



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2025 – 02:17 PM JST

PDB ID : 8Y7S
Title : Crystal structure of a benzaldehyde lyase mutant M6 from *Herbiconiux* sp. SALV-R1
Authors : Li, Y.; Zhang, Y.F.; Chen, Y.Y.; Liu, W.D.; Yao, P.Y.; Wu, Q.Q.; Zhu, D.M.
Deposited on : 2024-02-05
Resolution : 2.68 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:

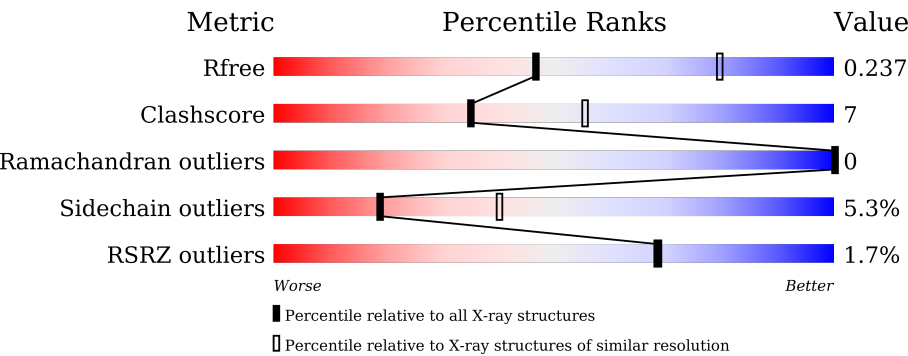
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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	558	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%85%14%.</div>
1	B	558	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%82%18%.</div>
1	C	558	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%82%17%.</div>
1	D	558	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%84%15%.</div>
1	E	558	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%84%15%..</div>
1	F	558	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%85%12%..</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	558	<div><div></div><div>2%84%15%.</div></div>
1	H	558	<div><div></div><div>%80%17%..</div></div>
1	I	558	<div><div></div><div>2%80%17%..</div></div>
1	J	558	<div><div></div><div>2%82%16%..</div></div>
1	K	558	<div><div></div><div>3%82%16%..</div></div>
1	L	558	<div><div></div><div>%78%20%..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 49634 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 Thiamine pyrophosphate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4064	2553	730	775	6			
1	B	557	Total	C	N	O	S	0	0	0
			4088	2566	733	783	6			
1	C	557	Total	C	N	O	S	0	0	0
			4085	2565	733	781	6			
1	D	557	Total	C	N	O	S	0	0	0
			4088	2566	733	783	6			
1	E	554	Total	C	N	O	S	0	0	0
			4054	2546	726	776	6			
1	F	554	Total	C	N	O	S	0	0	0
			4059	2549	730	774	6			
1	G	557	Total	C	N	O	S	0	0	0
			4066	2554	726	780	6			
1	H	553	Total	C	N	O	S	0	0	0
			4029	2530	722	771	6			
1	I	552	Total	C	N	O	S	0	0	0
			3963	2496	690	771	6			
1	J	553	Total	C	N	O	S	0	0	0
			4027	2534	720	767	6			
1	K	550	Total	C	N	O	S	0	0	0
			3980	2502	712	760	6			
1	L	553	Total	C	N	O	S	0	0	0
			4019	2530	720	763	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
A	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
A	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
A	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
A	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0

Continued on next page...

Continued from previous page...

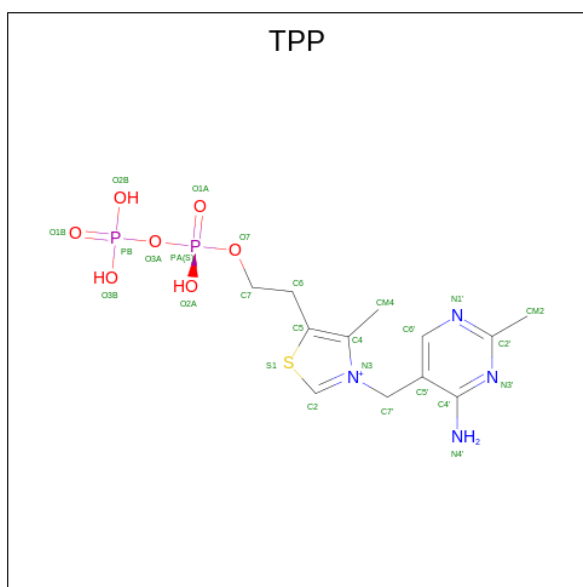
Chain	Residue	Modelled	Actual	Comment	Reference
A	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
B	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
B	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
B	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
B	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
B	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
B	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
C	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
C	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
C	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
C	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
C	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
C	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
D	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
D	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
D	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
D	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
D	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
D	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
E	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
E	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
E	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
E	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
E	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
E	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
F	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
F	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
F	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
F	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
F	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
F	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
G	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
G	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
G	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
G	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
G	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
G	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
H	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
H	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
H	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
H	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
H	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
I	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
I	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
I	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
I	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
I	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
I	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
J	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
J	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
J	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
J	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
J	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
J	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
K	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
K	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
K	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
K	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
K	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
K	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
L	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
L	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
L	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
L	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
L	552	LEU	ILE	engineered mutation	UNP A0A6M5J4S0
L	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	94	Total O 94 94	0	0
4	B	101	Total O 101 101	0	0
4	C	77	Total O 77 77	0	0
4	D	69	Total O 69 69	0	0
4	E	60	Total O 60 60	0	0
4	F	84	Total O 84 84	0	0
4	G	61	Total O 61 61	0	0
4	H	54	Total O 54 54	0	0

Continued on next page...

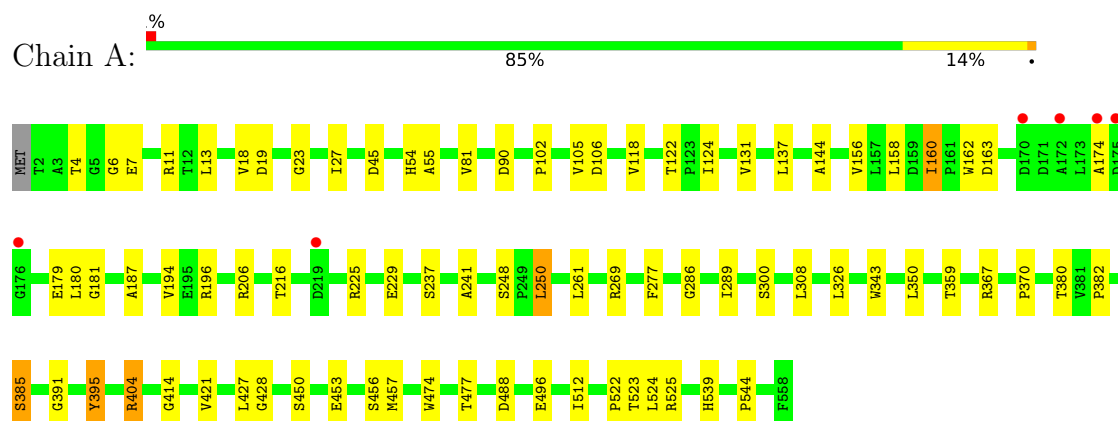
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	35	Total 35	O 35	0	0
4	J	58	Total 58	O 58	0	0
4	K	54	Total 54	O 54	0	0
4	L	41	Total 41	O 41	0	0

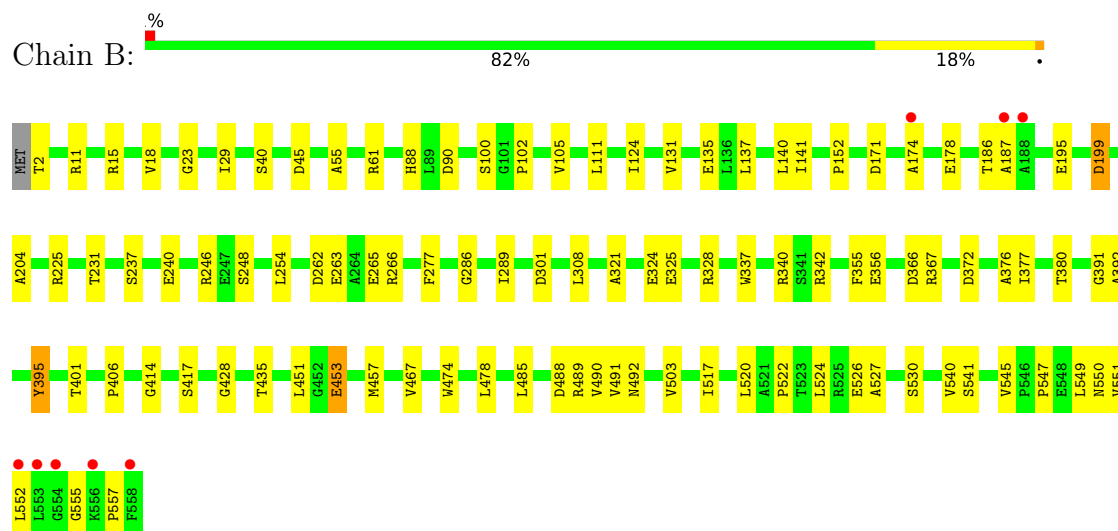
3 Residue-property plots [i](#)

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

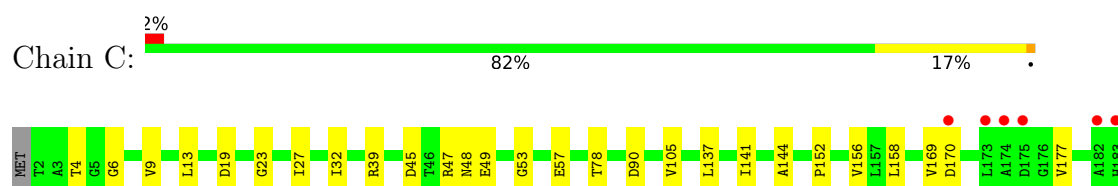
• Molecule 1: Thiamine pyrophosphate-binding protein

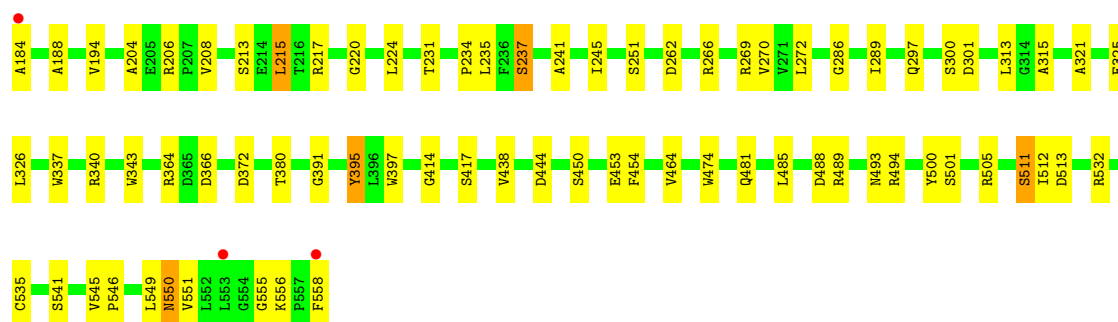


• Molecule 1: Thiamine pyrophosphate-binding protein

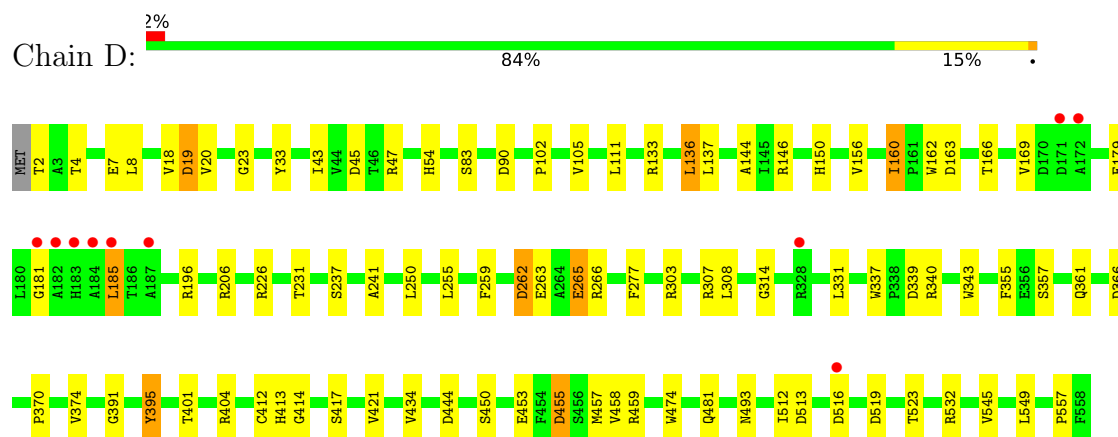


• Molecule 1: Thiamine pyrophosphate-binding protein

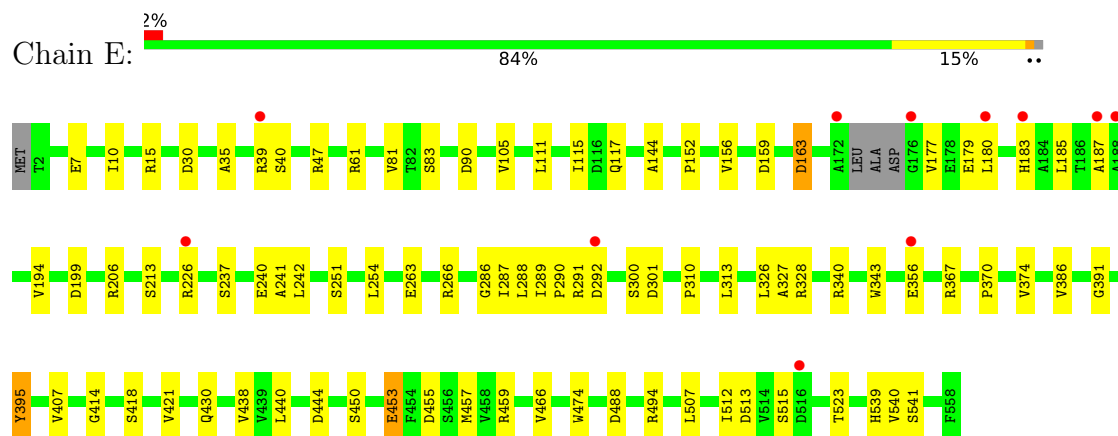




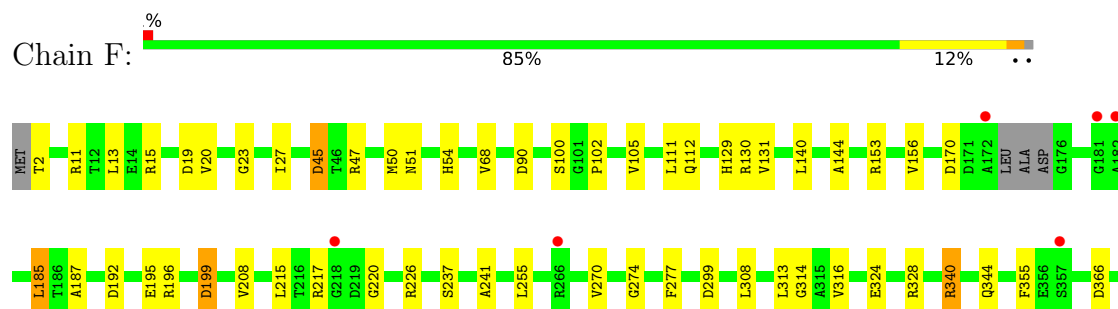
• Molecule 1: Thiamine pyrophosphate-binding protein



• Molecule 1: Thiamine pyrophosphate-binding protein

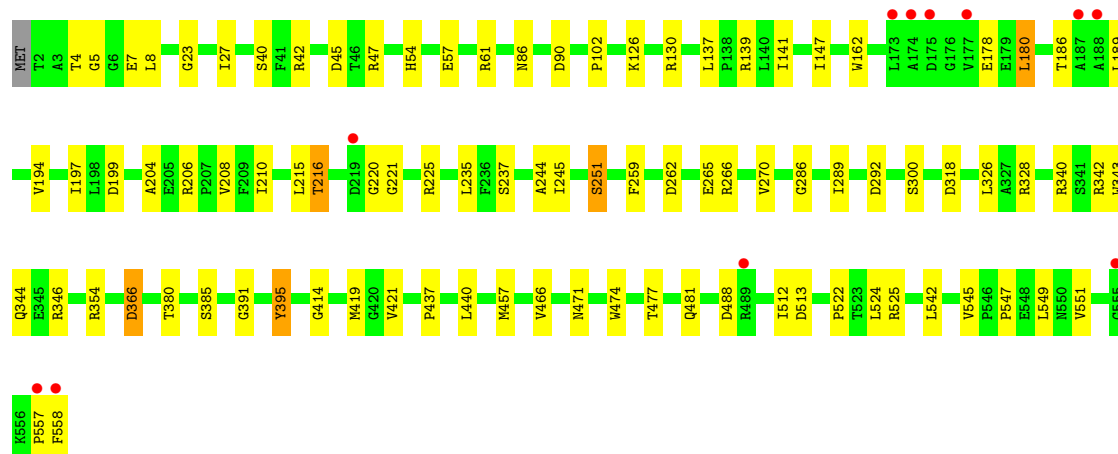
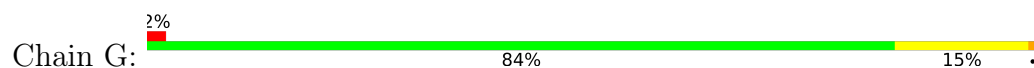


• Molecule 1: Thiamine pyrophosphate-binding protein

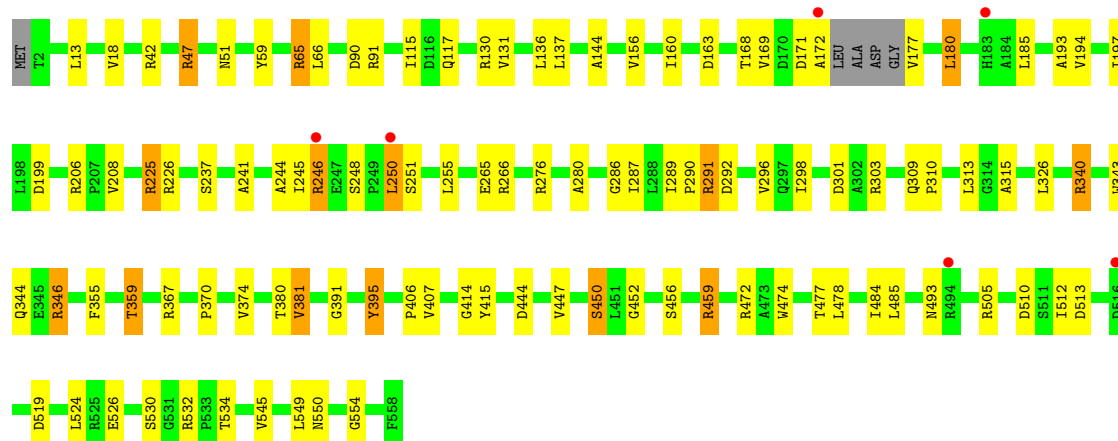
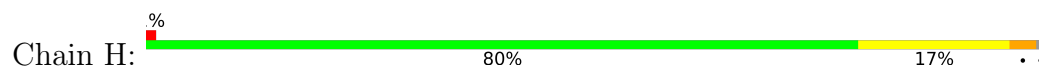




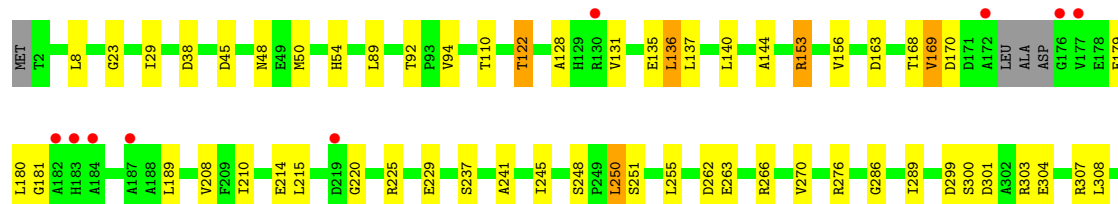
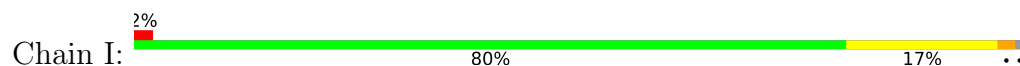
• Molecule 1: Thiamine pyrophosphate-binding protein

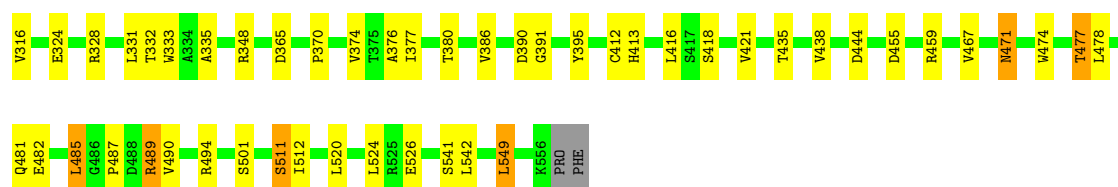


• Molecule 1: Thiamine pyrophosphate-binding protein

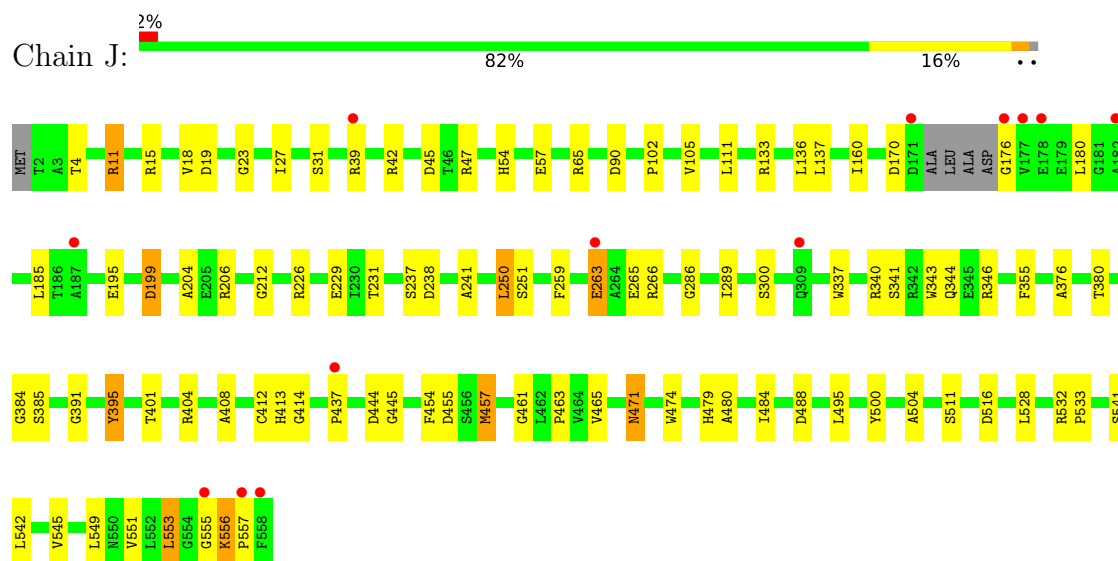


• Molecule 1: Thiamine pyrophosphate-binding protein

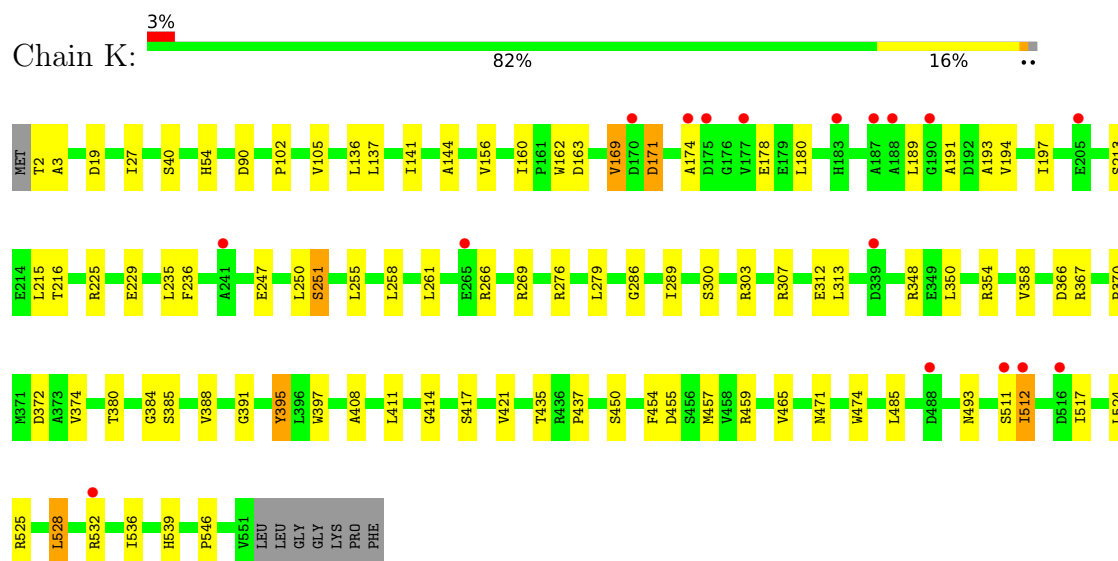




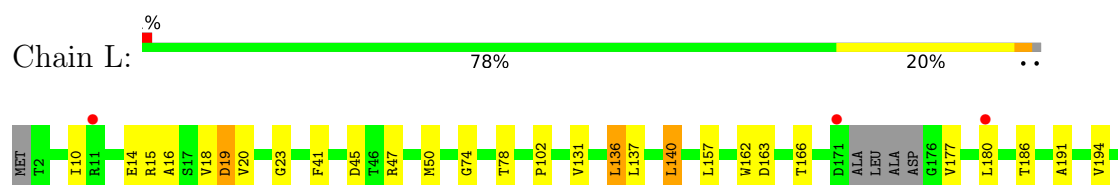
• Molecule 1: Thiamine pyrophosphate-binding protein

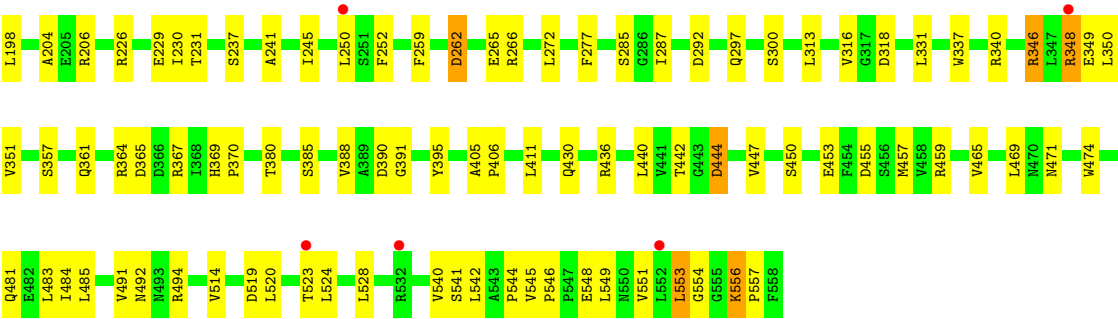


• Molecule 1: Thiamine pyrophosphate-binding protein



• Molecule 1: Thiamine pyrophosphate-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	333.79Å 98.70Å 231.65Å 90.00° 108.05° 90.00°	Depositor
Resolution (Å)	29.19 – 2.68 29.19 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.19-2.68) 99.1 (29.19-2.68)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.189 , 0.236 0.195 , 0.237	Depositor DCC
R_{free} test set	191266 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49634	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.31	0/4136	0.57	0/5654
1	B	0.35	0/4160	0.61	0/5684
1	C	0.34	0/4157	0.62	0/5680
1	D	0.34	0/4160	0.60	0/5684
1	E	0.37	0/4125	0.60	0/5637
1	F	0.36	0/4130	0.60	0/5642
1	G	0.35	0/4138	0.60	0/5657
1	H	0.37	0/4100	0.59	0/5606
1	I	0.37	0/4031	0.59	0/5522
1	J	0.36	0/4098	0.60	0/5602
1	K	0.34	0/4050	0.58	0/5544
1	L	0.38	0/4090	0.60	0/5592
All	All	0.35	0/49375	0.60	0/67504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4064	0	4052	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4088	0	4086	59	0
1	C	4085	0	4084	61	0
1	D	4088	0	4086	48	0
1	E	4054	0	4041	50	0
1	F	4059	0	4057	48	0
1	G	4066	0	4047	48	0
1	H	4029	0	3999	84	0
1	I	3963	0	3904	63	0
1	J	4027	0	4013	72	0
1	K	3980	0	3948	50	0
1	L	4019	0	4005	86	0
2	A	26	0	16	1	0
2	B	26	0	16	2	0
2	C	26	0	16	1	0
2	D	26	0	16	2	0
2	E	26	0	16	1	0
2	F	26	0	16	2	0
2	G	26	0	16	2	0
2	H	26	0	16	3	0
2	I	26	0	16	1	0
2	J	26	0	16	1	0
2	K	26	0	16	2	0
2	L	26	0	16	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	94	0	0	3	0
4	B	101	0	0	1	0
4	C	77	0	0	6	0
4	D	69	0	0	1	0
4	E	60	0	0	1	0
4	F	84	0	0	3	0
4	G	61	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	54	0	0	3	0
4	I	35	0	0	1	0
4	J	58	0	0	1	0
4	K	54	0	0	2	0
4	L	41	0	0	2	0
All	All	49634	0	48514	706	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 7.

All (706) 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:L:252:PHE:CE2	1:L:348:ARG:HD3	1.56	1.41
1:J:11:ARG:HG3	1:J:39:ARG:NH2	1.54	1.22
1:J:11:ARG:CG	1:J:39:ARG:HH22	1.55	1.19
1:A:11:ARG:HH11	1:A:174:ALA:HB1	1.18	1.08
1:H:340:ARG:HH11	1:H:340:ARG:CG	1.69	1.05
1:H:340:ARG:HH11	1:H:340:ARG:HG2	1.18	1.04
1:J:11:ARG:HG3	1:J:39:ARG:HH22	0.89	1.03
1:B:551:VAL:HA	1:B:555:GLY:HA2	1.42	1.00
1:B:11:ARG:NH1	1:B:174:ALA:HB1	1.80	0.97
1:L:252:PHE:CD2	1:L:348:ARG:HD3	2.02	0.95
1:A:11:ARG:NH1	1:A:174:ALA:CB	2.30	0.94
1:J:11:ARG:CB	1:J:39:ARG:HH12	1.81	0.93
1:A:11:ARG:NH1	1:A:174:ALA:HB1	1.83	0.93
1:H:291:ARG:HH11	1:H:291:ARG:CG	1.82	0.91
1:I:485:LEU:O	1:I:489:ARG:HG2	1.73	0.88
1:L:186:THR:CG2	1:L:318:ASP:HB2	2.03	0.88
1:A:11:ARG:HH11	1:A:174:ALA:CB	1.86	0.88
1:L:252:PHE:HE2	1:L:348:ARG:HD3	1.41	0.86
1:H:291:ARG:HH11	1:H:291:ARG:HG2	1.40	0.85
1:J:11:ARG:NE	1:J:39:ARG:NH2	2.26	0.84
1:B:266:ARG:HH11	1:B:266:ARG:HG2	1.43	0.84
1:H:291:ARG:HG2	1:H:291:ARG:NH1	1.93	0.81
1:J:11:ARG:CD	1:J:39:ARG:HH22	1.94	0.81
1:J:11:ARG:HB2	1:J:39:ARG:HH12	1.47	0.80
1:B:11:ARG:HH11	1:B:174:ALA:HB1	1.45	0.79
1:B:551:VAL:HA	1:B:555:GLY:CA	2.12	0.79
1:J:474:TRP:HB3	2:J:601:TPP:H61	1.64	0.78
1:H:340:ARG:HG2	1:H:340:ARG:NH1	1.97	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:GLU:HG2	1:E:39:ARG:HH21	1.48	0.77
1:L:252:PHE:CE2	1:L:348:ARG:CD	2.53	0.77
1:I:225:ARG:HG2	1:I:248:SER:HB2	1.64	0.77
1:L:186:THR:HG21	1:L:318:ASP:HB2	1.65	0.77
1:H:291:ARG:HH11	1:H:291:ARG:CB	1.98	0.75
1:I:136:LEU:HD12	1:I:140:LEU:HD11	1.68	0.74
1:J:11:ARG:CA	1:J:39:ARG:HH12	1.99	0.74
1:H:225:ARG:HD2	1:H:248:SER:H	1.53	0.74
1:D:455:ASP:OD2	1:D:459:ARG:NH1	2.21	0.74
1:C:27:ILE:HD12	1:C:27:ILE:H	1.53	0.73
1:K:266:ARG:HG2	1:K:266:ARG:HH11	1.53	0.73
1:G:215:LEU:HD22	1:G:220:GLY:HA3	1.69	0.73
1:A:179:GLU:HG3	1:A:181:GLY:H	1.53	0.72
1:H:276:ARG:NH2	1:H:415:TYR:CE2	2.58	0.72
1:H:459:ARG:HD2	4:H:728:HOH:O	1.88	0.71
1:J:340:ARG:O	1:J:344:GLN:HG3	1.89	0.71
1:H:266:ARG:HH11	1:H:290:PRO:HG3	1.56	0.70
1:D:4:THR:HG23	1:D:7:GLU:H	1.56	0.70
1:L:229:GLU:HG3	1:L:250:LEU:HD23	1.73	0.70
1:L:471:ASN:HB2	1:L:542:LEU:HB2	1.74	0.69
1:L:186:THR:HG22	1:L:318:ASP:HB2	1.74	0.69
1:I:455:ASP:OD2	1:I:459:ARG:NH1	2.26	0.69
1:J:11:ARG:CA	1:J:39:ARG:NH1	2.56	0.68
1:I:307:ARG:HB3	1:I:308:LEU:HD22	1.76	0.68
1:I:45:ASP:OD1	1:I:459:ARG:NH2	2.27	0.68
1:I:331:LEU:HD23	1:I:332:THR:HG23	1.76	0.68
1:L:206:ARG:NH2	4:L:701:HOH:O	2.27	0.68
1:L:444:ASP:OD1	1:L:444:ASP:N	2.20	0.67
1:L:15:ARG:HH21	1:L:177:VAL:HG22	1.59	0.67
1:C:208:VAL:HG12	1:C:234:PRO:HB2	1.76	0.67
1:D:54:HIS:CE1	1:D:421:VAL:HG12	2.30	0.67
1:A:144:ALA:HB1	1:A:156:VAL:HG11	1.77	0.66
1:B:266:ARG:NH2	1:B:286:GLY:O	2.29	0.66
1:C:474:TRP:HB3	2:C:601:TPP:H61	1.76	0.66
1:J:133:ARG:NH1	4:J:701:HOH:O	2.25	0.66
1:L:204:ALA:O	1:L:340:ARG:NH1	2.22	0.66
1:K:455:ASP:OD2	1:K:459:ARG:NH1	2.29	0.65
1:H:340:ARG:CG	1:H:340:ARG:NH1	2.40	0.65
1:L:262:ASP:HB2	1:L:265:GLU:OE2	1.96	0.65
1:C:315:ALA:HB2	1:D:185:LEU:HD12	1.79	0.65
1:G:208:VAL:HG22	1:G:270:VAL:HG22	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:454:PHE:HA	1:K:457:MET:HE2	1.80	0.64
1:D:90:ASP:OD1	1:D:414:GLY:HA3	1.97	0.64
1:G:189:LEU:HD21	1:G:197:ILE:HD12	1.79	0.64
1:K:266:ARG:NH2	1:K:286:GLY:O	2.30	0.64
1:H:291:ARG:HH12	1:H:310:PRO:CD	2.11	0.64
1:J:11:ARG:NE	1:J:39:ARG:HH22	1.88	0.64
1:K:27:ILE:HG12	1:K:162:TRP:CZ2	2.33	0.63
1:L:481:GLN:HA	1:L:485:LEU:HD12	1.80	0.63
1:B:262:ASP:HB2	1:B:265:GLU:HG3	1.80	0.63
1:G:137:LEU:O	1:G:141:ILE:HG13	1.98	0.63
1:A:131:VAL:HG11	1:A:137:LEU:HD13	1.80	0.63
1:A:269:ARG:NH1	4:A:701:HOH:O	2.31	0.63
1:H:266:ARG:NH1	1:H:290:PRO:HG3	2.12	0.63
1:L:348:ARG:NH1	1:L:351:VAL:HG11	2.13	0.62
1:F:340:ARG:O	1:F:344:GLN:HG3	1.99	0.62
1:E:179:GLU:OE2	1:E:183:HIS:HE1	1.82	0.62
1:F:226:ARG:NH1	1:F:324:GLU:OE1	2.32	0.62
1:C:266:ARG:NH2	1:C:286:GLY:O	2.32	0.62
1:A:4:THR:HG22	1:A:6:GLY:H	1.63	0.62
1:G:545:VAL:HG13	1:G:549:LEU:HD23	1.80	0.62
1:C:321:ALA:O	1:C:325:GLU:HG2	2.00	0.62
1:K:225:ARG:NH1	1:K:247:GLU:OE2	2.33	0.62
1:L:252:PHE:CD2	1:L:348:ARG:CD	2.81	0.62
1:D:144:ALA:HB1	1:D:156:VAL:HG11	1.80	0.62
1:J:11:ARG:HG3	1:J:39:ARG:CZ	2.29	0.62
1:H:291:ARG:HH12	1:H:310:PRO:HD2	1.64	0.61
1:L:186:THR:CG2	1:L:318:ASP:CB	2.76	0.61
1:L:453:GLU:O	1:L:457:MET:HG3	2.00	0.61
1:H:237:SER:HB2	1:H:241:ALA:HB3	1.82	0.61
1:K:261:LEU:HD13	1:K:350:LEU:HD22	1.83	0.61
1:L:186:THR:HG22	1:L:318:ASP:CB	2.30	0.61
1:I:136:LEU:HD12	1:I:140:LEU:CD1	2.31	0.60
1:J:11:ARG:HE	1:J:39:ARG:NH2	1.98	0.60
1:K:144:ALA:HB1	1:K:156:VAL:HG11	1.83	0.60
1:C:269:ARG:NH1	4:C:704:HOH:O	2.34	0.60
1:B:2:THR:N	1:B:171:ASP:OD1	2.34	0.60
1:B:453:GLU:O	1:B:457:MET:HG3	2.02	0.60
1:E:474:TRP:HB3	2:E:601:TPP:H61	1.83	0.60
1:B:11:ARG:NH1	1:B:174:ALA:CB	2.62	0.60
1:H:291:ARG:HH11	1:H:291:ARG:HB3	1.66	0.60
1:E:367:ARG:NH1	1:E:540:VAL:O	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:GLY:O	1:E:395:TYR:HD2	1.83	0.60
1:L:430:GLN:NE2	1:L:436:ARG:O	2.31	0.60
1:H:477:THR:HB	1:H:493:ASN:HD21	1.67	0.59
1:K:90:ASP:OD1	1:K:414:GLY:HA3	2.01	0.59
1:H:225:ARG:HG2	1:H:248:SER:CB	2.32	0.59
1:F:27:ILE:HD12	1:F:27:ILE:H	1.67	0.59
1:E:7:GLU:CG	1:E:39:ARG:HH21	2.15	0.59
1:J:471:ASN:HB2	1:J:542:LEU:HB2	1.84	0.59
1:L:390:ASP:OD1	1:L:391:GLY:N	2.28	0.59
1:E:194:VAL:HG23	1:E:326:LEU:HD23	1.84	0.59
1:H:484:ILE:HG22	1:H:485:LEU:HG	1.85	0.58
1:A:453:GLU:O	1:A:457:MET:HG3	2.03	0.58
1:E:313:LEU:HD21	1:F:185:LEU:HD23	1.85	0.58
1:C:235:LEU:HB3	1:C:251:SER:HA	1.85	0.58
1:J:90:ASP:OD1	1:J:414:GLY:HA3	2.04	0.58
1:F:90:ASP:OD1	1:F:414:GLY:HA3	2.03	0.58
1:J:11:ARG:N	1:J:39:ARG:NH1	2.51	0.58
1:H:225:ARG:HD2	1:H:248:SER:N	2.17	0.58
1:E:291:ARG:HH21	1:E:310:PRO:HD3	1.68	0.58
1:L:365:ASP:OD1	1:L:541:SER:OG	2.20	0.58
1:F:11:ARG:HH11	1:F:15:ARG:HH22	1.50	0.58
1:I:8:LEU:HD11	1:I:169:VAL:HG21	1.85	0.58
1:K:137:LEU:HD21	1:K:160:ILE:HD13	1.86	0.58
1:I:376:ALA:HB3	1:I:520:LEU:HD23	1.85	0.58
1:K:367:ARG:HH21	1:K:539:HIS:HB3	1.69	0.57
1:L:455:ASP:O	1:L:459:ARG:HG3	2.03	0.57
1:B:527:ALA:O	1:B:530:SER:OG	2.22	0.57
1:E:90:ASP:OD2	1:E:414:GLY:HA3	2.03	0.57
1:K:269:ARG:NH2	1:K:312:GLU:OE1	2.36	0.57
1:B:90:ASP:OD2	1:B:414:GLY:HA3	2.04	0.57
1:G:204:ALA:O	1:G:340:ARG:NH2	2.37	0.57
1:G:54:HIS:CE1	1:G:421:VAL:HG22	2.40	0.57
1:I:485:LEU:HB2	1:I:489:ARG:HG3	1.87	0.57
1:H:47:ARG:HG3	1:H:452:GLY:O	2.04	0.57
1:G:57:GLU:OE1	1:G:86:ASN:ND2	2.38	0.57
1:L:440:LEU:HD11	1:L:442:THR:HB	1.87	0.57
1:C:208:VAL:HG23	1:C:270:VAL:HG13	1.86	0.57
1:I:474:TRP:HB3	2:I:601:TPP:H61	1.86	0.57
1:C:49:GLU:HG2	4:C:708:HOH:O	2.04	0.56
1:H:355:PHE:O	1:H:359:THR:OG1	2.21	0.56
1:L:380:THR:HG21	1:L:524:LEU:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HH12	1:A:174:ALA:CB	2.19	0.56
1:A:90:ASP:OD1	1:A:414:GLY:HA3	2.06	0.56
1:D:453:GLU:O	1:D:457:MET:HG3	2.06	0.56
1:H:59:TYR:CE2	1:H:65:ARG:HD2	2.41	0.56
1:J:27:ILE:H	1:J:27:ILE:HD12	1.71	0.56
1:G:474:TRP:HB3	2:G:601:TPP:H61	1.87	0.55
1:I:263:GLU:HA	1:I:266:ARG:HG3	1.87	0.55
1:G:27:ILE:HG13	1:G:162:TRP:CZ2	2.40	0.55
1:I:391:GLY:O	1:I:395:TYR:HD2	1.89	0.55
1:J:266:ARG:NH1	1:J:286:GLY:O	2.29	0.55
1:L:380:THR:HB	1:L:524:LEU:HD23	1.87	0.55
1:J:15:ARG:NH2	1:J:176:GLY:O	2.39	0.55
1:A:7:GLU:O	1:A:11:ARG:HG3	2.06	0.55
1:G:340:ARG:O	1:G:344:GLN:HG3	2.06	0.55
1:H:225:ARG:HG2	1:H:248:SER:HB3	1.88	0.55
1:L:391:GLY:O	1:L:395:TYR:HD2	1.90	0.55
1:H:340:ARG:HH11	1:H:340:ARG:HG3	1.64	0.55
1:I:23:GLY:O	1:I:45:ASP:HA	2.06	0.55
1:I:131:VAL:HG22	1:I:140:LEU:HD12	1.87	0.55
1:E:237:SER:HB2	1:E:241:ALA:HB3	1.87	0.55
1:G:266:ARG:NH2	1:G:286:GLY:O	2.39	0.55
1:E:453:GLU:O	1:E:457:MET:HG3	2.07	0.55
1:A:4:THR:HG22	1:A:6:GLY:N	2.22	0.55
1:E:117:GLN:NE2	1:E:159:ASP:OD2	2.40	0.55
1:K:354:ARG:O	1:K:358:VAL:HG23	2.07	0.55
1:D:23:GLY:O	1:D:45:ASP:HA	2.07	0.54
1:L:364:ARG:HG2	1:L:369:HIS:HB2	1.89	0.54
1:G:215:LEU:CD2	1:G:220:GLY:HA3	2.37	0.54
1:I:54:HIS:CE1	1:I:421:VAL:HG12	2.42	0.54
1:E:10:ILE:HG21	1:E:39:ARG:HG3	1.89	0.54
1:F:47:ARG:NH1	1:F:455:ASP:OD1	2.35	0.54
1:F:131:VAL:HG13	1:F:140:LEU:HD12	1.89	0.54
1:G:221:GLY:O	1:G:225:ARG:HG3	2.08	0.54
1:G:391:GLY:O	1:G:395:TYR:HD2	1.89	0.54
1:J:212:GLY:HA2	1:J:238:ASP:OD1	2.08	0.54
1:L:367:ARG:NH1	1:L:540:VAL:O	2.40	0.54
1:I:262:ASP:O	1:I:266:ARG:HG2	2.07	0.54
1:K:512:ILE:HG13	1:K:536:ILE:HG12	1.90	0.54
1:H:545:VAL:HG13	1:H:549:LEU:HD23	1.90	0.54
1:A:23:GLY:O	1:A:45:ASP:HA	2.08	0.54
1:A:137:LEU:HD11	1:A:160:ILE:HD12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:GLY:O	1:C:395:TYR:HD2	1.91	0.54
1:F:355:PHE:HE1	1:F:401:THR:HG22	1.73	0.54
1:L:348:ARG:HH11	1:L:351:VAL:HG11	1.72	0.54
1:H:144:ALA:HB1	1:H:156:VAL:HG11	1.90	0.53
1:H:367:ARG:NH1	1:H:472:ARG:NE	2.55	0.53
1:B:372:ASP:HB3	1:B:517:ILE:HG12	1.89	0.53
1:F:474:TRP:HB3	2:F:601:TPP:H61	1.91	0.53
1:C:90:ASP:OD1	1:C:414:GLY:HA3	2.09	0.53
1:F:391:GLY:O	1:F:395:TYR:HD2	1.92	0.53
1:H:59:TYR:CE2	1:H:65:ARG:CD	2.92	0.53
1:B:367:ARG:NH1	1:B:540:VAL:O	2.42	0.53
1:G:551:VAL:HG22	1:G:557:PRO:HG3	1.91	0.53
1:I:237:SER:HB2	1:I:241:ALA:HB3	1.90	0.53
1:J:551:VAL:HA	1:J:555:GLY:HA2	1.91	0.53
1:B:23:GLY:O	1:B:45:ASP:HA	2.09	0.53
1:B:204:ALA:O	1:B:340:ARG:NH1	2.41	0.53
1:D:512:ILE:HG21	1:D:523:THR:CG2	2.39	0.53
1:I:299:ASP:O	1:I:316:VAL:HA	2.09	0.53
1:G:235:LEU:HB3	1:G:251:SER:HA	1.90	0.53
1:I:482:GLU:HG3	1:I:487:PRO:HA	1.91	0.53
1:J:237:SER:HB2	1:J:241:ALA:HB3	1.91	0.53
1:J:286:GLY:HA2	1:J:289:ILE:O	2.09	0.53
1:J:465:VAL:HG21	1:J:528:LEU:HD23	1.90	0.53
1:G:366:ASP:OD1	1:G:366:ASP:N	2.28	0.53
1:H:391:GLY:O	1:H:395:TYR:HD2	1.92	0.53
1:I:276:ARG:HG2	1:I:304:GLU:HG3	1.91	0.53
1:C:27:ILE:H	1:C:27:ILE:CD1	2.22	0.52
1:J:551:VAL:HA	1:J:555:GLY:CA	2.39	0.52
1:A:11:ARG:NH1	1:A:174:ALA:HB2	2.20	0.52
1:H:193:ALA:O	1:H:197:ILE:HG13	2.08	0.52
1:H:286:GLY:HA2	1:H:289:ILE:O	2.09	0.52
1:L:74:GLY:O	1:L:78:THR:HG23	2.09	0.52
1:B:451:LEU:HD13	1:B:503:VAL:HG11	1.90	0.52
1:D:162:TRP:O	1:D:166:THR:HG23	2.09	0.52
1:G:102:PRO:HG3	1:G:162:TRP:HB3	1.92	0.52
1:K:102:PRO:HB2	1:K:105:VAL:HG22	1.92	0.52
1:F:550:ASN:O	1:F:554:GLY:N	2.34	0.52
1:G:440:LEU:HD23	1:G:466:VAL:HG13	1.92	0.52
1:D:237:SER:HB2	1:D:241:ALA:HB3	1.90	0.52
1:F:277:PHE:HB3	1:F:308:LEU:HD12	1.91	0.52
1:D:266:ARG:HH11	1:D:266:ARG:HG2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:SER:HB3	1:G:437:PRO:HG2	1.92	0.52
1:J:545:VAL:HG13	1:J:549:LEU:HD23	1.91	0.52
1:G:265:GLU:OE2	1:G:346:ARG:NE	2.33	0.51
1:C:215:LEU:HG	1:C:220:GLY:HA3	1.91	0.51
1:G:5:GLY:HA2	1:G:8:LEU:HD12	1.92	0.51
1:H:194:VAL:HG13	1:H:326:LEU:HD23	1.91	0.51
1:B:225:ARG:HG2	1:B:248:SER:HB2	1.92	0.51
1:C:152:PRO:HG3	1:C:301:ASP:HB2	1.91	0.51
1:I:485:LEU:HB2	1:I:489:ARG:CG	2.41	0.51
1:J:385:SER:HB3	1:J:437:PRO:HG2	1.92	0.51
1:C:488:ASP:OD1	1:C:488:ASP:N	2.44	0.51
1:K:229:GLU:HG3	1:K:250:LEU:CD1	2.40	0.51
1:A:382:PRO:O	1:A:385:SER:HB2	2.11	0.51
1:F:23:GLY:O	1:F:45:ASP:HA	2.10	0.51
1:I:163:ASP:OD1	1:I:163:ASP:N	2.44	0.51
1:A:522:PRO:HA	1:A:525:ARG:NH1	2.26	0.51
1:E:440:LEU:HD23	1:E:466:VAL:HG13	1.91	0.51
2:F:601:TPP:H2	4:F:724:HOH:O	2.11	0.51
1:H:185:LEU:HD23	1:K:313:LEU:HD11	1.92	0.51
1:L:520:LEU:O	1:L:523:THR:OG1	2.23	0.51
1:H:91:ARG:CZ	1:H:276:ARG:HD3	2.41	0.51
1:I:48:ASN:ND2	1:I:50:MET:HB3	2.25	0.51
1:A:206:ARG:HB3	1:A:343:TRP:CE2	2.46	0.51
1:F:11:ARG:NH1	1:F:15:ARG:HH22	2.09	0.51
1:I:333:TRP:NE1	1:I:335:ALA:HB3	2.25	0.51
1:L:484:ILE:HG22	1:L:485:LEU:HG	1.91	0.51
1:A:124:ILE:HG22	1:E:115:ILE:HD12	1.93	0.51
1:D:146:ARG:NH1	1:D:179:GLU:O	2.37	0.51
1:H:59:TYR:OH	1:H:65:ARG:NH1	2.39	0.51
1:I:131:VAL:HG11	1:I:137:LEU:HG	1.93	0.51
1:D:163:ASP:OD2	1:D:163:ASP:N	2.38	0.51
1:E:455:ASP:OD2	1:E:459:ARG:NH1	2.42	0.51
1:G:90:ASP:OD1	1:G:414:GLY:HA3	2.11	0.51
1:G:262:ASP:O	1:G:266:ARG:HG2	2.11	0.51
1:H:530:SER:CB	4:H:705:HOH:O	2.59	0.51
1:A:54:HIS:CE1	1:A:421:VAL:HG12	2.46	0.50
1:L:388:VAL:HG12	1:L:440:LEU:HD13	1.93	0.50
1:G:237:SER:HB3	1:G:245:ILE:HD13	1.93	0.50
1:B:15:ARG:NH2	1:B:178:GLU:O	2.45	0.50
1:L:10:ILE:O	1:L:14:GLU:HG3	2.12	0.50
1:E:39:ARG:O	1:E:40:SER:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:GLY:O	1:L:45:ASP:HA	2.12	0.50
1:C:48:ASN:ND2	4:C:709:HOH:O	2.42	0.50
1:D:512:ILE:HG21	1:D:523:THR:HG21	1.92	0.50
1:C:286:GLY:HA2	1:C:289:ILE:O	2.11	0.50
1:H:477:THR:HB	1:H:493:ASN:ND2	2.26	0.50
1:C:313:LEU:HD21	1:D:185:LEU:HD11	1.94	0.50
1:G:259:PHE:CZ	1:G:557:PRO:HD2	2.47	0.50
1:L:465:VAL:HG21	1:L:528:LEU:HD22	1.94	0.50
1:J:265:GLU:OE2	1:J:346:ARG:NE	2.34	0.50
1:L:131:VAL:HG11	1:L:137:LEU:HG	1.94	0.50
1:L:551:VAL:HG12	1:L:557:PRO:HD3	1.94	0.50
1:A:450:SER:HB2	1:A:453:GLU:HG2	1.94	0.49
1:F:130:ARG:NH1	4:F:705:HOH:O	2.33	0.49
1:G:61:ARG:NH1	4:G:705:HOH:O	2.44	0.49
1:L:370:PRO:HD2	1:L:544:PRO:HG2	1.93	0.49
1:D:133:ARG:HB2	1:D:136:LEU:HD22	1.94	0.49
1:G:286:GLY:HA2	1:G:289:ILE:O	2.12	0.49
1:E:163:ASP:OD2	1:E:163:ASP:N	2.42	0.49
1:H:225:ARG:HG2	1:H:248:SER:HB2	1.94	0.49
1:J:444:ASP:HB2	1:J:500:TYR:CE2	2.47	0.49
1:H:246:ARG:NH1	1:H:407:VAL:O	2.46	0.49
1:C:272:LEU:HD12	1:C:297:GLN:HG3	1.95	0.49
1:D:150:HIS:HE1	1:D:181:GLY:HA3	1.76	0.49
1:H:367:ARG:HH12	1:H:472:ARG:NE	2.10	0.49
1:B:102:PRO:HB2	1:B:105:VAL:HG22	1.95	0.49
1:H:90:ASP:OD1	1:H:414:GLY:HA3	2.12	0.49
1:H:115:ILE:HG22	1:H:117:GLN:HG2	1.94	0.49
1:K:229:GLU:HG3	1:K:250:LEU:HD11	1.94	0.49
1:B:286:GLY:HA2	1:B:289:ILE:O	2.13	0.49
1:I:386:VAL:HB	1:I:438:VAL:HG22	1.94	0.49
1:I:412:CYS:SG	1:I:413:HIS:N	2.82	0.49
1:C:144:ALA:HB1	1:C:156:VAL:HG11	1.94	0.49
1:E:15:ARG:HB3	1:E:180:LEU:HD11	1.93	0.49
1:L:162:TRP:O	1:L:166:THR:HG23	2.13	0.49
1:L:237:SER:HB3	1:L:245:ILE:HG12	1.94	0.49
1:H:137:LEU:HD21	1:H:160:ILE:HD13	1.95	0.49
1:H:474:TRP:HB3	2:H:601:TPP:H61	1.95	0.49
1:L:186:THR:HG21	1:L:318:ASP:CB	2.38	0.49
1:F:111:LEU:HG	1:F:112:GLN:HG3	1.95	0.48
1:H:266:ARG:NH2	1:H:287:ILE:HA	2.28	0.48
1:J:474:TRP:CE2	1:J:495:LEU:HD11	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:388:VAL:HG22	1:K:411:LEU:HB2	1.94	0.48
1:L:546:PRO:HG2	1:L:549:LEU:HB2	1.95	0.48
1:A:187:ALA:HB1	1:B:187:ALA:HB1	1.95	0.48
1:H:265:GLU:OE1	1:H:346:ARG:NE	2.45	0.48
1:A:229:GLU:HA	1:A:250:LEU:HD23	1.93	0.48
1:C:188:ALA:HB2	1:C:321:ALA:CB	2.43	0.48
1:D:357:SER:O	1:D:361:GLN:HG3	2.13	0.48
1:H:291:ARG:NH1	1:H:309:GLN:HG2	2.29	0.48
1:K:367:ARG:NH2	1:K:539:HIS:HB3	2.27	0.48
1:E:35:ALA:O	1:E:39:ARG:HG2	2.14	0.48
1:J:488:ASP:OD1	1:J:488:ASP:N	2.46	0.48
1:L:50:MET:HB2	1:L:50:MET:HE2	1.76	0.48
1:L:483:LEU:HD11	1:L:545:VAL:HG11	1.94	0.48
1:C:237:SER:HB2	1:C:241:ALA:HB3	1.94	0.48
1:G:522:PRO:HA	1:G:525:ARG:CZ	2.44	0.48
1:I:229:GLU:HA	1:I:250:LEU:HD23	1.95	0.48
1:J:391:GLY:O	1:J:395:TYR:HD2	1.94	0.48
1:L:237:SER:HB2	1:L:241:ALA:HB3	1.96	0.48
1:B:392:ALA:HB2	2:B:601:TPP:S1	2.53	0.48
1:I:370:PRO:O	1:I:374:VAL:HG22	2.13	0.48
1:E:144:ALA:HB1	1:E:156:VAL:HG11	1.94	0.48
1:F:195:GLU:O	1:F:199:ASP:HB2	2.14	0.48
1:H:47:ARG:HG2	1:H:456:SER:OG	2.14	0.48
1:J:23:GLY:O	1:J:45:ASP:HA	2.13	0.48
1:K:276:ARG:NH1	4:K:709:HOH:O	2.46	0.48
1:L:548:GLU:O	1:L:551:VAL:HG22	2.14	0.48
1:D:262:ASP:O	1:D:266:ARG:HG3	2.13	0.48
1:F:274:GLY:O	4:F:701:HOH:O	2.20	0.48
1:I:501:SER:O	1:I:511:SER:OG	2.28	0.48
1:L:346:ARG:HH21	1:L:350:LEU:HB2	1.79	0.48
1:H:380:THR:HB	1:H:524:LEU:HD23	1.96	0.48
1:I:237:SER:HB3	1:I:245:ILE:HD13	1.95	0.48
1:K:178:GLU:HB3	4:K:724:HOH:O	2.14	0.48
1:B:135:GLU:CD	1:B:135:GLU:H	2.16	0.47
1:L:316:VAL:O	1:L:316:VAL:HG23	2.13	0.47
1:E:226:ARG:HE	1:E:327:ALA:HB1	1.79	0.47
1:K:137:LEU:HA	1:K:137:LEU:HD23	1.64	0.47
1:B:485:LEU:HB3	1:B:489:ARG:HG3	1.97	0.47
1:C:23:GLY:O	1:C:45:ASP:HA	2.15	0.47
1:C:206:ARG:HB3	1:C:343:TRP:CE2	2.50	0.47
1:F:51:ASN:OD1	1:F:450:SER:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:ILE:HD11	1:F:467:VAL:HG11	1.96	0.47
1:H:65:ARG:HG3	1:H:66:LEU:O	2.15	0.47
1:I:348:ARG:HA	1:I:348:ARG:HD3	1.56	0.47
1:C:262:ASP:O	1:C:266:ARG:HG2	2.13	0.47
1:H:459:ARG:NH1	1:H:459:ARG:HB3	2.30	0.47
1:I:481:GLN:OE1	1:I:490:VAL:HA	2.14	0.47
1:J:479:HIS:ND1	1:J:545:VAL:HG22	2.29	0.47
1:H:65:ARG:HG3	1:H:66:LEU:N	2.29	0.47
1:C:511:SER:C	1:C:512:ILE:HG13	2.34	0.47
1:D:277:PHE:HB3	1:D:308:LEU:HD12	1.96	0.47
1:G:186:THR:HG21	1:G:318:ASP:OD2	2.15	0.47
1:H:340:ARG:NH1	1:H:340:ARG:HG3	2.24	0.47
1:I:122:THR:HG23	1:I:128:ALA:HB3	1.96	0.47
1:J:355:PHE:HE1	1:J:401:THR:HG22	1.78	0.47
1:K:54:HIS:CE1	1:K:421:VAL:HG22	2.50	0.47
1:K:370:PRO:O	1:K:374:VAL:HG22	2.14	0.47
1:K:385:SER:HB3	1:K:437:PRO:HG2	1.96	0.47
1:B:61:ARG:NH2	1:B:240:GLU:OE2	2.46	0.47
1:B:391:GLY:O	1:B:395:TYR:HD2	1.98	0.47
1:B:478:LEU:HG	1:B:490:VAL:HG11	1.95	0.47
1:E:488:ASP:OD1	1:E:488:ASP:N	2.48	0.47
1:H:510:ASP:HB2	1:H:534:THR:HG23	1.97	0.47
1:A:27:ILE:HG12	1:A:162:TRP:CZ2	2.50	0.47
1:E:386:VAL:HG22	1:E:438:VAL:HG22	1.96	0.47
1:A:404:ARG:NH1	4:A:710:HOH:O	2.48	0.46
1:A:496:GLU:HB2	4:A:749:HOH:O	2.16	0.46
1:C:364:ARG:NH2	1:C:372:ASP:OD1	2.49	0.46
1:D:391:GLY:O	1:D:395:TYR:HD2	1.98	0.46
1:C:47:ARG:HD2	1:C:47:ARG:HA	1.68	0.46
1:G:126:LYS:HE3	1:G:147:ILE:HG22	1.96	0.46
1:H:250:LEU:HD11	1:H:344:GLN:NE2	2.30	0.46
1:H:478:LEU:N	1:H:493:ASN:HD22	2.12	0.46
1:J:384:GLY:HA2	1:J:408:ALA:HB2	1.97	0.46
1:L:551:VAL:CG1	1:L:557:PRO:HD3	2.45	0.46
1:D:545:VAL:HG13	1:D:549:LEU:HD23	1.97	0.46
1:E:286:GLY:HA2	1:E:289:ILE:O	2.16	0.46
1:F:377:ILE:O	1:F:381:VAL:HG13	2.14	0.46
1:H:59:TYR:CZ	1:H:65:ARG:HD2	2.51	0.46
1:A:81:VAL:HG21	1:E:81:VAL:HG11	1.97	0.46
1:F:19:ASP:OD2	1:F:20:VAL:HG23	2.15	0.46
1:A:225:ARG:HG2	1:A:248:SER:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:LEU:HD21	1:J:160:ILE:HD13	1.97	0.46
1:C:481:GLN:OE1	1:C:493:ASN:ND2	2.41	0.46
1:F:215:LEU:HG	1:F:220:GLY:HA3	1.97	0.46
1:H:225:ARG:HD3	1:H:244:ALA:O	2.16	0.46
1:I:304:GLU:OE2	1:I:307:ARG:NH1	2.49	0.46
1:J:259:PHE:CE2	1:J:556:LYS:HD2	2.49	0.46
1:L:474:TRP:HB3	2:L:601:TPP:H61	1.97	0.46
1:L:491:VAL:HG22	1:L:492:ASN:OD1	2.16	0.46
1:C:501:SER:O	1:C:511:SER:OG	2.33	0.46
1:C:549:LEU:HD12	1:C:549:LEU:O	2.16	0.46
1:E:370:PRO:O	1:E:374:VAL:HG22	2.15	0.46
1:J:504:ALA:HB3	1:J:511:SER:OG	2.16	0.46
1:B:474:TRP:HB3	2:B:601:TPP:H61	1.97	0.46
1:D:331:LEU:HD12	1:D:331:LEU:HA	1.77	0.46
1:B:266:ARG:HG2	1:B:266:ARG:NH1	2.20	0.46
1:G:512:ILE:HD12	1:G:513:ASP:H	1.80	0.46
1:K:397:TRP:CD1	1:K:546:PRO:HG3	2.50	0.46
1:B:376:ALA:HB3	1:B:520:LEU:HD23	1.98	0.46
1:G:47:ARG:HD2	1:G:47:ARG:HA	1.60	0.46
1:A:370:PRO:HD2	1:A:544:PRO:HG2	1.97	0.45
1:C:184:ALA:HA	1:D:314:GLY:O	2.16	0.45
1:L:262:ASP:HB2	1:L:265:GLU:HG3	1.98	0.45
1:B:195:GLU:O	1:B:199:ASP:HB2	2.15	0.45
1:C:245:ILE:HD12	1:C:251:SER:HB2	1.98	0.45
1:E:179:GLU:OE2	1:E:183:HIS:CE1	2.67	0.45
1:E:185:LEU:HD21	1:F:196:ARG:HH12	1.81	0.45
1:F:237:SER:HB2	1:F:241:ALA:HB3	1.98	0.45
1:F:556:LYS:HD2	1:F:556:LYS:HA	1.58	0.45
1:K:380:THR:HB	1:K:524:LEU:HD23	1.99	0.45
1:L:18:VAL:O	1:L:41:PHE:HE1	1.99	0.45
1:C:231:THR:HG22	1:C:337:TRP:CE2	2.51	0.45
1:E:47:ARG:NH1	1:E:455:ASP:OD2	2.48	0.45
1:I:380:THR:HB	1:I:524:LEU:HD23	1.99	0.45
1:J:445:GLY:HA2	1:L:47:ARG:NH2	2.32	0.45
1:D:512:ILE:HD12	1:D:512:ILE:HA	1.81	0.45
1:E:187:ALA:HB1	1:F:187:ALA:HB1	1.98	0.45
1:H:163:ASP:N	1:H:163:ASP:OD1	2.50	0.45
1:L:262:ASP:O	1:L:266:ARG:HG2	2.17	0.45
1:C:213:SER:HB3	4:C:703:HOH:O	2.16	0.45
1:E:287:ILE:HG13	1:E:288:LEU:N	2.32	0.45
1:C:505:ARG:NH1	1:C:511:SER:HB3	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:237:SER:HB3	1:H:245:ILE:HG21	1.97	0.45
1:L:136:LEU:HB3	1:L:140:LEU:HD22	1.98	0.45
1:E:242:LEU:HD22	1:E:254:LEU:HD21	1.99	0.45
1:F:144:ALA:HB1	1:F:156:VAL:HG11	1.99	0.45
1:K:189:LEU:HD23	1:K:189:LEU:HA	1.87	0.45
1:L:163:ASP:OD1	1:L:163:ASP:N	2.50	0.45
1:B:231:THR:HG22	1:B:337:TRP:CE2	2.51	0.45
1:E:367:ARG:NH2	1:E:539:HIS:HB3	2.32	0.45
1:I:144:ALA:HB1	1:I:156:VAL:HG11	1.99	0.45
1:J:47:ARG:HD2	1:J:47:ARG:HA	1.60	0.45
1:J:263:GLU:HA	1:J:266:ARG:HG3	1.98	0.45
1:A:102:PRO:HB2	1:A:105:VAL:HG22	1.98	0.45
1:F:299:ASP:O	1:F:316:VAL:HA	2.17	0.45
1:I:301:ASP:CG	1:I:303:ARG:HG2	2.36	0.45
1:J:15:ARG:NH1	1:J:176:GLY:O	2.50	0.45
1:K:384:GLY:HA2	1:K:408:ALA:HB2	1.98	0.45
1:K:474:TRP:CE3	2:K:601:TPP:HM41	2.52	0.45
1:L:226:ARG:HG2	1:L:230:ILE:HD11	1.99	0.45
1:A:512:ILE:HG21	1:A:523:THR:CG2	2.47	0.45
1:B:377:ILE:HD11	1:B:467:VAL:HG11	1.99	0.45
1:D:47:ARG:HD2	1:D:47:ARG:HA	1.74	0.45
1:C:485:LEU:HB3	1:C:489:ARG:HG3	1.99	0.44
1:D:102:PRO:HB2	1:D:105:VAL:HG22	1.98	0.44
1:G:419:MET:HG3	2:G:601:TPP:H72	1.99	0.44
1:H:180:LEU:HD13	1:H:180:LEU:HA	1.74	0.44
1:H:246:ARG:HD2	1:H:407:VAL:O	2.18	0.44
1:I:135:GLU:CD	1:I:135:GLU:H	2.20	0.44
1:J:11:ARG:HA	1:J:39:ARG:NH1	2.29	0.44
1:B:355:PHE:HE1	1:B:401:THR:HG22	1.82	0.44
1:D:33:TYR:CE2	1:D:43:ILE:HG21	2.52	0.44
1:I:266:ARG:NH2	1:I:286:GLY:O	2.49	0.44
1:L:469:LEU:HG	1:L:540:VAL:HG11	1.99	0.44
1:B:246:ARG:HD2	1:B:406:PRO:HA	1.98	0.44
1:D:259:PHE:CZ	1:D:557:PRO:HD2	2.52	0.44
1:F:102:PRO:HB2	1:F:105:VAL:HG22	1.99	0.44
1:H:245:ILE:O	1:H:251:SER:HB2	2.17	0.44
1:L:229:GLU:CG	1:L:250:LEU:HD23	2.44	0.44
1:H:291:ARG:HH12	1:H:310:PRO:HD3	1.80	0.44
1:I:549:LEU:HD23	1:I:549:LEU:HA	1.84	0.44
1:J:461:GLY:O	1:J:463:PRO:HD3	2.18	0.44
1:A:367:ARG:NH2	1:A:539:HIS:HB3	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ASP:OD2	1:B:366:ASP:N	2.40	0.44
1:C:39:ARG:HG3	1:C:39:ARG:HH11	1.83	0.44
1:H:301:ASP:CG	1:H:303:ARG:HG2	2.37	0.44
1:I:286:GLY:HA2	1:I:289:ILE:O	2.17	0.44
1:K:465:VAL:HG21	1:K:528:LEU:HD13	2.00	0.44
1:L:524:LEU:HG	1:L:528:LEU:HD23	2.00	0.44
1:B:545:VAL:HG13	1:B:549:LEU:HD23	1.98	0.44
1:C:6:GLY:HA2	1:C:32:ILE:HG12	2.00	0.44
1:C:234:PRO:HG2	1:C:343:TRP:NE1	2.33	0.44
1:C:397:TRP:CD1	1:C:546:PRO:HG3	2.53	0.44
1:E:263:GLU:HA	1:E:266:ARG:HD2	2.00	0.44
1:E:328:ARG:NH1	1:F:192:ASP:OD2	2.50	0.44
1:H:474:TRP:CE3	2:H:601:TPP:HM41	2.53	0.44
1:J:457:MET:HE3	1:J:533:PRO:HB3	1.99	0.44
1:K:191:ALA:O	1:K:194:VAL:HG22	2.18	0.44
1:K:372:ASP:HB3	1:K:517:ILE:HG12	1.99	0.44
1:L:277:PHE:N	4:L:706:HOH:O	2.38	0.44
1:A:391:GLY:O	1:A:395:TYR:HD2	2.00	0.44
1:D:262:ASP:HB2	1:D:265:GLU:HG3	2.00	0.44
1:D:340:ARG:NE	4:D:704:HOH:O	2.32	0.44
1:D:412:CYS:SG	1:D:413:HIS:N	2.88	0.44
1:E:266:ARG:NH1	1:E:290:PRO:HG3	2.32	0.44
1:C:49:GLU:CG	4:C:708:HOH:O	2.64	0.44
1:D:458:VAL:HG13	1:D:532:ARG:HH22	1.82	0.44
1:F:45:ASP:OD1	1:F:45:ASP:N	2.35	0.44
1:I:89:LEU:HD12	1:I:416:LEU:HB2	1.99	0.44
1:L:15:ARG:NH2	1:L:177:VAL:HG22	2.31	0.44
1:L:553:LEU:HB2	1:L:554:GLY:H	1.64	0.44
1:C:105:VAL:HG12	1:C:105:VAL:O	2.17	0.43
1:F:185:LEU:HD13	1:F:185:LEU:HA	1.82	0.43
1:I:179:GLU:HG3	1:I:181:GLY:H	1.82	0.43
1:I:215:LEU:HG	1:I:220:GLY:HA3	1.99	0.43
1:J:47:ARG:NH1	1:J:455:ASP:OD2	2.44	0.43
1:J:206:ARG:HB3	1:J:343:TRP:CZ2	2.53	0.43
1:L:405:ALA:HA	1:L:406:PRO:HD3	1.86	0.43
1:B:503:VAL:HG13	1:F:503:VAL:HG13	2.01	0.43
1:E:185:LEU:HD11	1:F:313:LEU:HD21	1.99	0.43
1:E:187:ALA:HB1	1:F:187:ALA:CB	2.48	0.43
1:G:23:GLY:O	1:G:45:ASP:HA	2.17	0.43
1:G:139:ARG:HG3	1:G:178:GLU:OE1	2.18	0.43
1:H:51:ASN:OD1	1:H:450:SER:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:PRO:HB2	1:J:105:VAL:HG22	1.99	0.43
1:J:204:ALA:O	1:J:340:ARG:NH1	2.37	0.43
1:J:265:GLU:CD	1:J:346:ARG:HE	2.20	0.43
1:J:11:ARG:CB	1:J:39:ARG:NH1	2.64	0.43
1:C:194:VAL:HG13	1:C:326:LEU:HD23	2.01	0.43
1:I:208:VAL:HG22	1:I:270:VAL:HG22	2.00	0.43
1:I:210:ILE:HG21	1:I:255:LEU:HD13	1.99	0.43
1:I:444:ASP:OD1	1:I:444:ASP:N	2.50	0.43
1:K:391:GLY:O	1:K:395:TYR:HD2	2.01	0.43
1:A:13:LEU:O	1:A:18:VAL:HG13	2.19	0.43
1:B:547:PRO:HD2	4:B:701:HOH:O	2.18	0.43
1:C:444:ASP:HB2	1:C:500:TYR:CE2	2.54	0.43
1:J:54:HIS:HA	1:J:57:GLU:HG3	2.01	0.43
1:J:454:PHE:HA	1:J:457:MET:HE2	2.00	0.43
1:F:328:ARG:HG2	1:F:328:ARG:HH11	1.82	0.43
1:H:255:LEU:HD21	1:H:280:ALA:O	2.19	0.43
1:J:19:ASP:OD1	1:J:65:ARG:NH2	2.50	0.43
1:L:45:ASP:OD2	1:L:459:ARG:NH2	2.41	0.43
1:B:491:VAL:HG22	1:B:492:ASN:OD1	2.18	0.43
1:J:532:ARG:HB3	1:J:532:ARG:CZ	2.48	0.43
1:L:19:ASP:OD2	1:L:20:VAL:HG23	2.19	0.43
1:A:286:GLY:HA2	1:A:289:ILE:O	2.19	0.43
1:C:9:VAL:O	1:C:13:LEU:HG	2.18	0.43
1:C:206:ARG:HB3	1:C:343:TRP:CD2	2.53	0.43
1:K:474:TRP:HB3	2:K:601:TPP:H61	1.99	0.43
1:C:215:LEU:HD13	1:C:224:LEU:HD22	2.01	0.43
1:D:481:GLN:OE1	1:D:493:ASN:ND2	2.50	0.43
1:D:519:ASP:O	1:D:523:THR:OG1	2.21	0.43
1:F:153:ARG:CZ	1:F:217:ARG:HB3	2.49	0.43
1:G:380:THR:HB	1:G:524:LEU:HD23	2.01	0.43
1:I:390:ASP:OD1	1:I:391:GLY:N	2.49	0.43
1:J:445:GLY:HA2	1:L:47:ARG:HH21	1.84	0.43
1:D:355:PHE:HE1	1:D:401:THR:HG22	1.83	0.42
1:F:50:MET:HG3	1:F:54:HIS:CE1	2.54	0.42
1:F:366:ASP:OD1	1:F:366:ASP:N	2.42	0.42
1:L:348:ARG:HD2	1:L:348:ARG:HA	1.71	0.42
1:A:106:ASP:OD2	1:F:129:HIS:NE2	2.51	0.42
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.83	0.42
1:B:11:ARG:HH12	1:B:174:ALA:CB	2.30	0.42
1:C:438:VAL:HG12	1:C:464:VAL:HG13	2.01	0.42
1:D:444:ASP:OD1	1:D:444:ASP:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:VAL:HG13	1:F:270:VAL:HG13	2.00	0.42
1:J:412:CYS:SG	1:J:413:HIS:N	2.92	0.42
1:J:551:VAL:HG22	1:J:557:PRO:HD3	2.01	0.42
1:L:231:THR:HG22	1:L:337:TRP:CE2	2.53	0.42
1:A:237:SER:HB2	1:A:241:ALA:HB3	2.02	0.42
1:I:153:ARG:HG2	1:I:214:GLU:OE2	2.20	0.42
1:I:477:THR:O	1:I:481:GLN:HG3	2.18	0.42
1:C:217:ARG:H	1:C:217:ARG:HG2	1.71	0.42
1:D:370:PRO:O	1:D:374:VAL:HG22	2.19	0.42
1:G:194:VAL:HG13	1:G:326:LEU:HD23	2.01	0.42
1:G:216:THR:HG23	1:G:244:ALA:HB2	2.01	0.42
1:G:471:ASN:HB2	1:G:542:LEU:HB2	2.02	0.42
1:H:512:ILE:HG13	1:H:513:ASP:N	2.34	0.42
2:H:601:TPP:C2	2:H:601:TPP:HN42	2.33	0.42
1:K:235:LEU:HB3	1:K:251:SER:HA	2.01	0.42
1:K:286:GLY:HA2	1:K:289:ILE:O	2.20	0.42
1:B:137:LEU:O	1:B:141:ILE:HG13	2.20	0.42
1:C:266:ARG:NH1	4:C:702:HOH:O	2.33	0.42
1:C:545:VAL:HG13	1:C:549:LEU:HD23	2.01	0.42
1:D:19:ASP:OD2	1:D:20:VAL:HG23	2.19	0.42
1:G:180:LEU:HD13	1:G:180:LEU:HA	1.83	0.42
1:L:131:VAL:HG13	1:L:140:LEU:HD23	2.00	0.42
1:B:324:GLU:O	1:B:328:ARG:HG3	2.19	0.42
1:C:45:ASP:OD2	1:C:45:ASP:N	2.42	0.42
1:C:141:ILE:HG12	1:C:158:LEU:HD23	2.01	0.42
1:G:206:ARG:HB3	1:G:343:TRP:CZ2	2.55	0.42
1:H:296:VAL:HG22	1:H:313:LEU:HB3	2.02	0.42
1:K:193:ALA:O	1:K:197:ILE:HG13	2.20	0.42
1:L:191:ALA:O	1:L:194:VAL:HG22	2.19	0.42
1:A:488:ASP:OD2	1:A:488:ASP:N	2.40	0.42
1:H:474:TRP:HD1	1:H:493:ASN:HA	1.84	0.42
1:K:137:LEU:HD22	1:K:141:ILE:HD11	2.01	0.42
2:L:601:TPP:HN42	2:L:601:TPP:C2	2.32	0.42
1:C:204:ALA:O	1:C:340:ARG:NH1	2.39	0.42
1:C:454:PHE:CZ	1:C:535:CYS:HB2	2.53	0.42
1:D:137:LEU:HD21	1:D:160:ILE:HD13	2.02	0.42
1:H:381:VAL:HG12	1:H:406:PRO:HD2	2.01	0.42
1:D:259:PHE:CE2	1:D:557:PRO:HD2	2.55	0.42
1:F:376:ALA:HB3	1:F:520:LEU:HD23	2.02	0.42
1:H:131:VAL:HG11	1:H:137:LEU:HG	2.02	0.42
1:I:189:LEU:N	4:I:709:HOH:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:512:ILE:HD12	1:I:512:ILE:HA	1.86	0.42
1:K:525:ARG:NH2	1:K:525:ARG:HB2	2.34	0.42
1:L:16:ALA:HB2	1:L:180:LEU:HD22	2.02	0.42
1:L:388:VAL:HG22	1:L:411:LEU:HB2	2.02	0.42
1:A:277:PHE:HB3	1:A:308:LEU:HD12	2.01	0.42
1:B:131:VAL:HG22	1:B:140:LEU:HD12	2.01	0.42
1:E:430:GLN:HA	1:E:438:VAL:HG21	2.02	0.42
1:E:512:ILE:HG21	1:E:523:THR:CG2	2.50	0.42
1:H:206:ARG:HB3	1:H:343:TRP:CZ2	2.55	0.42
1:K:454:PHE:HA	1:K:457:MET:CE	2.49	0.42
1:L:285:SER:OG	1:L:287:ILE:HG12	2.20	0.42
1:L:455:ASP:OD2	1:L:459:ARG:NH1	2.52	0.42
1:A:118:VAL:O	1:A:122:THR:OG1	2.35	0.41
1:A:380:THR:HB	1:A:524:LEU:HD23	2.00	0.41
1:D:8:LEU:HD11	1:D:169:VAL:HG21	2.02	0.41
1:K:474:TRP:N	1:K:493:ASN:O	2.52	0.41
1:A:474:TRP:CE3	2:A:601:TPP:HM41	2.55	0.41
1:B:488:ASP:OD1	1:B:488:ASP:N	2.48	0.41
1:B:550:ASN:HB2	1:B:557:PRO:HA	2.01	0.41
1:E:418:SER:O	1:E:421:VAL:HG13	2.20	0.41
1:F:508:GLY:O	1:F:532:ARG:NH2	2.43	0.41
1:G:354:ARG:HH21	1:G:547:PRO:HB2	1.86	0.41
1:J:259:PHE:CE2	1:J:557:PRO:HD2	2.55	0.41
1:J:556:LYS:HA	1:J:556:LYS:HD3	1.32	0.41
1:L:313:LEU:HA	1:L:313:LEU:HD12	1.83	0.41
1:D:339:ASP:OD2	1:J:226:ARG:NE	2.54	0.41
1:E:185:LEU:N	1:F:314:GLY:O	2.52	0.41
1:H:298:ILE:HG23	1:H:315:ALA:HB3	2.02	0.41
1:J:11:ARG:CG	1:J:39:ARG:NH2	2.37	0.41
1:K:279:LEU:HD12	1:K:279:LEU:HA	1.87	0.41
1:A:163:ASP:N	1:A:163:ASP:OD1	2.50	0.41
1:B:152:PRO:HG3	1:B:301:ASP:HB2	2.03	0.41
1:B:380:THR:HB	1:B:524:LEU:HD23	2.01	0.41
1:E:152:PRO:CG	1:E:301:ASP:HB2	2.50	0.41
1:G:42:ARG:N	4:G:707:HOH:O	2.51	0.41
1:J:195:GLU:O	1:J:199:ASP:HB2	2.21	0.41
1:C:550:ASN:OD1	1:C:550:ASN:N	2.53	0.41
1:D:206:ARG:HG2	1:D:343:TRP:CE3	2.55	0.41
1:H:266:ARG:HH22	1:H:287:ILE:HA	1.85	0.41
1:J:553:LEU:H	1:J:553:LEU:HG	1.54	0.41
1:L:250:LEU:HD13	1:L:250:LEU:HA	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:471:ASN:HB2	1:I:542:LEU:HD13	2.02	0.41
1:J:480:ALA:O	1:J:484:ILE:HG12	2.20	0.41
1:K:3:ALA:O	1:K:169:VAL:N	2.51	0.41
1:K:54:HIS:NE2	1:K:421:VAL:HG22	2.36	0.41
1:L:272:LEU:HD12	1:L:297:GLN:HG3	2.02	0.41
1:L:514:VAL:HG13	1:L:519:ASP:HB2	2.02	0.41
1:C:137:LEU:O	1:C:141:ILE:HG13	2.21	0.41
1:F:27:ILE:H	1:F:27:ILE:CD1	2.31	0.41
1:I:92:THR:HG22	1:I:94:VAL:HG23	2.02	0.41
1:L:140:LEU:HD12	1:L:140:LEU:HA	1.71	0.41
1:A:55:ALA:O	1:A:428:GLY:HA3	2.20	0.41
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.89	0.41
1:A:261:LEU:HG	1:A:350:LEU:HD22	2.03	0.41
1:B:88:HIS:HB2	1:B:124:ILE:O	2.21	0.41
1:D:404:ARG:H	1:D:404:ARG:HG3	1.71	0.41
1:E:61:ARG:NE	1:E:240:GLU:OE2	2.50	0.41
1:E:206:ARG:HG2	1:E:343:TRP:CE3	2.56	0.41
1:G:235:LEU:HG	1:G:245:ILE:HB	2.02	0.41
1:G:488:ASP:OD1	1:G:488:ASP:N	2.54	0.41
1:H:367:ARG:HH22	1:H:472:ARG:HG3	1.86	0.41
1:I:324:GLU:O	1:I:328:ARG:HG3	2.20	0.41
1:I:377:ILE:HD11	1:I:467:VAL:HG11	2.03	0.41
1:I:455:ASP:O	1:I:459:ARG:HG3	2.20	0.41
1:J:376:ALA:O	1:J:380:THR:OG1	2.22	0.41
1:K:236:PHE:CE2	1:K:258:LEU:HG	2.56	0.41
1:L:102:PRO:HG3	1:L:162:TRP:CE3	2.56	0.41
1:A:512:ILE:HG21	1:A:523:THR:HG21	2.02	0.41
1:B:29:ILE:HG13	1:B:29:ILE:O	2.21	0.41
1:H:550:ASN:O	1:H:554:GLY:N	2.54	0.41
1:K:163:ASP:OD1	1:K:163:ASP:N	2.53	0.41
1:K:171:ASP:HA	1:K:174:ALA:HB3	2.02	0.41
1:B:237:SER:O	1:B:254:LEU:HA	2.21	0.40
1:C:551:VAL:HA	1:C:555:GLY:O	2.22	0.40
2:D:601:TPP:C2	2:D:601:TPP:HN42	2.35	0.40
1:J:229:GLU:HA	1:J:250:LEU:HD23	2.03	0.40
1:L:259:PHE:CZ	1:L:556:LYS:HB2	2.56	0.40
1:A:427:LEU:HD11	1:A:456:SER:HB2	2.03	0.40
1:E:494:ARG:NH2	4:E:709:HOH:O	2.53	0.40
1:I:245:ILE:O	1:I:251:SER:HB2	2.21	0.40
1:J:133:ARG:HB2	1:J:136:LEU:HG	2.03	0.40
1:B:522:PRO:O	1:B:526:GLU:HG3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLY:O	1:C:57:GLU:HG3	2.21	0.40
1:E:152:PRO:HG3	1:E:301:ASP:HB2	2.03	0.40
1:F:13:LEU:HD22	1:F:68:VAL:HG21	2.04	0.40
1:H:65:ARG:HD3	4:H:718:HOH:O	2.21	0.40
1:I:478:LEU:HD22	1:I:542:LEU:HD21	2.04	0.40
1:K:348:ARG:HE	1:K:348:ARG:HB2	1.66	0.40
1:A:187:ALA:HB1	1:B:187:ALA:CB	2.52	0.40
1:A:187:ALA:CB	1:B:187:ALA:HB1	2.51	0.40
1:A:194:VAL:HG13	1:A:326:LEU:HD23	2.04	0.40
1:B:55:ALA:O	1:B:428:GLY:HA3	2.21	0.40
1:B:478:LEU:HG	1:B:490:VAL:CG1	2.51	0.40
1:D:474:TRP:HB3	2:D:601:TPP:H61	2.02	0.40
1:E:367:ARG:HH21	1:E:539:HIS:HB3	1.87	0.40
1:G:477:THR:O	1:G:481:GLN:HG3	2.22	0.40
1:H:13:LEU:HB3	1:H:18:VAL:CG2	2.52	0.40
1:H:171:ASP:O	1:H:172:ALA:C	2.59	0.40
1:H:370:PRO:O	1:H:374:VAL:HG22	2.22	0.40
1:J:231:THR:HG22	1:J:337:TRP:CE2	2.57	0.40
1:B:277:PHE:HB3	1:B:308:LEU:HD12	2.03	0.40
1:B:321:ALA:O	1:B:325:GLU:HG2	2.22	0.40
1:D:231:THR:HG22	1:D:337:TRP:CE2	2.57	0.40
1:I:136:LEU:HD23	1:I:136:LEU:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/558 (100%)	542 (98%)	13 (2%)	0	100	100
1	B	555/558 (100%)	542 (98%)	13 (2%)	0	100	100
1	C	555/558 (100%)	543 (98%)	12 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	555/558 (100%)	544 (98%)	11 (2%)	0	100	100
1	E	550/558 (99%)	533 (97%)	17 (3%)	0	100	100
1	F	550/558 (99%)	535 (97%)	15 (3%)	0	100	100
1	G	555/558 (100%)	541 (98%)	14 (2%)	0	100	100
1	H	549/558 (98%)	539 (98%)	10 (2%)	0	100	100
1	I	548/558 (98%)	532 (97%)	16 (3%)	0	100	100
1	J	549/558 (98%)	537 (98%)	12 (2%)	0	100	100
1	K	548/558 (98%)	538 (98%)	10 (2%)	0	100	100
1	L	549/558 (98%)	535 (97%)	14 (3%)	0	100	100
All	All	6618/6696 (99%)	6461 (98%)	157 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/415 (98%)	393 (97%)	12 (3%)	36	63
1	B	411/415 (99%)	396 (96%)	15 (4%)	30	55
1	C	410/415 (99%)	387 (94%)	23 (6%)	17	37
1	D	411/415 (99%)	386 (94%)	25 (6%)	15	34
1	E	406/415 (98%)	384 (95%)	22 (5%)	18	39
1	F	407/415 (98%)	390 (96%)	17 (4%)	25	49
1	G	406/415 (98%)	389 (96%)	17 (4%)	25	49
1	H	401/415 (97%)	371 (92%)	30 (8%)	11	25
1	I	392/415 (94%)	368 (94%)	24 (6%)	15	34
1	J	401/415 (97%)	378 (94%)	23 (6%)	17	37
1	K	393/415 (95%)	367 (93%)	26 (7%)	14	30
1	L	399/415 (96%)	378 (95%)	21 (5%)	19	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4842/4980 (97%)	4587 (95%)	255 (5%)	19	40

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	160	ILE
1	A	180	LEU
1	A	196	ARG
1	A	216	THR
1	A	250	LEU
1	A	300	SER
1	A	359	THR
1	A	385	SER
1	A	395	TYR
1	A	404	ARG
1	A	477	THR
1	B	18	VAL
1	B	40	SER
1	B	100	SER
1	B	111	LEU
1	B	186	THR
1	B	199	ASP
1	B	263	GLU
1	B	342	ARG
1	B	356	GLU
1	B	395	TYR
1	B	417	SER
1	B	435	THR
1	B	453	GLU
1	B	541	SER
1	B	552	LEU
1	C	4	THR
1	C	19	ASP
1	C	78	THR
1	C	169	VAL
1	C	170	ASP
1	C	177	VAL
1	C	215	LEU
1	C	237	SER
1	C	300	SER
1	C	366	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	380	THR
1	C	395	TYR
1	C	417	SER
1	C	450	SER
1	C	453	GLU
1	C	494	ARG
1	C	511	SER
1	C	513	ASP
1	C	532	ARG
1	C	541	SER
1	C	550	ASN
1	C	556	LYS
1	C	558	PHE
1	D	2	THR
1	D	18	VAL
1	D	19	ASP
1	D	83	SER
1	D	111	LEU
1	D	136	LEU
1	D	160	ILE
1	D	185	LEU
1	D	196	ARG
1	D	226	ARG
1	D	250	LEU
1	D	255	LEU
1	D	262	ASP
1	D	263	GLU
1	D	265	GLU
1	D	303	ARG
1	D	307	ARG
1	D	366	ASP
1	D	395	TYR
1	D	417	SER
1	D	434	VAL
1	D	450	SER
1	D	455	ASP
1	D	513	ASP
1	D	516	ASP
1	E	30	ASP
1	E	83	SER
1	E	105	VAL
1	E	111	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	163	ASP
1	E	177	VAL
1	E	199	ASP
1	E	213	SER
1	E	251	SER
1	E	292	ASP
1	E	300	SER
1	E	340	ARG
1	E	356	GLU
1	E	395	TYR
1	E	407	VAL
1	E	444	ASP
1	E	450	SER
1	E	453	GLU
1	E	507	LEU
1	E	513	ASP
1	E	515	SER
1	E	541	SER
1	F	2	THR
1	F	45	ASP
1	F	100	SER
1	F	170	ASP
1	F	185	LEU
1	F	199	ASP
1	F	255	LEU
1	F	340	ARG
1	F	395	TYR
1	F	407	VAL
1	F	447	VAL
1	F	450	SER
1	F	455	ASP
1	F	472	ARG
1	F	477	THR
1	F	532	ARG
1	F	556	LYS
1	G	4	THR
1	G	7	GLU
1	G	40	SER
1	G	130	ARG
1	G	180	LEU
1	G	199	ASP
1	G	210	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	216	THR
1	G	251	SER
1	G	292	ASP
1	G	300	SER
1	G	328	ARG
1	G	342	ARG
1	G	366	ASP
1	G	395	TYR
1	G	457	MET
1	G	558	PHE
1	H	42	ARG
1	H	47	ARG
1	H	65	ARG
1	H	130	ARG
1	H	136	LEU
1	H	168	THR
1	H	169	VAL
1	H	177	VAL
1	H	180	LEU
1	H	199	ASP
1	H	208	VAL
1	H	225	ARG
1	H	226	ARG
1	H	246	ARG
1	H	250	LEU
1	H	291	ARG
1	H	292	ASP
1	H	340	ARG
1	H	346	ARG
1	H	359	THR
1	H	381	VAL
1	H	395	TYR
1	H	444	ASP
1	H	447	VAL
1	H	450	SER
1	H	459	ARG
1	H	505	ARG
1	H	519	ASP
1	H	526	GLU
1	H	532	ARG
1	I	29	ILE
1	I	38	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	110	THR
1	I	122	THR
1	I	136	LEU
1	I	153	ARG
1	I	168	THR
1	I	169	VAL
1	I	170	ASP
1	I	180	LEU
1	I	250	LEU
1	I	300	SER
1	I	365	ASP
1	I	418	SER
1	I	435	THR
1	I	471	ASN
1	I	477	THR
1	I	485	LEU
1	I	489	ARG
1	I	494	ARG
1	I	511	SER
1	I	526	GLU
1	I	541	SER
1	I	549	LEU
1	J	4	THR
1	J	11	ARG
1	J	18	VAL
1	J	31	SER
1	J	42	ARG
1	J	111	LEU
1	J	170	ASP
1	J	180	LEU
1	J	185	LEU
1	J	199	ASP
1	J	250	LEU
1	J	251	SER
1	J	263	GLU
1	J	300	SER
1	J	341	SER
1	J	395	TYR
1	J	404	ARG
1	J	457	MET
1	J	471	ASN
1	J	516	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	541	SER
1	J	553	LEU
1	J	556	LYS
1	K	2	THR
1	K	19	ASP
1	K	40	SER
1	K	136	LEU
1	K	169	VAL
1	K	171	ASP
1	K	180	LEU
1	K	213	SER
1	K	215	LEU
1	K	216	THR
1	K	251	SER
1	K	255	LEU
1	K	300	SER
1	K	303	ARG
1	K	307	ARG
1	K	366	ASP
1	K	395	TYR
1	K	417	SER
1	K	435	THR
1	K	450	SER
1	K	471	ASN
1	K	485	LEU
1	K	511	SER
1	K	512	ILE
1	K	528	LEU
1	K	532	ARG
1	L	19	ASP
1	L	136	LEU
1	L	140	LEU
1	L	157	LEU
1	L	198	LEU
1	L	262	ASP
1	L	292	ASP
1	L	300	SER
1	L	331	LEU
1	L	346	ARG
1	L	348	ARG
1	L	349	GLU
1	L	357	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	361	GLN
1	L	385	SER
1	L	444	ASP
1	L	447	VAL
1	L	450	SER
1	L	494	ARG
1	L	553	LEU
1	L	556	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	413	HIS
1	C	361	GLN
1	E	183	HIS
1	G	129	HIS
1	H	481	GLN
1	H	493	ASN
1	I	413	HIS
1	J	309	GLN
1	K	470	ASN
1	L	309	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPP	C	601	3	22,27,27	1.10	2 (9%)	29,40,40	1.11	2 (6%)
2	TPP	B	601	3	22,27,27	1.05	1 (4%)	29,40,40	1.03	2 (6%)
2	TPP	D	601	3	22,27,27	1.03	2 (9%)	29,40,40	1.14	2 (6%)
2	TPP	F	601	3	22,27,27	1.03	2 (9%)	29,40,40	1.36	2 (6%)
2	TPP	K	601	3	22,27,27	1.05	2 (9%)	29,40,40	1.26	2 (6%)
2	TPP	L	601	3	22,27,27	1.07	2 (9%)	29,40,40	1.42	2 (6%)
2	TPP	A	601	3	22,27,27	1.13	2 (9%)	29,40,40	1.39	2 (6%)
2	TPP	E	601	3	22,27,27	1.13	2 (9%)	29,40,40	1.32	2 (6%)
2	TPP	G	601	3	22,27,27	1.15	1 (4%)	29,40,40	1.44	2 (6%)
2	TPP	H	601	3	22,27,27	1.13	1 (4%)	29,40,40	1.00	2 (6%)
2	TPP	J	601	3	22,27,27	1.09	2 (9%)	29,40,40	1.34	2 (6%)
2	TPP	I	601	3	22,27,27	1.15	2 (9%)	29,40,40	1.48	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	C	601	3	-	1/16/17/17	0/2/2/2
2	TPP	B	601	3	-	0/16/17/17	0/2/2/2
2	TPP	D	601	3	-	1/16/17/17	0/2/2/2
2	TPP	F	601	3	-	1/16/17/17	0/2/2/2
2	TPP	K	601	3	-	0/16/17/17	0/2/2/2
2	TPP	L	601	3	-	0/16/17/17	0/2/2/2
2	TPP	A	601	3	-	0/16/17/17	0/2/2/2
2	TPP	E	601	3	-	0/16/17/17	0/2/2/2
2	TPP	G	601	3	-	1/16/17/17	0/2/2/2
2	TPP	H	601	3	-	0/16/17/17	0/2/2/2
2	TPP	J	601	3	-	0/16/17/17	0/2/2/2
2	TPP	I	601	3	-	1/16/17/17	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	TPP	C6-C5	-4.35	1.49	1.50
2	H	601	TPP	C6-C5	-4.23	1.49	1.50
2	I	601	TPP	C6-C5	-4.20	1.49	1.50
2	A	601	TPP	C6-C5	-3.96	1.49	1.50
2	B	601	TPP	C6-C5	-3.91	1.49	1.50
2	C	601	TPP	C6-C5	-3.88	1.49	1.50
2	E	601	TPP	C6-C5	-3.80	1.49	1.50
2	J	601	TPP	C6-C5	-3.78	1.49	1.50
2	K	601	TPP	C6-C5	-3.72	1.49	1.50
2	L	601	TPP	C6-C5	-3.58	1.49	1.50
2	D	601	TPP	C6-C5	-3.47	1.49	1.50
2	F	601	TPP	C6-C5	-3.33	1.49	1.50
2	E	601	TPP	C4-N3	2.66	1.42	1.39
2	A	601	TPP	C4-N3	2.63	1.42	1.39
2	L	601	TPP	C4-N3	2.54	1.41	1.39
2	F	601	TPP	C4-N3	2.44	1.41	1.39
2	J	601	TPP	C4-N3	2.32	1.41	1.39
2	I	601	TPP	C4-N3	2.19	1.41	1.39
2	D	601	TPP	C4-N3	2.17	1.41	1.39
2	K	601	TPP	C4-N3	2.10	1.41	1.39
2	C	601	TPP	C4-N3	2.10	1.41	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	601	TPP	C6-C5-C4	6.56	132.70	127.43
2	G	601	TPP	C6-C5-C4	6.28	132.47	127.43
2	L	601	TPP	C6-C5-C4	6.06	132.30	127.43
2	A	601	TPP	C6-C5-C4	5.80	132.09	127.43
2	F	601	TPP	C6-C5-C4	5.69	132.00	127.43
2	J	601	TPP	C6-C5-C4	5.55	131.89	127.43
2	E	601	TPP	C6-C5-C4	5.36	131.74	127.43
2	K	601	TPP	C6-C5-C4	4.86	131.33	127.43
2	C	601	TPP	C6-C5-C4	3.82	130.50	127.43
2	D	601	TPP	C6-C5-C4	3.48	130.22	127.43
2	D	601	TPP	C5-C4-N3	3.24	114.06	107.57
2	J	601	TPP	C5-C4-N3	3.19	113.95	107.57
2	B	601	TPP	C5-C4-N3	3.17	113.91	107.57
2	F	601	TPP	C5-C4-N3	3.12	113.81	107.57
2	K	601	TPP	C5-C4-N3	3.11	113.80	107.57
2	C	601	TPP	C5-C4-N3	3.09	113.76	107.57
2	A	601	TPP	C5-C4-N3	3.08	113.73	107.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	601	TPP	C5-C4-N3	3.07	113.72	107.57
2	H	601	TPP	C5-C4-N3	3.03	113.64	107.57
2	I	601	TPP	C5-C4-N3	2.99	113.56	107.57
2	E	601	TPP	C5-C4-N3	2.98	113.54	107.57
2	G	601	TPP	C5-C4-N3	2.98	113.53	107.57
2	B	601	TPP	C6-C5-C4	2.86	129.73	127.43
2	H	601	TPP	C6-C5-C4	2.74	129.63	127.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	601	TPP	C5-C6-C7-O7
2	I	601	TPP	C5-C6-C7-O7
2	C	601	TPP	PA-O3A-PB-O1B
2	D	601	TPP	PA-O3A-PB-O1B
2	F	601	TPP	PA-O3A-PB-O1B

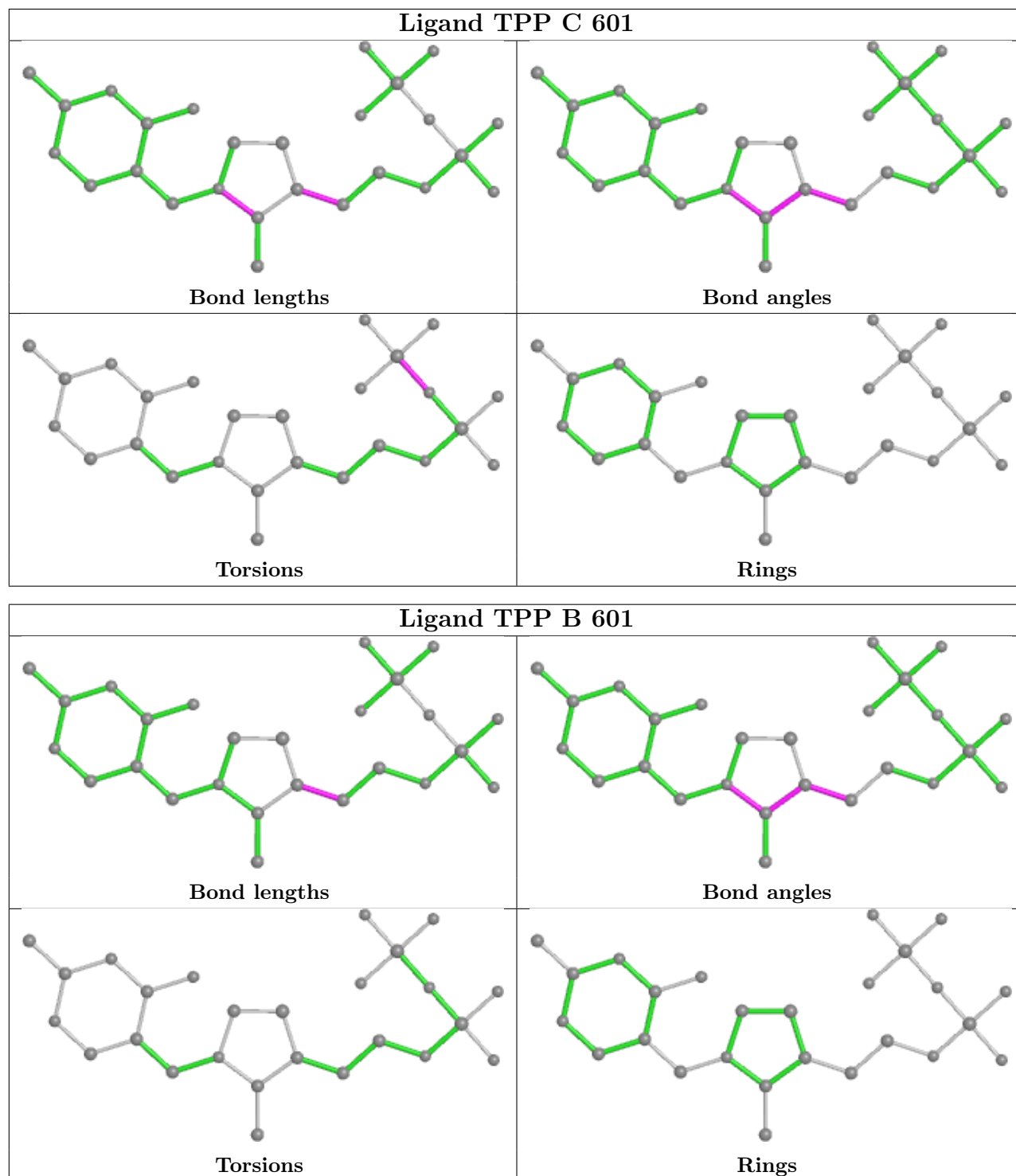
There are no ring outliers.

12 monomers are involved in 20 short contacts:

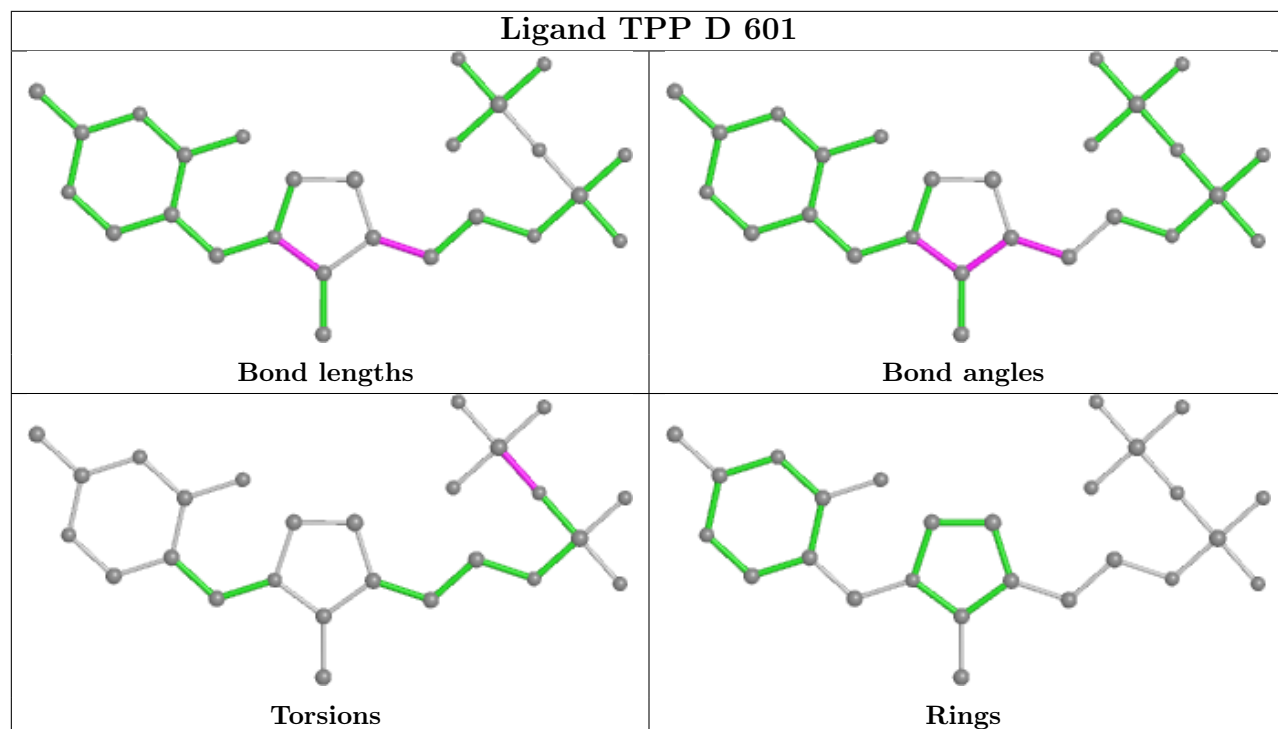
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	TPP	1	0
2	B	601	TPP	2	0
2	D	601	TPP	2	0
2	F	601	TPP	2	0
2	K	601	TPP	2	0
2	L	601	TPP	2	0
2	A	601	TPP	1	0
2	E	601	TPP	1	0
2	G	601	TPP	2	0
2	H	601	TPP	3	0
2	J	601	TPP	1	0
2	I	601	TPP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

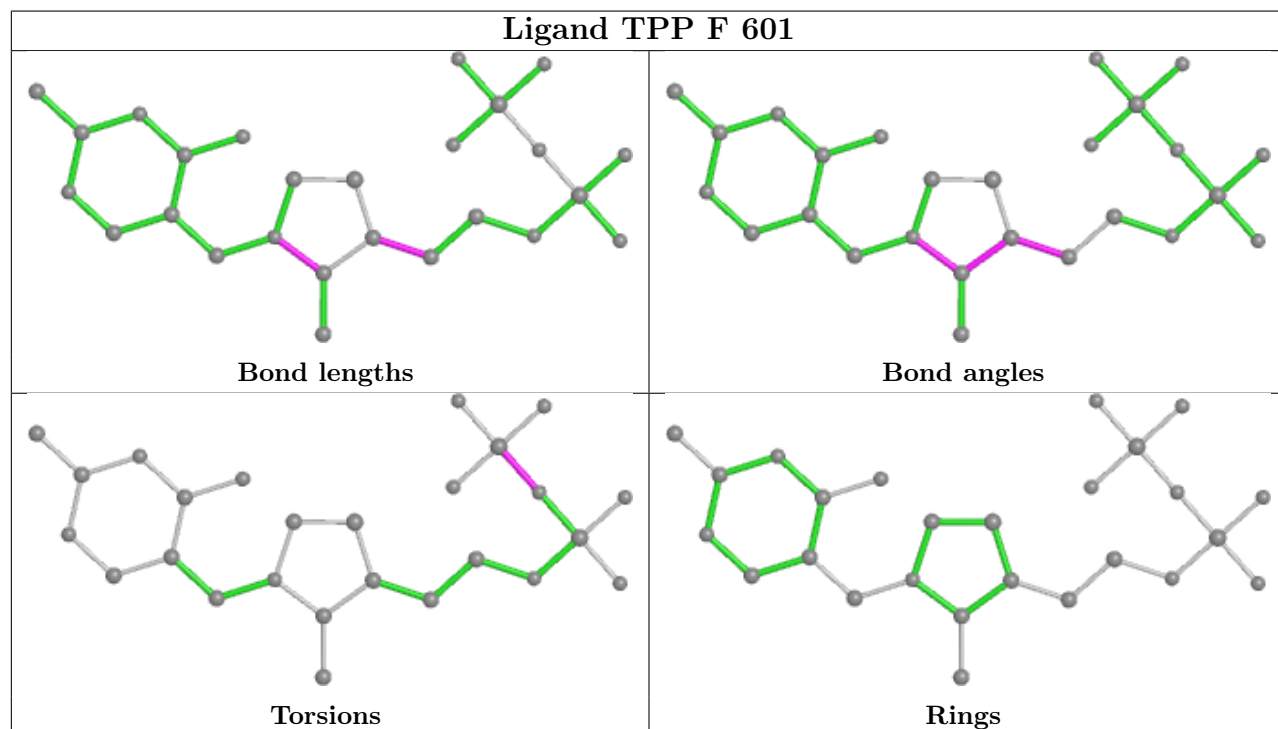
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



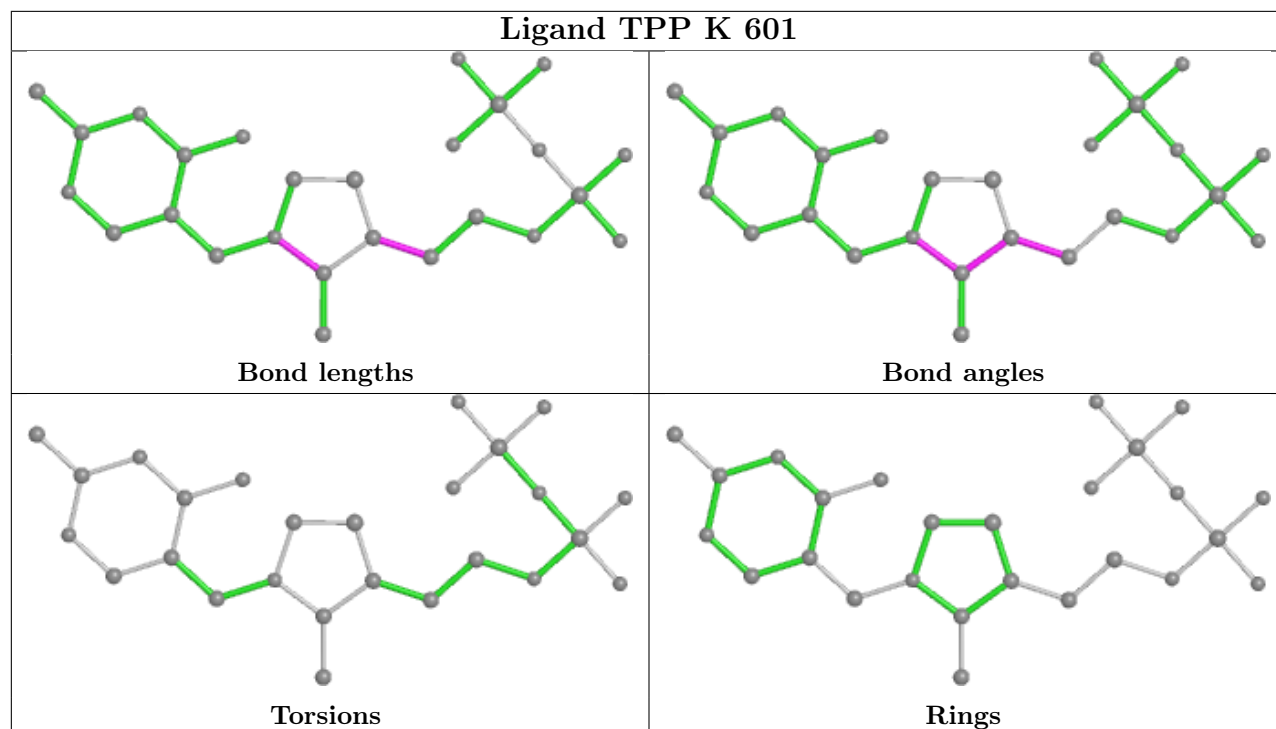
Ligand TPP D 601



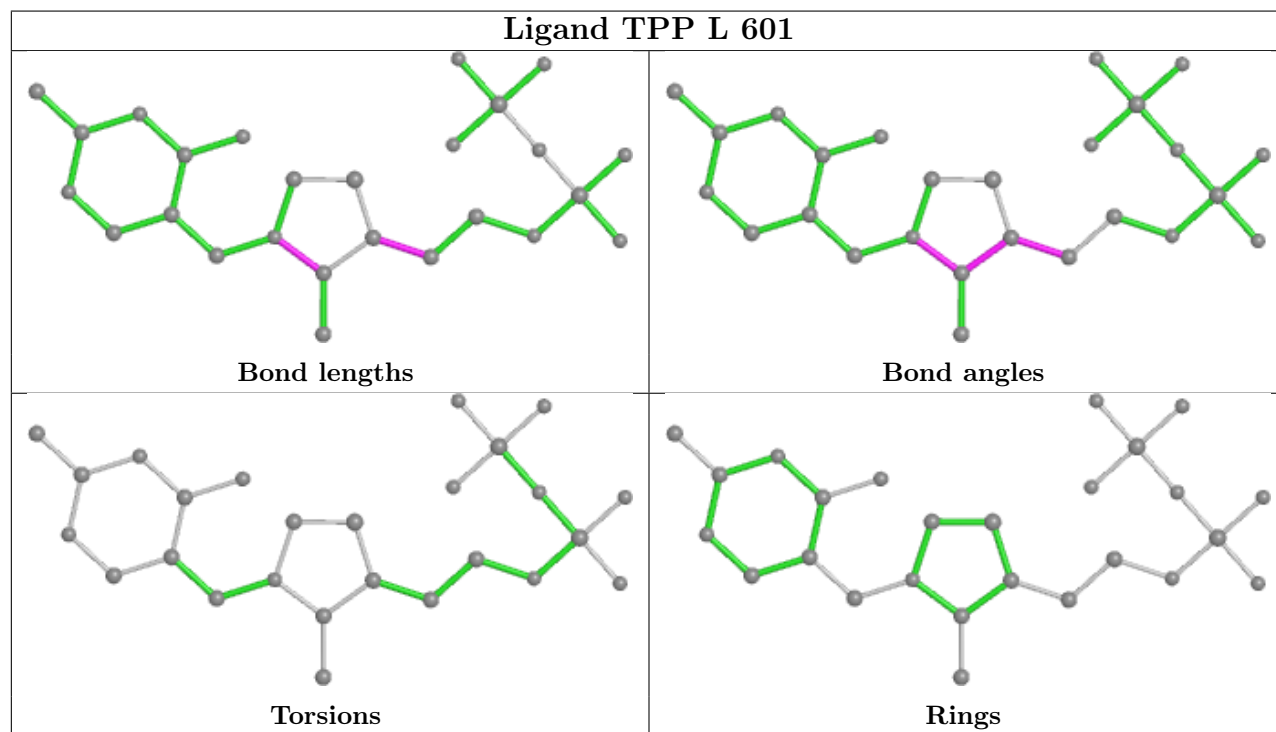
Ligand TPP F 601



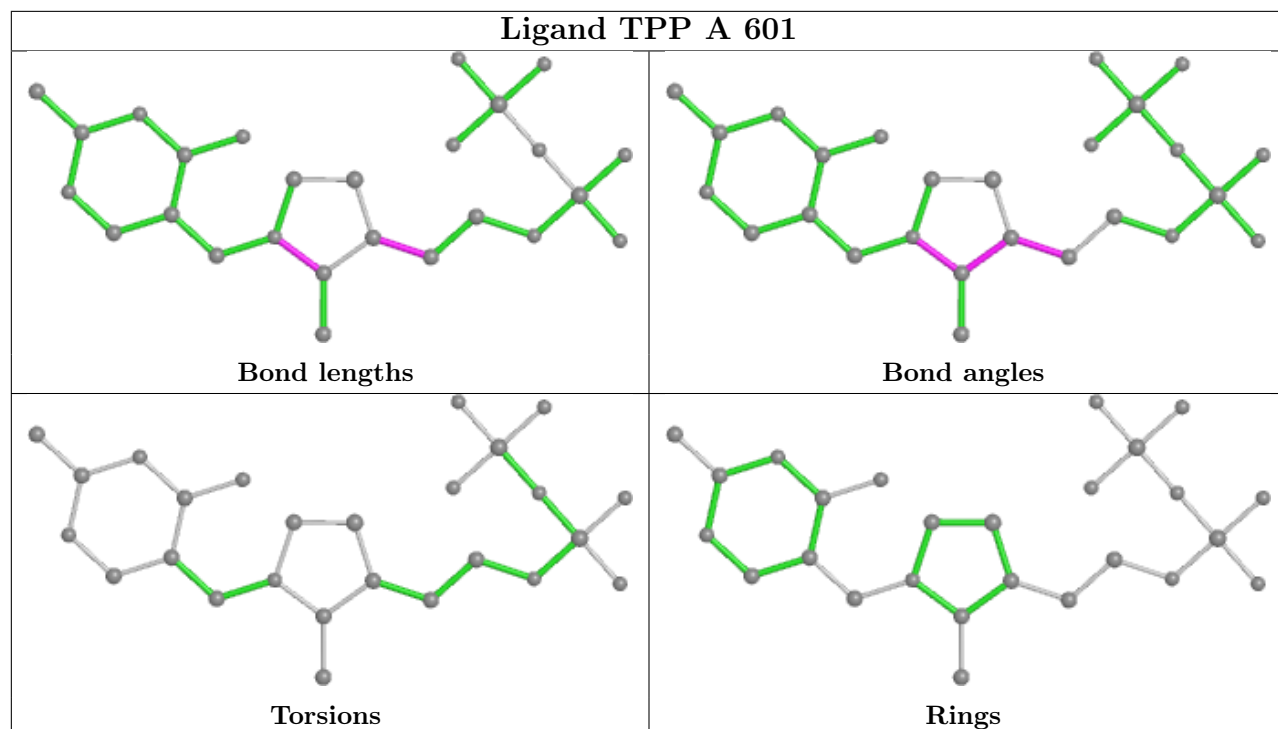
Ligand TPP K 601



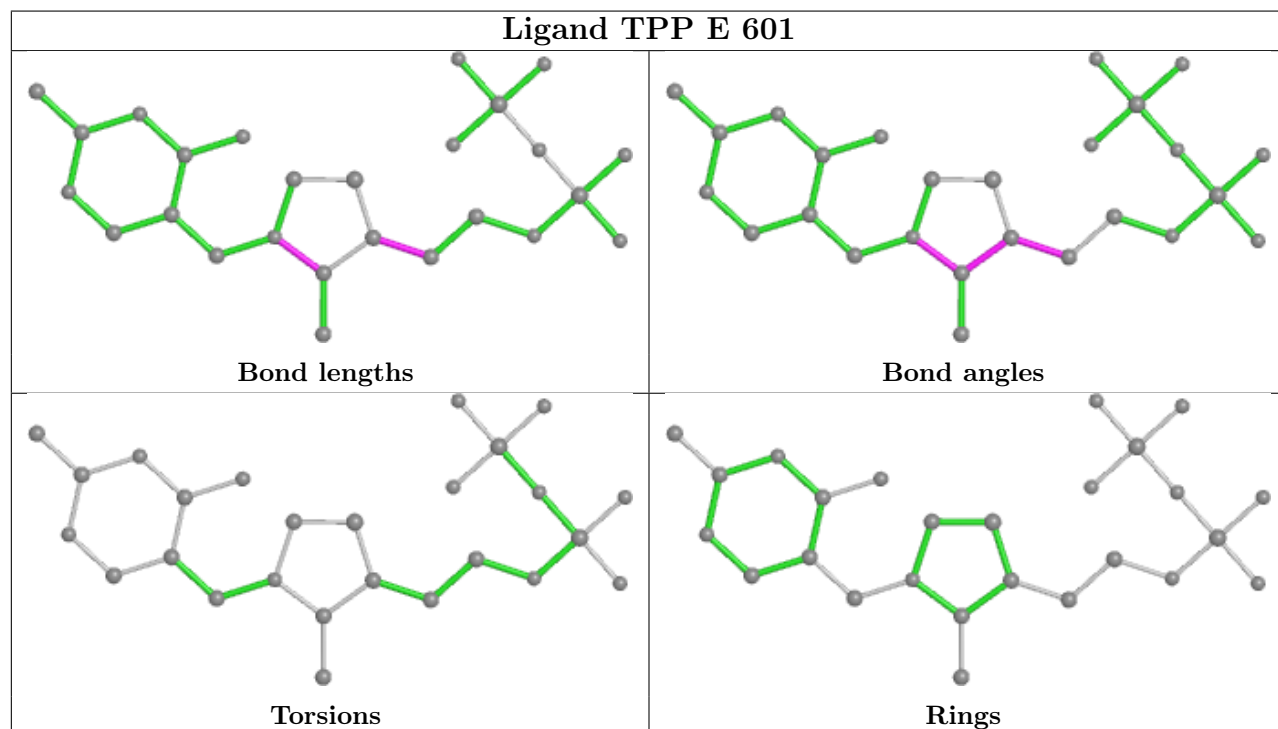
Ligand TPP L 601



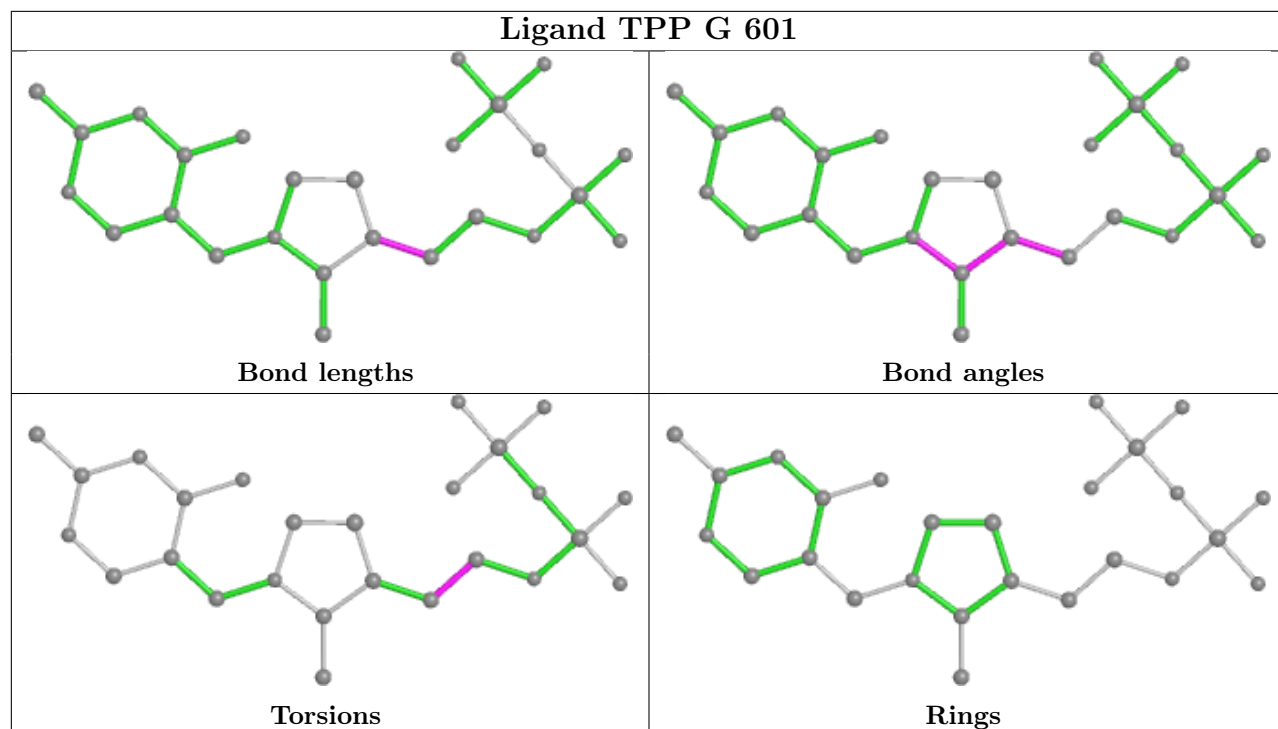
Ligand TPP A 601



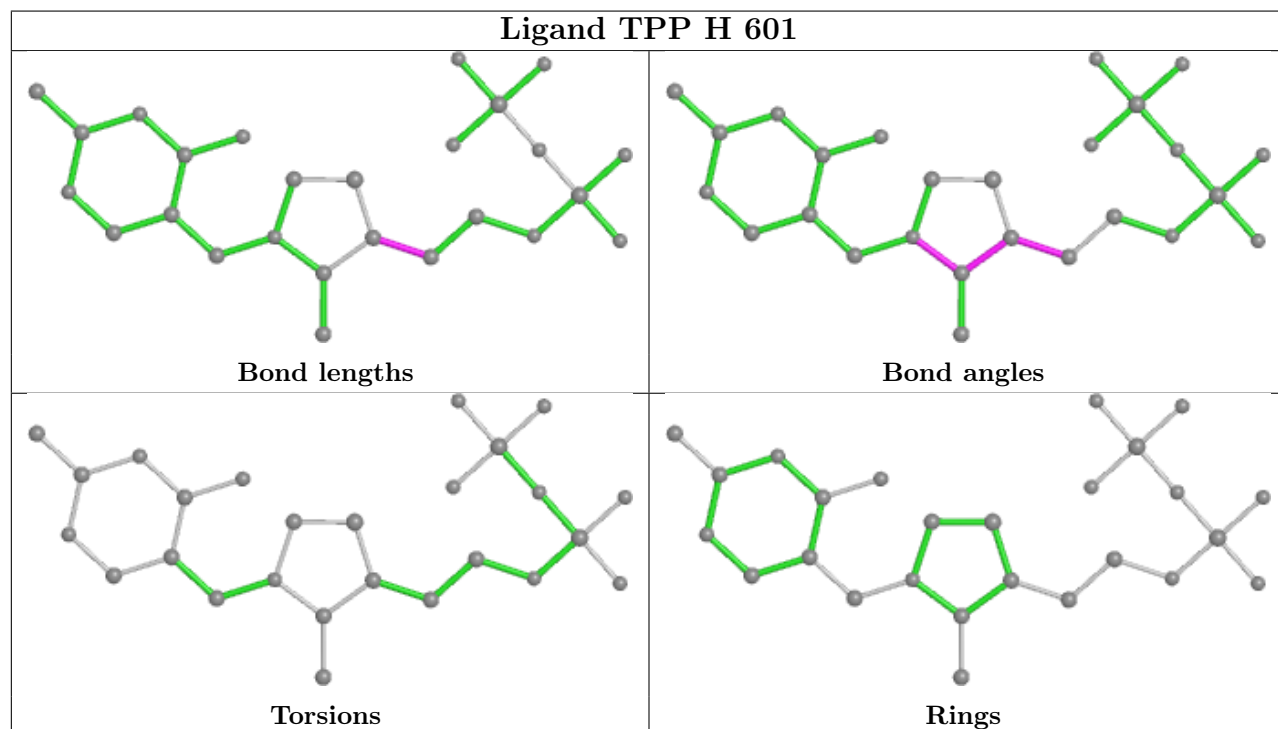
Ligand TPP E 601

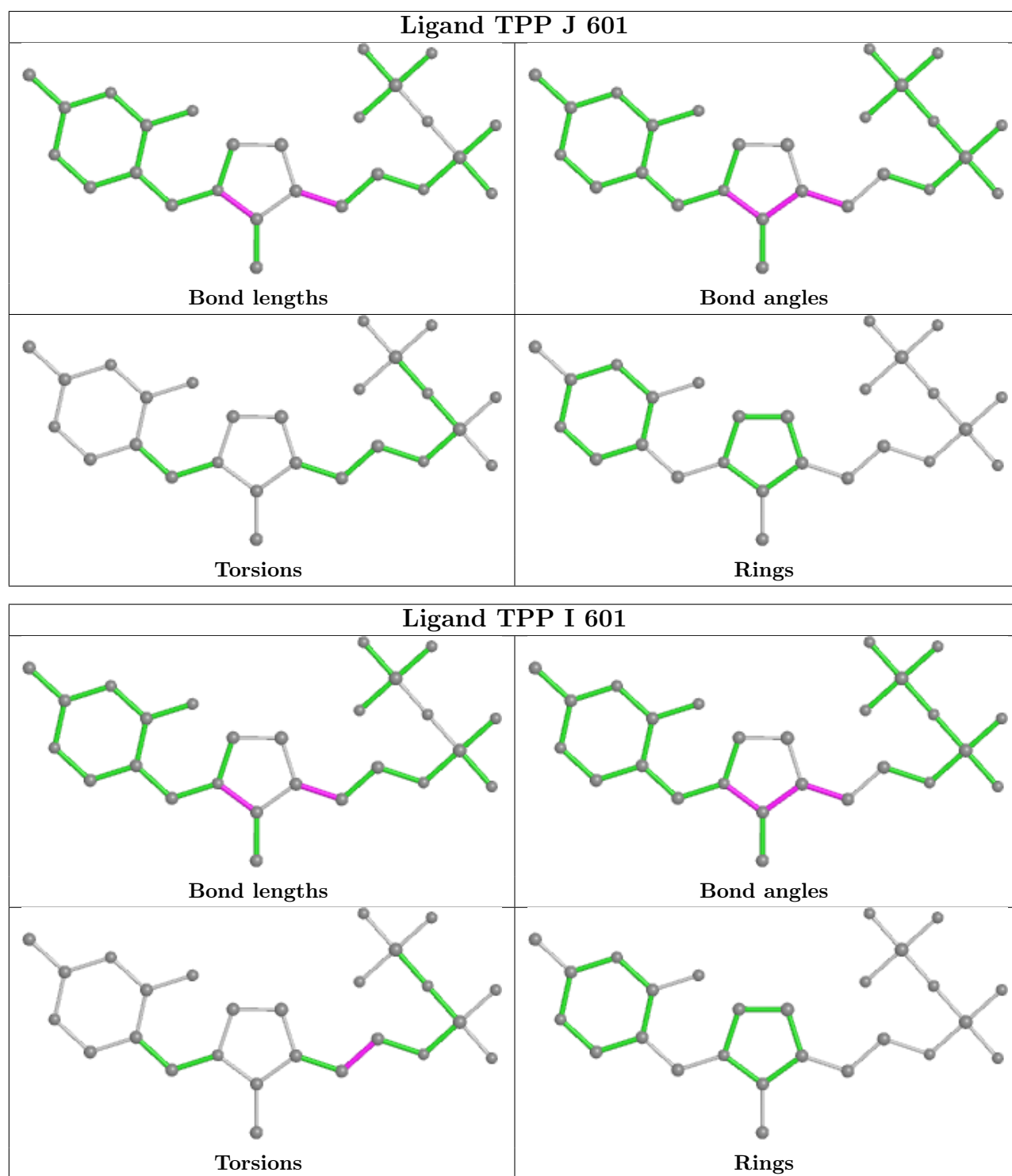


Ligand TPP G 601



Ligand TPP H 601





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/558 (99%)	-0.34	6 (1%) 77 77	20, 34, 52, 85	0
1	B	557/558 (99%)	-0.31	8 (1%) 73 72	20, 34, 54, 92	0
1	C	557/558 (99%)	-0.27	9 (1%) 70 70	23, 35, 56, 91	0
1	D	557/558 (99%)	-0.25	10 (1%) 67 67	23, 37, 57, 88	0
1	E	554/558 (99%)	-0.04	11 (1%) 64 64	22, 39, 63, 93	0
1	F	554/558 (99%)	-0.18	7 (1%) 74 74	21, 39, 62, 86	0
1	G	557/558 (99%)	-0.11	11 (1%) 64 64	24, 39, 61, 99	0
1	H	553/558 (99%)	0.00	6 (1%) 77 77	26, 42, 63, 92	0
1	I	552/558 (98%)	0.09	9 (1%) 70 70	27, 44, 68, 95	0
1	J	553/558 (99%)	-0.12	13 (2%) 59 58	25, 39, 57, 89	0
1	K	550/558 (98%)	0.13	17 (3%) 51 50	25, 46, 70, 85	0
1	L	553/558 (99%)	0.16	8 (1%) 73 72	29, 49, 68, 89	0
All	All	6654/6696 (99%)	-0.10	115 (1%) 69 68	20, 39, 63, 99	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	GLY	7.4
1	L	171	ASP	6.8
1	C	174	ALA	5.0
1	C	558	PHE	4.6
1	J	176	GLY	4.4
1	G	173	LEU	4.2
1	J	558	PHE	4.1
1	E	188	ALA	4.0
1	F	181	GLY	4.0
1	I	183	HIS	3.7
1	I	182	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	558	PHE	3.5
1	K	170	ASP	3.5
1	C	184	ALA	3.5
1	A	174	ALA	3.4
1	B	558	PHE	3.4
1	E	39	ARG	3.4
1	H	172	ALA	3.4
1	G	489	ARG	3.4
1	D	183	HIS	3.4
1	K	339	ASP	3.3
1	E	176	GLY	3.3
1	F	218	GLY	3.3
1	G	557	PRO	3.3
1	C	183	HIS	3.3
1	E	180	LEU	3.3
1	I	172	ALA	3.2
1	J	39	ARG	3.2
1	A	176	GLY	3.2
1	D	182	ALA	3.1
1	D	328	ARG	3.1
1	F	556	LYS	3.1
1	G	555	GLY	3.0
1	D	187	ALA	3.0
1	E	292	ASP	3.0
1	E	187	ALA	3.0
1	J	263	GLU	2.9
1	J	557	PRO	2.9
1	E	172	ALA	2.9
1	A	175	ASP	2.9
1	E	183	HIS	2.9
1	B	552	LEU	2.9
1	E	516	ASP	2.8
1	C	182	ALA	2.8
1	J	187	ALA	2.8
1	C	175	ASP	2.8
1	J	555	GLY	2.8
1	F	182	ALA	2.8
1	K	187	ALA	2.8
1	C	553	LEU	2.7
1	K	532	ARG	2.7
1	C	170	ASP	2.7
1	I	184	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	250	LEU	2.6
1	A	172	ALA	2.6
1	B	187	ALA	2.6
1	K	241	ALA	2.6
1	E	356	GLU	2.6
1	A	219	ASP	2.6
1	J	309	GLN	2.6
1	L	348	ARG	2.5
1	L	532	ARG	2.5
1	H	516	ASP	2.5
1	F	357	SER	2.5
1	B	553	LEU	2.5
1	H	183	HIS	2.5
1	B	556	LYS	2.5
1	G	219	ASP	2.5
1	I	219	ASP	2.5
1	K	512	ILE	2.5
1	K	188	ALA	2.4
1	F	266	ARG	2.4
1	I	177	VAL	2.4
1	D	516	ASP	2.4
1	G	175	ASP	2.4
1	J	171	ASP	2.4
1	E	226	ARG	2.4
1	K	175	ASP	2.4
1	C	173	LEU	2.3
1	B	188	ALA	2.3
1	H	494	ARG	2.3
1	I	130	ARG	2.3
1	K	183	HIS	2.3
1	H	246	ARG	2.3
1	I	187	ALA	2.2
1	L	180	LEU	2.2
1	F	172	ALA	2.2
1	G	188	ALA	2.2
1	I	176	GLY	2.2
1	L	552	LEU	2.2
1	J	177	VAL	2.2
1	G	177	VAL	2.2
1	D	172	ALA	2.2
1	D	185	LEU	2.2
1	G	187	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	554	GLY	2.2
1	L	523	THR	2.1
1	D	184	ALA	2.1
1	G	174	ALA	2.1
1	K	205	GLU	2.1
1	K	265	GLU	2.1
1	K	511	SER	2.1
1	K	177	VAL	2.1
1	L	250	LEU	2.1
1	K	190	GLY	2.1
1	L	11	ARG	2.0
1	A	170	ASP	2.0
1	K	488	ASP	2.0
1	K	516	ASP	2.0
1	B	174	ALA	2.0
1	K	174	ALA	2.0
1	J	437	PRO	2.0
1	J	178	GLU	2.0
1	D	171	ASP	2.0
1	J	182	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	F	602	1/1	0.77	0.15	36,36,36,36	0
3	MG	E	602	1/1	0.81	0.19	70,70,70,70	0
3	MG	H	602	1/1	0.85	0.12	39,39,39,39	0

Continued on next page...

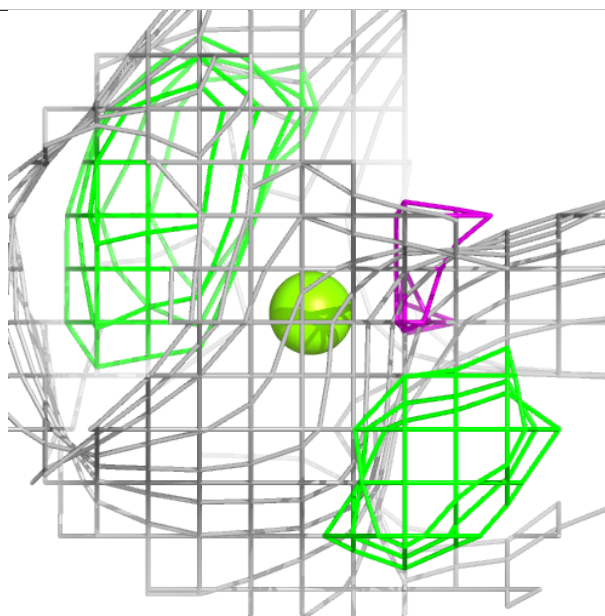
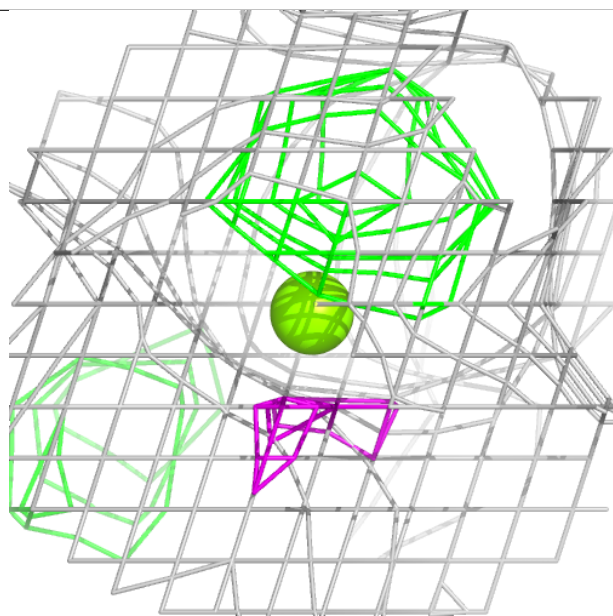
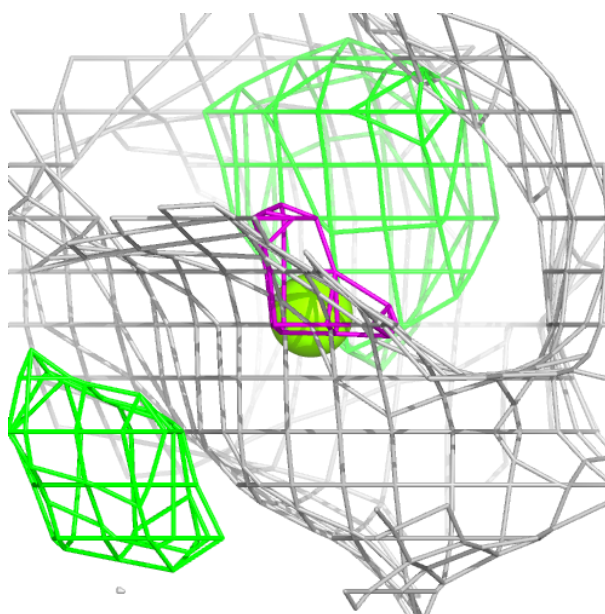
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	D	602	1/1	0.90	0.10	38,38,38,38	0
3	MG	B	602	1/1	0.90	0.09	41,41,41,41	0
3	MG	J	602	1/1	0.90	0.09	39,39,39,39	0
3	MG	K	602	1/1	0.91	0.07	42,42,42,42	0
3	MG	L	602	1/1	0.91	0.09	45,45,45,45	0
2	TPP	I	601	26/26	0.93	0.10	30,42,48,50	0
2	TPP	B	601	26/26	0.93	0.14	16,31,39,312	0
3	MG	I	602	1/1	0.93	0.08	42,42,42,42	0
2	TPP	L	601	26/26	0.95	0.09	29,45,55,56	0
2	TPP	E	601	26/26	0.95	0.09	22,37,45,96	0
2	TPP	C	601	26/26	0.96	0.08	18,31,45,80	0
2	TPP	G	601	26/26	0.96	0.08	27,33,40,43	0
3	MG	A	602	1/1	0.96	0.06	35,35,35,35	0
2	TPP	D	601	26/26	0.97	0.07	27,32,43,50	0
2	TPP	H	601	26/26	0.97	0.07	21,33,43,50	0
2	TPP	F	601	26/26	0.97	0.07	25,31,37,55	0
3	MG	C	602	1/1	0.97	0.05	32,32,32,32	0
2	TPP	J	601	26/26	0.97	0.07	25,34,39,40	0
2	TPP	K	601	26/26	0.97	0.08	31,42,48,52	0
3	MG	G	602	1/1	0.98	0.06	30,30,30,30	0
2	TPP	A	601	26/26	0.98	0.06	17,31,39,45	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.

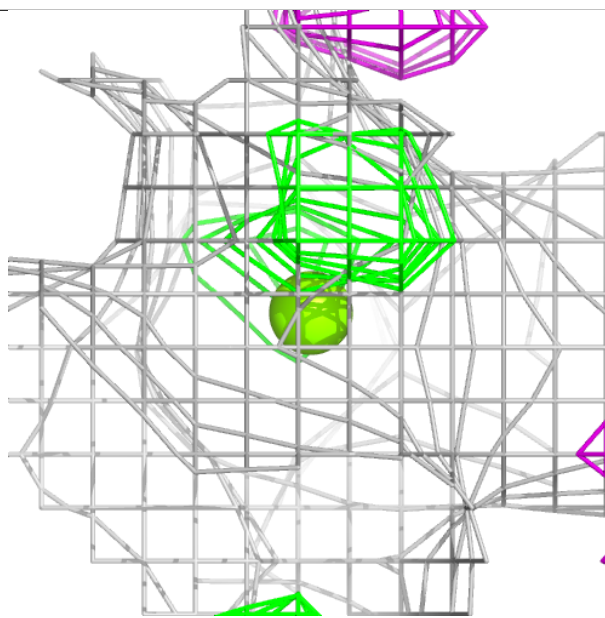
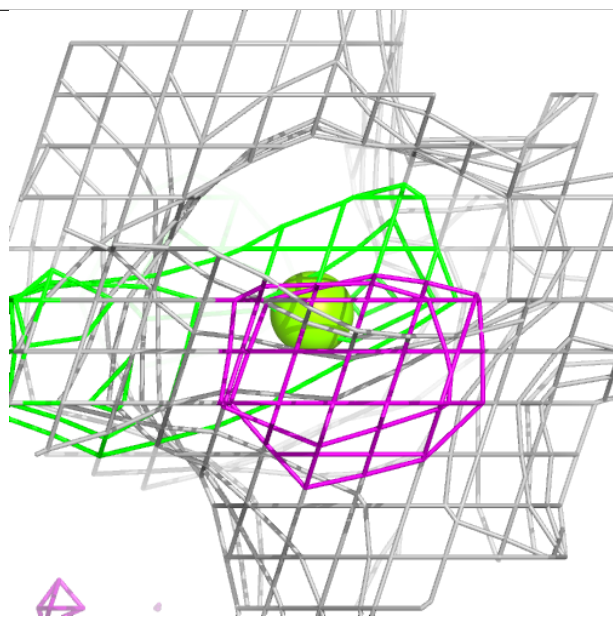
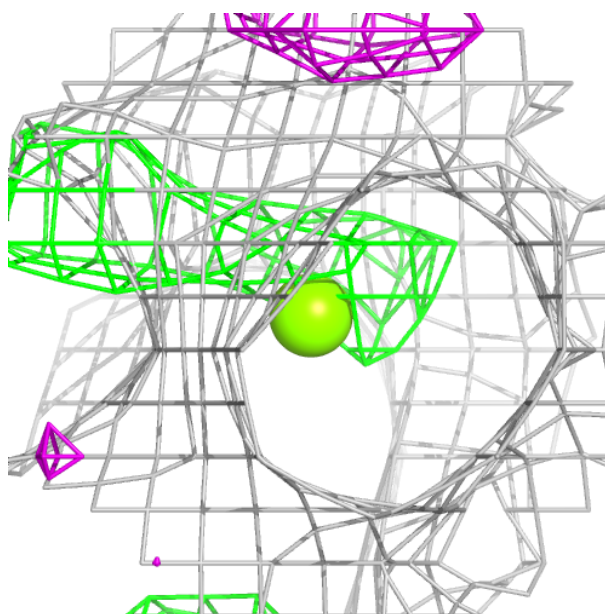
Electron density around MG F 602:

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



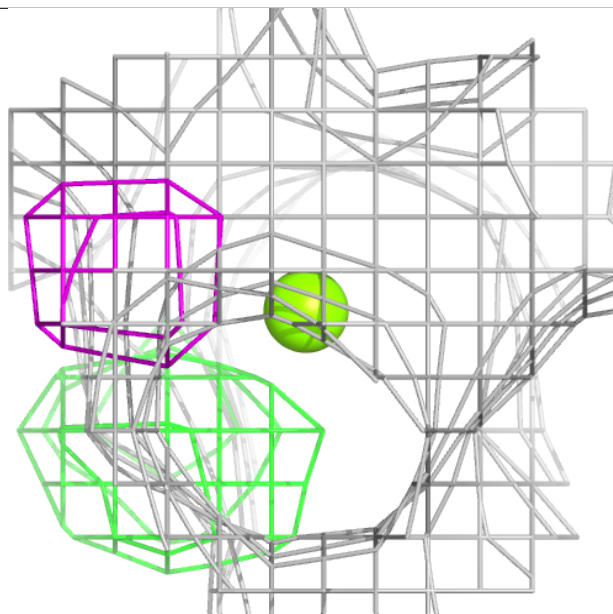
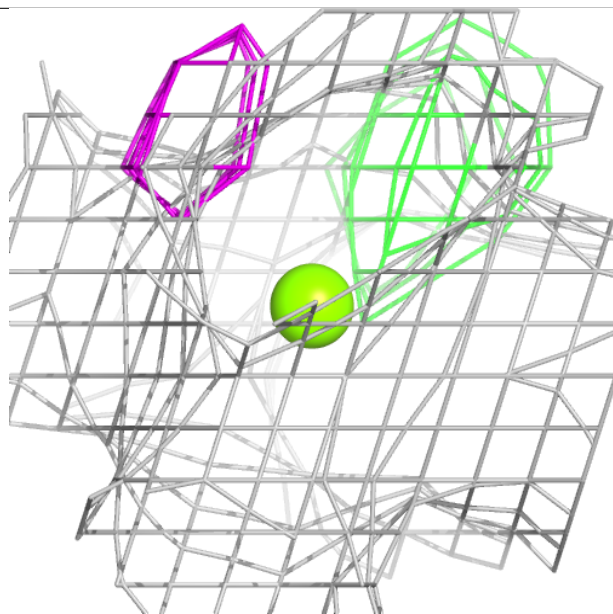
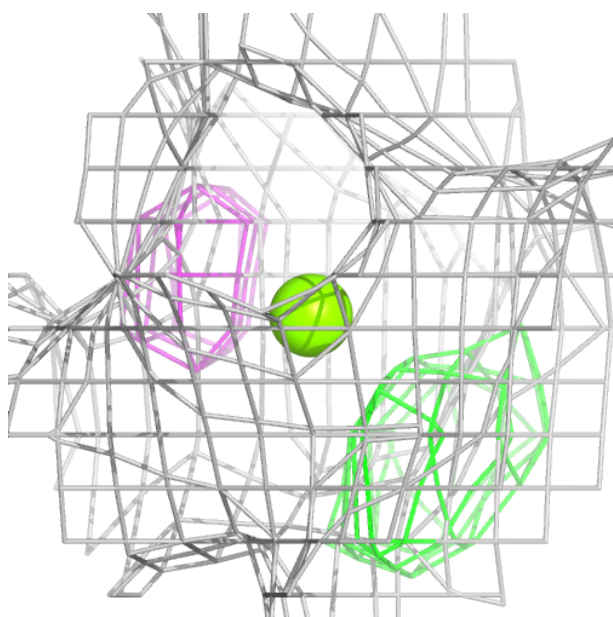
Electron density around MG E 602:

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



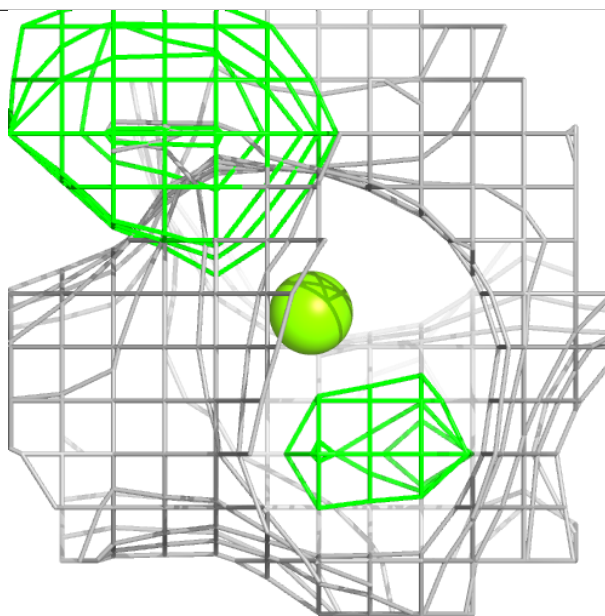
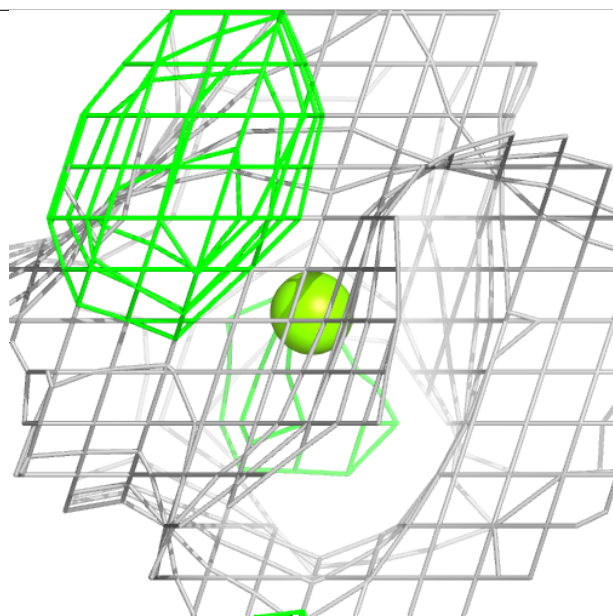
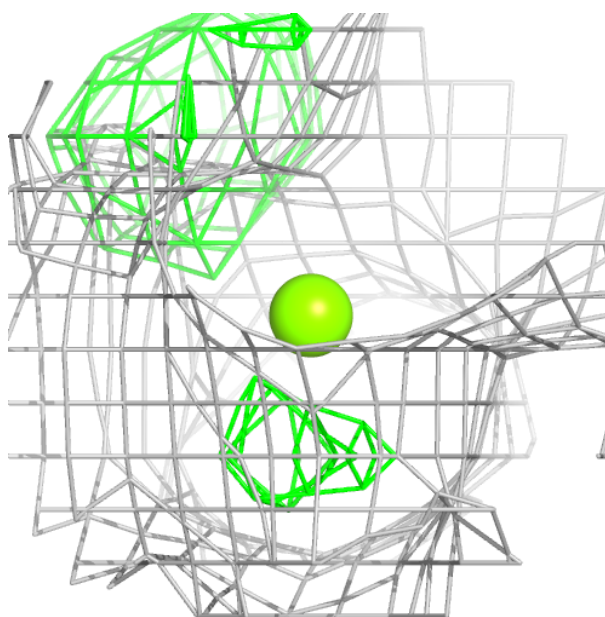
Electron density around MG H 602:

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



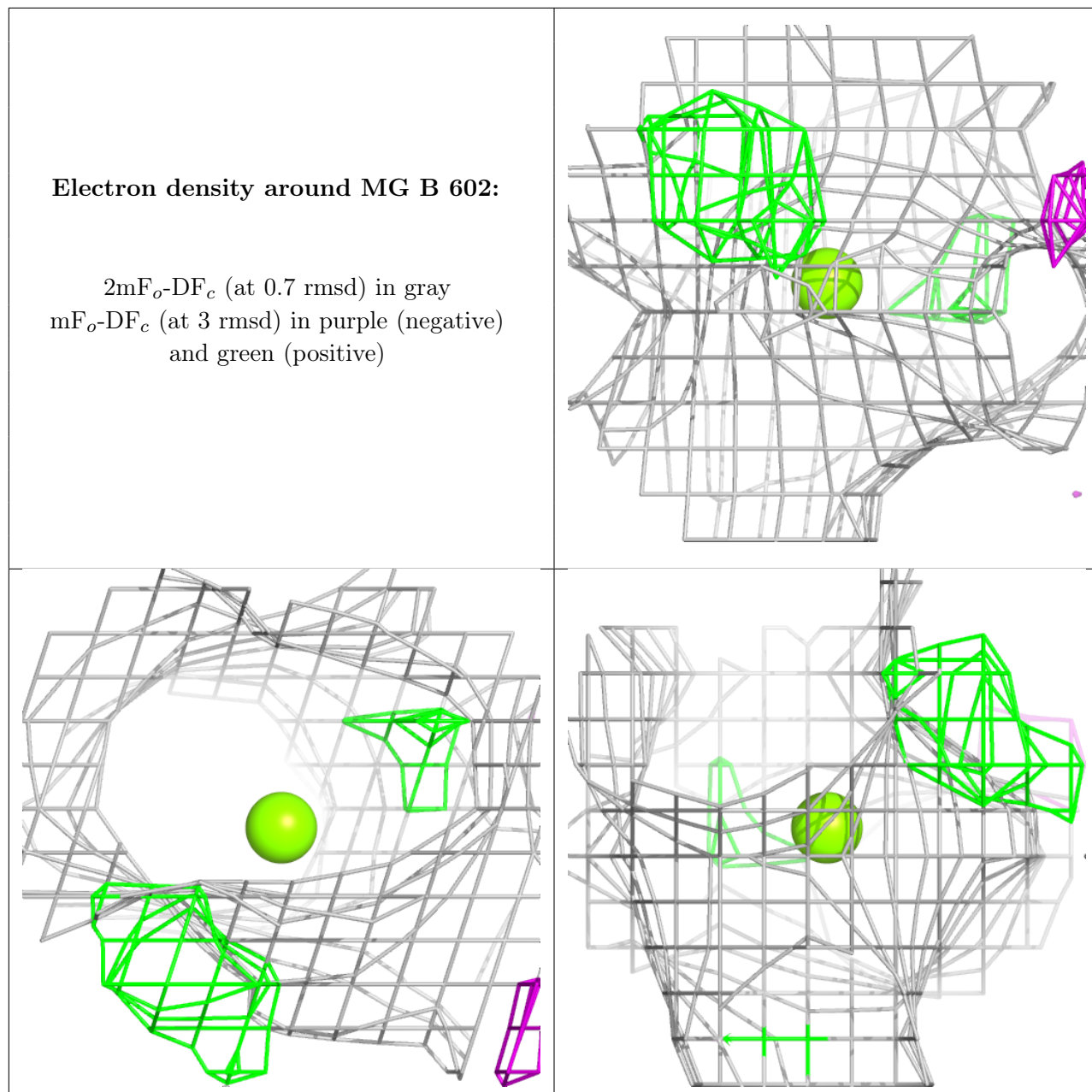
Electron density around MG D 602:

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



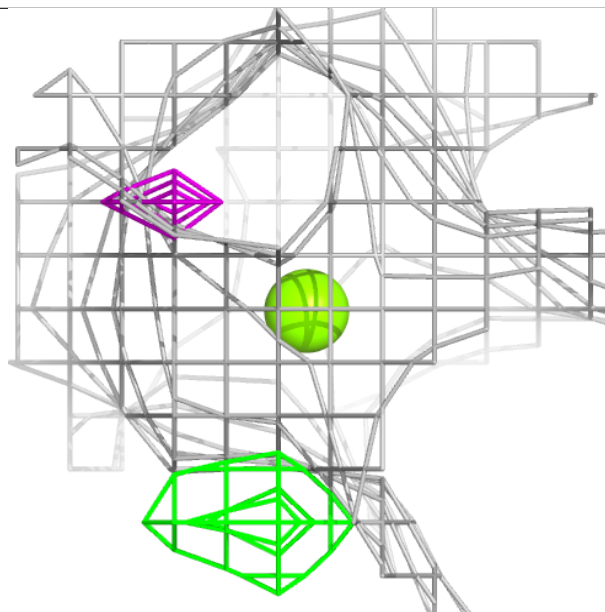
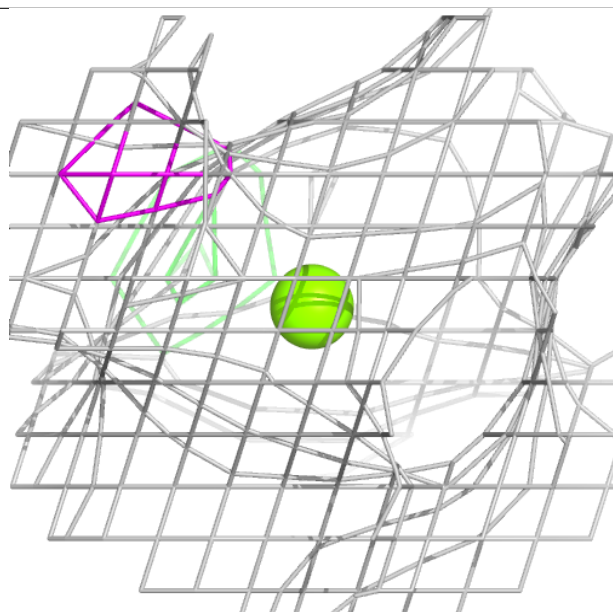
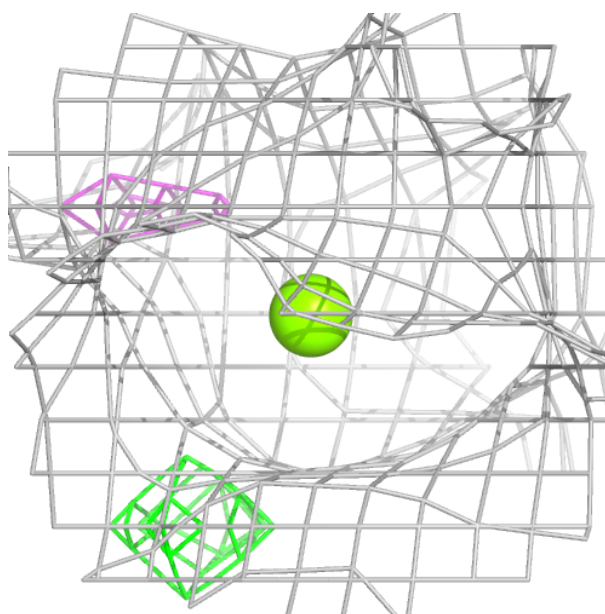
Electron density around MG B 602:

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



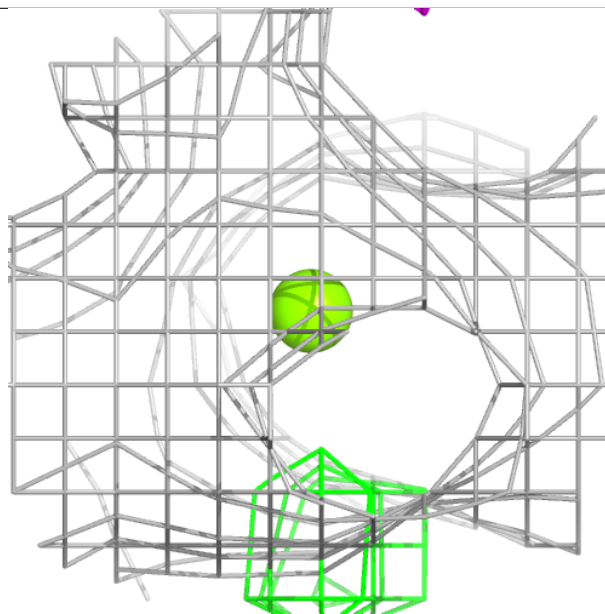
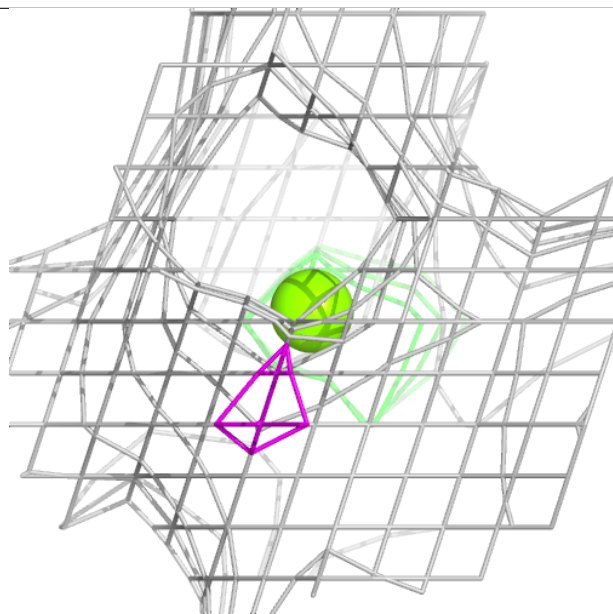
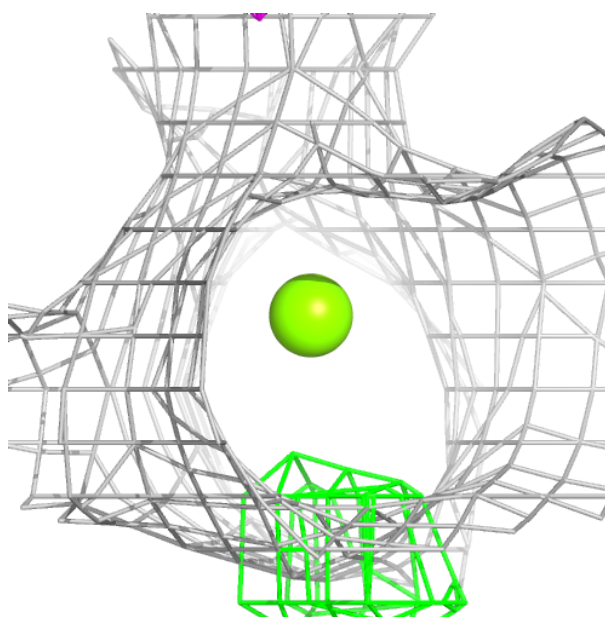
Electron density around MG J 602:

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



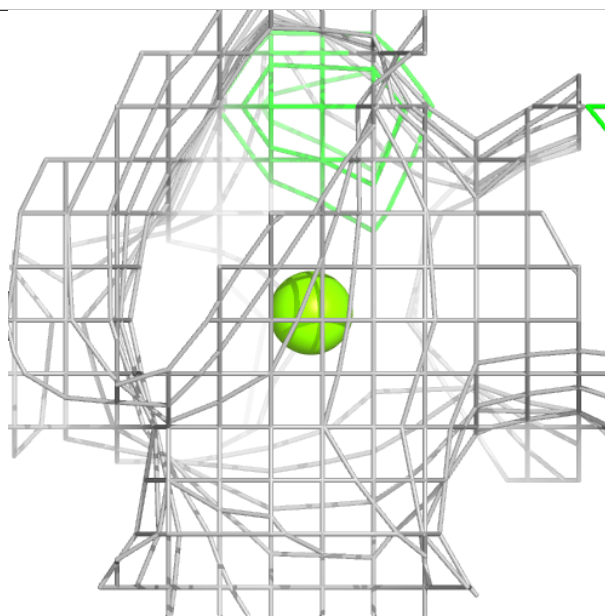
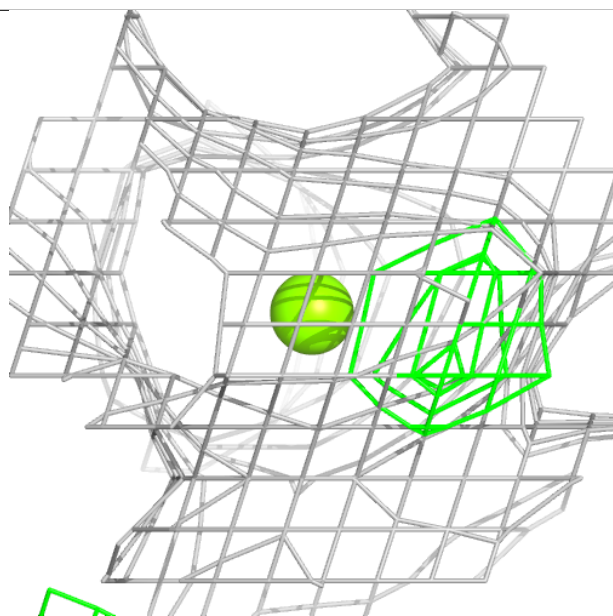
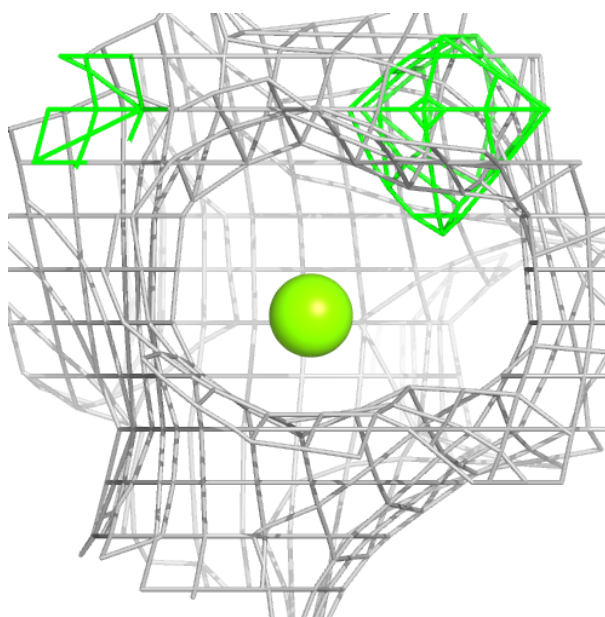
Electron density around MG K 602:

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



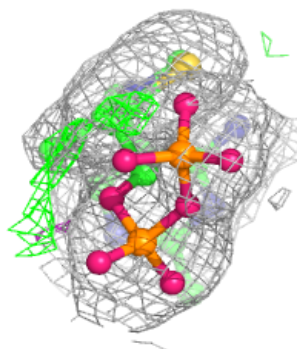
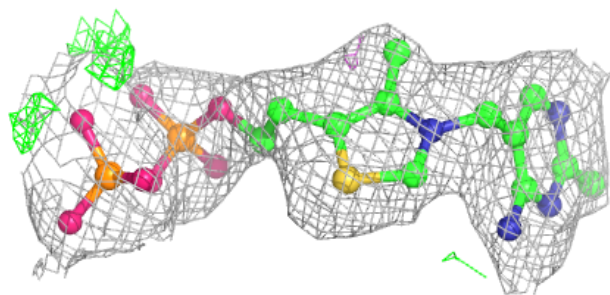
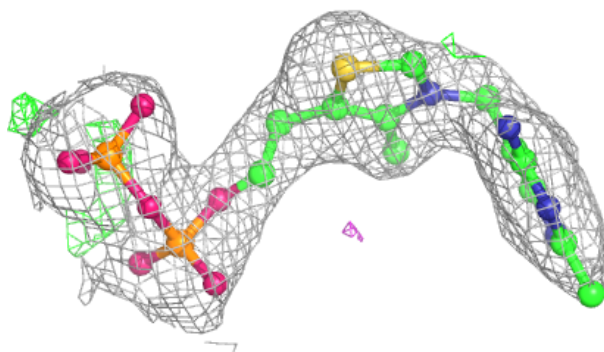
Electron density around MG L 602:

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

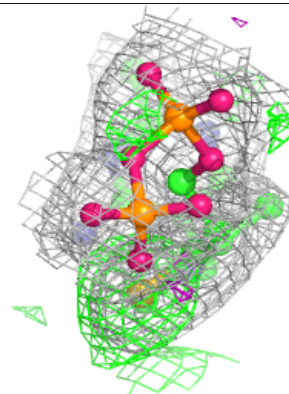
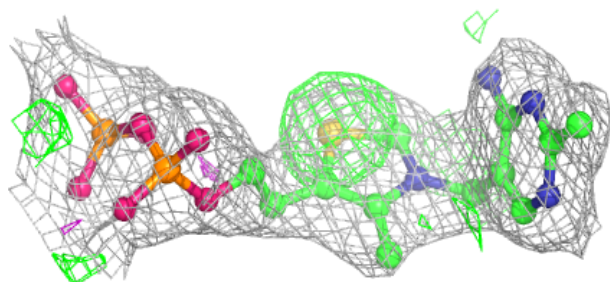
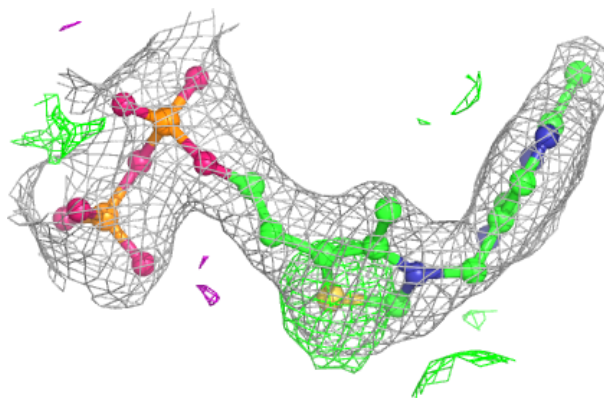


Electron density around TPP I 601:

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

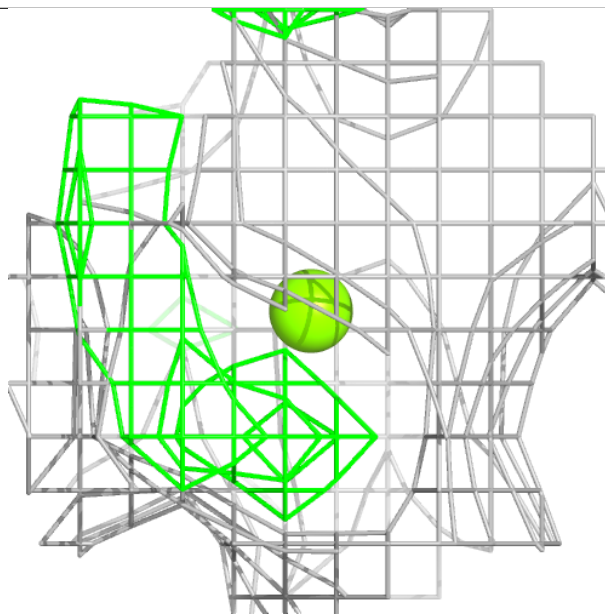
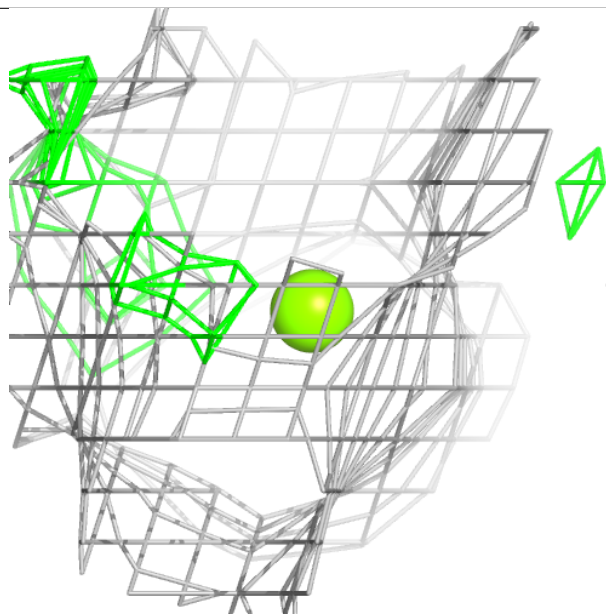
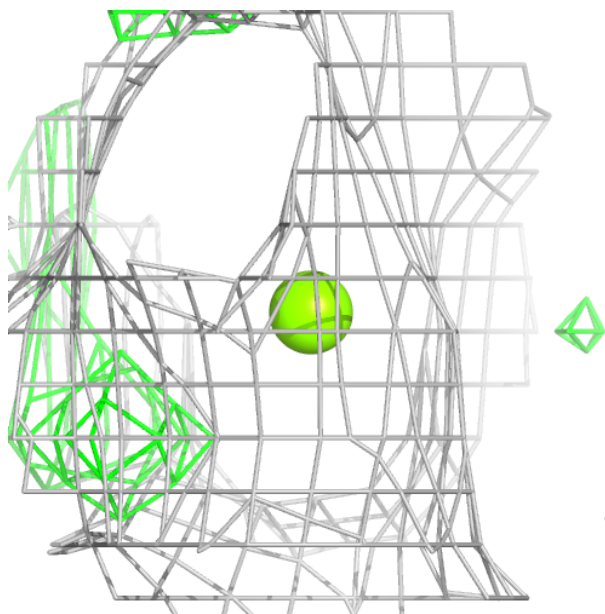
**Electron density around TPP B 601:**

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



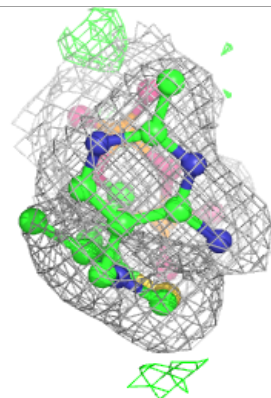
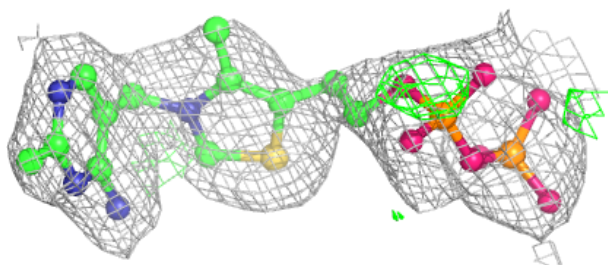
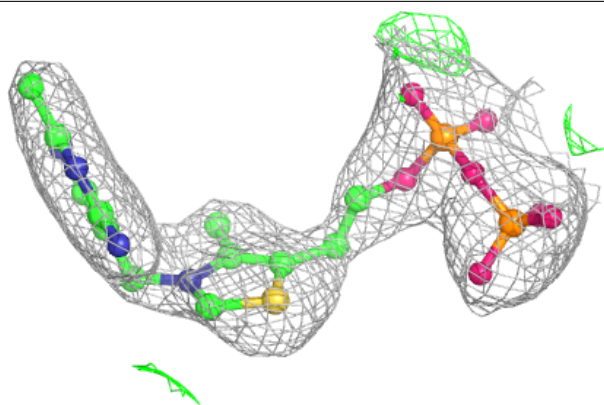
Electron density around MG I 602:

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

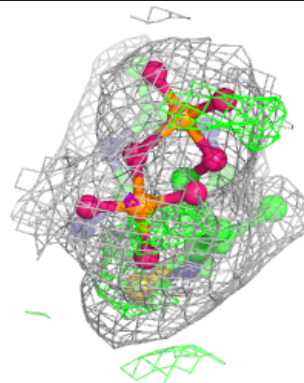
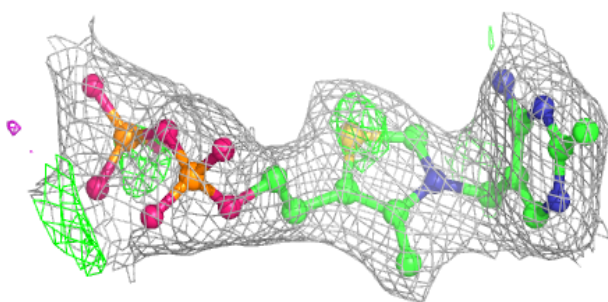
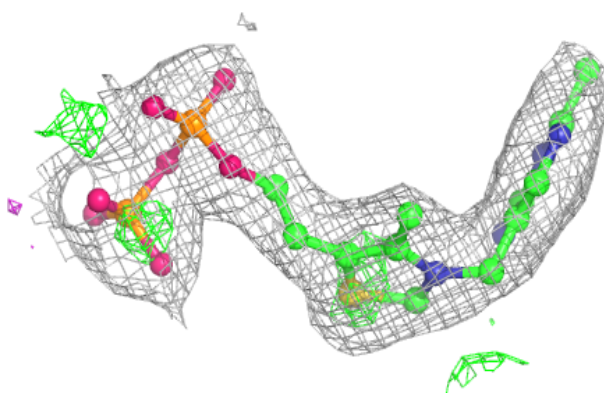


Electron density around TPP L 601:

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

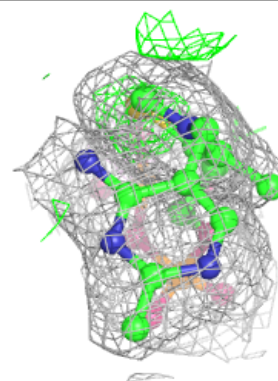
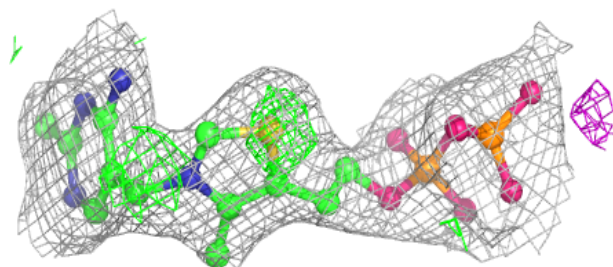
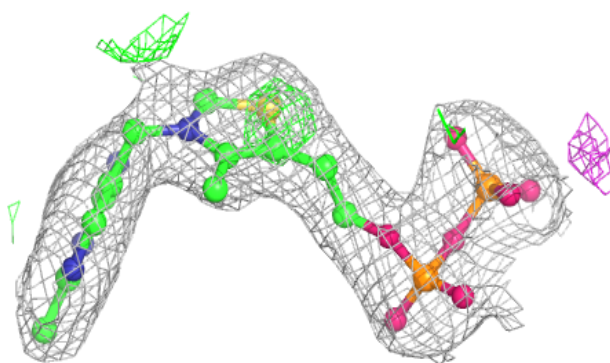
**Electron density around TPP E 601:**

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

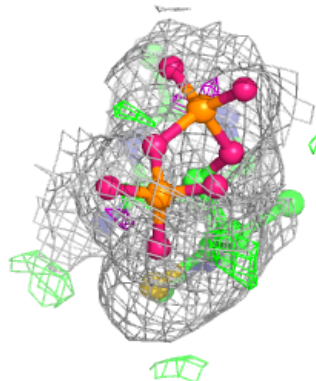
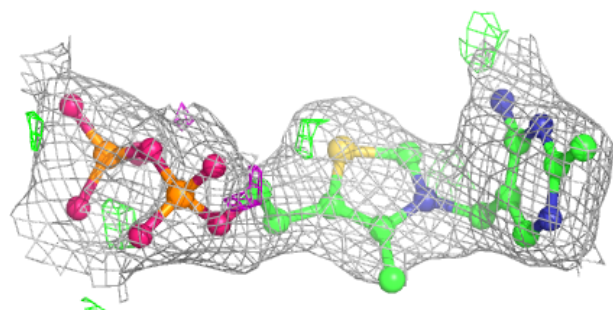
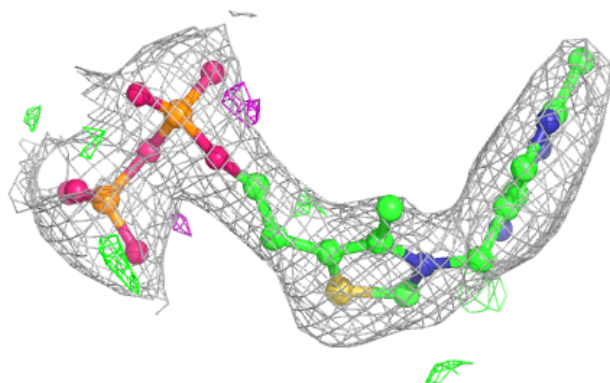


Electron density around TPP C 601:

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

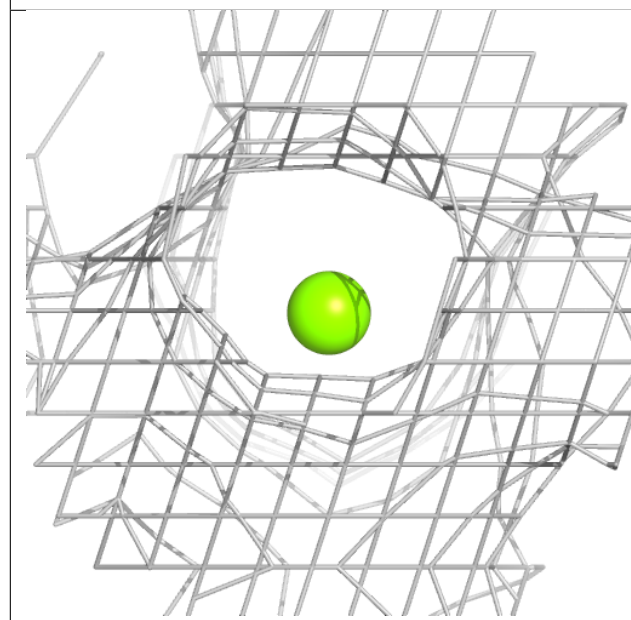
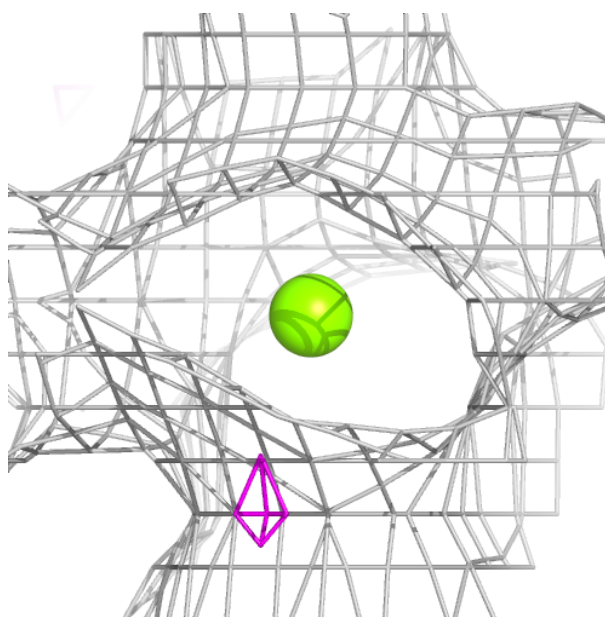
**Electron density around TPP G 601:**

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



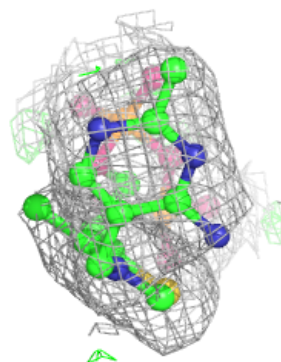
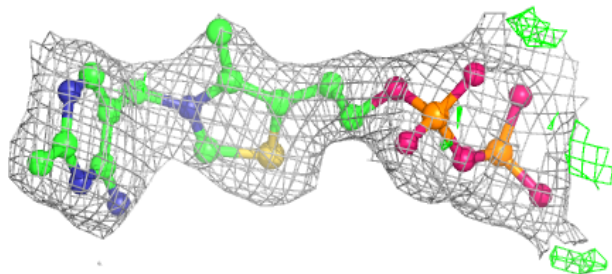
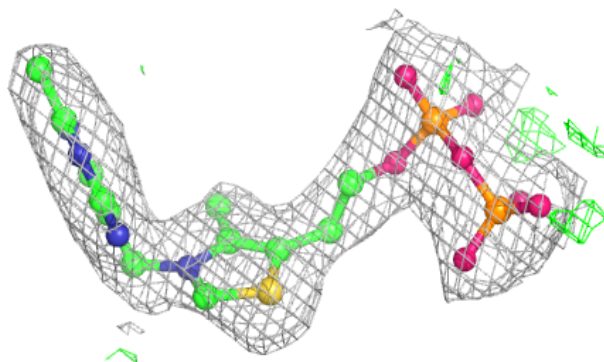
Electron density around MG A 602:

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

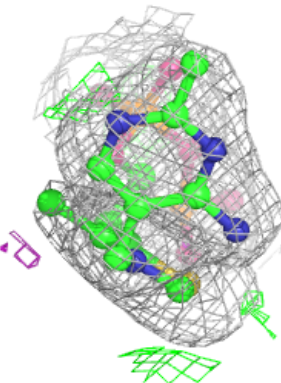
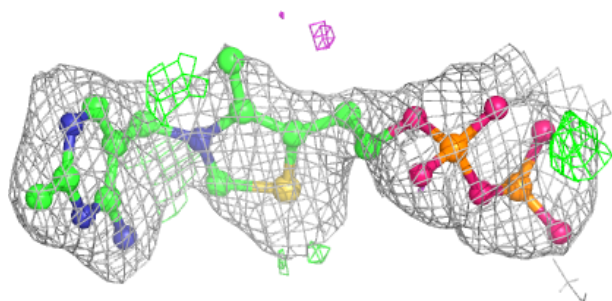
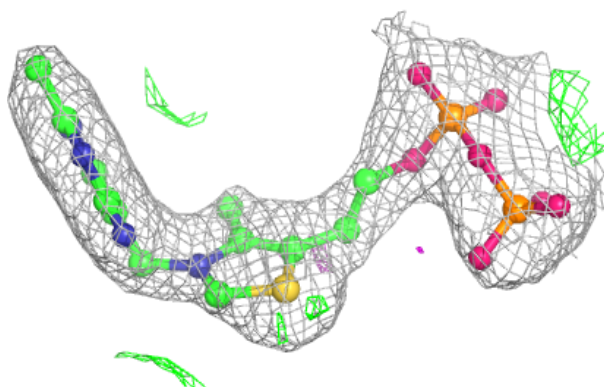


Electron density around TPP D 601:

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

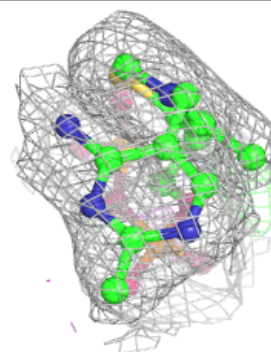
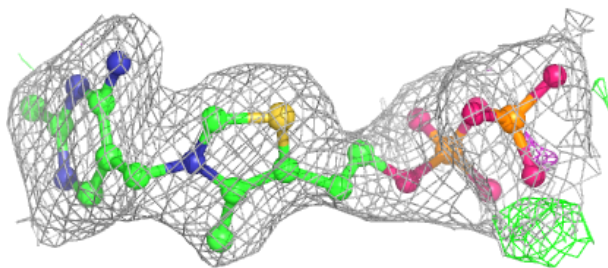
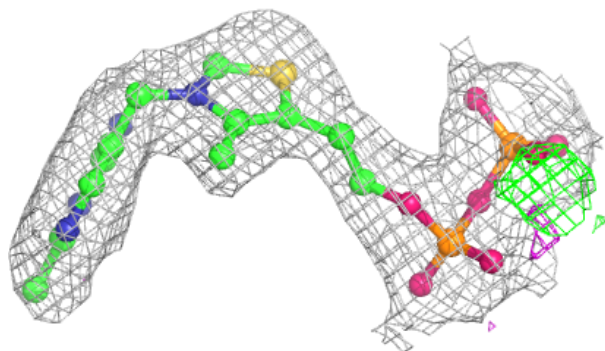
**Electron density around TPP H 601:**

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



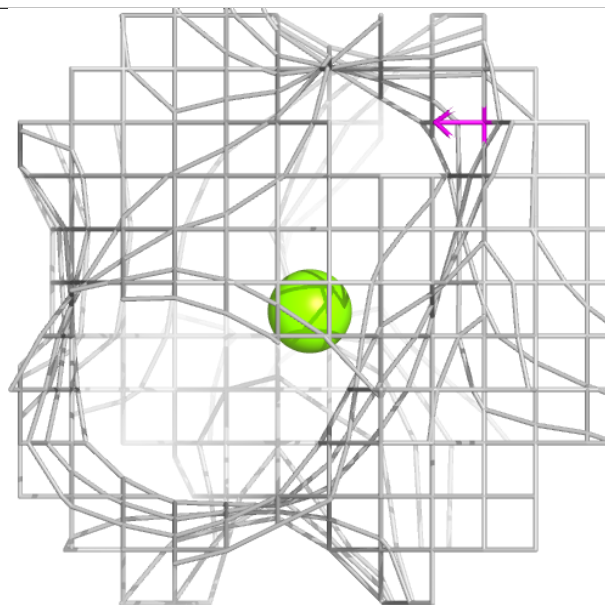
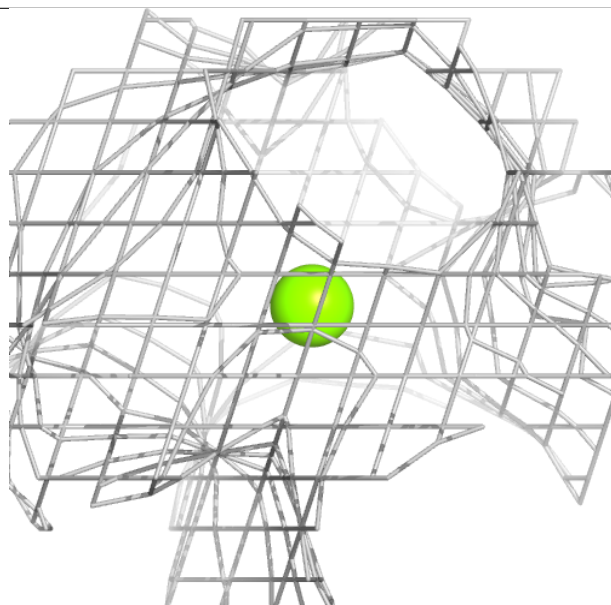
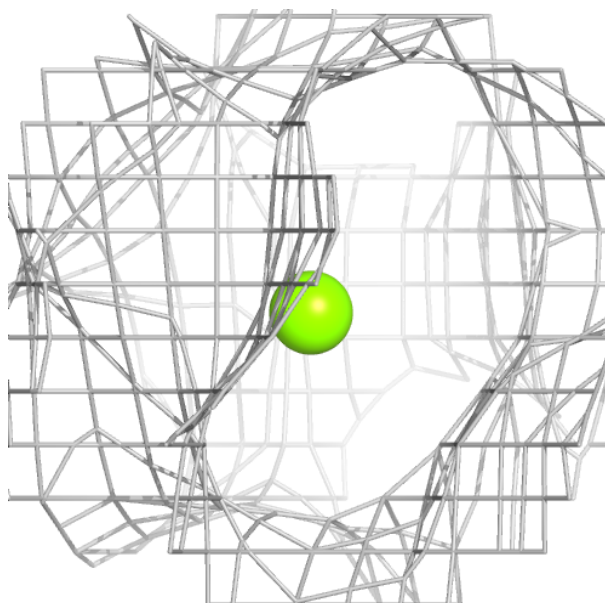
Electron density around TPP F 601:

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



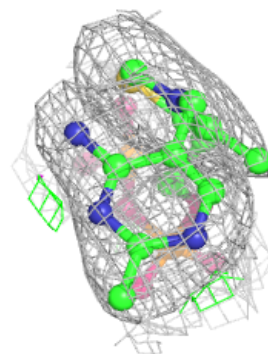
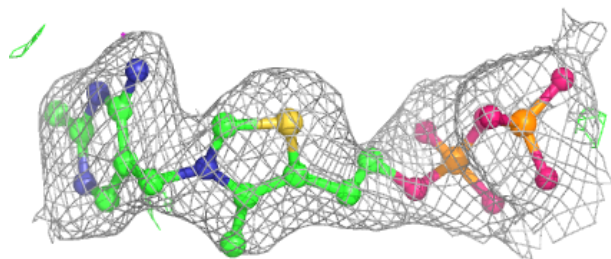
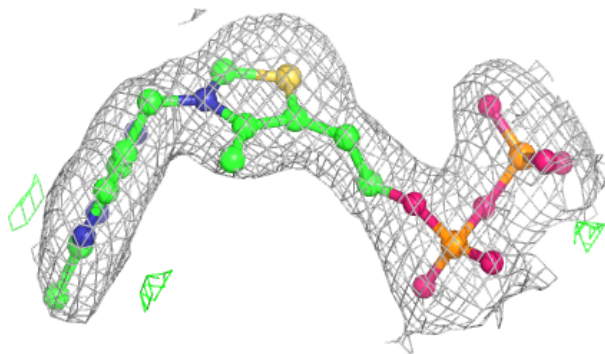
Electron density around MG C 602:

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

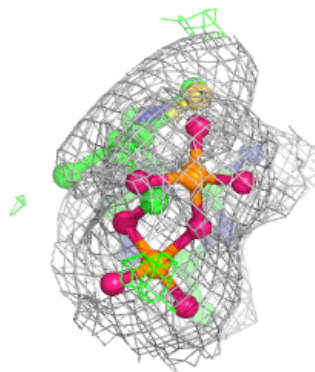
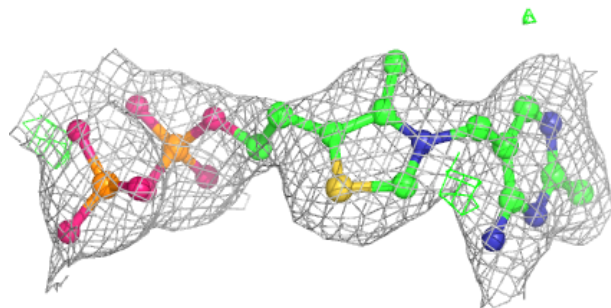
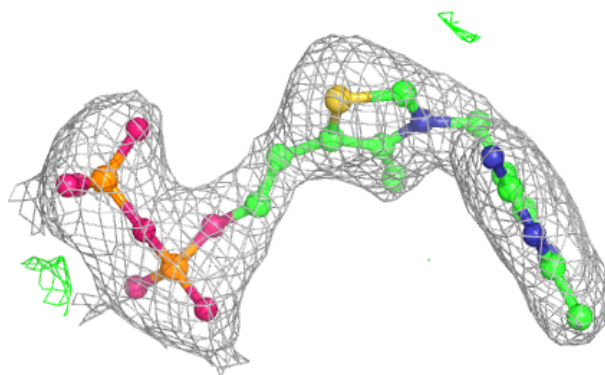


Electron density around TPP J 601:

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

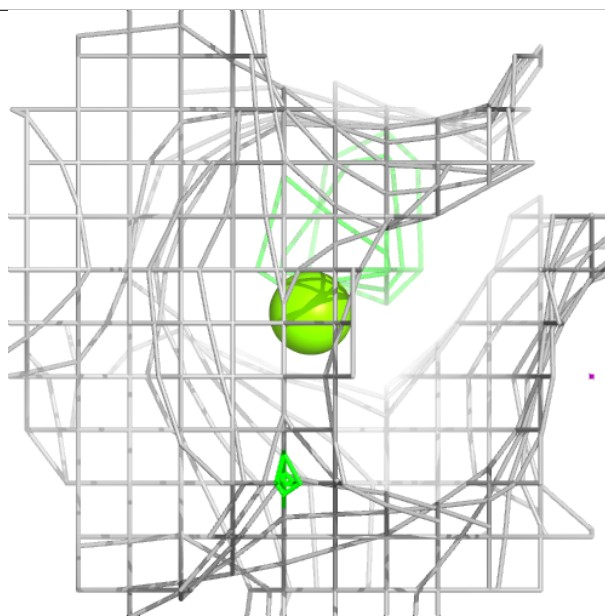
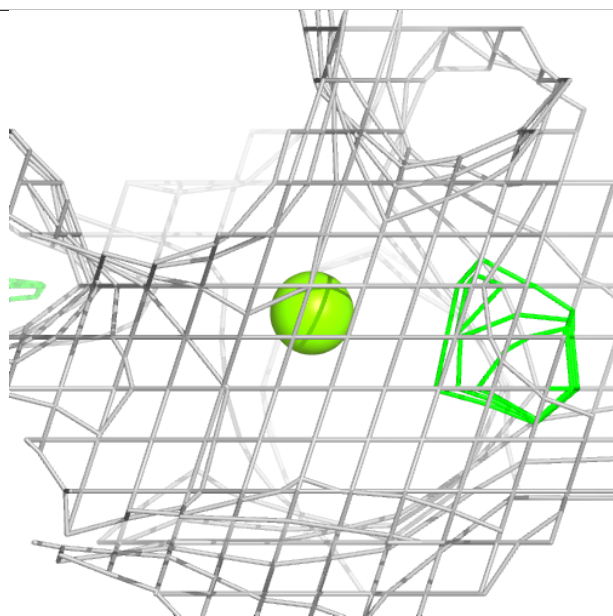
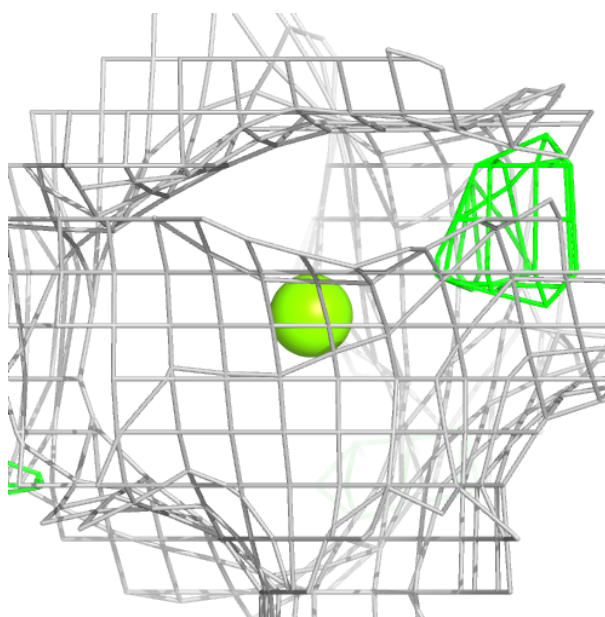
**Electron density around TPP K 601:**

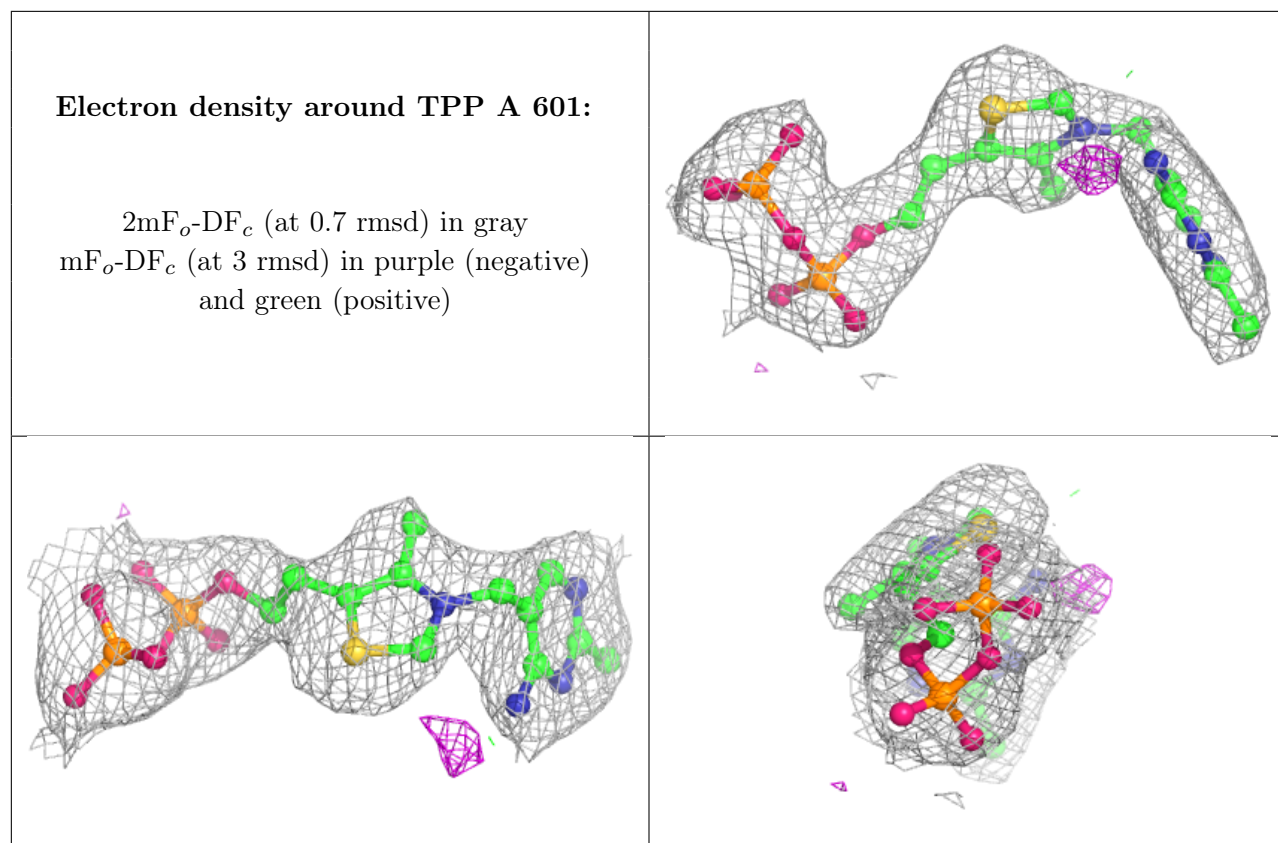
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.