497	HIS
1	K	532	GLN

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Mol	Chain	Res	Type
1	K	555	GLN
1	L	43	GLN
1	L	81	ASN
1	L	121	ASN
1	M	81	ASN
1	M	181	ASN
1	M	316	GLN
1	M	555	GLN
1	O	43	GLN
1	O	81	ASN
1	O	295	ASN
1	O	461	ASN
1	O	497	HIS
1	O	532	GLN
1	Q	43	GLN
1	R	34	GLN
1	R	295	ASN
1	S	34	GLN
1	S	43	GLN
1	S	81	ASN
1	S	121	ASN
1	S	210	ASN
1	S	497	HIS
1	T	38	ASN
1	T	532	GLN
1	U	34	GLN
1	U	43	GLN
1	U	121	ASN
1	U	316	GLN
1	U	362	ASN
1	U	389	ASN
1	U	439	GLN
1	V	34	GLN
1	V	43	GLN
1	V	81	ASN
1	V	121	ASN
1	V	295	ASN
1	V	439	GLN
1	W	34	GLN
1	W	38	ASN
1	W	121	ASN
1	W	210	ASN

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Mol	Chain	Res	Type
1	W	295	ASN
1	W	443	GLN
1	X	121	ASN
1	X	295	ASN
1	X	302	ASN
1	X	439	GLN
1	X	443	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 54 ligands modelled in this entry, 24 are monoatomic - leaving 30 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
3	TPP	E	602	2	26,27,27	1.84	4 (15%)	38,40,40	3.03	9 (23%)
3	TPP	Q	602	2	26,27,27	1.81	4 (15%)	38,40,40	2.36	9 (23%)
4	EDO	Q	603	-	3,3,3	0.45	0	2,2,2	0.10	0
4	EDO	R	603	-	3,3,3	0.54	0	2,2,2	0.06	0
3	TPP	A	602	2	26,27,27	1.84	4 (15%)	38,40,40	2.30	12 (31%)
3	TPP	S	602	2	26,27,27	1.95	4 (15%)	38,40,40	2.41	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	I	603	-	3,3,3	0.50	0	2,2,2	0.22	0
3	TPP	P	602	2	26,27,27	1.76	4 (15%)	38,40,40	2.31	8 (21%)
3	TPP	R	602	2	26,27,27	1.86	5 (19%)	38,40,40	2.53	9 (23%)
3	TPP	H	602	2	26,27,27	1.82	4 (15%)	38,40,40	2.58	10 (26%)
3	TPP	X	602	2	26,27,27	1.85	4 (15%)	38,40,40	2.41	11 (28%)
3	TPP	B	602	2	26,27,27	1.79	4 (15%)	38,40,40	2.28	7 (18%)
3	TPP	T	602	2	26,27,27	1.85	4 (15%)	38,40,40	2.19	8 (21%)
3	TPP	J	602	2	26,27,27	1.72	4 (15%)	38,40,40	2.61	10 (26%)
3	TPP	G	602	2	26,27,27	1.71	4 (15%)	38,40,40	2.36	7 (18%)
3	TPP	K	602	2	26,27,27	1.88	5 (19%)	38,40,40	2.16	7 (18%)
3	TPP	F	603	2	26,27,27	1.88	5 (19%)	38,40,40	2.62	10 (26%)
3	TPP	V	602	2	26,27,27	1.80	3 (11%)	38,40,40	2.03	7 (18%)
3	TPP	L	602	2	26,27,27	1.84	4 (15%)	38,40,40	2.16	7 (18%)
3	TPP	O	602	2	26,27,27	1.74	4 (15%)	38,40,40	2.13	8 (21%)
3	TPP	I	602	2	26,27,27	1.84	4 (15%)	38,40,40	2.85	9 (23%)
3	TPP	W	602	2	26,27,27	1.77	3 (11%)	38,40,40	2.25	9 (23%)
3	TPP	C	602	2	26,27,27	1.77	5 (19%)	38,40,40	2.28	9 (23%)
3	TPP	U	602	2	26,27,27	1.75	3 (11%)	38,40,40	2.18	10 (26%)
4	EDO	A	603	-	3,3,3	0.57	0	2,2,2	0.21	0
4	EDO	F	601	-	3,3,3	0.45	0	2,2,2	0.25	0
3	TPP	D	602	2	26,27,27	1.85	5 (19%)	38,40,40	2.59	11 (28%)
3	TPP	M	602	2	26,27,27	1.92	4 (15%)	38,40,40	2.66	9 (23%)
4	EDO	N	603	-	3,3,3	0.45	0	2,2,2	0.37	0
3	TPP	N	602	2	26,27,27	1.92	5 (19%)	38,40,40	3.12	10 (26%)

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
3	TPP	E	602	2	-	1/17/17/17	0/2/2/2
3	TPP	Q	602	2	-	2/17/17/17	0/2/2/2
4	EDO	Q	603	-	-	1/1/1/1	-
4	EDO	R	603	-	-	1/1/1/1	-
3	TPP	A	602	2	-	4/17/17/17	0/2/2/2
3	TPP	S	602	2	-	0/17/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	I	603	-	-	0/1/1/1	-
3	TPP	P	602	2	-	2/17/17/17	0/2/2/2
3	TPP	R	602	2	-	0/17/17/17	0/2/2/2
3	TPP	H	602	2	-	2/17/17/17	0/2/2/2
3	TPP	X	602	2	-	0/17/17/17	0/2/2/2
3	TPP	B	602	2	-	0/17/17/17	0/2/2/2
3	TPP	T	602	2	-	1/17/17/17	0/2/2/2
3	TPP	J	602	2	-	0/17/17/17	0/2/2/2
3	TPP	G	602	2	-	0/17/17/17	0/2/2/2
3	TPP	K	602	2	-	0/17/17/17	0/2/2/2
3	TPP	F	603	2	-	0/17/17/17	0/2/2/2
3	TPP	V	602	2	-	1/17/17/17	0/2/2/2
3	TPP	L	602	2	-	4/17/17/17	0/2/2/2
3	TPP	O	602	2	-	0/17/17/17	0/2/2/2
3	TPP	I	602	2	-	0/17/17/17	0/2/2/2
3	TPP	W	602	2	-	0/17/17/17	0/2/2/2
3	TPP	C	602	2	-	0/17/17/17	0/2/2/2
3	TPP	U	602	2	-	2/17/17/17	0/2/2/2
4	EDO	A	603	-	-	1/1/1/1	-
4	EDO	F	601	-	-	1/1/1/1	-
3	TPP	D	602	2	-	4/17/17/17	0/2/2/2
3	TPP	M	602	2	-	0/17/17/17	0/2/2/2
4	EDO	N	603	-	-	1/1/1/1	-
3	TPP	N	602	2	-	0/17/17/17	0/2/2/2

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	602	TPP	C5-C4	7.26	1.50	1.35
3	S	602	TPP	C5-C4	7.25	1.50	1.35
3	B	602	TPP	C5-C4	7.08	1.50	1.35
3	L	602	TPP	C5-C4	7.08	1.50	1.35
3	I	602	TPP	C5-C4	7.02	1.50	1.35
3	U	602	TPP	C5-C4	6.93	1.49	1.35
3	V	602	TPP	C5-C4	6.92	1.49	1.35
3	P	602	TPP	C5-C4	6.90	1.49	1.35
3	A	602	TPP	C5-C4	6.88	1.49	1.35
3	T	602	TPP	C5-C4	6.88	1.49	1.35
3	K	602	TPP	C5-C4	6.88	1.49	1.35
3	H	602	TPP	C5-C4	6.83	1.49	1.35
3	M	602	TPP	C5-C4	6.81	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	602	TPP	C5-C4	6.81	1.49	1.35
3	N	602	TPP	C5-C4	6.79	1.49	1.35
3	E	602	TPP	C5-C4	6.78	1.49	1.35
3	D	602	TPP	C5-C4	6.77	1.49	1.35
3	W	602	TPP	C5-C4	6.71	1.49	1.35
3	C	602	TPP	C5-C4	6.71	1.49	1.35
3	F	603	TPP	C5-C4	6.62	1.49	1.35
3	O	602	TPP	C5-C4	6.57	1.49	1.35
3	R	602	TPP	C5-C4	6.54	1.49	1.35
3	G	602	TPP	C5-C4	6.54	1.49	1.35
3	J	602	TPP	C5-C4	6.23	1.48	1.35
3	M	602	TPP	C5'-C4'	4.50	1.50	1.42
3	A	602	TPP	C5'-C4'	4.29	1.49	1.42
3	K	602	TPP	C5'-C4'	4.13	1.49	1.42
3	F	603	TPP	C5'-C4'	4.11	1.49	1.42
3	X	602	TPP	C5'-C4'	4.07	1.49	1.42
3	T	602	TPP	C5'-C4'	4.03	1.49	1.42
3	R	602	TPP	C5'-C4'	4.00	1.49	1.42
3	W	602	TPP	C5'-C4'	4.00	1.49	1.42
3	S	602	TPP	C5'-C4'	4.00	1.49	1.42
3	D	602	TPP	C5'-C4'	3.97	1.49	1.42
3	N	602	TPP	C5'-C4'	3.93	1.49	1.42
3	O	602	TPP	C5'-C4'	3.93	1.49	1.42
3	V	602	TPP	C5'-C4'	3.86	1.49	1.42
3	I	602	TPP	C5'-C4'	3.79	1.49	1.42
3	L	602	TPP	C5'-C4'	3.77	1.49	1.42
3	J	602	TPP	C5'-C4'	3.76	1.49	1.42
3	B	602	TPP	C5'-C4'	3.69	1.48	1.42
3	U	602	TPP	C5'-C4'	3.64	1.48	1.42
3	G	602	TPP	C5'-C4'	3.58	1.48	1.42
3	Q	602	TPP	C5'-C4'	3.58	1.48	1.42
3	H	602	TPP	C5'-C4'	3.42	1.48	1.42
3	E	602	TPP	C5'-C4'	3.35	1.48	1.42
3	C	602	TPP	C5'-C4'	3.35	1.48	1.42
3	P	602	TPP	C5'-C4'	3.23	1.48	1.42
3	E	602	TPP	C4-N3	-3.02	1.33	1.39
3	N	602	TPP	C4-N3	-2.92	1.33	1.39
3	M	602	TPP	C4-N3	-2.75	1.34	1.39
3	R	602	TPP	C4-N3	-2.67	1.34	1.39
3	R	602	TPP	PA-O3A	2.66	1.62	1.59
3	H	602	TPP	C4-N3	-2.63	1.34	1.39
3	N	602	TPP	C2-S1	2.61	1.77	1.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	602	TPP	C4-N3	-2.60	1.34	1.39
3	I	602	TPP	C4-N3	-2.57	1.34	1.39
3	P	602	TPP	C4-N3	-2.52	1.34	1.39
3	C	602	TPP	C4-N3	-2.49	1.34	1.39
3	D	602	TPP	C4-N3	-2.49	1.34	1.39
3	L	602	TPP	C2-S1	2.49	1.76	1.69
3	F	603	TPP	C4-N3	-2.48	1.34	1.39
3	D	602	TPP	C2-S1	2.47	1.76	1.69
3	Q	602	TPP	C4-N3	-2.46	1.34	1.39
3	H	602	TPP	C2-S1	2.43	1.76	1.69
3	G	602	TPP	C4-N3	-2.43	1.34	1.39
3	T	602	TPP	C4-N3	-2.43	1.34	1.39
3	M	602	TPP	C2-S1	2.38	1.76	1.69
3	L	602	TPP	C4-N3	-2.35	1.35	1.39
3	F	603	TPP	PA-O3A	2.35	1.62	1.59
3	E	602	TPP	PA-O3A	2.34	1.62	1.59
3	S	602	TPP	C2-S1	2.33	1.76	1.69
3	Q	602	TPP	C2-S1	2.33	1.76	1.69
3	K	602	TPP	PA-O3A	2.31	1.62	1.59
3	W	602	TPP	PA-O3A	2.31	1.62	1.59
3	O	602	TPP	C2-S1	2.30	1.76	1.69
3	X	602	TPP	C2-S1	2.29	1.76	1.69
3	C	602	TPP	C2-S1	2.28	1.76	1.69
3	N	602	TPP	PB-O2B	-2.24	1.46	1.54
3	K	602	TPP	C2-S1	2.24	1.76	1.69
3	I	602	TPP	C2-S1	2.21	1.75	1.69
3	F	603	TPP	C2-S1	2.21	1.75	1.69
3	A	602	TPP	C2-S1	2.21	1.75	1.69
3	O	602	TPP	C4-N3	-2.20	1.35	1.39
3	S	602	TPP	C4-N3	-2.20	1.35	1.39
3	P	602	TPP	C2-S1	2.19	1.75	1.69
3	G	602	TPP	C2-S1	2.17	1.75	1.69
3	B	602	TPP	C4-N3	-2.16	1.35	1.39
3	B	602	TPP	C2-S1	2.15	1.75	1.69
3	V	602	TPP	C4-N3	-2.14	1.35	1.39
3	X	602	TPP	C4-N3	-2.13	1.35	1.39
3	T	602	TPP	C2-S1	2.12	1.75	1.69
3	A	602	TPP	PA-O3A	2.10	1.61	1.59
3	J	602	TPP	C2-S1	2.09	1.75	1.69
3	R	602	TPP	C2-S1	2.08	1.75	1.69
3	C	602	TPP	C2-N3	2.06	1.37	1.32
3	K	602	TPP	C4-N3	-2.06	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	602	TPP	C4-N3	-2.03	1.35	1.39
3	D	602	TPP	C2-N3	2.02	1.37	1.32

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	602	TPP	C2-S1-C5	-14.32	81.73	91.22
3	E	602	TPP	C2-S1-C5	-13.79	82.08	91.22
3	I	602	TPP	C2-S1-C5	-12.52	82.92	91.22
3	F	603	TPP	C2-S1-C5	-11.74	83.44	91.22
3	M	602	TPP	C2-S1-C5	-11.70	83.47	91.22
3	H	602	TPP	C2-S1-C5	-11.54	83.57	91.22
3	J	602	TPP	C2-S1-C5	-11.39	83.67	91.22
3	D	602	TPP	C2-S1-C5	-11.27	83.75	91.22
3	R	602	TPP	C2-S1-C5	-10.92	83.98	91.22
3	G	602	TPP	C2-S1-C5	-10.08	84.54	91.22
3	P	602	TPP	C2-S1-C5	-9.83	84.70	91.22
3	X	602	TPP	C2-S1-C5	-9.77	84.74	91.22
3	S	602	TPP	C2-S1-C5	-9.74	84.77	91.22
3	C	602	TPP	C2-S1-C5	-9.68	84.80	91.22
3	Q	602	TPP	C2-S1-C5	-9.63	84.84	91.22
3	B	602	TPP	C2-S1-C5	-9.45	84.96	91.22
3	A	602	TPP	C2-S1-C5	-9.06	85.22	91.22
3	O	602	TPP	C2-S1-C5	-9.04	85.23	91.22
3	T	602	TPP	C2-S1-C5	-8.79	85.39	91.22
3	L	602	TPP	C2-S1-C5	-8.73	85.43	91.22
3	K	602	TPP	C2-S1-C5	-8.60	85.52	91.22
3	E	602	TPP	S1-C2-N3	8.37	122.89	112.30
3	W	602	TPP	C2-S1-C5	-8.37	85.67	91.22
3	U	602	TPP	C2-S1-C5	-8.17	85.81	91.22
3	N	602	TPP	S1-C2-N3	8.04	122.47	112.30
3	I	602	TPP	S1-C2-N3	7.62	121.94	112.30
3	V	602	TPP	C2-S1-C5	-7.55	86.21	91.22
3	M	602	TPP	S1-C2-N3	6.72	120.81	112.30
3	F	603	TPP	S1-C2-N3	6.54	120.58	112.30
3	D	602	TPP	S1-C2-N3	6.47	120.49	112.30
3	H	602	TPP	S1-C2-N3	6.31	120.28	112.30
3	Q	602	TPP	S1-C2-N3	6.20	120.14	112.30
3	J	602	TPP	S1-C2-N3	6.19	120.14	112.30
3	S	602	TPP	S1-C2-N3	6.19	120.13	112.30
3	R	602	TPP	S1-C2-N3	6.17	120.10	112.30
3	A	602	TPP	S1-C2-N3	5.87	119.73	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TPP	S1-C2-N3	5.79	119.63	112.30
3	X	602	TPP	S1-C2-N3	5.65	119.45	112.30
3	G	602	TPP	S1-C2-N3	5.65	119.45	112.30
3	P	602	TPP	S1-C2-N3	5.63	119.42	112.30
3	C	602	TPP	S1-C2-N3	5.45	119.20	112.30
3	T	602	TPP	S1-C2-N3	5.45	119.20	112.30
3	K	602	TPP	S1-C2-N3	5.44	119.18	112.30
3	W	602	TPP	S1-C2-N3	5.37	119.09	112.30
3	L	602	TPP	S1-C2-N3	5.34	119.06	112.30
3	O	602	TPP	S1-C2-N3	5.26	118.96	112.30
3	U	602	TPP	S1-C2-N3	5.26	118.95	112.30
3	V	602	TPP	S1-C2-N3	4.66	118.20	112.30
3	C	602	TPP	C6'-N1'-C2'	4.26	123.07	116.07
3	D	602	TPP	C6'-N1'-C2'	4.09	122.79	116.07
3	E	602	TPP	C6'-N1'-C2'	4.07	122.77	116.07
3	S	602	TPP	CM2-C2'-N1'	4.07	121.53	117.20
3	F	603	TPP	C6'-N1'-C2'	4.02	122.67	116.07
3	J	602	TPP	C6'-N1'-C2'	4.00	122.64	116.07
3	V	602	TPP	C6'-N1'-C2'	3.98	122.60	116.07
3	U	602	TPP	C6'-N1'-C2'	3.97	122.60	116.07
3	R	602	TPP	C6'-N1'-C2'	3.97	122.59	116.07
3	T	602	TPP	C6'-N1'-C2'	3.97	122.59	116.07
3	K	602	TPP	C6'-N1'-C2'	3.94	122.55	116.07
3	W	602	TPP	C6'-N1'-C2'	3.90	122.48	116.07
3	A	602	TPP	C6'-N1'-C2'	3.84	122.38	116.07
3	I	602	TPP	C6'-N1'-C2'	3.83	122.37	116.07
3	P	602	TPP	C6'-N1'-C2'	3.83	122.36	116.07
3	X	602	TPP	C6'-N1'-C2'	3.77	122.27	116.07
3	O	602	TPP	C6'-N1'-C2'	3.77	122.26	116.07
3	X	602	TPP	CM2-C2'-N1'	3.74	121.18	117.20
3	E	602	TPP	C2-N3-C4	-3.72	109.03	114.06
3	B	602	TPP	C6'-N1'-C2'	3.70	122.15	116.07
3	Q	602	TPP	C6'-N1'-C2'	3.67	122.10	116.07
3	M	602	TPP	C6'-N1'-C2'	3.58	121.95	116.07
3	L	602	TPP	C6'-N1'-C2'	3.56	121.92	116.07
3	N	602	TPP	C4-C5-S1	3.53	116.07	110.56
3	S	602	TPP	C6'-N1'-C2'	3.52	121.86	116.07
3	N	602	TPP	C6'-N1'-C2'	3.49	121.81	116.07
3	G	602	TPP	C6'-N1'-C2'	3.48	121.79	116.07
3	T	602	TPP	CM2-C2'-N1'	3.37	120.79	117.20
3	C	602	TPP	N1'-C2'-N3'	-3.30	120.04	125.53
3	N	602	TPP	C2-N3-C4	-3.28	109.63	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	TPP	C6'-N1'-C2'	3.26	121.42	116.07
3	U	602	TPP	C6-C5-S1	-3.25	113.29	120.90
3	I	602	TPP	CM2-C2'-N1'	3.24	120.65	117.20
3	I	602	TPP	C2-N3-C4	-3.23	109.69	114.06
3	E	602	TPP	C4-C5-S1	3.22	115.59	110.56
3	N	602	TPP	CM2-C2'-N1'	3.19	120.60	117.20
3	I	602	TPP	C6-C5-S1	-3.19	113.44	120.90
3	V	602	TPP	CM2-C2'-N1'	3.11	120.52	117.20
3	K	602	TPP	N1'-C2'-N3'	-3.10	120.37	125.53
3	J	602	TPP	C4-C5-S1	3.07	115.35	110.56
3	K	602	TPP	CM2-C2'-N1'	3.06	120.46	117.20
3	X	602	TPP	N1'-C2'-N3'	-3.03	120.48	125.53
3	D	602	TPP	CM2-C2'-N1'	3.02	120.42	117.20
3	D	602	TPP	C2-N3-C4	-3.01	109.99	114.06
3	E	602	TPP	CM2-C2'-N1'	3.00	120.39	117.20
3	J	602	TPP	CM4-C4-N3	2.99	127.47	120.57
3	A	602	TPP	CM4-C4-N3	2.98	127.44	120.57
3	M	602	TPP	C2-N3-C4	-2.96	110.05	114.06
3	H	602	TPP	C4-C5-S1	2.96	115.17	110.56
3	H	602	TPP	O2A-PA-O3A	2.95	115.25	107.27
3	N	602	TPP	N1'-C2'-N3'	-2.95	120.62	125.53
3	X	602	TPP	C6-C5-S1	-2.95	114.00	120.90
3	U	602	TPP	N1'-C2'-N3'	-2.95	120.63	125.53
3	R	602	TPP	O2A-PA-O3A	2.94	115.22	107.27
3	I	602	TPP	C4-C5-S1	2.94	115.15	110.56
3	S	602	TPP	C2-N3-C4	-2.93	110.10	114.06
3	F	603	TPP	C4-C5-S1	2.92	115.12	110.56
3	R	602	TPP	N1'-C2'-N3'	-2.92	120.68	125.53
3	L	602	TPP	N1'-C2'-N3'	-2.89	120.73	125.53
3	N	602	TPP	C6-C5-S1	-2.88	114.15	120.90
3	D	602	TPP	N1'-C2'-N3'	-2.88	120.73	125.53
3	H	602	TPP	N1'-C2'-N3'	-2.88	120.74	125.53
3	M	602	TPP	CM2-C2'-N1'	2.88	120.26	117.20
3	J	602	TPP	N1'-C2'-N3'	-2.87	120.75	125.53
3	L	602	TPP	CM2-C2'-N1'	2.87	120.26	117.20
3	V	602	TPP	N1'-C2'-N3'	-2.86	120.77	125.53
3	P	602	TPP	N1'-C2'-N3'	-2.85	120.78	125.53
3	B	602	TPP	C6-C5-S1	-2.85	114.22	120.90
3	W	602	TPP	N1'-C2'-N3'	-2.85	120.79	125.53
3	E	602	TPP	N1'-C2'-N3'	-2.83	120.82	125.53
3	M	602	TPP	N1'-C2'-N3'	-2.83	120.82	125.53
3	M	602	TPP	C4-C5-S1	2.82	114.97	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	602	TPP	C6-C5-S1	-2.81	114.31	120.90
3	G	602	TPP	N1'-C2'-N3'	-2.81	120.86	125.53
3	W	602	TPP	CM4-C4-N3	2.80	127.04	120.57
3	I	602	TPP	N1'-C2'-N3'	-2.80	120.87	125.53
3	D	602	TPP	C4-C5-S1	2.79	114.92	110.56
3	W	602	TPP	CM2-C2'-N1'	2.77	120.15	117.20
3	T	602	TPP	N1'-C2'-N3'	-2.76	120.93	125.53
3	A	602	TPP	C2-N3-C4	-2.73	110.36	114.06
3	A	602	TPP	C6-C5-S1	-2.73	114.50	120.90
3	F	603	TPP	N1'-C2'-N3'	-2.73	120.99	125.53
3	V	602	TPP	C6-C5-S1	-2.72	114.53	120.90
3	G	602	TPP	C6-C5-S1	-2.71	114.55	120.90
3	R	602	TPP	C4-C5-S1	2.71	114.78	110.56
3	E	602	TPP	C6-C5-S1	-2.69	114.60	120.90
3	Q	602	TPP	C2-N3-C4	-2.69	110.43	114.06
3	R	602	TPP	C6-C5-S1	-2.68	114.62	120.90
3	Q	602	TPP	C6-C5-S1	-2.68	114.62	120.90
3	B	602	TPP	N1'-C2'-N3'	-2.68	121.08	125.53
3	Q	602	TPP	N1'-C2'-N3'	-2.65	121.12	125.53
3	T	602	TPP	C6-C5-S1	-2.65	114.71	120.90
3	S	602	TPP	N1'-C2'-N3'	-2.61	121.18	125.53
3	D	602	TPP	CM4-C4-N3	2.59	126.55	120.57
3	F	603	TPP	CM4-C4-N3	2.55	126.46	120.57
3	X	602	TPP	C4-C5-S1	2.54	114.52	110.56
3	A	602	TPP	N1'-C2'-N3'	-2.52	121.34	125.53
3	G	602	TPP	C4-C5-S1	2.52	114.49	110.56
3	O	602	TPP	N1'-C2'-N3'	-2.51	121.35	125.53
3	P	602	TPP	C6-C5-S1	-2.51	115.03	120.90
3	J	602	TPP	C6-C5-S1	-2.50	115.04	120.90
3	O	602	TPP	C6-C5-S1	-2.50	115.04	120.90
3	L	602	TPP	C6-C5-S1	-2.49	115.07	120.90
3	G	602	TPP	CM2-C2'-N1'	2.47	119.83	117.20
3	M	602	TPP	C6-C5-S1	-2.47	115.13	120.90
3	Q	602	TPP	O2A-PA-O3A	2.45	113.88	107.27
3	V	602	TPP	C5'-C6'-N1'	-2.42	119.89	123.83
3	N	602	TPP	O3B-PB-O2B	2.42	116.86	107.80
3	F	603	TPP	C5'-C6'-N1'	-2.38	119.96	123.83
3	F	603	TPP	C6-C5-S1	-2.38	115.33	120.90
3	B	602	TPP	C2-N3-C4	-2.38	110.85	114.06
3	K	602	TPP	C2-N3-C4	-2.36	110.87	114.06
3	C	602	TPP	C4-C5-S1	2.36	114.24	110.56
3	I	602	TPP	C5'-C6'-N1'	-2.36	120.00	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	602	TPP	CM2-C2'-N1'	2.35	119.70	117.20
3	P	602	TPP	C4-C5-S1	2.35	114.22	110.56
3	M	602	TPP	O3B-PB-O2B	2.34	116.59	107.80
3	F	603	TPP	CM2-C2'-N1'	2.34	119.69	117.20
3	C	602	TPP	CM2-C2'-N1'	2.33	119.68	117.20
3	N	602	TPP	C2'-N3'-C4'	2.33	121.67	118.10
3	X	602	TPP	C2-N3-C4	-2.32	110.92	114.06
3	E	602	TPP	C5'-C6'-N1'	-2.32	120.06	123.83
3	B	602	TPP	C4-C5-S1	2.32	114.18	110.56
3	J	602	TPP	C2-N3-C4	-2.31	110.94	114.06
3	C	602	TPP	C6-C5-S1	-2.30	115.51	120.90
3	A	602	TPP	CM4-C4-C5	-2.30	121.85	127.75
3	H	602	TPP	C2-N3-C4	-2.28	110.98	114.06
3	U	602	TPP	CM2-C2'-N1'	2.28	119.62	117.20
3	J	602	TPP	C5'-C6'-N1'	-2.24	120.19	123.83
3	C	602	TPP	C2-N3-C4	-2.24	111.04	114.06
3	U	602	TPP	O3B-PB-O2B	2.22	116.14	107.80
3	D	602	TPP	C5'-C6'-N1'	-2.22	120.23	123.83
3	D	602	TPP	C6-C5-S1	-2.21	115.72	120.90
3	R	602	TPP	O3B-PB-O2B	2.21	116.10	107.80
3	F	603	TPP	C2-N3-C4	-2.21	111.08	114.06
3	S	602	TPP	C4-C5-S1	2.21	114.00	110.56
3	U	602	TPP	C5'-C6'-N1'	-2.21	120.24	123.83
3	A	602	TPP	C5'-C6'-N1'	-2.20	120.25	123.83
3	L	602	TPP	C2-N3-C4	-2.20	111.08	114.06
3	H	602	TPP	C6-C5-S1	-2.20	115.75	120.90
3	T	602	TPP	C5'-C6'-N1'	-2.20	120.25	123.83
3	A	602	TPP	CM2-C2'-N1'	2.19	119.53	117.20
3	A	602	TPP	O2A-PA-O3A	2.19	113.18	107.27
3	A	602	TPP	C4-C5-S1	2.18	113.97	110.56
3	O	602	TPP	C2-N3-C4	-2.15	111.15	114.06
3	T	602	TPP	C2-N3-C4	-2.13	111.18	114.06
3	P	602	TPP	C5'-C6'-N1'	-2.13	120.37	123.83
3	R	602	TPP	C2-N3-C4	-2.13	111.19	114.06
3	O	602	TPP	CM2-C2'-N1'	2.13	119.46	117.20
3	S	602	TPP	C5'-C6'-N1'	-2.11	120.40	123.83
3	Q	602	TPP	C5'-C6'-N1'	-2.11	120.40	123.83
3	C	602	TPP	CM2-C2'-N3'	2.11	120.28	117.13
3	X	602	TPP	C5'-C6'-N1'	-2.10	120.41	123.83
3	K	602	TPP	C6-C5-S1	-2.08	116.02	120.90
3	H	602	TPP	C2'-N3'-C4'	2.08	121.30	118.10
3	O	602	TPP	C4-C5-S1	2.07	113.80	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	602	TPP	C4-C5-S1	2.07	113.79	110.56
3	P	602	TPP	CM2-C2'-N1'	2.07	119.40	117.20
3	X	602	TPP	C2'-N3'-C4'	2.06	121.27	118.10
3	H	602	TPP	CM2-C2'-N1'	2.03	119.37	117.20
3	X	602	TPP	CM4-C4-N3	2.03	125.26	120.57
3	Q	602	TPP	CM2-C2'-N1'	2.03	119.36	117.20
3	W	602	TPP	C2'-N3'-C4'	2.03	121.22	118.10
3	U	602	TPP	CM4-C4-N3	2.02	125.23	120.57
3	W	602	TPP	O3B-PB-O2B	2.02	115.36	107.80
3	D	602	TPP	CM4-C4-C5	-2.01	122.61	127.75
3	W	602	TPP	C6-C5-S1	-2.00	116.22	120.90

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	TPP	PA-O3A-PB-O3B
3	L	602	TPP	PA-O3A-PB-O2B
3	L	602	TPP	PA-O3A-PB-O3B
3	P	602	TPP	PA-O3A-PB-O2B
4	A	603	EDO	O1-C1-C2-O2
4	R	603	EDO	O1-C1-C2-O2
3	V	602	TPP	PB-O3A-PA-O7
3	D	602	TPP	PA-O3A-PB-O1B
3	A	602	TPP	PA-O3A-PB-O2B
3	H	602	TPP	PA-O3A-PB-O3B
3	Q	602	TPP	C5-C6-C7-O7
3	U	602	TPP	C5-C6-C7-O7
4	F	601	EDO	O1-C1-C2-O2
4	Q	603	EDO	O1-C1-C2-O2
3	A	602	TPP	PA-O3A-PB-O1B
3	L	602	TPP	PA-O3A-PB-O1B
3	D	602	TPP	PA-O3A-PB-O2B
3	D	602	TPP	PA-O3A-PB-O3B
3	H	602	TPP	PA-O3A-PB-O2B
3	Q	602	TPP	PA-O3A-PB-O2B
3	U	602	TPP	PA-O3A-PB-O2B
4	N	603	EDO	O1-C1-C2-O2
3	A	602	TPP	C5-C6-C7-O7
3	D	602	TPP	C5-C6-C7-O7
3	E	602	TPP	C5-C6-C7-O7
3	L	602	TPP	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
3	P	602	TPP	C5-C6-C7-O7
3	T	602	TPP	C5-C6-C7-O7

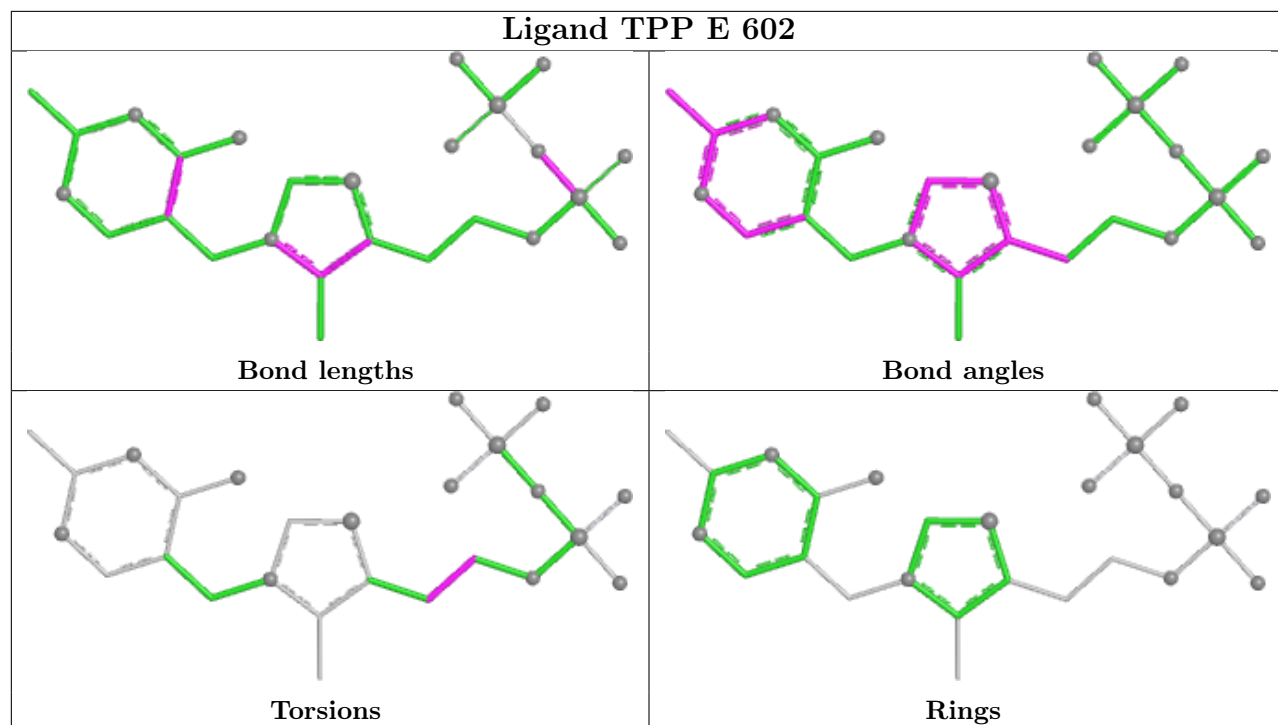
There are no ring outliers.

22 monomers are involved in 41 short contacts:

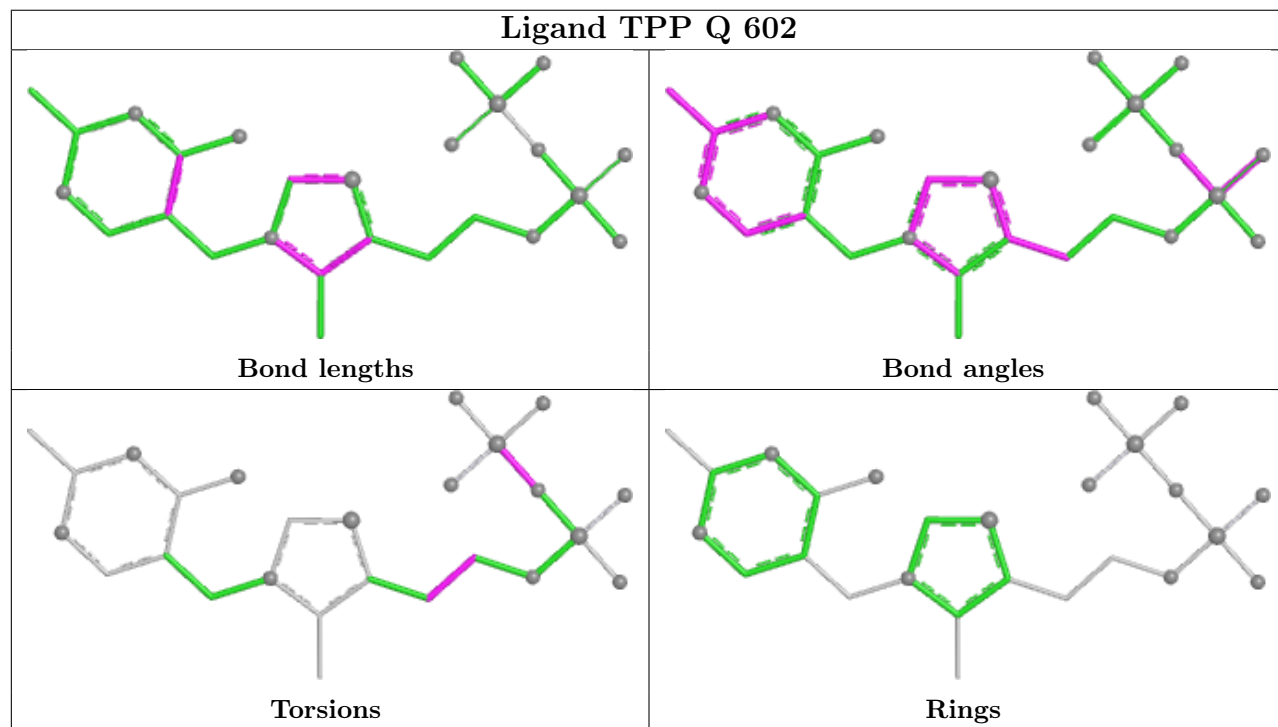
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	TPP	4	0
3	Q	602	TPP	2	0
3	A	602	TPP	1	0
3	P	602	TPP	2	0
3	R	602	TPP	2	0
3	H	602	TPP	2	0
3	X	602	TPP	2	0
3	T	602	TPP	1	0
3	J	602	TPP	2	0
3	G	602	TPP	3	0
3	K	602	TPP	2	0
3	F	603	TPP	1	0
3	L	602	TPP	2	0
3	O	602	TPP	2	0
3	I	602	TPP	2	0
3	W	602	TPP	1	0
3	C	602	TPP	2	0
3	U	602	TPP	1	0
4	F	601	EDO	2	0
3	D	602	TPP	2	0
3	M	602	TPP	2	0
3	N	602	TPP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

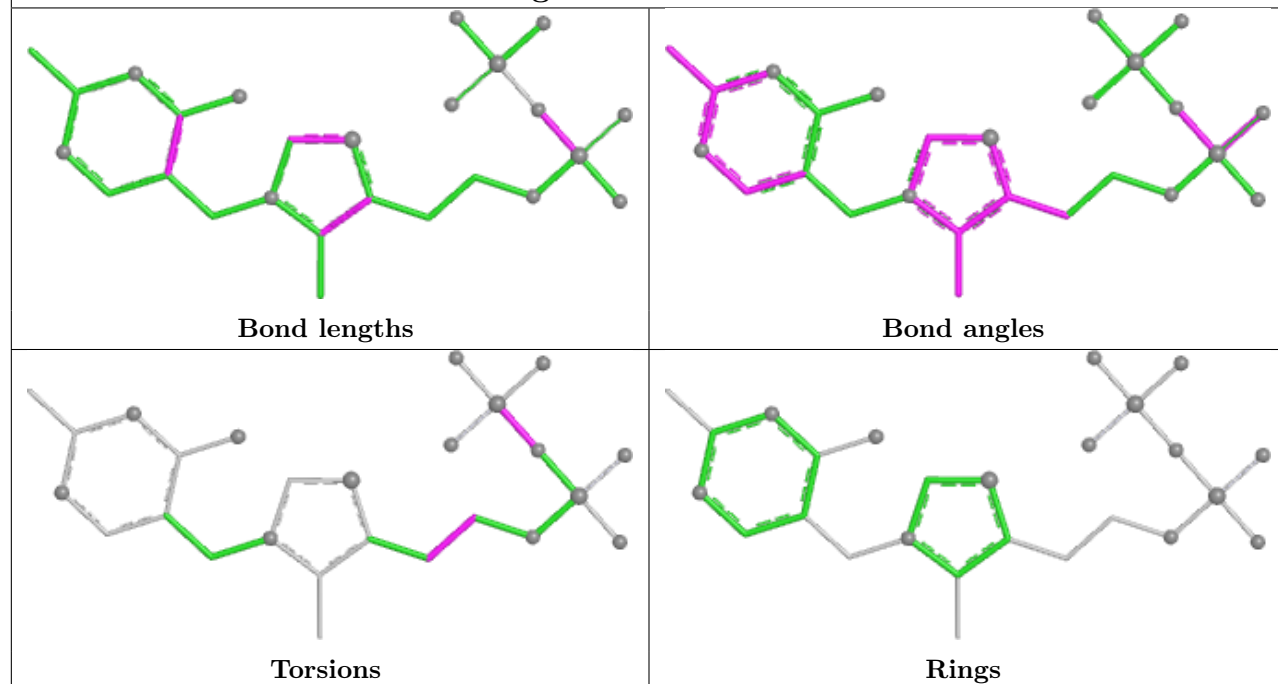
Ligand TPP E 602



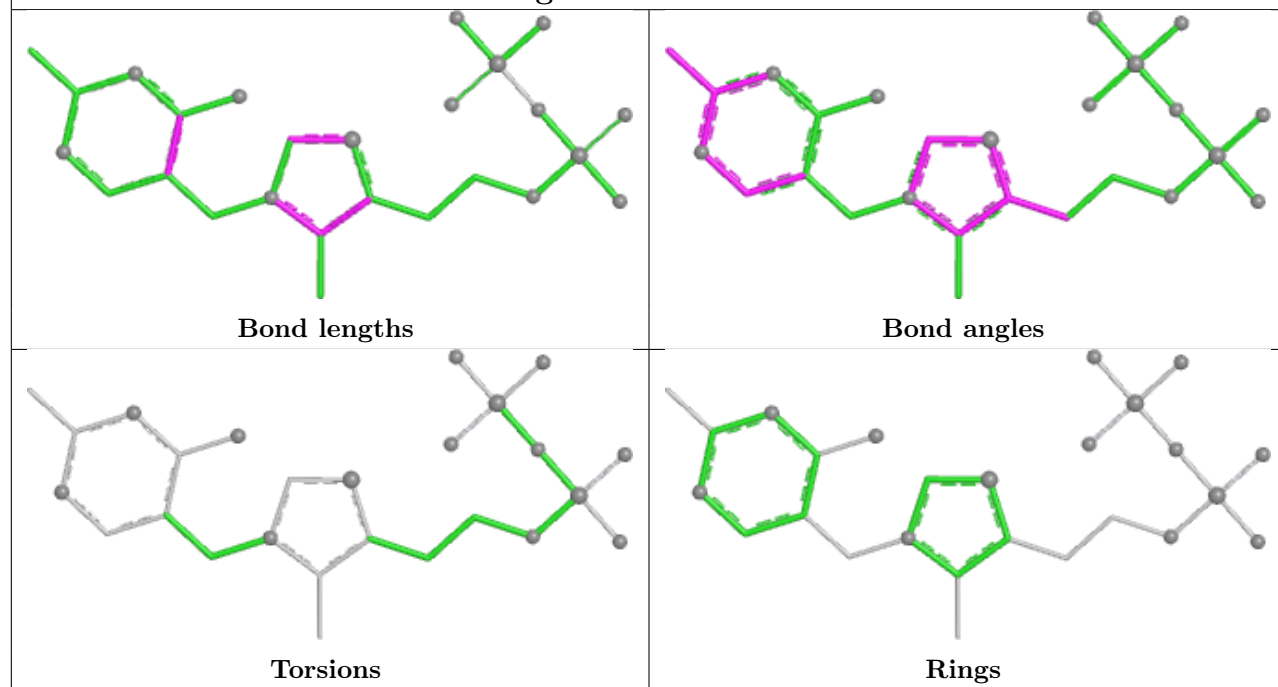
Ligand TPP Q 602



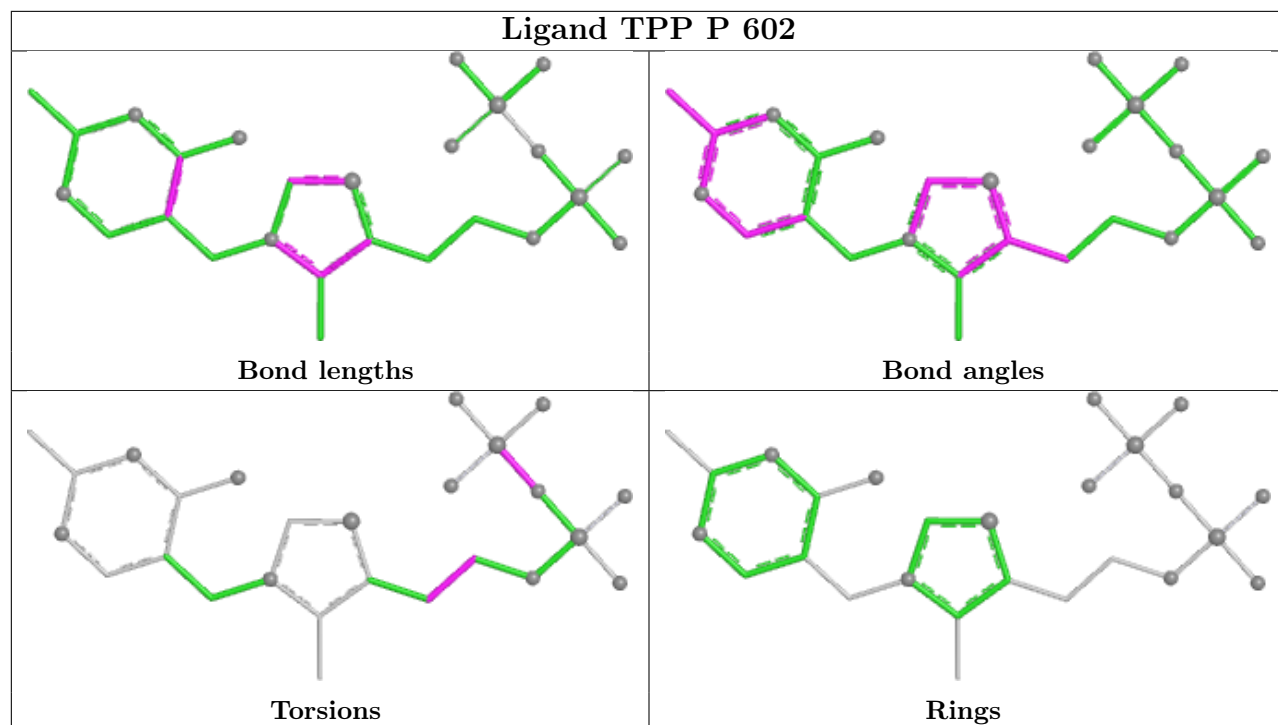
Ligand TPP A 602



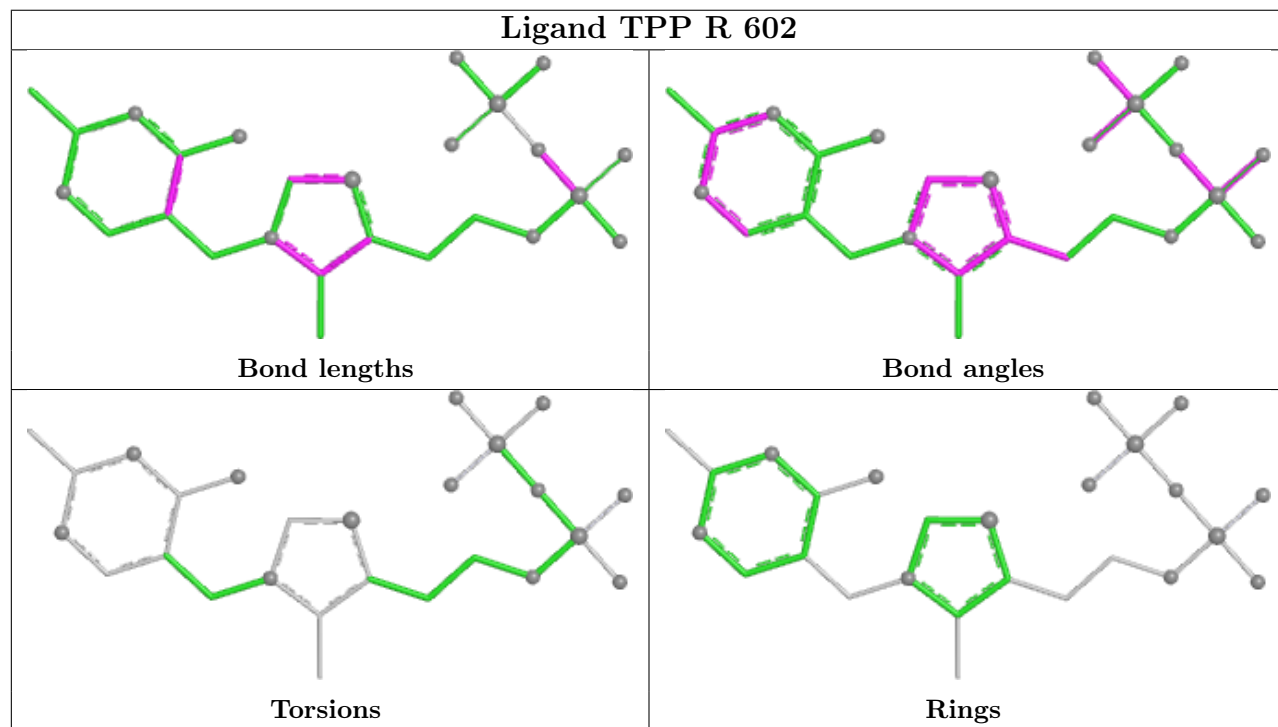
Ligand TPP S 602



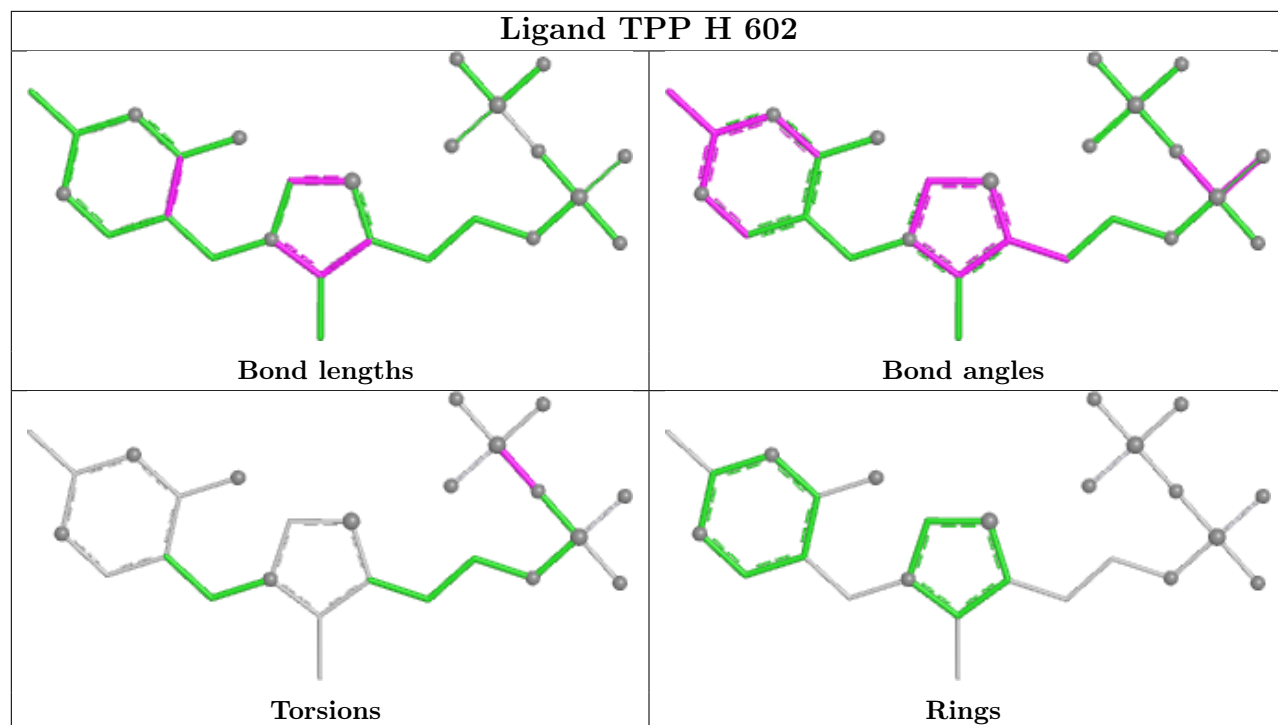
Ligand TPP P 602



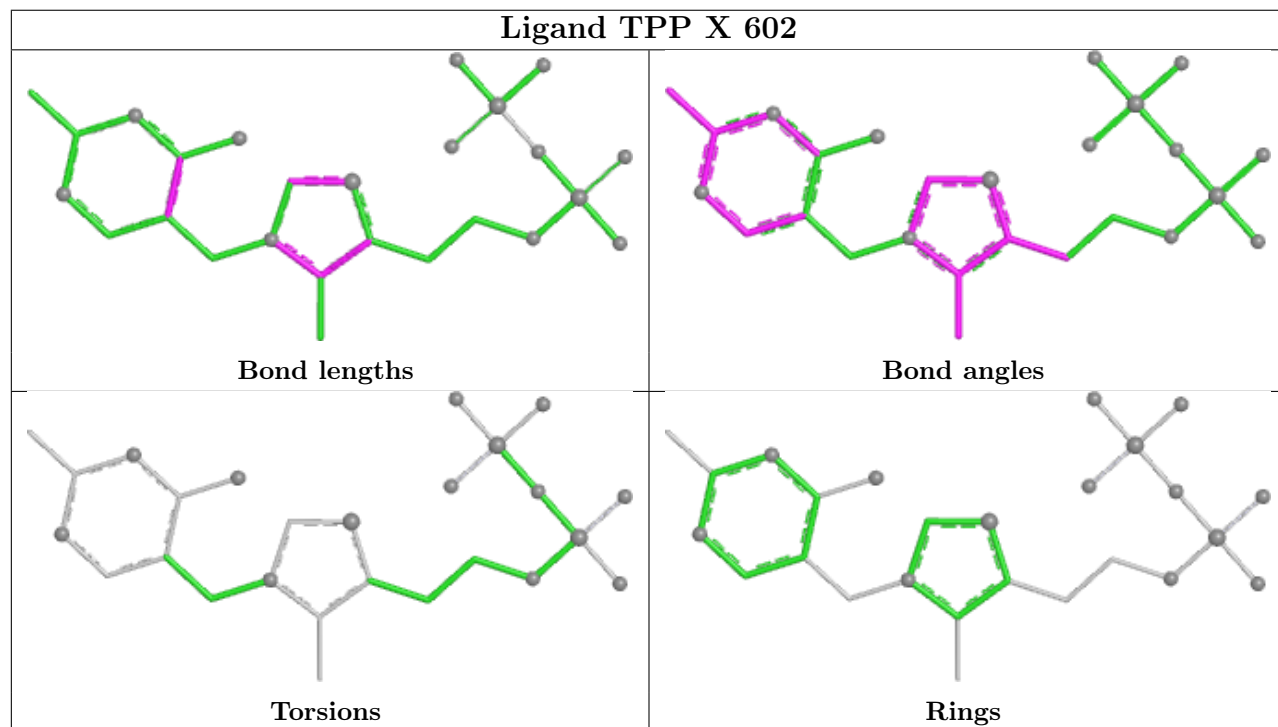
Ligand TPP R 602



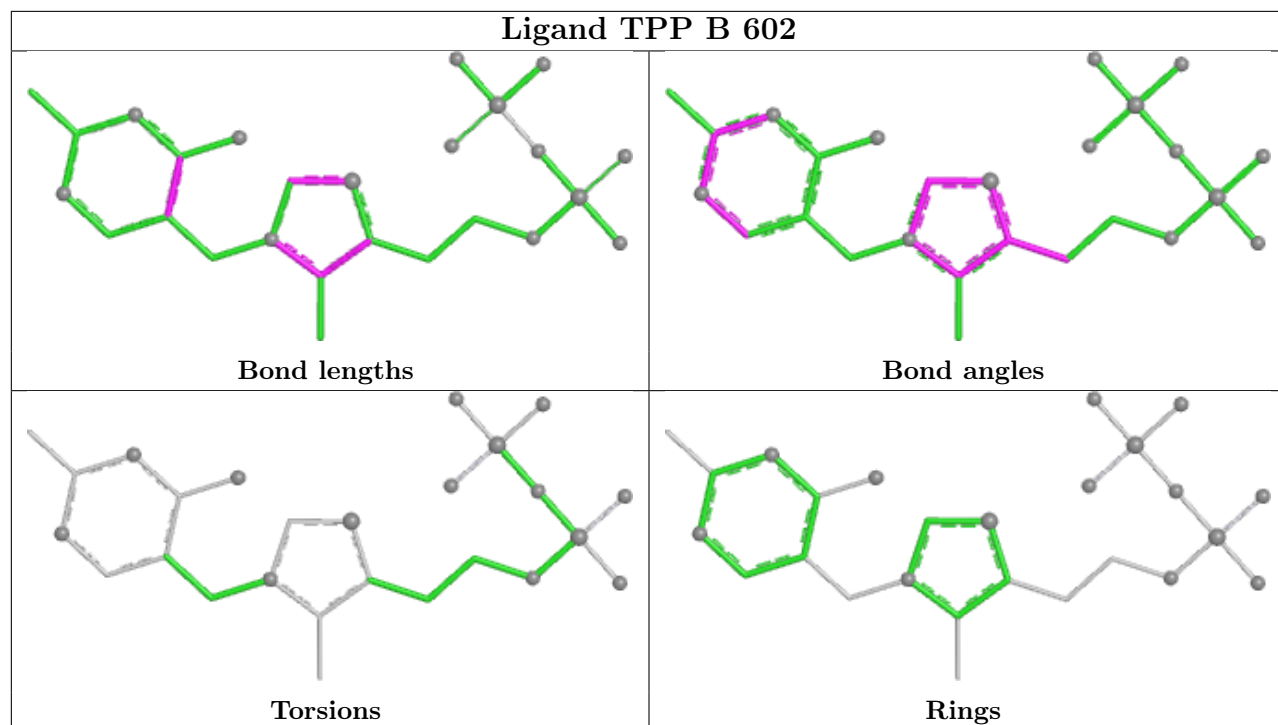
Ligand TPP H 602



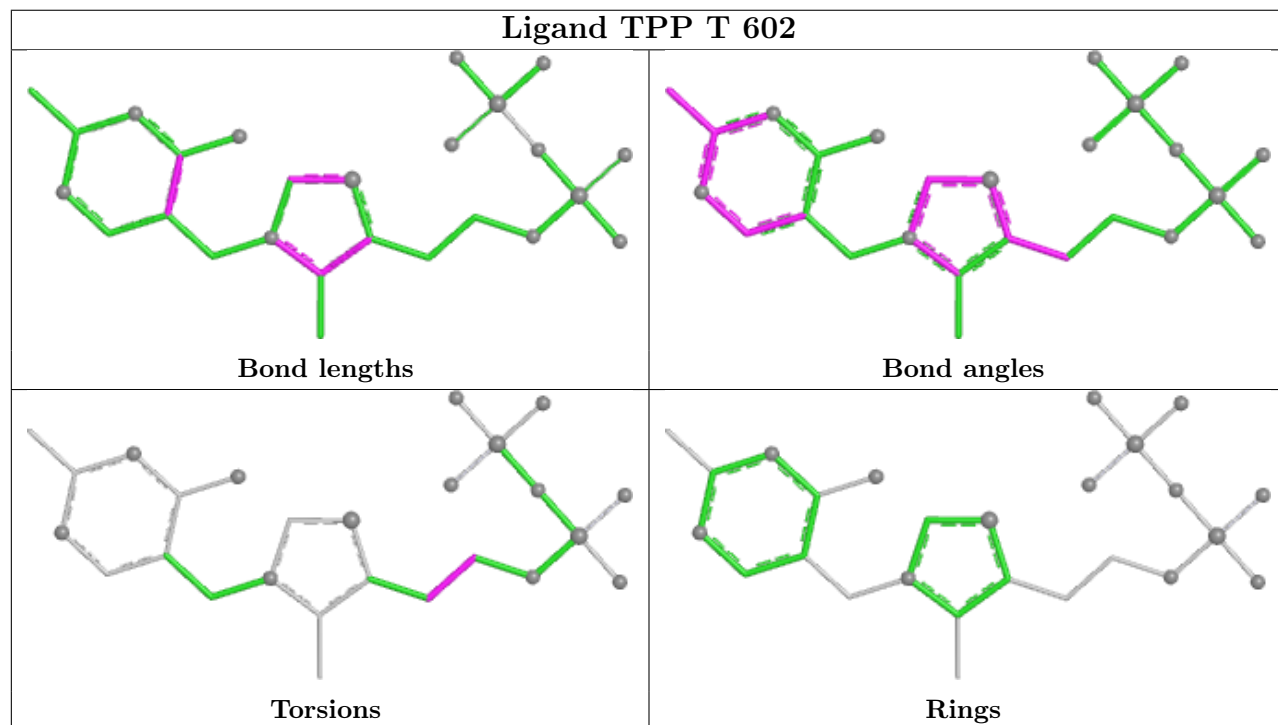
Ligand TPP X 602



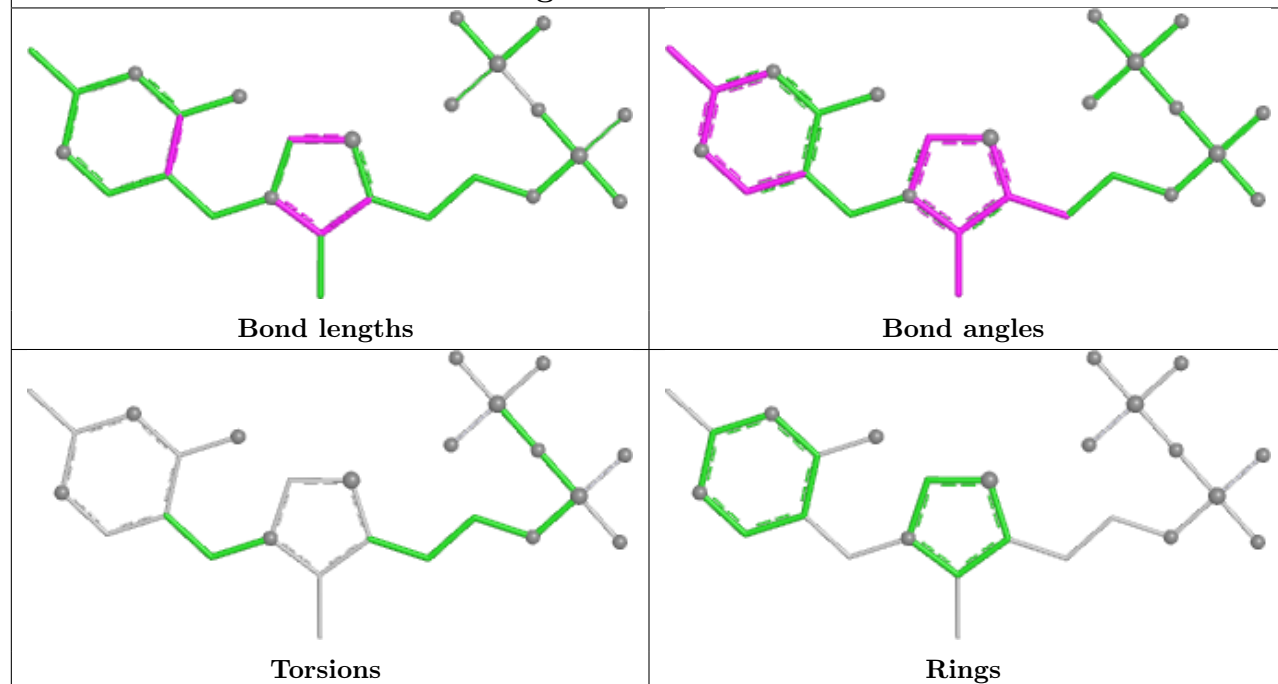
Ligand TPP B 602



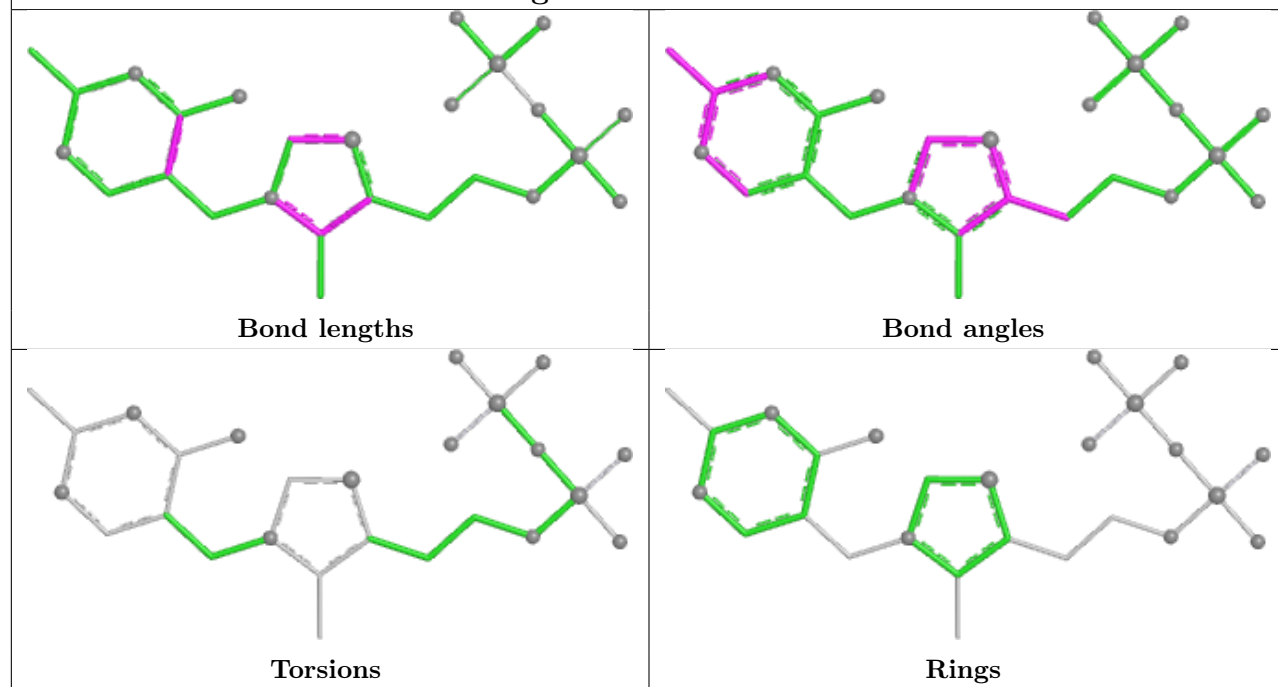
Ligand TPP T 602



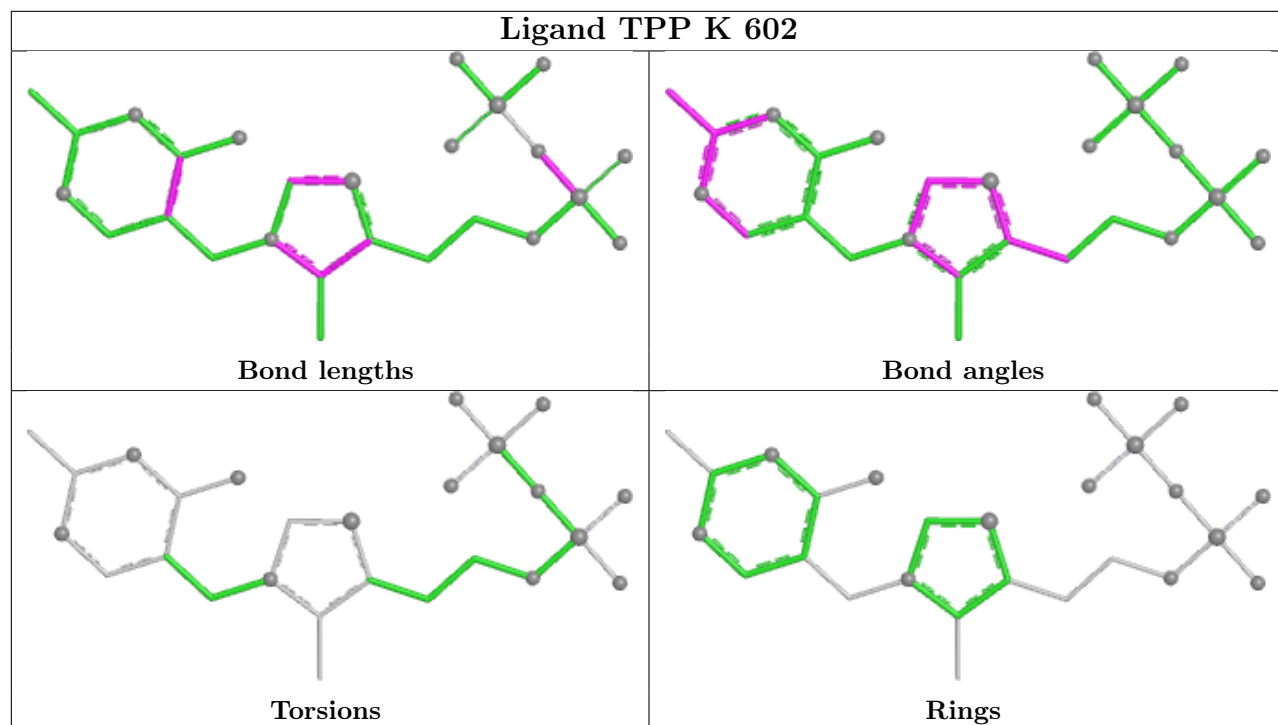
Ligand TPP J 602



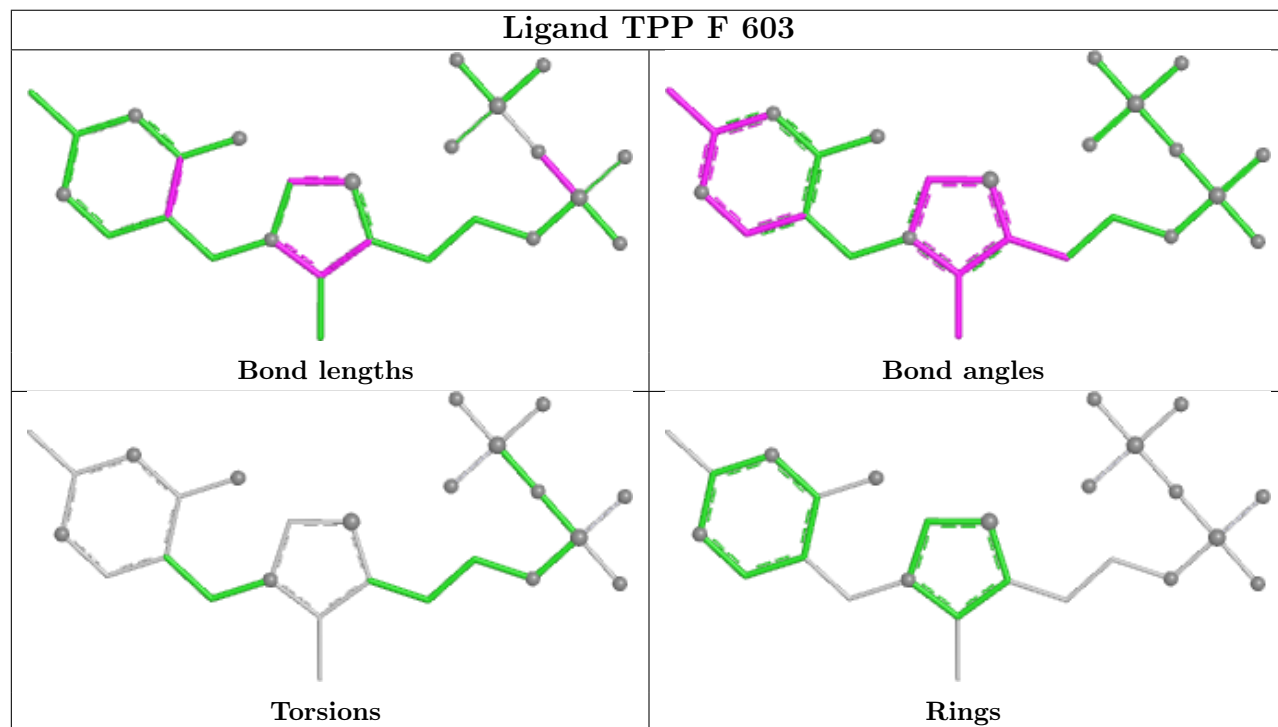
Ligand TPP G 602



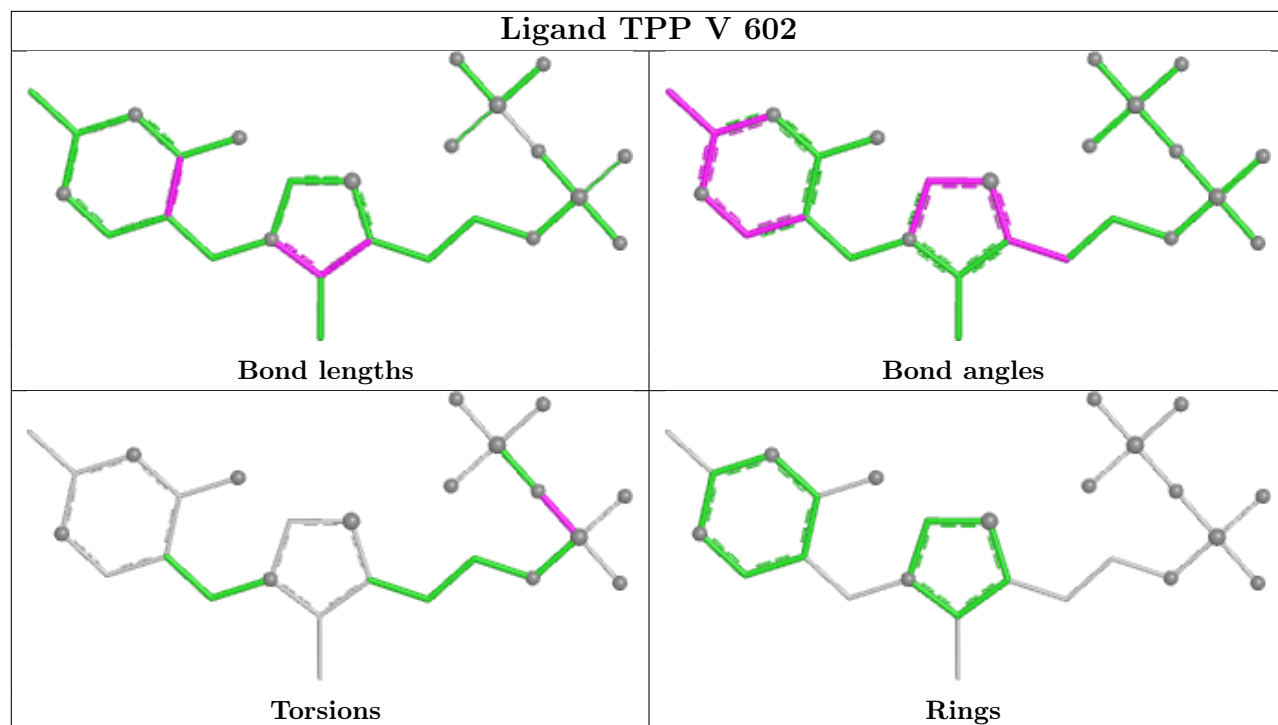
Ligand TPP K 602



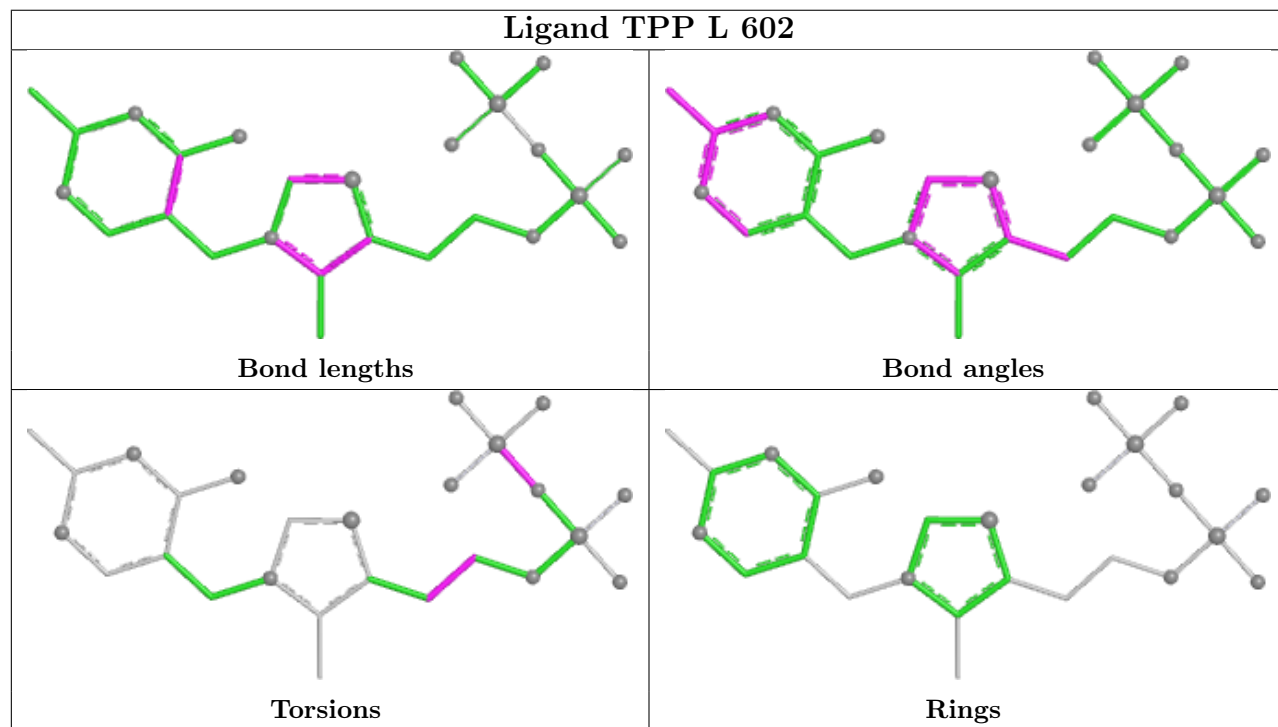
Ligand TPP F 603



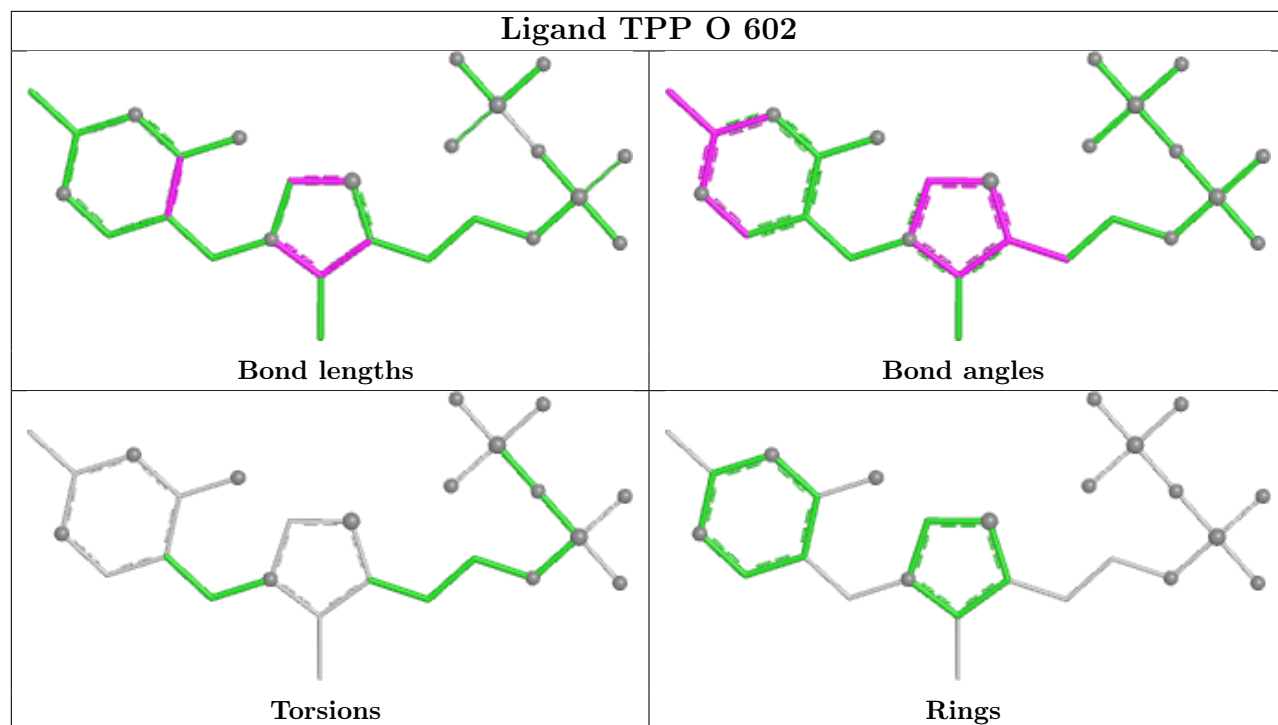
Ligand TPP V 602



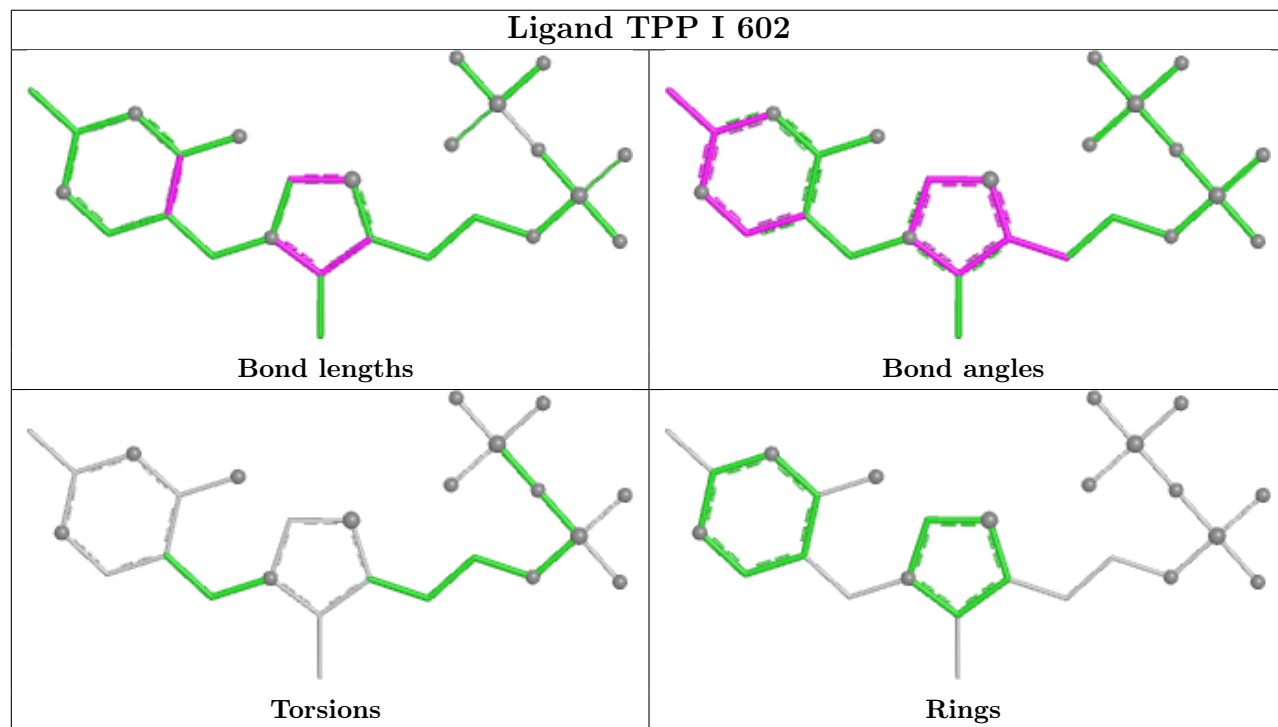
Ligand TPP L 602

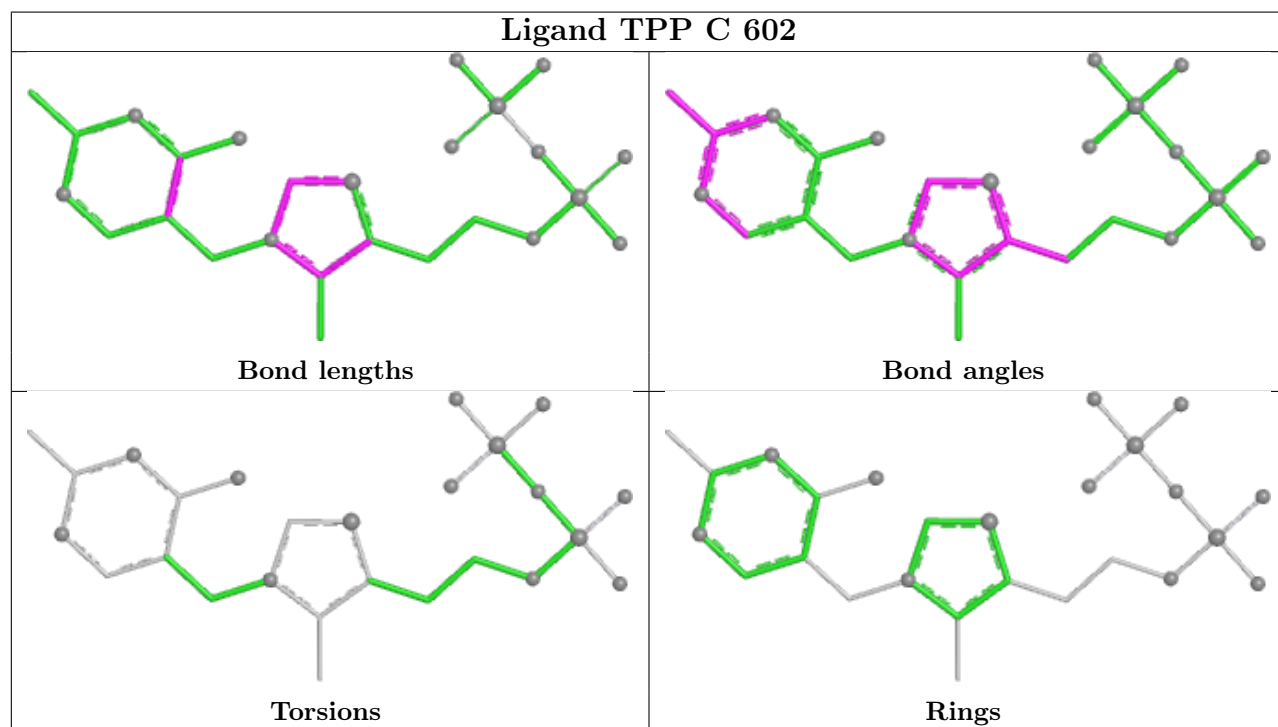
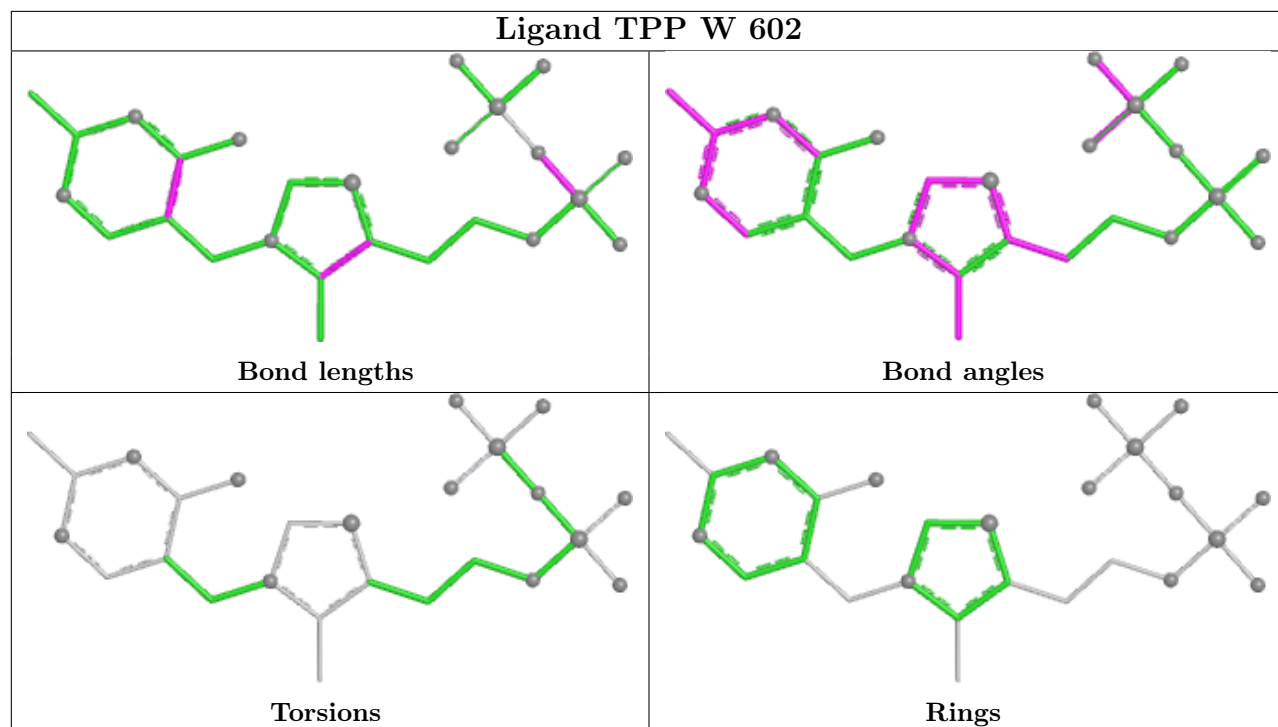


Ligand TPP O 602

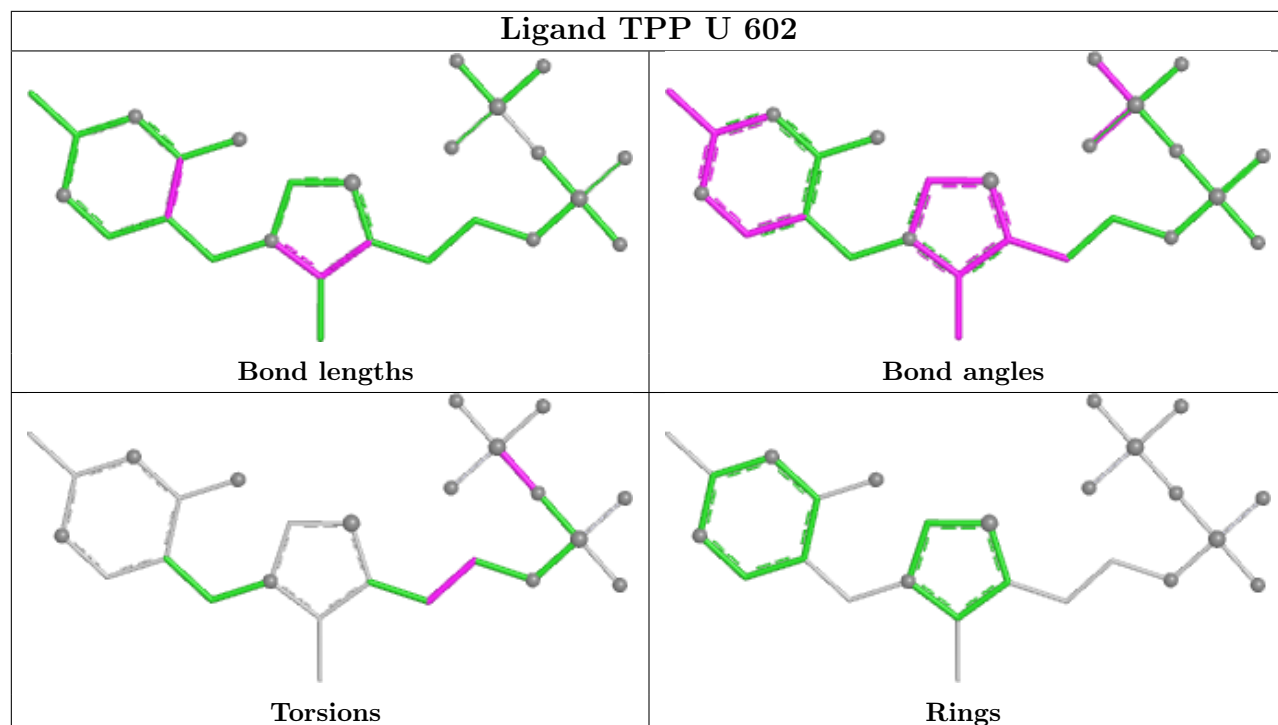


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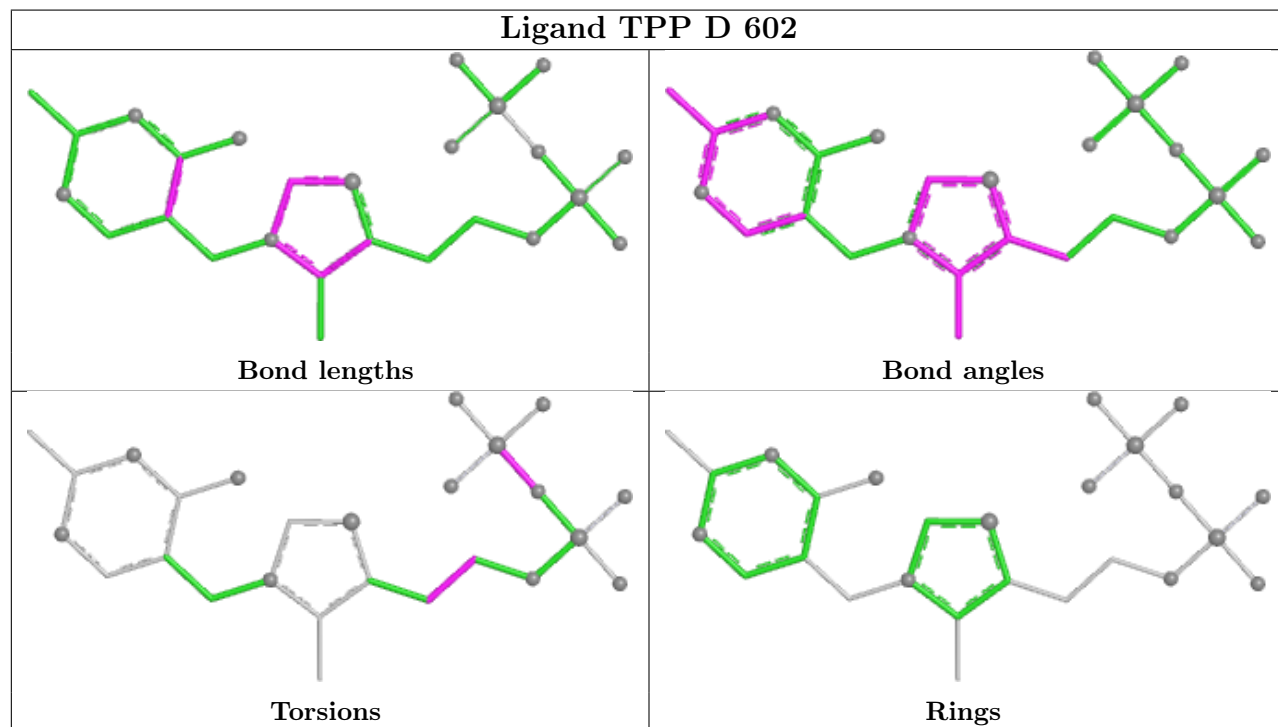


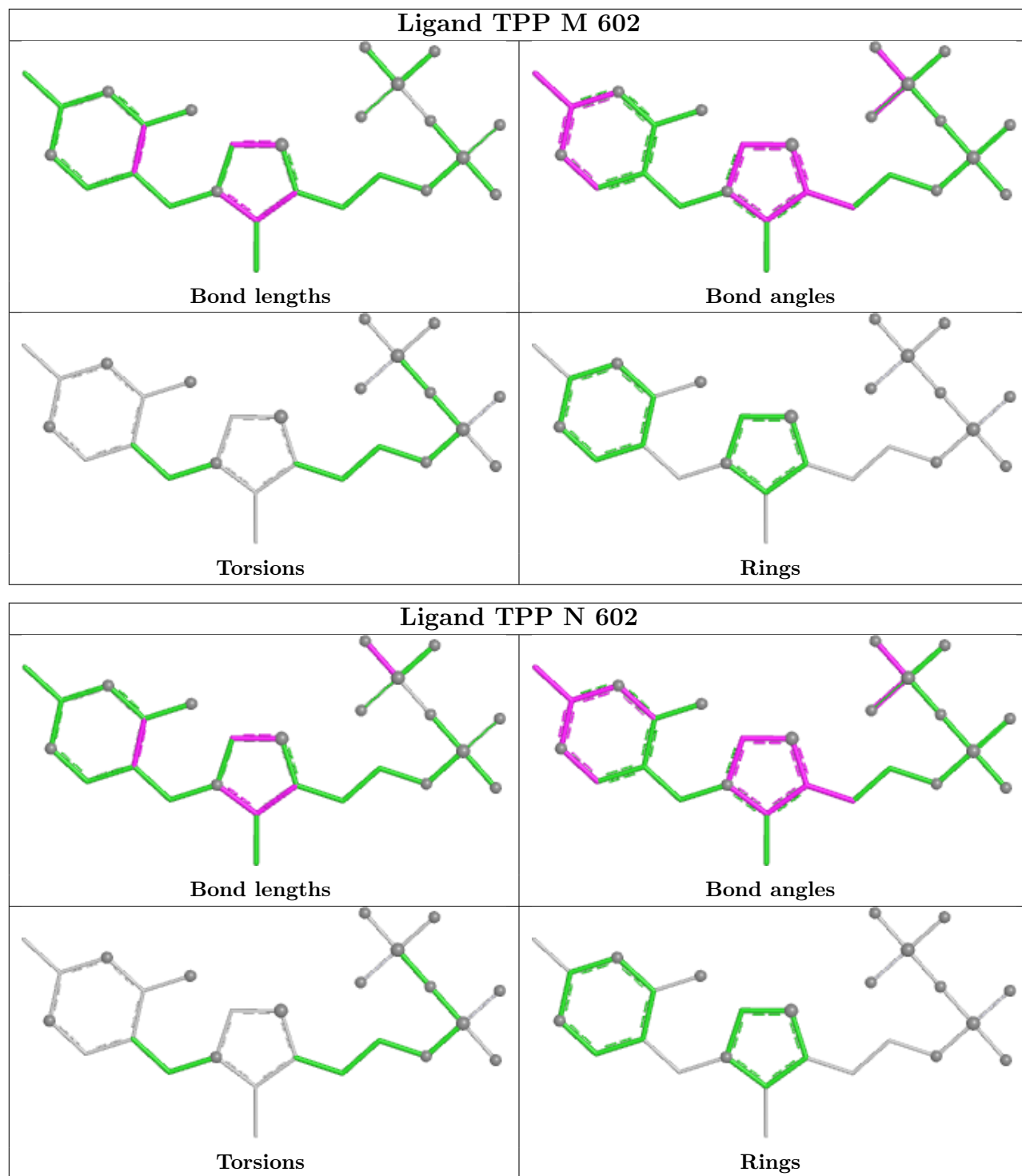


Ligand TPP U 602



Ligand TPP D 602





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	555:GLN	C	556:ALA	N	5.35
1	E	555:GLN	C	556:ALA	N	3.78

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	555/573 (96%)	0.37	21 (3%)	44	49	12, 27, 43, 68	5 (0%)
1	B	555/573 (96%)	0.31	22 (3%)	42	47	12, 25, 44, 66	4 (0%)
1	C	555/573 (96%)	-0.02	11 (1%)	65	69	10, 19, 36, 57	6 (1%)
1	D	555/573 (96%)	0.04	11 (1%)	65	69	11, 21, 36, 58	5 (0%)
1	E	556/573 (97%)	-0.04	13 (2%)	61	64	10, 20, 35, 76	4 (0%)
1	F	555/573 (96%)	-0.21	7 (1%)	75	78	7, 17, 31, 55	9 (1%)
1	G	555/573 (96%)	0.20	18 (3%)	50	54	8, 24, 41, 62	7 (1%)
1	H	555/573 (96%)	0.34	16 (2%)	53	57	10, 26, 43, 66	6 (1%)
1	I	556/573 (97%)	0.21	24 (4%)	40	45	9, 23, 44, 88	6 (1%)
1	J	555/573 (96%)	-0.00	13 (2%)	61	64	12, 21, 37, 66	4 (0%)
1	K	555/573 (96%)	0.11	17 (3%)	51	55	11, 22, 40, 58	7 (1%)
1	L	555/573 (96%)	0.05	10 (1%)	67	71	10, 21, 37, 58	9 (1%)
1	M	555/573 (96%)	-0.22	9 (1%)	70	74	6, 16, 32, 50	7 (1%)
1	N	555/573 (96%)	-0.16	6 (1%)	78	80	8, 17, 31, 51	7 (1%)
1	O	555/573 (96%)	0.14	16 (2%)	53	57	12, 23, 41, 62	3 (0%)
1	P	555/573 (96%)	0.07	19 (3%)	48	52	8, 22, 42, 63	7 (1%)
1	Q	555/573 (96%)	0.24	22 (3%)	42	47	12, 25, 43, 63	5 (0%)
1	R	555/573 (96%)	0.23	20 (3%)	46	50	10, 25, 44, 74	8 (1%)
1	S	555/573 (96%)	0.10	17 (3%)	51	55	13, 23, 42, 64	2 (0%)
1	T	555/573 (96%)	0.09	9 (1%)	70	74	12, 23, 40, 59	4 (0%)
1	U	555/573 (96%)	1.76	225 (40%)	0	1	18, 42, 72, 94	4 (0%)
1	V	555/573 (96%)	1.38	148 (26%)	1	1	18, 41, 68, 98	4 (0%)
1	W	555/573 (96%)	1.88	250 (45%)	0	1	21, 47, 72, 97	3 (0%)
1	X	555/573 (96%)	0.52	26 (4%)	36	41	13, 31, 50, 77	3 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	13322/13752 (96%)	0.31	950 (7%)	22	25	6, 24, 52, 98	129 (0%)

All (950) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	556	ALA	9.3
1	I	556	ALA	9.0
1	U	348	VAL	7.7
1	W	348	VAL	7.3
1	W	346	ALA	6.7
1	U	349	LEU	6.7
1	W	344	THR	6.6
1	W	351	ILE	6.3
1	U	269	ALA	5.6
1	U	517	LEU	5.5
1	V	349	LEU	5.5
1	W	249	PHE	5.3
1	W	347	PRO	5.3
1	W	269	ALA	5.3
1	W	290	ALA	5.3
1	U	268	GLY	5.3
1	V	348	VAL	5.2
1	X	348	VAL	5.2
1	U	351	ILE	5.2
1	W	354	ALA	5.2
1	U	372	LEU	5.2
1	W	391[A]	SER	5.1
1	U	354	ALA	5.1
1	V	353	ALA	5.1
1	V	355[A]	GLU	5.1
1	W	355[A]	GLU	5.0
1	V	1	MET	5.0
1	U	299	LYS	5.0
1	W	211	VAL	5.0
1	X	1	MET	4.9
1	W	333	LYS	4.9
1	W	205	LEU	4.9
1	U	344	THR	4.9
1	U	369	ILE	4.8
1	U	300	GLY	4.8
1	U	353	ALA	4.8
1	V	354	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	U	347	PRO	4.8
1	W	268	GLY	4.8
1	W	353	ALA	4.7
1	I	344	THR	4.7
1	U	346	ALA	4.6
1	W	349	LEU	4.6
1	U	355[A]	GLU	4.5
1	U	343	GLY	4.5
1	V	198	VAL	4.5
1	U	339	ALA	4.5
1	U	540	ILE	4.5
1	U	471	ILE	4.4
1	U	250	PRO	4.4
1	U	390	ALA	4.4
1	U	514	LYS	4.4
1	V	278	ALA	4.4
1	V	346	ALA	4.4
1	Q	1	MET	4.4
1	W	546	VAL	4.4
1	W	341	THR	4.3
1	U	249	PHE	4.3
1	W	358	ALA	4.3
1	W	343	GLY	4.3
1	U	359	PRO	4.3
1	W	256	PHE	4.3
1	B	348	VAL	4.3
1	W	466	VAL	4.3
1	U	256	PHE	4.2
1	U	277	ASP	4.2
1	W	539	LEU	4.2
1	U	555	GLN	4.2
1	W	544	LYS	4.2
1	W	538	THR	4.2
1	W	469	ILE	4.2
1	U	296	SER	4.2
1	U	391[A]	SER	4.2
1	Q	348	VAL	4.2
1	U	238	ALA	4.1
1	V	351	ILE	4.1
1	V	347	PRO	4.1
1	X	349	LEU	4.1
1	S	344	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	1	MET	4.1
1	U	356	PRO	4.1
1	U	426[A]	GLU	4.1
1	W	204	TRP	4.0
1	U	276	ALA	4.0
1	W	1	MET	4.0
1	U	338	PRO	4.0
1	W	350	GLY	4.0
1	U	528	CYS	4.0
1	U	333	LYS	4.0
1	V	205	LEU	4.0
1	W	272	LEU	4.0
1	V	469	ILE	4.0
1	T	1	MET	4.0
1	W	278	ALA	3.9
1	W	273	VAL	3.9
1	R	349	LEU	3.9
1	K	1	MET	3.9
1	W	233	ASP	3.9
1	U	358	ALA	3.9
1	W	548	ALA	3.9
1	W	265	SER	3.9
1	W	517	LEU	3.9
1	U	393	MET	3.9
1	R	350	GLY	3.9
1	W	315	GLY	3.9
1	U	375	SER	3.9
1	W	470	ALA	3.9
1	F	1	MET	3.9
1	W	248	PHE	3.8
1	U	376	ASP	3.8
1	U	518	ASP	3.8
1	W	369	ILE	3.8
1	U	401	VAL	3.8
1	A	343	GLY	3.8
1	U	350	GLY	3.8
1	W	237	CYS	3.8
1	U	212	VAL	3.8
1	U	273	VAL	3.8
1	U	258	GLY	3.8
1	V	297	TRP	3.8
1	W	297	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	W	345	GLN	3.8
1	W	392	ARG	3.8
1	K	346	ALA	3.8
1	Q	346	ALA	3.8
1	V	200	ALA	3.8
1	U	272	LEU	3.8
1	U	539	LEU	3.8
1	W	340	THR	3.8
1	U	370	GLN	3.8
1	N	343	GLY	3.8
1	U	395	ILE	3.7
1	W	280	LEU	3.7
1	I	495	ASP	3.7
1	D	555	GLN	3.7
1	U	373	ILE	3.7
1	K	344	THR	3.7
1	U	509	LEU	3.7
1	U	345	GLN	3.7
1	F	555	GLN	3.7
1	U	397	GLY	3.7
1	W	239	VAL	3.7
1	U	513	ILE	3.7
1	R	346	ALA	3.7
1	U	341	THR	3.7
1	V	358	ALA	3.7
1	W	399	ALA	3.7
1	W	187	LEU	3.6
1	W	18	LYS	3.6
1	V	344	THR	3.6
1	U	541	ALA	3.6
1	U	515	LYS	3.6
1	V	555	GLN	3.6
1	B	344	THR	3.6
1	U	1	MET	3.6
1	U	496	GLY	3.6
1	C	345	GLN	3.6
1	V	345	GLN	3.6
1	G	1	MET	3.6
1	R	344	THR	3.6
1	U	230	ALA	3.6
1	W	224	ALA	3.6
1	W	250	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	W	359	PRO	3.6
1	P	355[A]	GLU	3.6
1	U	237	CYS	3.6
1	U	266	SER	3.6
1	R	495	ASP	3.5
1	P	1	MET	3.5
1	U	211	VAL	3.5
1	U	264	VAL	3.5
1	A	346	ALA	3.5
1	U	396	PRO	3.5
1	U	214	LEU	3.5
1	V	211	VAL	3.5
1	W	264	VAL	3.5
1	V	331	ALA	3.5
1	D	495	ASP	3.5
1	V	202	VAL	3.5
1	V	204	TRP	3.5
1	W	240	THR	3.5
1	X	345	GLN	3.5
1	W	467	ILE	3.5
1	U	531	ALA	3.5
1	W	516	ALA	3.5
1	W	541	ALA	3.5
1	I	349	LEU	3.5
1	P	495	ASP	3.5
1	O	1	MET	3.5
1	G	355[A]	GLU	3.5
1	U	267	GLU	3.5
1	W	251	GLU	3.5
1	W	267	GLU	3.5
1	R	345	GLN	3.5
1	Q	344	THR	3.5
1	V	359	PRO	3.4
1	V	369	ILE	3.4
1	M	345	GLN	3.4
1	U	209	GLN	3.4
1	U	550	ASN	3.4
1	U	340	THR	3.4
1	R	1	MET	3.4
1	U	306	MET	3.4
1	V	531	ALA	3.4
1	W	301	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	W	360	LEU	3.4
1	A	355[A]	GLU	3.4
1	B	533	ASP	3.4
1	I	352	GLU	3.4
1	U	252	ASP	3.4
1	U	456	ILE	3.4
1	W	42[A]	GLU	3.4
1	U	297	TRP	3.4
1	U	535	CYS	3.4
1	W	393	MET	3.4
1	W	518	ASP	3.4
1	H	555	GLN	3.4
1	W	282	LEU	3.4
1	W	261	TRP	3.3
1	U	352	GLU	3.3
1	U	365	MET	3.3
1	B	495	ASP	3.3
1	M	495	ASP	3.3
1	U	39	LYS	3.3
1	A	348	VAL	3.3
1	Q	350	GLY	3.3
1	W	236	GLY	3.3
1	N	555	GLN	3.3
1	W	555	GLN	3.3
1	V	339	ALA	3.3
1	W	330	LEU	3.3
1	W	302	ASN	3.3
1	W	39	LYS	3.3
1	U	505	THR	3.3
1	U	371	SER	3.3
1	W	339	ALA	3.3
1	U	501	LEU	3.3
1	V	234	ARG	3.3
1	U	544	LYS	3.3
1	J	495	ASP	3.3
1	V	495	ASP	3.3
1	W	209	GLN	3.3
1	W	536	THR	3.3
1	W	335	PRO	3.3
1	W	512	ALA	3.3
1	U	360	LEU	3.3
1	V	499	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	355[A]	GLU	3.3
1	W	362	ASN	3.3
1	W	342	GLN	3.3
1	W	300	GLY	3.2
1	V	212	VAL	3.2
1	V	273	VAL	3.2
1	U	278	ALA	3.2
1	V	334	ALA	3.2
1	Q	349	LEU	3.2
1	H	495[A]	ASP	3.2
1	J	345	GLN	3.2
1	U	301	ASP	3.2
1	W	504	SER	3.2
1	S	343	GLY	3.2
1	W	423	GLY	3.2
1	W	294	TRP	3.2
1	U	271	GLU	3.2
1	I	348	VAL	3.2
1	W	189	VAL	3.2
1	U	275	ASN	3.2
1	U	512	ALA	3.2
1	V	328	ALA	3.2
1	W	499	LEU	3.2
1	W	509	LEU	3.2
1	U	286	PHE	3.2
1	L	343	GLY	3.2
1	V	350	GLY	3.2
1	W	210	ASN	3.2
1	U	546	VAL	3.2
1	W	198	VAL	3.2
1	A	555	GLN	3.2
1	U	467	ILE	3.2
1	V	343	GLY	3.2
1	W	308	THR	3.2
1	D	345	GLN	3.2
1	V	546	VAL	3.1
1	W	542	TRP	3.1
1	G	533	ASP	3.1
1	U	259	LEU	3.1
1	V	301	ASP	3.1
1	W	323	LEU	3.1
1	D	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	U	229	VAL	3.1
1	U	399	ALA	3.1
1	W	352	GLU	3.1
1	U	458	PHE	3.1
1	U	538	THR	3.1
1	V	356	PRO	3.1
1	E	533	ASP	3.1
1	Q	533	ASP	3.1
1	U	314	ALA	3.1
1	W	212	VAL	3.1
1	J	1	MET	3.1
1	K	555	GLN	3.1
1	Q	345	GLN	3.1
1	W	554	PRO	3.1
1	B	346	ALA	3.1
1	U	331	ALA	3.1
1	U	516	ALA	3.1
1	V	547	ALA	3.1
1	W	547	ALA	3.1
1	X	346	ALA	3.1
1	U	403	LEU	3.1
1	V	280	LEU	3.1
1	U	213	MET	3.1
1	U	430	ILE	3.1
1	V	540	ILE	3.1
1	O	555	GLN	3.1
1	H	344	THR	3.0
1	V	254	PRO	3.0
1	W	388	PHE	3.0
1	V	189	VAL	3.0
1	U	530	ILE	3.0
1	W	336	SER	3.0
1	W	540	ILE	3.0
1	L	344	THR	3.0
1	U	240	THR	3.0
1	W	312	THR	3.0
1	V	335	PRO	3.0
1	V	494	GLU	3.0
1	S	533	ASP	3.0
1	W	253	HIS	3.0
1	R	555	GLN	3.0
1	W	314	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	W	16	GLY	3.0
1	W	511	GLY	3.0
1	T	494	GLU	3.0
1	U	534	ASP	3.0
1	U	542	TRP	3.0
1	W	260	TYR	3.0
1	W	299	LYS	3.0
1	W	514	LYS	3.0
1	M	1	MET	3.0
1	U	200	ALA	3.0
1	U	235	LEU	3.0
1	U	305	VAL	3.0
1	A	352	GLU	3.0
1	V	258	GLY	3.0
1	C	344	THR	3.0
1	P	533	ASP	3.0
1	U	298	PRO	3.0
1	V	515	LYS	3.0
1	V	533	ASP	3.0
1	W	338	PRO	3.0
1	W	385	ASP	3.0
1	W	515	LYS	3.0
1	C	555	GLN	2.9
1	W	387	TRP	3.0
1	V	314	ALA	2.9
1	W	266	SER	2.9
1	W	332	GLU	2.9
1	B	349	LEU	2.9
1	U	303	VAL	2.9
1	W	241	ILE	2.9
1	U	377	THR	2.9
1	U	385	ASP	2.9
1	W	497	HIS	2.9
1	J	555	GLN	2.9
1	W	506	GLY	2.9
1	V	239	VAL	2.9
1	I	1	MET	2.9
1	U	394	PRO	2.9
1	U	521	ARG	2.9
1	U	289	TYR	2.9
1	J	346	ALA	2.9
1	W	200	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	343	GLY	2.9
1	V	235	LEU	2.9
1	U	47	CYS	2.9
1	U	495	ASP	2.9
1	V	47	CYS	2.9
1	V	237	CYS	2.9
1	W	303	VAL	2.9
1	A	351	ILE	2.9
1	H	1	MET	2.9
1	U	206	GLN	2.9
1	J	344	THR	2.9
1	U	469	ILE	2.9
1	W	213	MET	2.9
1	W	520	ARG	2.9
1	U	251	GLU	2.9
1	W	226	LYS	2.9
1	W	232	ALA	2.9
1	P	345	GLN	2.8
1	T	555	GLN	2.8
1	U	205	LEU	2.8
1	V	330	LEU	2.8
1	X	301	ASP	2.8
1	U	202	VAL	2.8
1	U	453	ILE	2.8
1	U	526	ILE	2.8
1	V	279	ILE	2.8
1	C	494	GLU	2.8
1	W	254	PRO	2.8
1	W	289	TYR	2.8
1	G	555	GLN	2.8
1	O	345	GLN	2.8
1	R	533	ASP	2.8
1	U	257	ARG	2.8
1	U	520	ARG	2.8
1	W	320	GLY	2.8
1	W	507	ALA	2.8
1	V	517	LEU	2.8
1	O	344	THR	2.8
1	V	536	THR	2.8
1	W	401	VAL	2.8
1	U	362	ASN	2.8
1	U	234	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	V	209	GLN	2.8
1	W	545	ARG	2.8
1	T	495	ASP	2.8
1	Q	494	GLU	2.8
1	R	352	GLU	2.8
1	U	203	GLU	2.8
1	W	222	ALA	2.8
1	W	334	ALA	2.8
1	X	141	GLU	2.8
1	W	17	LEU	2.8
1	B	347	PRO	2.8
1	U	18	LYS	2.8
1	V	530	ILE	2.8
1	W	15	ILE	2.8
1	V	463	ARG	2.8
1	G	345	GLN	2.8
1	Q	555	GLN	2.8
1	V	206	GLN	2.8
1	F	533	ASP	2.8
1	I	301	ASP	2.8
1	W	494	GLU	2.8
1	G	343	GLY	2.8
1	W	245	ALA	2.8
1	V	214	LEU	2.8
1	W	235	LEU	2.8
1	W	321	LEU	2.8
1	U	241	ILE	2.8
1	U	357	ASN	2.7
1	A	1	MET	2.7
1	P	332	GLU	2.7
1	Q	495	ASP	2.7
1	U	506	GLY	2.7
1	U	507	ALA	2.7
1	V	276	ALA	2.7
1	P	344	THR	2.7
1	W	356	PRO	2.7
1	B	345	GLN	2.7
1	S	555	GLN	2.7
1	W	194	VAL	2.7
1	W	279	ILE	2.7
1	W	430	ILE	2.7
1	R	42[A]	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	V	332	GLU	2.7
1	V	207	ASP	2.7
1	X	39	LYS	2.7
1	V	232	ALA	2.7
1	V	256	PHE	2.7
1	V	507	ALA	2.7
1	W	329	ALA	2.7
1	D	344	THR	2.7
1	U	366	THR	2.7
1	W	183	LEU	2.7
1	X	344	THR	2.7
1	U	302	ASN	2.7
1	B	1	MET	2.7
1	B	332	GLU	2.7
1	D	189	VAL	2.7
1	U	455	VAL	2.7
1	B	469	ILE	2.7
1	A	489	ASP	2.7
1	B	119	ASP	2.7
1	N	495	ASP	2.7
1	U	392	ARG	2.7
1	W	328	ALA	2.7
1	U	499	LEU	2.7
1	Q	355[A]	GLU	2.7
1	W	203	GLU	2.7
1	R	348	VAL	2.7
1	V	535	CYS	2.7
1	V	333	LYS	2.7
1	U	511	GLY	2.7
1	W	384	GLY	2.7
1	W	398	GLY	2.7
1	H	345	GLN	2.6
1	A	494	GLU	2.6
1	H	267	GLU	2.6
1	R	353	ALA	2.6
1	V	468	GLU	2.6
1	U	219	LEU	2.6
1	U	379	LEU	2.6
1	V	272	LEU	2.6
1	V	321	LEU	2.6
1	W	37	LEU	2.6
1	A	252	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	489	ASP	2.6
1	U	504	SER	2.6
1	W	215	VAL	2.6
1	E	343	GLY	2.6
1	S	350	GLY	2.6
1	K	355[A]	GLU	2.6
1	V	203	GLU	2.6
1	W	537	GLU	2.6
1	W	243	ALA	2.6
1	E	344	THR	2.6
1	V	340	THR	2.6
1	K	347	PRO	2.6
1	W	259	LEU	2.6
1	M	207	ASP	2.6
1	W	229	VAL	2.6
1	W	471	ILE	2.6
1	A	350	GLY	2.6
1	L	345	GLN	2.6
1	A	271	GLU	2.6
1	U	42[A]	GLU	2.6
1	W	468	GLU	2.6
1	S	1	MET	2.6
1	W	529	ASN	2.6
1	U	290	ALA	2.6
1	W	361	THR	2.6
1	P	301	ASP	2.6
1	U	282	LEU	2.6
1	U	553	LYS	2.6
1	P	555	GLN	2.6
1	W	175	VAL	2.6
1	W	395	ILE	2.6
1	G	350	GLY	2.6
1	W	281	CYS	2.6
1	U	210	ASN	2.6
1	W	255	ASN	2.6
1	V	541	ALA	2.6
1	K	533	ASP	2.6
1	U	533	ASP	2.6
1	W	199	ASP	2.6
1	W	184	LEU	2.6
1	I	345	GLN	2.5
1	G	468	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	494	GLU	2.5
1	W	202	VAL	2.5
1	U	236	GLY	2.5
1	A	347	PRO	2.5
1	I	358	ALA	2.5
1	V	548	ALA	2.5
1	X	347	PRO	2.5
1	A	345	GLN	2.5
1	V	183	LEU	2.5
1	X	37	LEU	2.5
1	C	203	GLU	2.5
1	N	203	GLU	2.5
1	U	468	GLU	2.5
1	X	355[A]	GLU	2.5
1	W	373	ILE	2.5
1	W	460	ILE	2.5
1	U	255	ASN	2.5
1	B	555	GLN	2.5
1	U	361	THR	2.5
1	B	267	GLU	2.5
1	U	265	SER	2.5
1	U	381	ALA	2.5
1	U	537	GLU	2.5
1	W	271	GLU	2.5
1	U	253	HIS	2.5
1	V	229	VAL	2.5
1	U	519	ASN	2.5
1	W	535	CYS	2.5
1	I	207	ASP	2.5
1	K	301	ASP	2.5
1	U	363	ASP	2.5
1	W	252	ASP	2.5
1	W	495	ASP	2.5
1	L	555	GLN	2.5
1	P	342	GLN	2.5
1	U	342	GLN	2.5
1	W	225	GLU	2.5
1	W	172	ALA	2.5
1	W	238	ALA	2.5
1	W	331	ALA	2.5
1	W	36	LEU	2.5
1	U	497	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	343	GLY	2.5
1	C	343	GLY	2.5
1	H	343	GLY	2.5
1	Q	343	GLY	2.5
1	U	498	GLY	2.5
1	V	293	GLY	2.5
1	U	294	TRP	2.5
1	E	355[A]	GLU	2.4
1	H	489	ASP	2.4
1	I	307	ASP	2.4
1	P	119	ASP	2.4
1	U	494	GLU	2.4
1	W	309	ASP	2.4
1	X	555	GLN	2.4
1	V	238	ALA	2.4
1	W	432	MET	2.4
1	O	350	GLY	2.4
1	D	355[A]	GLU	2.4
1	I	355	GLU	2.4
1	O	352	GLU	2.4
1	B	376	ASP	2.4
1	H	301	ASP	2.4
1	U	460	ILE	2.4
1	W	364	GLU	2.4
1	W	510	GLU	2.4
1	X	351	ILE	2.4
1	U	261	TRP	2.4
1	A	344	THR	2.4
1	U	454	PRO	2.4
1	V	554	PRO	2.4
1	W	394	PRO	2.4
1	S	39	LYS	2.4
1	U	329	ALA	2.4
1	U	470	ALA	2.4
1	V	196	ALA	2.4
1	W	390	ALA	2.4
1	X	544	LYS	2.4
1	W	214	LEU	2.4
1	W	372	LEU	2.4
1	I	343	GLY	2.4
1	S	355[A]	GLU	2.4
1	U	368	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	W	489	ASP	2.4
1	W	453	ILE	2.4
1	W	456	ILE	2.4
1	E	1	MET	2.4
1	W	365	MET	2.4
1	W	431	MET	2.4
1	U	337	ARG	2.4
1	X	520	ARG	2.4
1	V	329	ALA	2.4
1	W	379	LEU	2.4
1	J	468	GLU	2.4
1	P	271	GLU	2.4
1	U	225	GLU	2.4
1	V	506	GLY	2.4
1	C	495	ASP	2.4
1	H	533	ASP	2.4
1	W	286	PHE	2.4
1	R	15	ILE	2.4
1	S	348	VAL	2.4
1	U	215	VAL	2.4
1	U	279	ILE	2.4
1	W	305	VAL	2.4
1	V	391[A]	SER	2.4
1	U	536	THR	2.4
1	V	195	THR	2.4
1	U	254	PRO	2.4
1	V	260	TYR	2.3
1	B	353	ALA	2.3
1	P	188	GLU	2.3
1	V	231	LEU	2.3
1	W	219	LEU	2.3
1	M	343	GLY	2.3
1	E	301	ASP	2.3
1	V	337	ARG	2.3
1	W	521	ARG	2.3
1	U	239	VAL	2.3
1	U	524	THR	2.3
1	V	549	THR	2.3
1	W	325	THR	2.3
1	W	377	THR	2.3
1	T	271	GLU	2.3
1	V	342	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	531	ALA	2.3
1	U	503	ALA	2.3
1	W	283	ALA	2.3
1	V	262	GLY	2.3
1	V	539	LEU	2.3
1	F	252	ASP	2.3
1	L	533	ASP	2.3
1	U	463	ARG	2.3
1	V	39	LYS	2.3
1	W	306	MET	2.3
1	V	336	SER	2.3
1	V	180	ILE	2.3
1	X	469	ILE	2.3
1	A	267	GLU	2.3
1	T	355[A]	GLU	2.3
1	U	325	THR	2.3
1	O	354	ALA	2.3
1	F	495	ASP	2.3
1	J	533	ASP	2.3
1	K	343	GLY	2.3
1	K	495	ASP	2.3
1	O	495	ASP	2.3
1	Q	252	ASP	2.3
1	W	376	ASP	2.3
1	F	494	GLU	2.3
1	G	42[A]	GLU	2.3
1	M	494	GLU	2.3
1	R	332	GLU	2.3
1	V	504	SER	2.3
1	W	296	SER	2.3
1	W	386	SER	2.3
1	V	249	PHE	2.3
1	E	555	GLN	2.3
1	I	555	GLN	2.3
1	W	532	GLN	2.3
1	X	471	ILE	2.3
1	O	348	VAL	2.3
1	W	455	VAL	2.3
1	U	312	THR	2.3
1	V	338	PRO	2.3
1	W	192	THR	2.3
1	W	366	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	W	337	ARG	2.3
1	A	533	ASP	2.3
1	G	495	ASP	2.3
1	I	353	ALA	2.3
1	I	376	ASP	2.3
1	M	301	ASP	2.3
1	Q	301	ASP	2.3
1	S	495	ASP	2.3
1	S	518	ASP	2.3
1	V	252	ASP	2.3
1	V	493	ASP	2.3
1	W	197	ALA	2.3
1	W	230	ALA	2.3
1	W	276	ALA	2.3
1	U	35	LEU	2.3
1	U	280	LEU	2.3
1	D	352	GLU	2.2
1	R	469	ILE	2.2
1	U	457	ILE	2.2
1	V	366	THR	2.2
1	W	505	THR	2.2
1	B	463	ARG	2.2
1	W	208	ARG	2.2
1	E	495	ASP	2.2
1	R	518	ASP	2.2
1	H	350	GLY	2.2
1	Q	354	ALA	2.2
1	V	300	GLY	2.2
1	W	262	GLY	2.2
1	W	464	GLY	2.2
1	X	343	GLY	2.2
1	U	459	LEU	2.2
1	Q	42[A]	GLU	2.2
1	U	508	GLU	2.2
1	U	429	HIS	2.2
1	V	497	HIS	2.2
1	W	322	SER	2.2
1	G	348	VAL	2.2
1	H	546	VAL	2.2
1	Q	347	PRO	2.2
1	Q	351	ILE	2.2
1	T	469	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	492	ASN	2.2
1	V	430	ILE	2.2
1	V	544	LYS	2.2
1	W	311	VAL	2.2
1	C	207	ASP	2.2
1	N	1	MET	2.2
1	V	199	ASP	2.2
1	V	518	ASP	2.2
1	V	496	GLY	2.2
1	I	331	ALA	2.2
1	Q	353	ALA	2.2
1	S	468	GLU	2.2
1	T	353	ALA	2.2
1	V	245	ALA	2.2
1	W	141	GLU	2.2
1	W	201	ALA	2.2
1	X	271	GLU	2.2
1	V	253	HIS	2.2
1	A	463	ARG	2.2
1	V	367	ARG	2.2
1	W	234	ARG	2.2
1	E	39	LYS	2.2
1	W	553	LYS	2.2
1	V	255	ASN	2.2
1	W	389	ASN	2.2
1	C	1	MET	2.2
1	H	252	ASP	2.2
1	P	189	VAL	2.2
1	V	194	VAL	2.2
1	W	44	VAL	2.2
1	E	188	GLU	2.2
1	L	355[A]	GLU	2.2
1	R	355[A]	GLU	2.2
1	S	271	GLU	2.2
1	S	494	GLU	2.2
1	U	522	GLY	2.2
1	V	236	GLY	2.2
1	V	537	GLU	2.2
1	W	426	GLU	2.2
1	U	367	ARG	2.2
1	V	266	SER	2.2
1	W	182	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	389	ASN	2.2
1	V	357	ASN	2.2
1	W	357	ASN	2.2
1	M	344	THR	2.2
1	U	307	ASP	2.2
1	V	489	ASP	2.2
1	V	538	THR	2.2
1	X	252	ASP	2.2
1	C	469	ILE	2.1
1	G	494	GLU	2.1
1	U	388	PHE	2.1
1	U	402	GLU	2.1
1	U	449	ILE	2.1
1	V	251	GLU	2.1
1	V	267	GLU	2.1
1	P	348	VAL	2.1
1	U	466	VAL	2.1
1	X	175	VAL	2.1
1	O	343	GLY	2.1
1	W	293	GLY	2.1
1	I	346	ALA	2.1
1	L	346	ALA	2.1
1	P	353	ALA	2.1
1	U	548	ALA	2.1
1	V	327	ALA	2.1
1	U	330	LEU	2.1
1	W	304	MET	2.1
1	D	301	ASP	2.1
1	G	301	ASP	2.1
1	O	518	ASP	2.1
1	V	271	GLU	2.1
1	W	173	GLU	2.1
1	W	207	ASP	2.1
1	W	277	ASP	2.1
1	O	347	PRO	2.1
1	W	378	THR	2.1
1	G	471	ILE	2.1
1	I	351	ILE	2.1
1	M	555	GLN	2.1
1	U	248	PHE	2.1
1	W	313	PHE	2.1
1	W	513	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	189	VAL	2.1
1	K	348	VAL	2.1
1	L	348	VAL	2.1
1	U	315	GLY	2.1
1	V	311	VAL	2.1
1	B	354	ALA	2.1
1	U	547	ALA	2.1
1	V	390	ALA	2.1
1	V	470	ALA	2.1
1	W	65	ALA	2.1
1	W	223	ALA	2.1
1	U	226	LYS	2.1
1	W	459	LEU	2.1
1	J	352	GLU	2.1
1	J	494	GLU	2.1
1	P	267	GLU	2.1
1	U	332	GLU	2.1
1	U	510	GLU	2.1
1	X	267	GLU	2.1
1	A	376	ASP	2.1
1	E	207	ASP	2.1
1	K	119	ASP	2.1
1	P	199	ASP	2.1
1	Q	518	ASP	2.1
1	R	252	ASP	2.1
1	S	119	ASP	2.1
1	U	207	ASP	2.1
1	U	549	THR	2.1
1	V	471	ILE	2.1
1	W	400	ARG	2.1
1	U	204	TRP	2.1
1	I	189	VAL	2.1
1	U	194	VAL	2.1
1	T	333	LYS	2.1
1	H	358	ALA	2.1
1	K	353	ALA	2.1
1	V	269	ALA	2.1
1	V	512	ALA	2.1
1	V	360	LEU	2.1
1	J	355[A]	GLU	2.1
1	K	468	GLU	2.1
1	K	537[A]	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	352	GLU	2.1
1	W	47	CYS	2.1
1	X	207	ASP	2.1
1	U	532	GLN	2.1
1	V	478	TYR	2.1
1	V	545	ARG	2.1
1	W	463	ARG	2.1
1	U	500	GLY	2.1
1	W	397	GLY	2.1
1	C	467	ILE	2.1
1	F	469	ILE	2.1
1	W	457	ILE	2.1
1	W	326	PHE	2.1
1	W	458	PHE	2.1
1	V	482	TRP	2.1
1	G	346	ALA	2.1
1	J	188	GLU	2.0
1	O	203	GLU	2.0
1	O	355	GLU	2.0
1	W	62	ALA	2.1
1	W	242	MET	2.0
1	S	349	LEU	2.0
1	U	36	LEU	2.0
1	V	259	LEU	2.0
1	U	529	ASN	2.0
1	W	181	ASN	2.0
1	K	207	ASP	2.0
1	K	345	GLN	2.0
1	V	119	ASP	2.0
1	V	281	CYS	2.0
1	W	528	CYS	2.0
1	X	47	CYS	2.0
1	R	520	ARG	2.0
1	U	428	ARG	2.0
1	U	335	PRO	2.0
1	X	179	PRO	2.0
1	V	553	LYS	2.0
1	U	262	GLY	2.0
1	D	467	ILE	2.0
1	I	467	ILE	2.0
1	U	15	ILE	2.0
1	G	271	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	468	GLU	2.0
1	O	267	GLU	2.0
1	U	274	GLU	2.0
1	V	188	GLU	2.0
1	V	303	VAL	2.0
1	W	285	VAL	2.0
1	W	508	GLU	2.0
1	O	346	ALA	2.0
1	Q	358	ALA	2.0
1	W	244	ALA	2.0
1	W	503	ALA	2.0
1	W	531	ALA	2.0
1	V	210	ASN	2.0
1	E	345	GLN	2.0
1	I	209	GLN	2.0
1	S	342	GLN	2.0
1	U	487	LEU	2.0
1	V	282	LEU	2.0
1	B	252	ASP	2.0
1	H	518	ASP	2.0
1	J	301	ASP	2.0
1	P	39	LYS	2.0
1	V	226	LYS	2.0
1	V	514	LYS	2.0
1	G	344	THR	2.0
1	V	505	THR	2.0
1	I	350	GLY	2.0
1	U	474	GLY	2.0
1	U	543	GLY	2.0
1	W	543	GLY	2.0
1	V	2	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	I	603	4/4	0.75	0.29	56,58,58,58	0
4	EDO	A	603	4/4	0.76	0.29	42,42,43,44	0
4	EDO	R	603	4/4	0.76	0.29	53,55,55,57	0
4	EDO	N	603	4/4	0.77	0.27	48,51,52,54	0
4	EDO	Q	603	4/4	0.79	0.29	57,59,60,60	0
4	EDO	F	601	4/4	0.87	0.20	50,50,51,51	0
3	TPP	W	602	26/26	0.89	0.14	34,39,50,53	0
3	TPP	V	602	26/26	0.92	0.11	27,38,41,45	0
3	TPP	U	602	26/26	0.92	0.11	27,36,42,46	0
3	TPP	X	602	26/26	0.94	0.09	23,27,32,35	0
3	TPP	K	602	26/26	0.94	0.09	19,21,29,34	0
3	TPP	L	602	26/26	0.94	0.09	17,20,24,27	0
3	TPP	Q	602	26/26	0.94	0.09	17,22,27,30	0
3	TPP	A	602	26/26	0.94	0.10	19,23,31,36	0
3	TPP	B	602	26/26	0.94	0.10	21,27,32,36	0
3	TPP	D	602	26/26	0.94	0.09	15,17,22,25	0
3	TPP	G	602	26/26	0.95	0.09	18,23,27,29	0
3	TPP	P	602	26/26	0.95	0.08	16,22,26,29	0
3	TPP	H	602	26/26	0.95	0.09	19,23,27,30	0
3	TPP	R	602	26/26	0.95	0.09	17,22,27,32	0
3	TPP	S	602	26/26	0.95	0.08	18,20,26,30	0
3	TPP	T	602	26/26	0.95	0.09	19,23,28,34	0
3	TPP	I	602	26/26	0.95	0.08	16,19,25,29	0
3	TPP	F	603	26/26	0.95	0.08	13,16,20,24	0
3	TPP	J	602	26/26	0.96	0.07	16,18,22,25	0
2	MG	W	601	1/1	0.96	0.05	37,37,37,37	0
3	TPP	E	602	26/26	0.96	0.07	13,15,21,23	0
3	TPP	M	602	26/26	0.96	0.08	13,15,19,22	0
3	TPP	N	602	26/26	0.96	0.08	12,14,19,24	0
3	TPP	O	602	26/26	0.96	0.08	18,19,25,27	0
3	TPP	C	602	26/26	0.96	0.07	14,16,20,23	0
2	MG	P	601	1/1	0.97	0.04	21,21,21,21	0
2	MG	S	601	1/1	0.97	0.03	23,23,23,23	0
2	MG	U	601	1/1	0.97	0.04	31,31,31,31	0
2	MG	V	601	1/1	0.97	0.04	34,34,34,34	0
2	MG	D	601	1/1	0.97	0.03	22,22,22,22	0
2	MG	E	601	1/1	0.97	0.02	14,14,14,14	0

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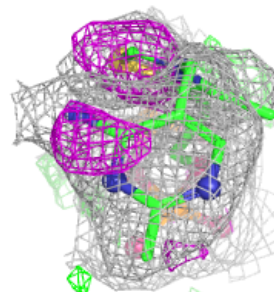
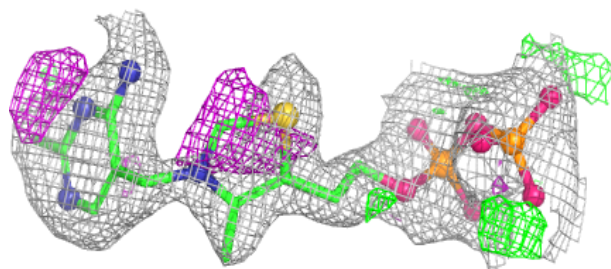
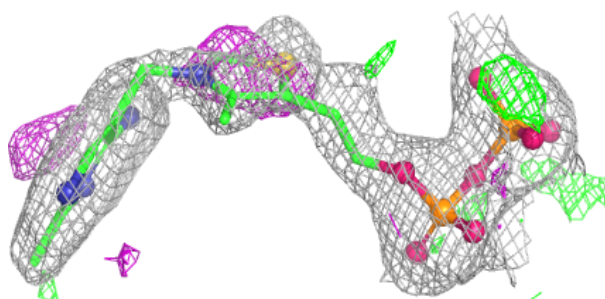
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	H	601	1/1	0.97	0.04	19,19,19,19	0
2	MG	A	601	1/1	0.98	0.04	25,25,25,25	0
2	MG	T	601	1/1	0.98	0.03	19,19,19,19	0
2	MG	M	601	1/1	0.98	0.02	13,13,13,13	0
2	MG	B	601	1/1	0.98	0.04	25,25,25,25	0
2	MG	R	601	1/1	0.98	0.04	25,25,25,25	0
2	MG	X	601	1/1	0.98	0.04	32,32,32,32	0
2	MG	O	601	1/1	0.99	0.03	17,17,17,17	0
2	MG	G	601	1/1	0.99	0.03	21,21,21,21	0
2	MG	Q	601	1/1	0.99	0.02	22,22,22,22	0
2	MG	C	601	1/1	0.99	0.04	13,13,13,13	0
2	MG	I	601	1/1	0.99	0.03	19,19,19,19	0
2	MG	J	601	1/1	0.99	0.04	15,15,15,15	0
2	MG	K	601	1/1	0.99	0.02	23,23,23,23	0
2	MG	L	601	1/1	0.99	0.02	24,24,24,24	0
2	MG	F	602	1/1	0.99	0.02	15,15,15,15	0
2	MG	N	601	1/1	0.99	0.01	11,11,11,11	0

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

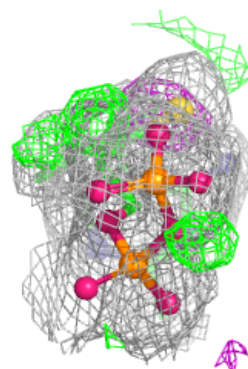
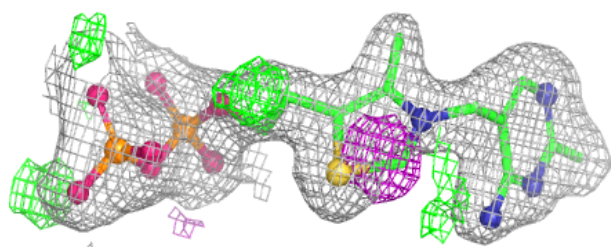
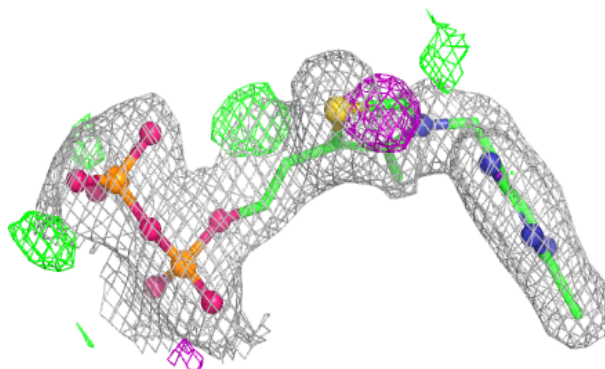
Electron density around TPP W 602:

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

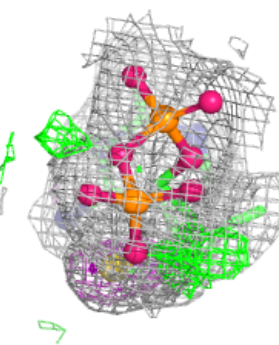
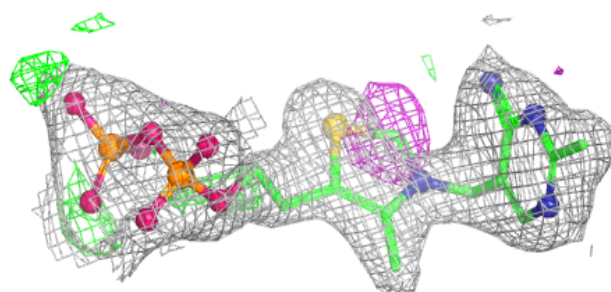
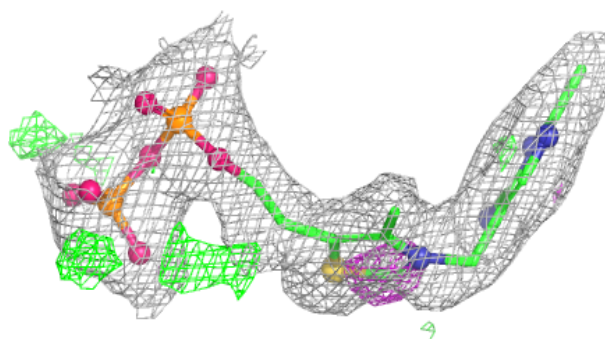


Electron density around TPP V 602:

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

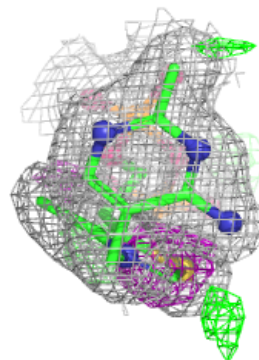
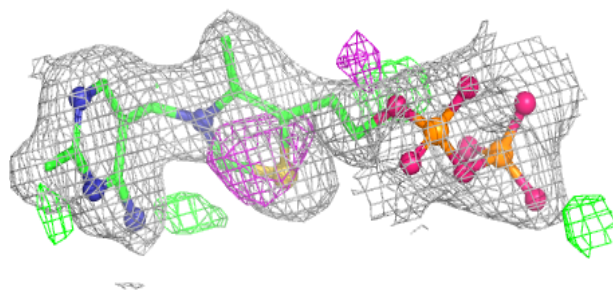
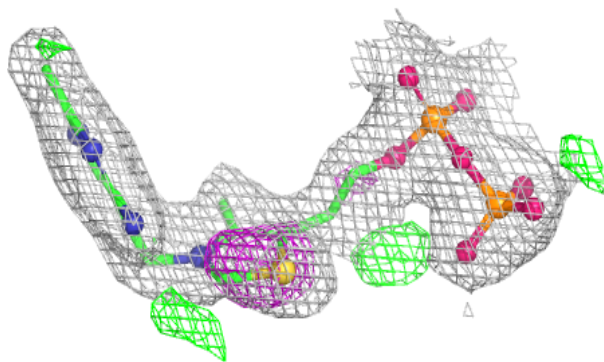
**Electron density around TPP U 602:**

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

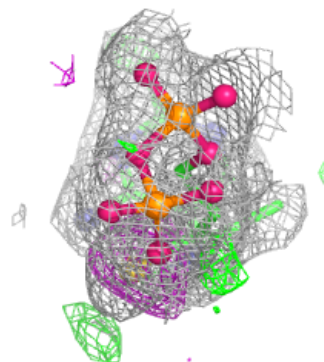
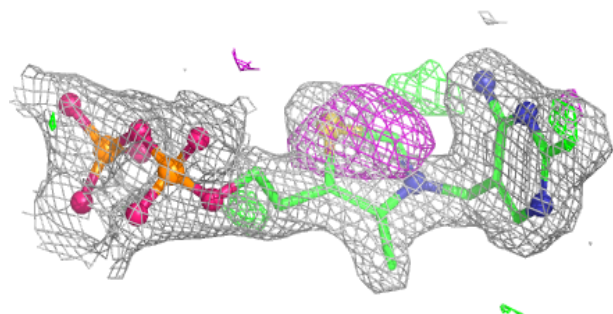
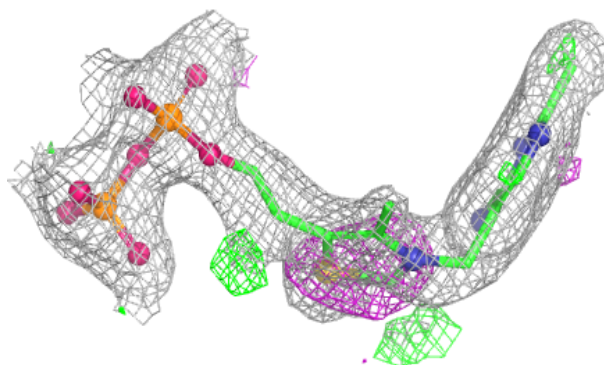


Electron density around TPP X 602:

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

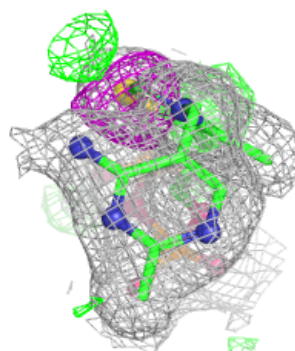
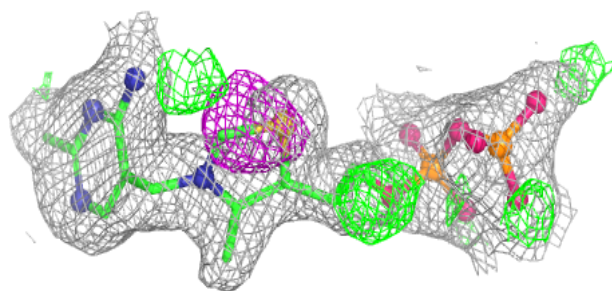
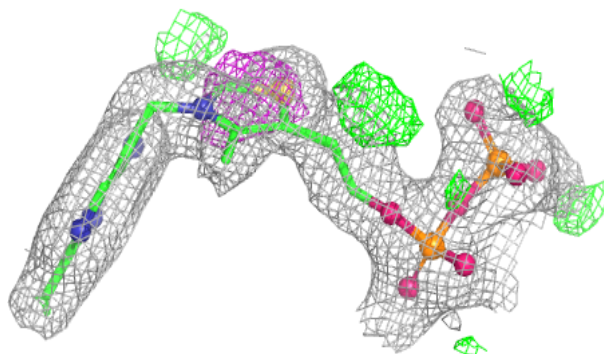
**Electron density around TPP K 602:**

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

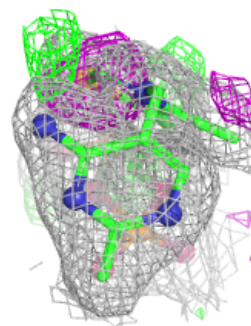
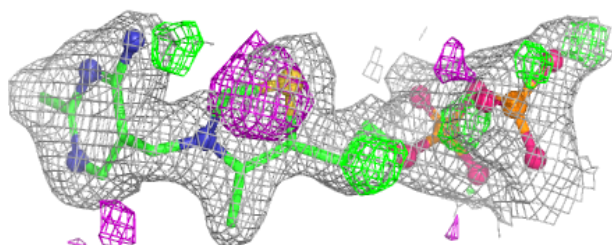
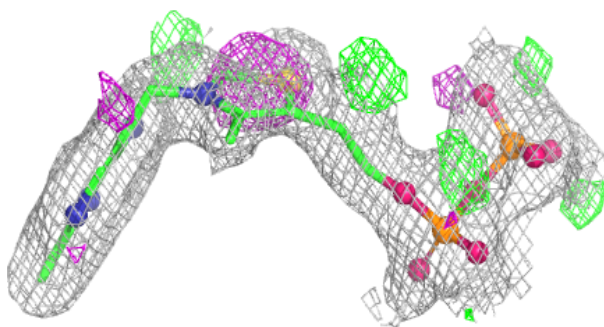


Electron density around TPP L 602:

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

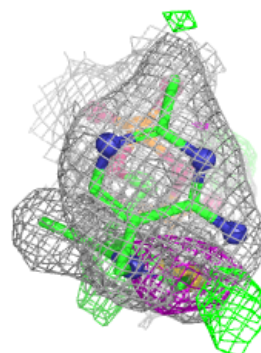
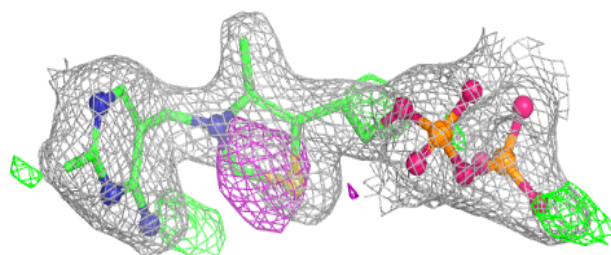
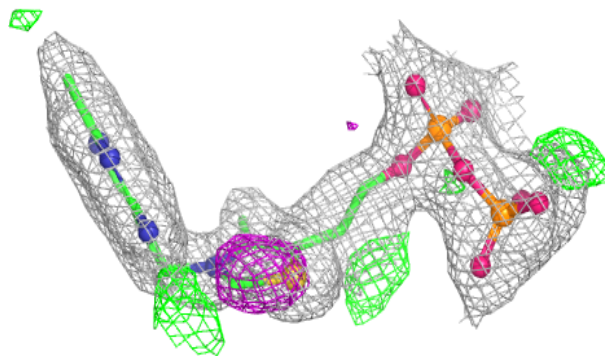
**Electron density around TPP Q 602:**

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

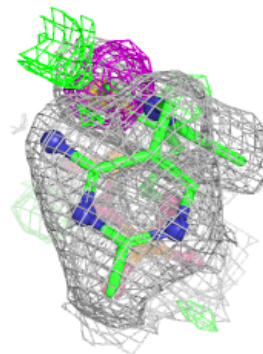
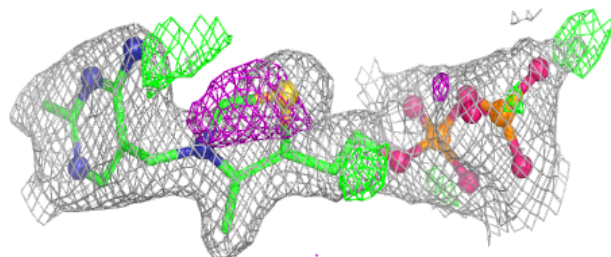
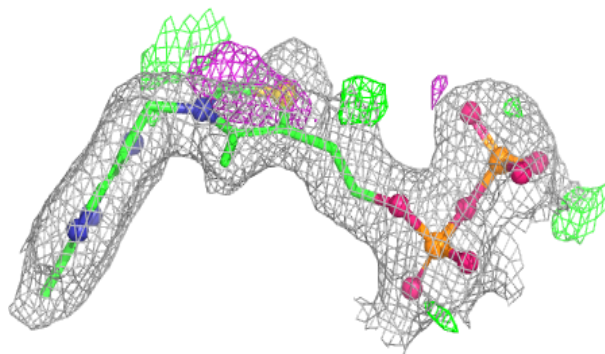


Electron density around TPP A 602:

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

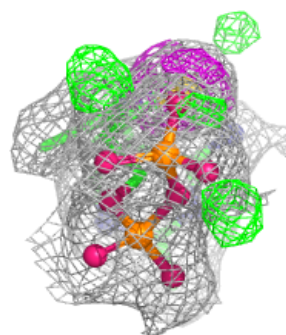
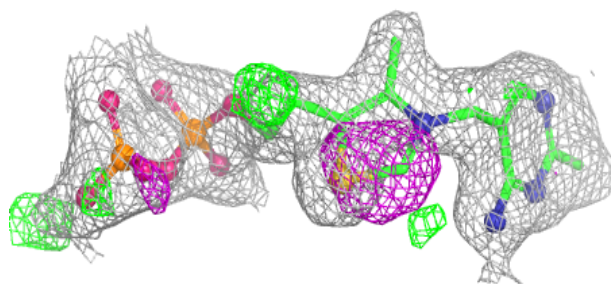
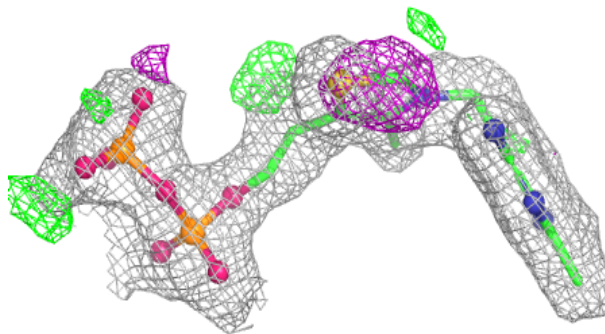
**Electron density around TPP B 602:**

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

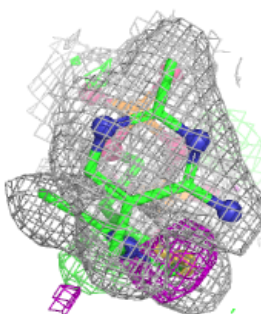
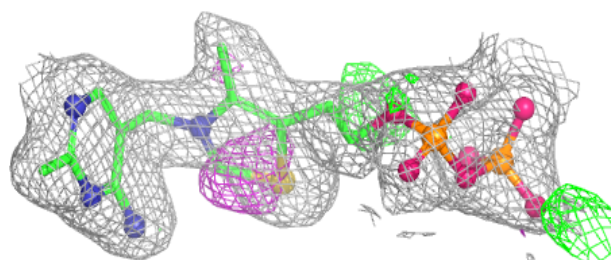
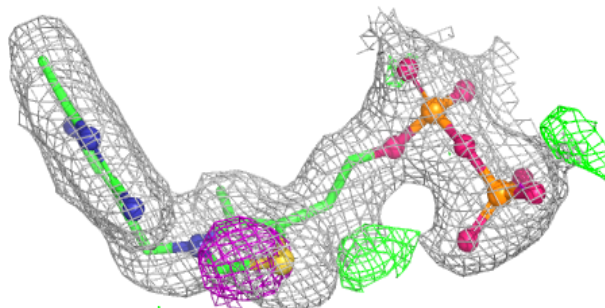


Electron density around TPP D 602:

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

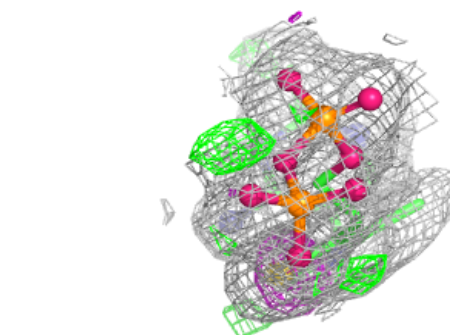
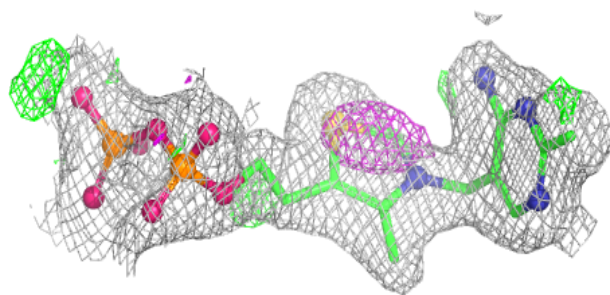
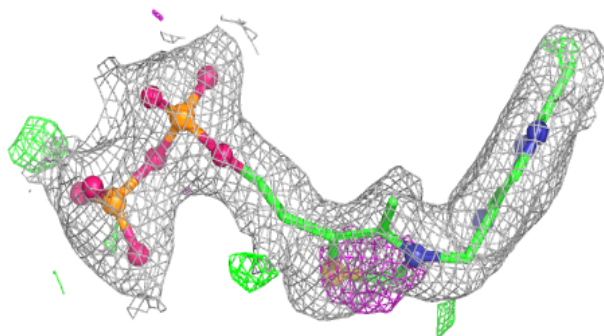
**Electron density around TPP G 602:**

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

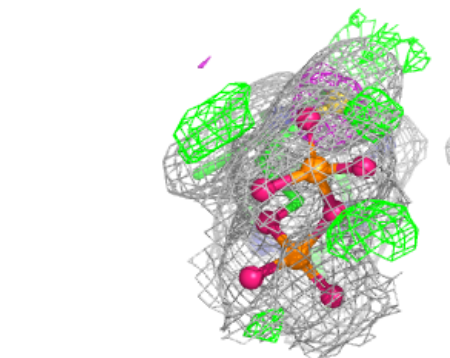
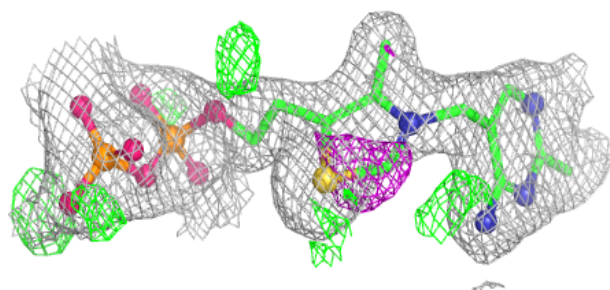
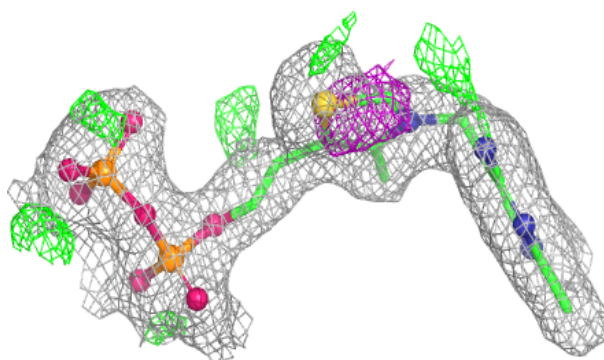


Electron density around TPP P 602:

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

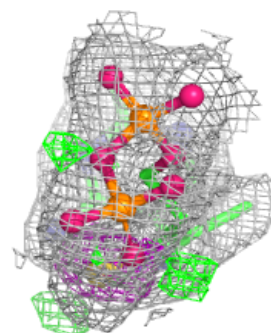
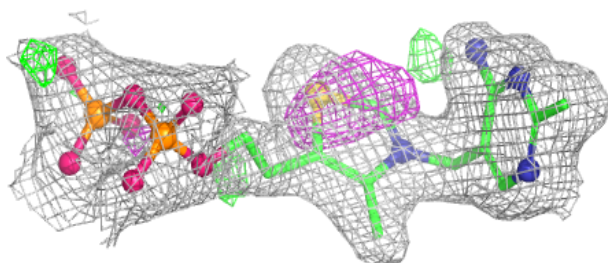
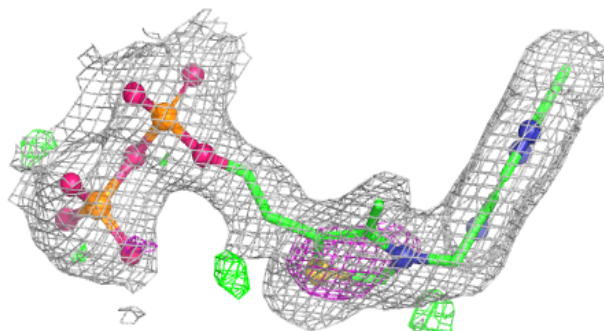
**Electron density around TPP H 602:**

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

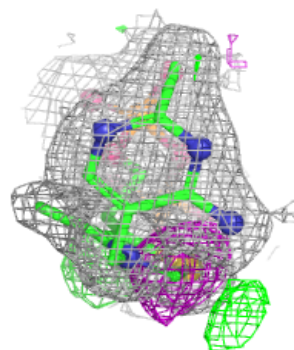
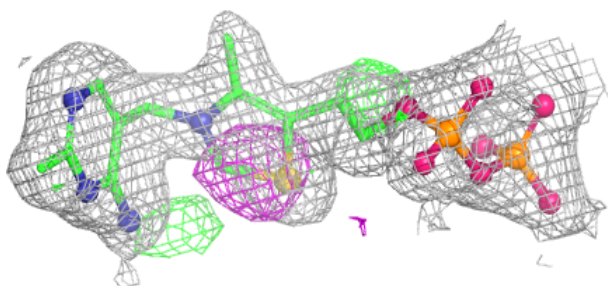
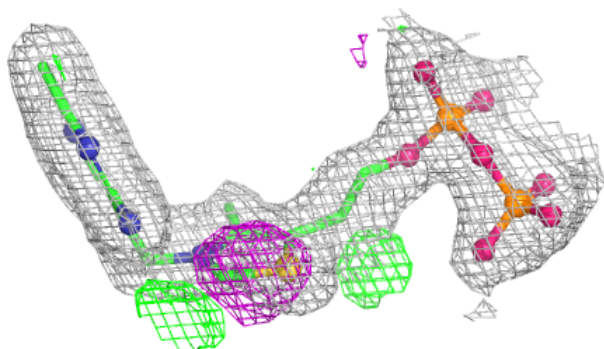


Electron density around TPP R 602:

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

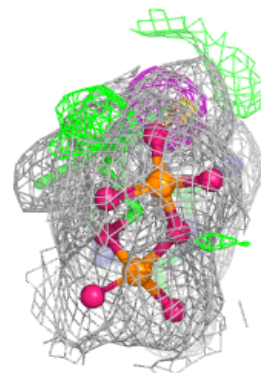
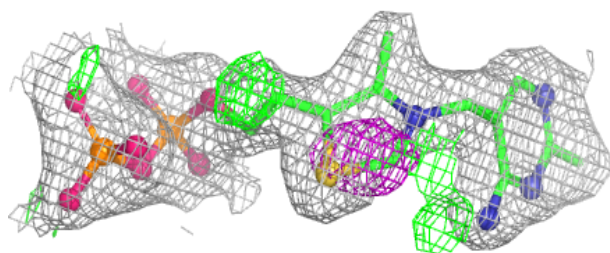
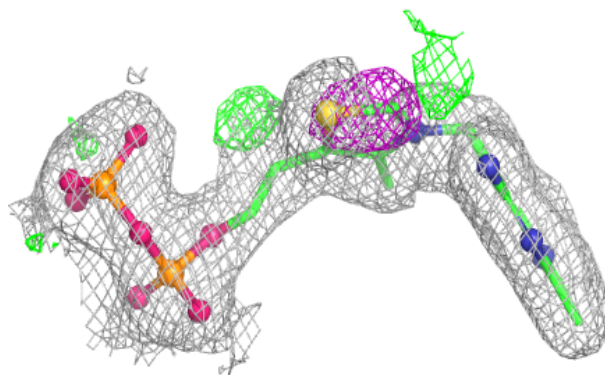
**Electron density around TPP S 602:**

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

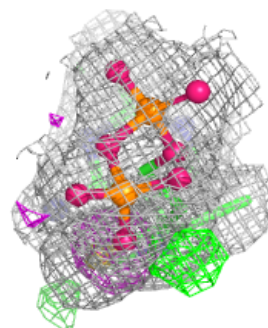
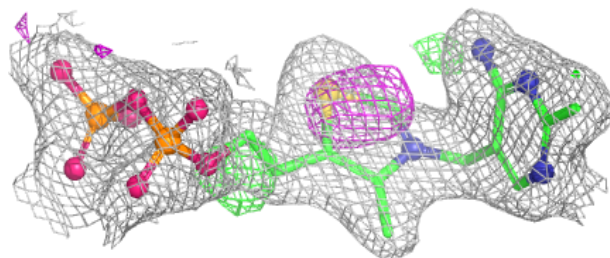
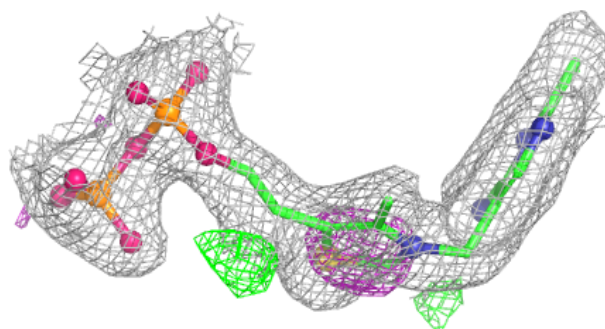


Electron density around TPP T 602:

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

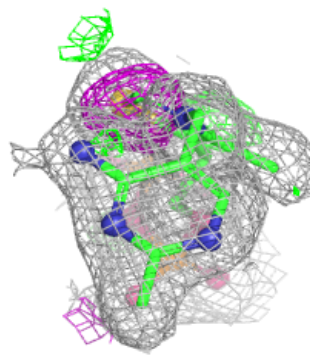
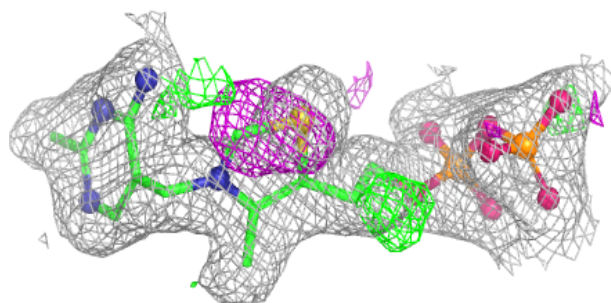
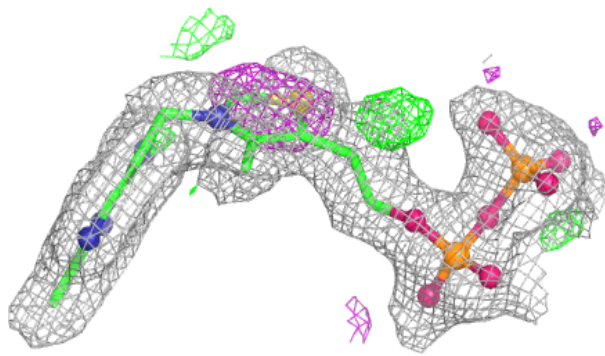
**Electron density around TPP I 602:**

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

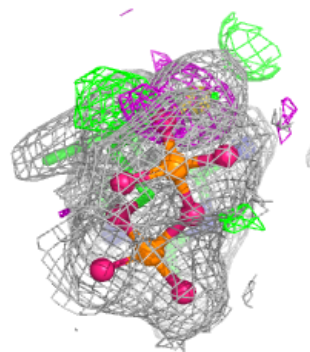
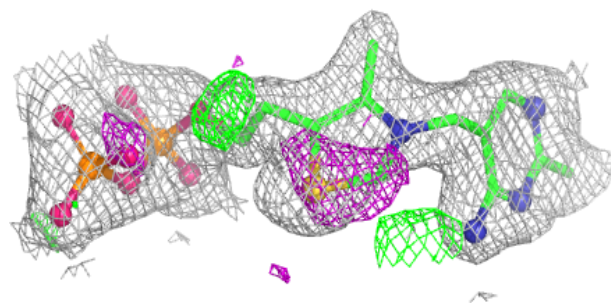
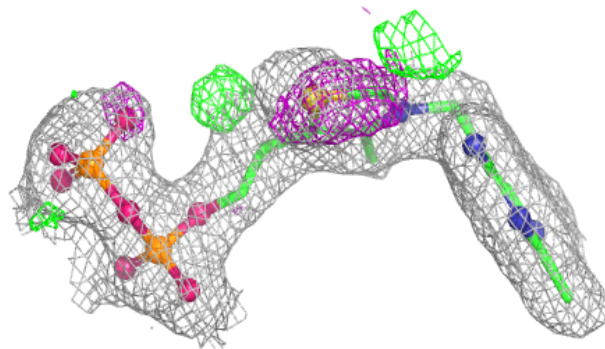


Electron density around TPP F 603:

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

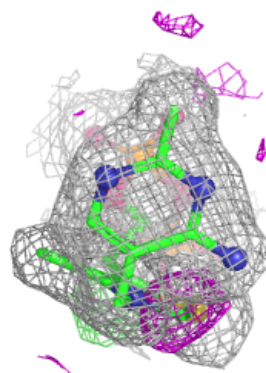
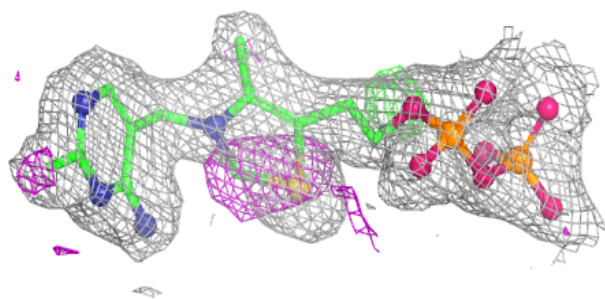
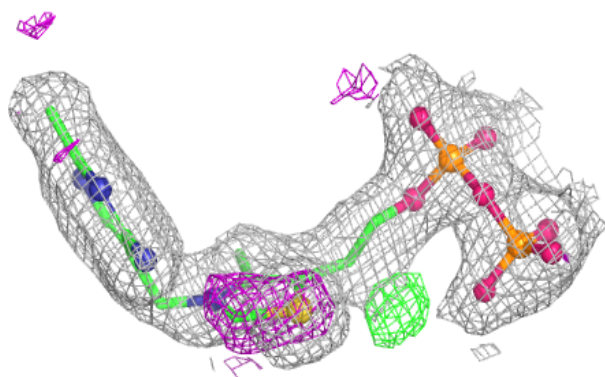
**Electron density around TPP J 602:**

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

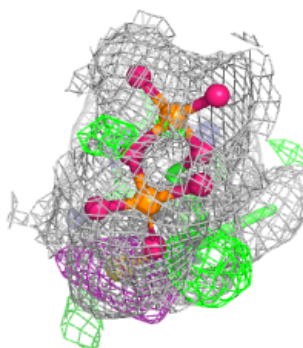
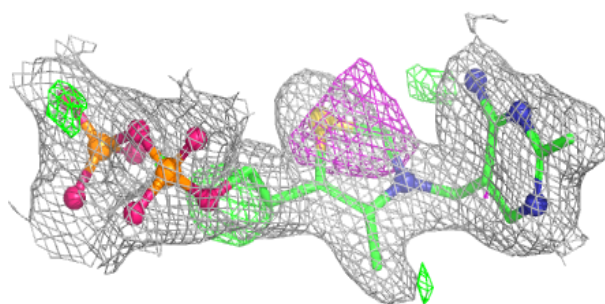
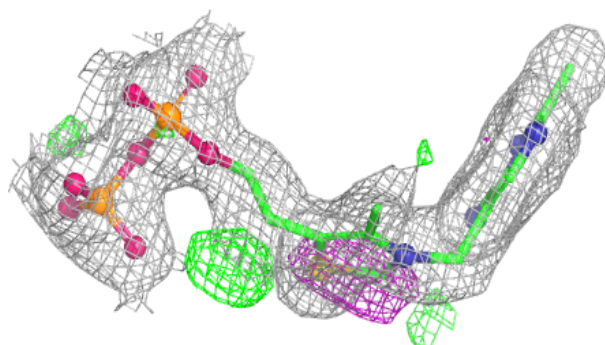


Electron density around TPP E 602:

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

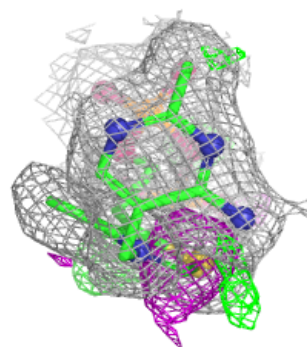
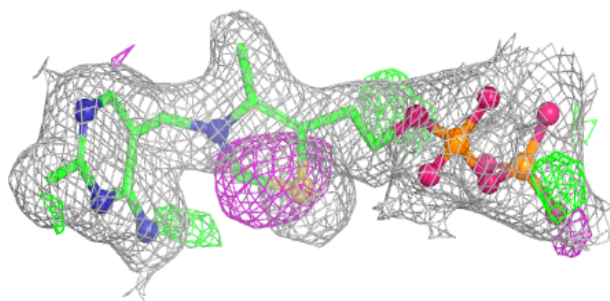
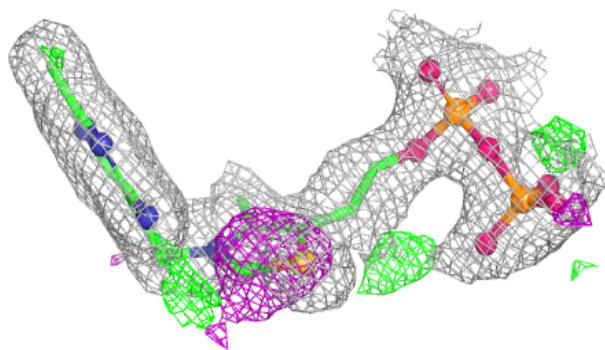
**Electron density around TPP M 602:**

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

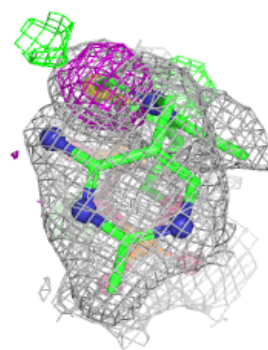
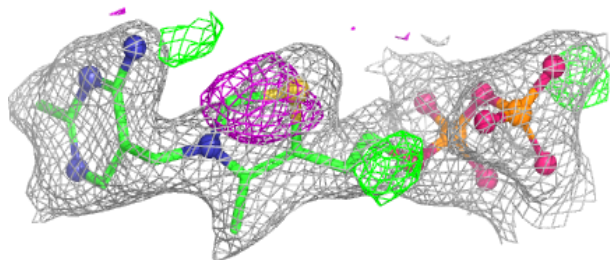
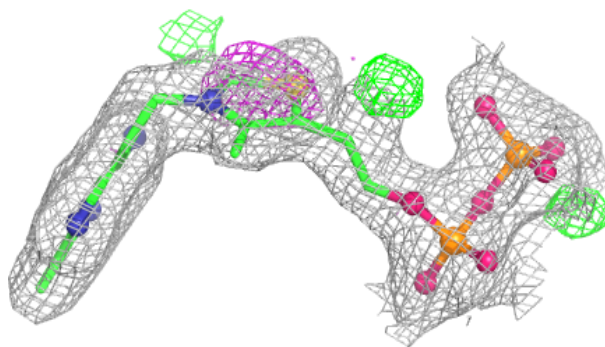


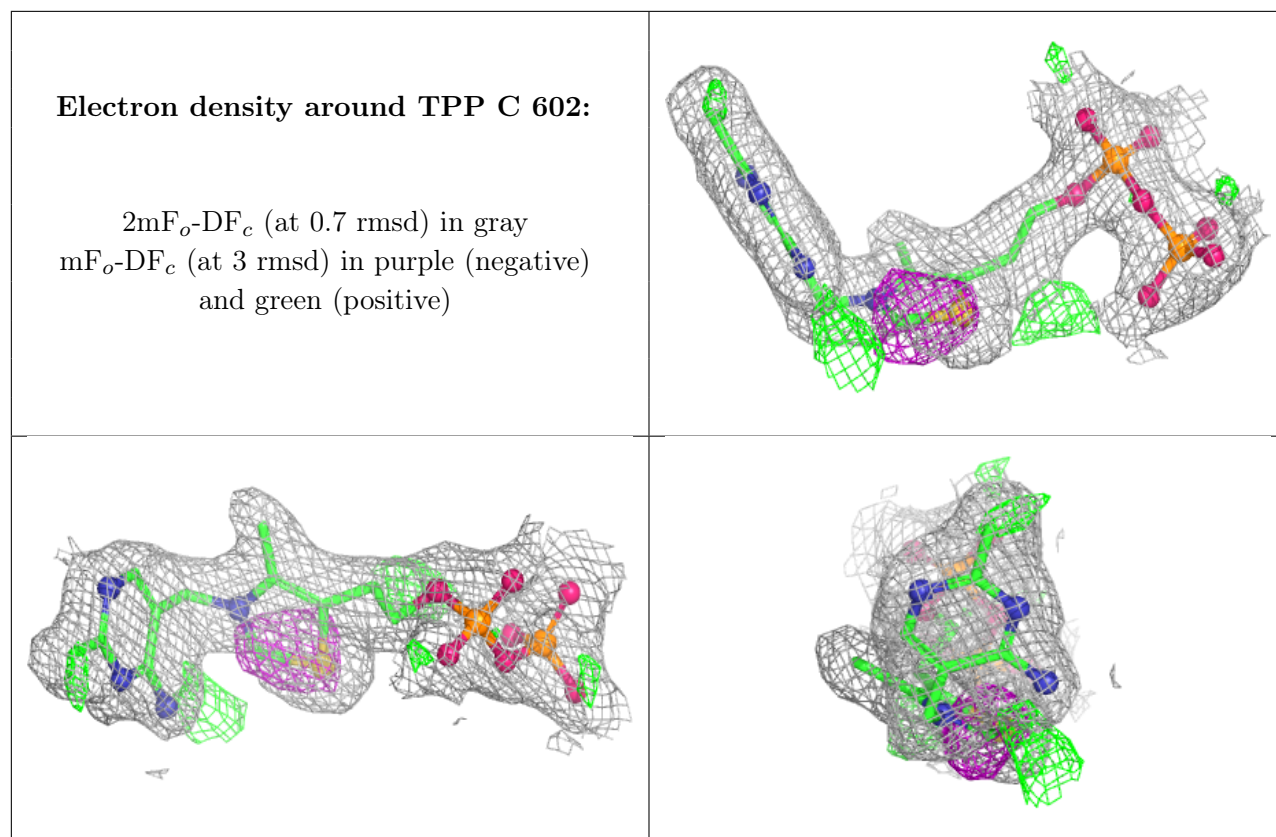
Electron density around TPP N 602:

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

**Electron density around TPP O 602:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.