



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:26 PM UTC

PDB ID : 8Y7S / pdb_00008y7s
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:

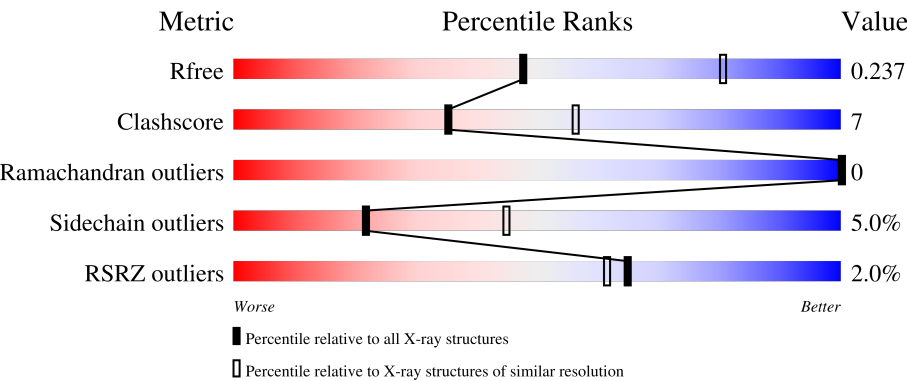
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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	2% 85% 14% .
1	B	558	% 81% 18% .
1	C	558	2% 81% 19% .
1	D	558	2% 84% 15% .
1	E	558	2% 84% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	558	% 85% 13% ..
1	G	558	2% 83% 16% .
1	H	558	% 79% 17% ..
1	I	558	2% 79% 18% ..
1	J	558	3% 81% 17% ..
1	K	558	3% 81% 16% ..
1	L	558	2% 77% 20% ..

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

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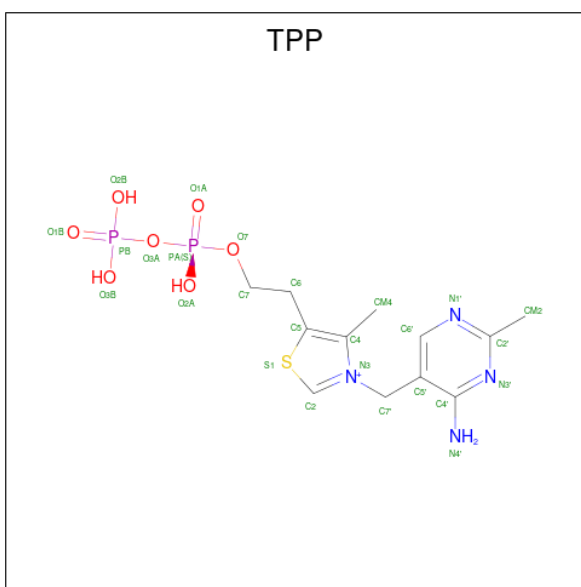
Chain	Residue	Modelled	Actual	Comment	Reference
A	553	LEU	MET	engineered mutation	UNP A0A6M5J4S0
B	27	ILE	ALA	engineered mutation	UNP A0A6M5J4S0
B	29	ILE	VAL	engineered mutation	UNP A0A6M5J4S0
B	417	SER	GLY	engineered mutation	UNP A0A6M5J4S0
B	549	LEU	GLU	engineered mutation	UNP A0A6M5J4S0
B	552	LEU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

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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 (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: 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

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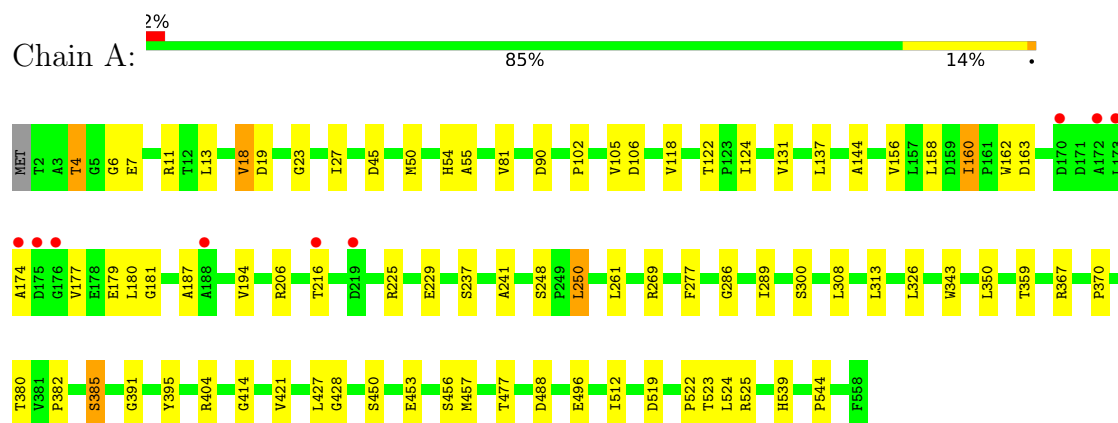
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	35	Total 35	O 35	0	0
4	J	58	Total 58	O 58	0	0
4	K	54	Total 54	O 54	0	0
4	L	41	Total 41	O 41	0	0

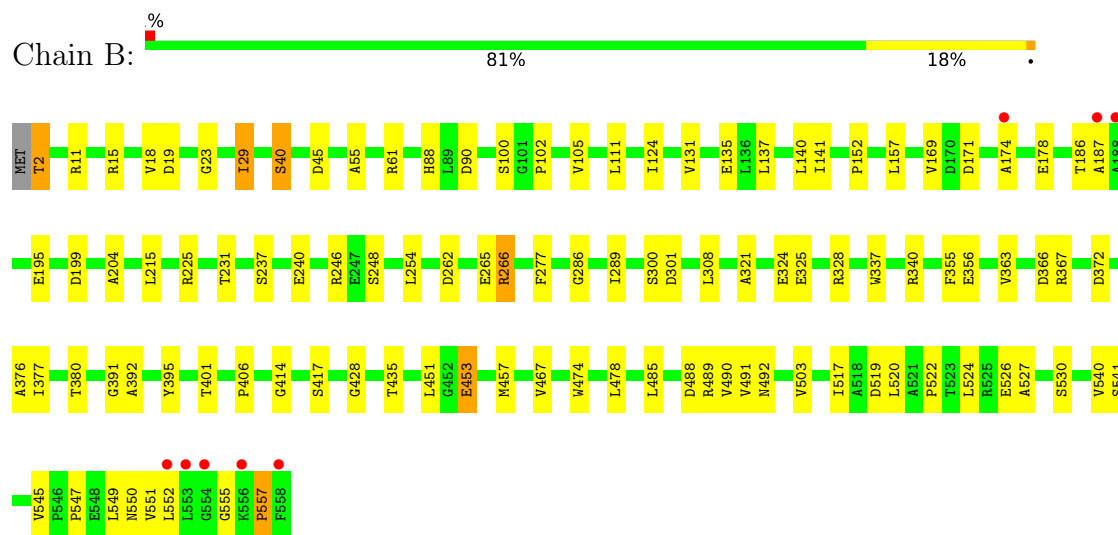
3 Residue-property plots [i](#)

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.

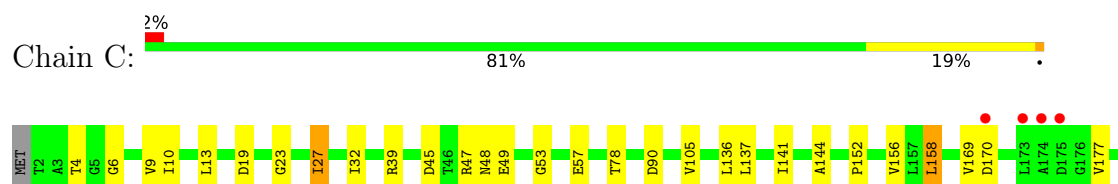
• Molecule 1: Thiamine pyrophosphate-binding protein

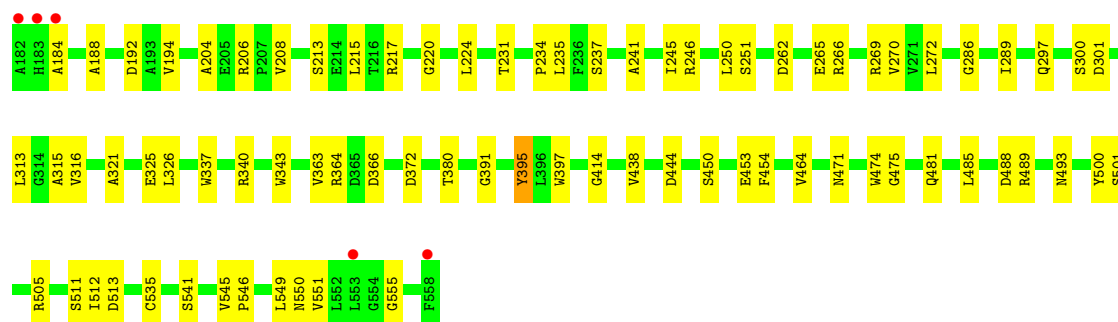


• Molecule 1: Thiamine pyrophosphate-binding protein

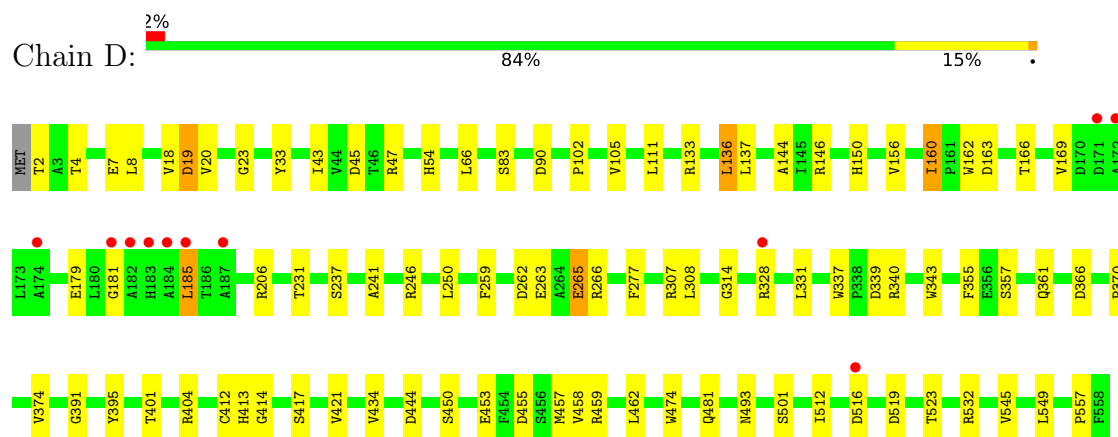


• Molecule 1: Thiamine pyrophosphate-binding protein

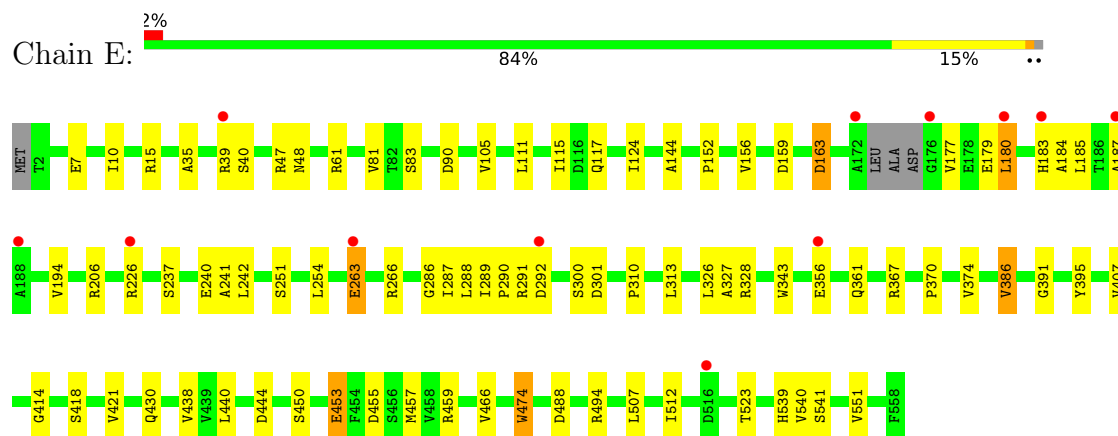




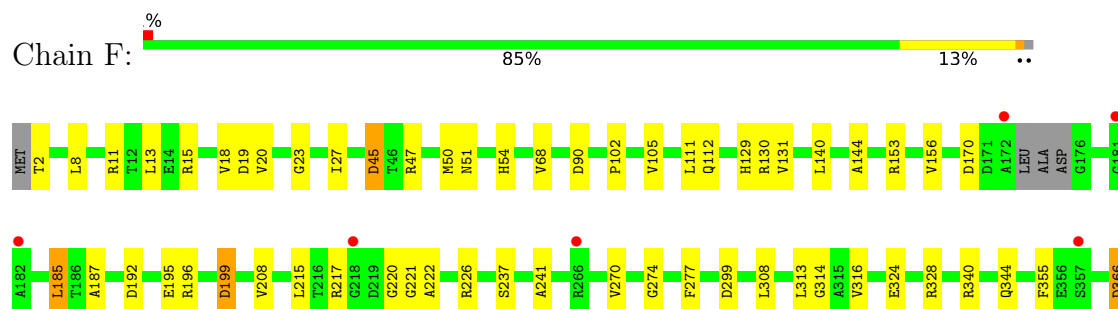
• Molecule 1: Thiamine pyrophosphate-binding protein



• Molecule 1: Thiamine pyrophosphate-binding protein

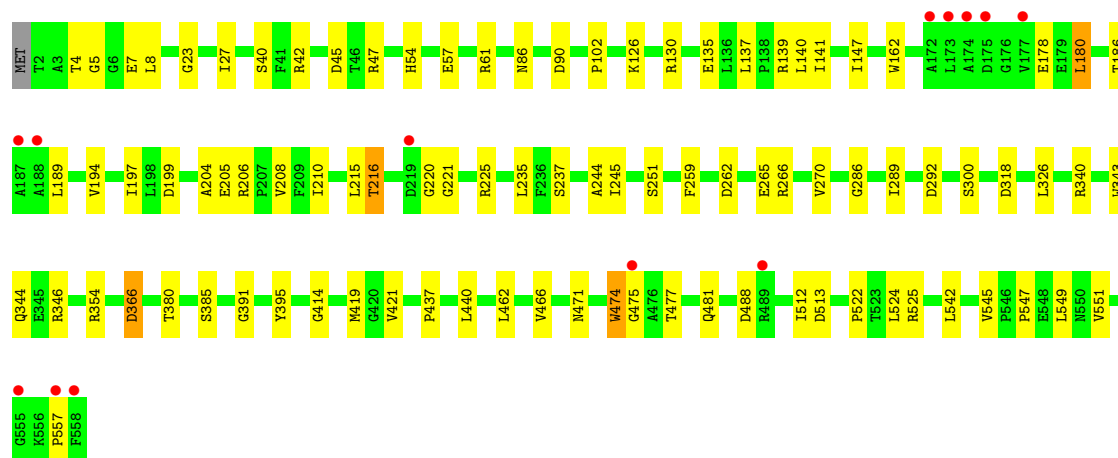
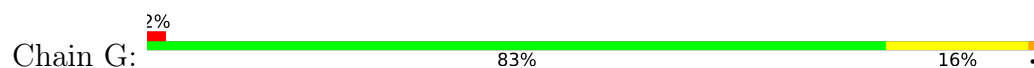


• Molecule 1: Thiamine pyrophosphate-binding protein

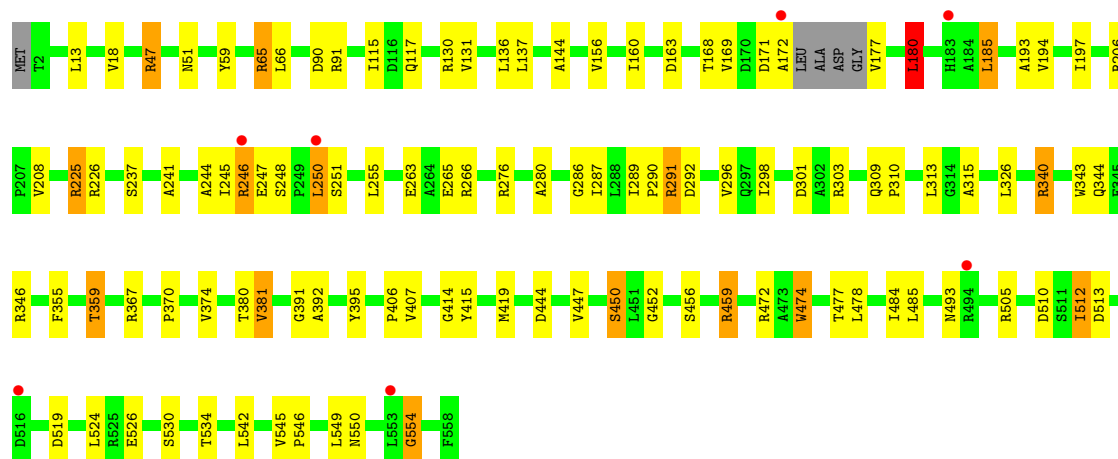
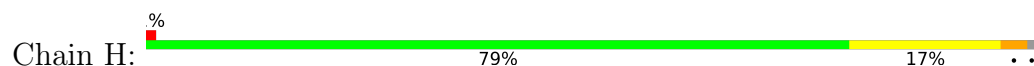




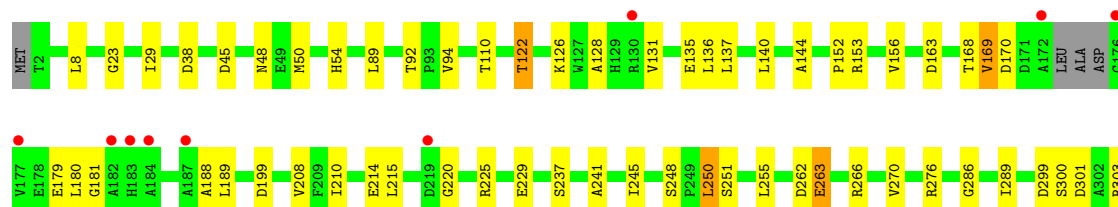
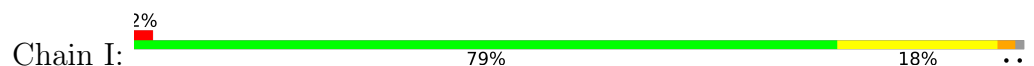
• Molecule 1: Thiamine pyrophosphate-binding protein

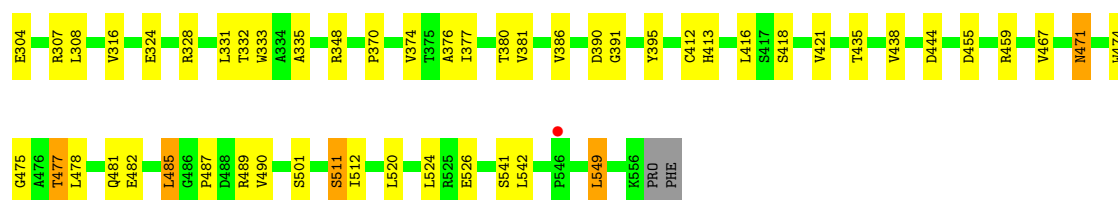


• Molecule 1: Thiamine pyrophosphate-binding protein

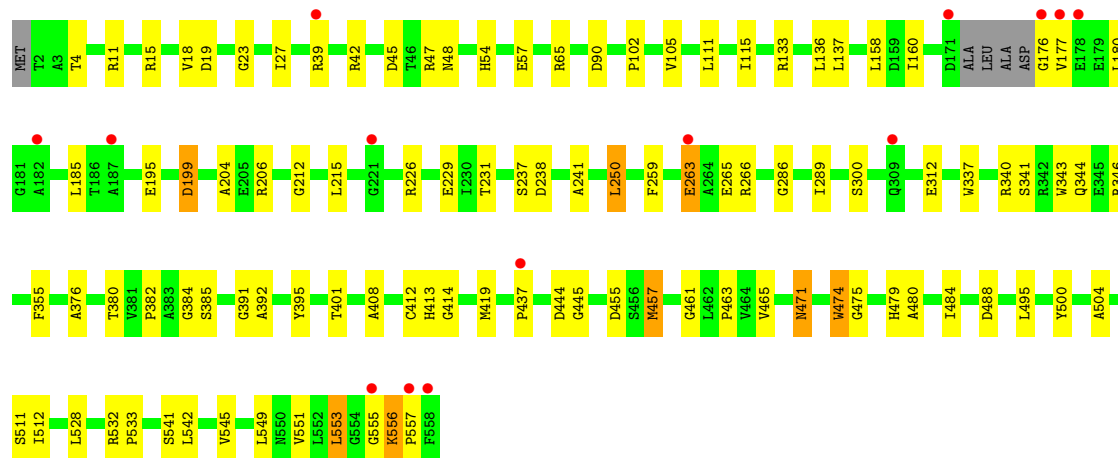
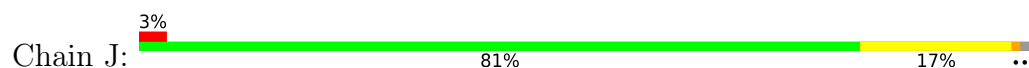


• Molecule 1: Thiamine pyrophosphate-binding protein

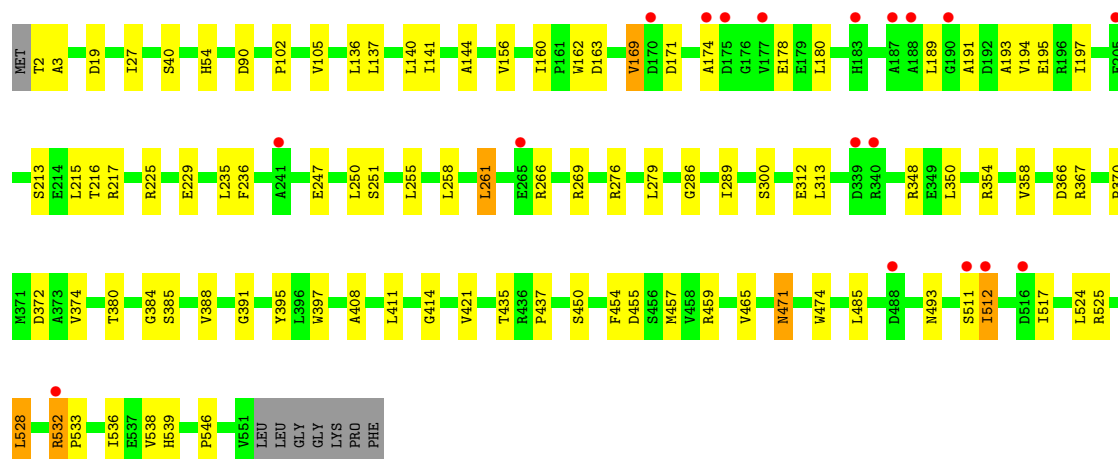
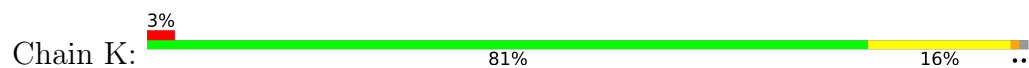




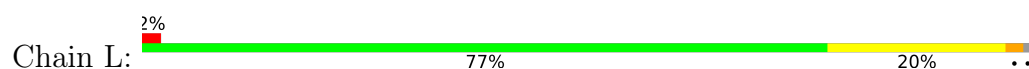
• Molecule 1: Thiamine pyrophosphate-binding protein

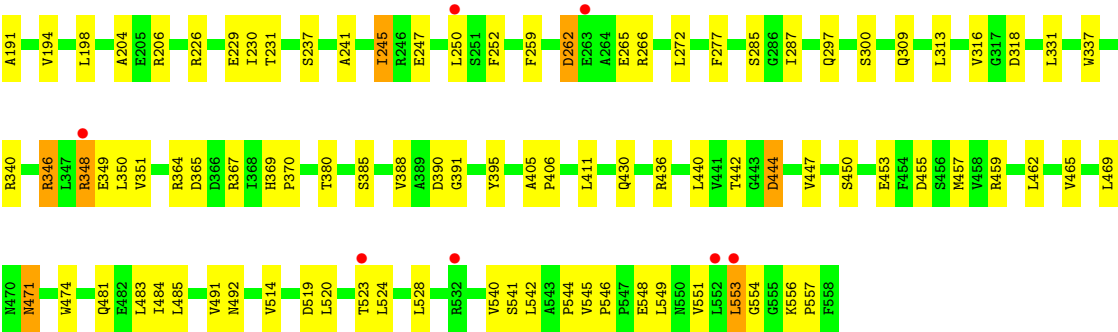


• Molecule 1: Thiamine pyrophosphate-binding protein



• 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	10023 reflections (4.96%)	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 ⓘ

5.1 Standard geometry ⓘ

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	0.28	0/4136	0.49	0/5654
1	B	0.32	0/4160	0.56	3/5684 (0.1%)
1	C	0.33	0/4157	0.57	1/5680 (0.0%)
1	D	0.33	0/4160	0.55	1/5684 (0.0%)
1	E	0.42	0/4125	0.63	1/5637 (0.0%)
1	F	0.41	2/4130 (0.0%)	0.60	1/5642 (0.0%)
1	G	0.37	0/4138	0.61	2/5657 (0.0%)
1	H	0.44	1/4100 (0.0%)	0.68	5/5606 (0.1%)
1	I	0.43	0/4031	0.67	1/5522 (0.0%)
1	J	0.37	0/4098	0.59	2/5602 (0.0%)
1	K	0.37	0/4050	0.57	1/5544 (0.0%)
1	L	0.42	0/4090	0.64	2/5592 (0.0%)
All	All	0.38	3/49375 (0.0%)	0.60	20/67504 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	546	PRO	CA-C	14.71	1.62	1.52
1	H	546	PRO	CA-C	5.51	1.55	1.52
1	F	546	PRO	C-O	-5.50	1.20	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	546	PRO	O-C-N	15.92	128.63	121.15
1	G	475	GLY	N-CA-C	6.75	120.83	112.73
1	H	180	LEU	N-CA-C	-6.66	105.31	113.50
1	J	475	GLY	N-CA-C	6.53	120.56	112.73
1	C	475	GLY	N-CA-C	6.39	120.40	112.73
1	B	557	PRO	N-CA-C	6.27	122.11	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	263	GLU	CB-CA-C	-6.06	100.73	110.79
1	B	40	SER	CA-C-N	5.96	129.34	120.87
1	B	40	SER	C-N-CA	5.96	129.34	120.87
1	H	554	GLY	CA-C-O	-5.92	118.37	122.22
1	I	475	GLY	N-CA-C	5.82	119.72	112.73
1	L	471	ASN	N-CA-C	-5.71	106.22	112.72
1	H	546	PRO	O-C-N	5.67	123.81	121.15
1	K	471	ASN	N-CA-C	-5.62	106.01	112.92
1	L	186	THR	OG1-CB-CG2	5.60	120.50	109.30
1	E	474	TRP	N-CA-C	-5.48	99.12	110.80
1	J	474	TRP	N-CA-C	-5.48	98.81	108.23
1	H	474	TRP	N-CA-C	-5.24	100.25	108.63
1	G	474	TRP	N-CA-C	-5.14	98.94	107.99
1	D	516	ASP	CB-CA-C	-5.04	101.44	109.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4064	0	4052	55	0
1	B	4088	0	4086	59	0
1	C	4085	0	4084	63	0
1	D	4088	0	4086	49	0
1	E	4054	0	4041	53	0
1	F	4059	0	4057	49	0
1	G	4066	0	4047	49	0
1	H	4029	0	3999	86	0
1	I	3963	0	3904	66	0
1	J	4027	0	4013	75	0
1	K	3980	0	3948	50	0
1	L	4019	0	4005	87	0
2	A	26	0	16	0	0
2	B	26	0	16	2	0
2	C	26	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
2	I	26	0	16	1	0
2	J	26	0	16	1	0
2	K	26	0	16	1	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
4	H	54	0	0	3	0
4	I	35	0	0	2	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	721	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 (721) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:454:PHE:HA	1:K:457:MET:HE2	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:48:ASN:HD21	1:L:50:MET:HE1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:MET:HE1	1:E:48:ASN:HD21	1.73	0.54
1:A:137:LEU:HD11	1:A:160:ILE:HD12	1.90	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:135:GLU:CD	1:B:135:GLU:H	2.16	0.51
1:C:488:ASP:OD1	1:C:488:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:511:SER:C	1:C:512:ILE:HG13	2.34	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:I:126:LYS:NZ	1:I:152:PRO:O	2.39	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:I:301:ASP:CG	1:I:303:ARG:HG2	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:GLU:CD	1:I:135:GLU:H	2.20	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:H:301:ASP:CG	1:H:303:ARG:HG2	2.37	0.48
1:J:474:TRP:CE2	1:J:495:LEU:HD11	2.48	0.48
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:J:382:PRO:O	1:J:385:SER:OG	2.31	0.48
1:A:229:GLU:HA	1:A:250:LEU:HD23	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:392:ALA:HB2	1:J:419:MET:HE3	1.95	0.48
1:J:488:ASP:OD1	1:J:488:ASP:N	2.46	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:J:265:GLU:CD	1:J:346:ARG:HE	2.20	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:501:SER:O	1:C:511:SER:OG	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:OD1	1:H:163:ASP:N	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
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:H:171:ASP:O	1:H:172:ALA:C	2.59	0.45
1:K:189:LEU:HD23	1:K:189:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:J:11:ARG:HA	1:J:39:ARG:NH1	2.29	0.44
1:L:48:ASN:ND2	1:L:50:MET:HE3	2.32	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:C:192:ASP:CG	1:D:328:ARG:HH12	2.24	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
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:266:ARG:HH22	1:H:287:ILE:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:163:ASP:OD1	1:L:163:ASP:N	2.50	0.43
1:L:405:ALA:HA	1:L:406:PRO:HD3	1.86	0.43
1:A:519:ASP:C	1:A:522:PRO:HD2	2.43	0.43
1:B:503:VAL:HG13	1:F:503:VAL:HG13	2.01	0.43
1:H:392:ALA:HB2	1:H:419:MET:HE3	1.99	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:183:HIS:O	1:E:184:ALA:C	2.61	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:221:GLY:O	1:F:222:ALA:C	2.62	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:246:ARG:C	1:C:246:ARG:HD2	2.44	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
1:F:208:VAL:HG13	1:F:270:VAL:HG13	2.00	0.42
1:H:225:ARG:NH1	1:H:247:GLU:CD	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:188:ALA:C	4:I:709:HOH:O	2.62	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:511:SER:C	1:J:512:ILE:HG13	2.45	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:G:135:GLU:CD	1:G:135:GLU:H	2.27	0.41
1:K:474:TRP:N	1:K:493:ASN:O	2.52	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:457:MET:HE3	1:J:533:PRO:HB3	2.03	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:K:532:ARG:O	1:K:533:PRO:C	2.62	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

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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: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:I:455:ASP:CG	1:I:459:ARG:HH11	2.29	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:G:488:ASP:OD1	1:G:488:ASP:N	2.54	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:179:GLU:CD	1:E:183:HIS:HE1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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 [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	555/558 (100%)	542 (98%)	13 (2%)	0	100	100
1	B	555/558 (100%)	542 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	555/558 (100%)	543 (98%)	12 (2%)	0	100	100
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%)	392 (97%)	13 (3%)	34	61
1	B	411/415 (99%)	390 (95%)	21 (5%)	21	44
1	C	410/415 (99%)	387 (94%)	23 (6%)	19	40
1	D	411/415 (99%)	391 (95%)	20 (5%)	22	46
1	E	406/415 (98%)	385 (95%)	21 (5%)	21	43
1	F	407/415 (98%)	393 (97%)	14 (3%)	32	59
1	G	406/415 (98%)	392 (97%)	14 (3%)	32	59
1	H	401/415 (97%)	373 (93%)	28 (7%)	14	31
1	I	392/415 (94%)	370 (94%)	22 (6%)	19	40
1	J	401/415 (97%)	380 (95%)	21 (5%)	21	43
1	K	393/415 (95%)	368 (94%)	25 (6%)	16	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	399/415 (96%)	378 (95%)	21 (5%)	20	43
All	All	4842/4980 (97%)	4599 (95%)	243 (5%)	22	45

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	18	VAL
1	A	19	ASP
1	A	160	ILE
1	A	177	VAL
1	A	180	LEU
1	A	216	THR
1	A	250	LEU
1	A	300	SER
1	A	313	LEU
1	A	359	THR
1	A	385	SER
1	A	477	THR
1	B	2	THR
1	B	18	VAL
1	B	19	ASP
1	B	29	ILE
1	B	40	SER
1	B	100	SER
1	B	111	LEU
1	B	157	LEU
1	B	169	VAL
1	B	186	THR
1	B	215	LEU
1	B	266	ARG
1	B	300	SER
1	B	356	GLU
1	B	363	VAL
1	B	417	SER
1	B	435	THR
1	B	453	GLU
1	B	519	ASP
1	B	541	SER
1	B	552	LEU
1	C	4	THR
1	C	10	ILE

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Mol	Chain	Res	Type
1	C	19	ASP
1	C	27	ILE
1	C	78	THR
1	C	136	LEU
1	C	158	LEU
1	C	169	VAL
1	C	170	ASP
1	C	177	VAL
1	C	250	LEU
1	C	265	GLU
1	C	300	SER
1	C	316	VAL
1	C	363	VAL
1	C	366	ASP
1	C	380	THR
1	C	395	TYR
1	C	450	SER
1	C	453	GLU
1	C	471	ASN
1	C	513	ASP
1	C	541	SER
1	D	2	THR
1	D	18	VAL
1	D	19	ASP
1	D	66	LEU
1	D	83	SER
1	D	111	LEU
1	D	136	LEU
1	D	160	ILE
1	D	185	LEU
1	D	246	ARG
1	D	250	LEU
1	D	263	GLU
1	D	265	GLU
1	D	307	ARG
1	D	366	ASP
1	D	417	SER
1	D	434	VAL
1	D	450	SER
1	D	462	LEU
1	D	501	SER
1	E	83	SER

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Mol	Chain	Res	Type
1	E	105	VAL
1	E	111	LEU
1	E	124	ILE
1	E	163	ASP
1	E	177	VAL
1	E	180	LEU
1	E	251	SER
1	E	263	GLU
1	E	292	ASP
1	E	300	SER
1	E	356	GLU
1	E	361	GLN
1	E	386	VAL
1	E	407	VAL
1	E	444	ASP
1	E	450	SER
1	E	453	GLU
1	E	507	LEU
1	E	541	SER
1	E	551	VAL
1	F	2	THR
1	F	8	LEU
1	F	18	VAL
1	F	45	ASP
1	F	170	ASP
1	F	185	LEU
1	F	199	ASP
1	F	366	ASP
1	F	407	VAL
1	F	447	VAL
1	F	450	SER
1	F	455	ASP
1	F	477	THR
1	F	556	LYS
1	G	4	THR
1	G	7	GLU
1	G	40	SER
1	G	130	ARG
1	G	140	LEU
1	G	180	LEU
1	G	199	ASP
1	G	205	GLU

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Mol	Chain	Res	Type
1	G	210	ILE
1	G	216	THR
1	G	292	ASP
1	G	300	SER
1	G	366	ASP
1	G	462	LEU
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	185	LEU
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	359	THR
1	H	381	VAL
1	H	444	ASP
1	H	447	VAL
1	H	450	SER
1	H	459	ARG
1	H	505	ARG
1	H	512	ILE
1	H	519	ASP
1	H	526	GLU
1	H	542	LEU
1	I	29	ILE
1	I	38	ASP
1	I	110	THR
1	I	122	THR
1	I	168	THR
1	I	169	VAL
1	I	170	ASP
1	I	180	LEU

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Mol	Chain	Res	Type
1	I	199	ASP
1	I	250	LEU
1	I	263	GLU
1	I	300	SER
1	I	381	VAL
1	I	418	SER
1	I	435	THR
1	I	471	ASN
1	I	477	THR
1	I	485	LEU
1	I	511	SER
1	I	526	GLU
1	I	541	SER
1	I	549	LEU
1	J	4	THR
1	J	18	VAL
1	J	42	ARG
1	J	111	LEU
1	J	115	ILE
1	J	158	LEU
1	J	177	VAL
1	J	180	LEU
1	J	185	LEU
1	J	199	ASP
1	J	215	LEU
1	J	250	LEU
1	J	263	GLU
1	J	300	SER
1	J	312	GLU
1	J	341	SER
1	J	457	MET
1	J	471	ASN
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	140	LEU
1	K	169	VAL
1	K	180	LEU

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Mol	Chain	Res	Type
1	K	195	GLU
1	K	213	SER
1	K	215	LEU
1	K	216	THR
1	K	217	ARG
1	K	255	LEU
1	K	261	LEU
1	K	300	SER
1	K	366	ASP
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	K	538	VAL
1	L	71	LEU
1	L	136	LEU
1	L	140	LEU
1	L	157	LEU
1	L	158	LEU
1	L	198	LEU
1	L	245	ILE
1	L	247	GLU
1	L	262	ASP
1	L	300	SER
1	L	309	GLN
1	L	331	LEU
1	L	346	ARG
1	L	348	ARG
1	L	349	GLU
1	L	385	SER
1	L	444	ASP
1	L	447	VAL
1	L	450	SER
1	L	462	LEU
1	L	553	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	361	GLN
1	A	413	HIS
1	A	492	ASN
1	B	64	HIS
1	C	86	ASN
1	C	117	GLN
1	C	256	GLN
1	C	361	GLN
1	D	143	GLN
1	D	150	HIS
1	D	256	GLN
1	E	183	HIS
1	F	25	ASN
1	F	112	GLN
1	G	51	ASN
1	G	64	HIS
1	G	129	HIS
1	H	88	HIS
1	H	481	GLN
1	H	493	ASN
1	H	550	ASN
1	I	34	GLN
1	I	86	ASN
1	I	413	HIS
1	I	492	ASN
1	I	497	ASN
1	I	550	ASN
1	J	54	HIS
1	J	309	GLN
1	J	344	GLN
1	J	550	ASN
1	K	129	HIS
1	K	283	HIS
1	K	413	HIS
1	L	88	HIS
1	L	309	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	E	601	3	26,27,27	0.96	2 (7%)	38,40,40	1.51	1 (2%)
2	TPP	L	601	3	26,27,27	0.97	1 (3%)	38,40,40	1.55	2 (5%)
2	TPP	C	601	3	26,27,27	0.94	2 (7%)	38,40,40	1.49	1 (2%)
2	TPP	A	601	3	26,27,27	0.92	2 (7%)	38,40,40	1.52	1 (2%)
2	TPP	K	601	3	26,27,27	0.93	1 (3%)	38,40,40	1.60	2 (5%)
2	TPP	I	601	3	26,27,27	0.95	2 (7%)	38,40,40	1.55	1 (2%)
2	TPP	H	601	3	26,27,27	0.92	1 (3%)	38,40,40	1.18	1 (2%)
2	TPP	D	601	3	26,27,27	0.93	1 (3%)	38,40,40	1.54	2 (5%)
2	TPP	B	601	3	26,27,27	0.87	1 (3%)	38,40,40	1.62	3 (7%)
2	TPP	J	601	3	26,27,27	0.96	1 (3%)	38,40,40	1.70	3 (7%)
2	TPP	G	601	3	26,27,27	0.95	2 (7%)	38,40,40	1.49	1 (2%)
2	TPP	F	601	3	26,27,27	0.95	2 (7%)	38,40,40	1.53	1 (2%)

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	E	601	3	-	0/17/17/17	0/2/2/2
2	TPP	L	601	3	-	0/17/17/17	0/2/2/2
2	TPP	C	601	3	-	1/17/17/17	0/2/2/2
2	TPP	A	601	3	-	0/17/17/17	0/2/2/2
2	TPP	K	601	3	-	0/17/17/17	0/2/2/2
2	TPP	I	601	3	-	1/17/17/17	0/2/2/2
2	TPP	H	601	3	-	0/17/17/17	0/2/2/2
2	TPP	D	601	3	-	1/17/17/17	0/2/2/2
2	TPP	B	601	3	-	0/17/17/17	0/2/2/2
2	TPP	J	601	3	-	0/17/17/17	0/2/2/2
2	TPP	G	601	3	-	1/17/17/17	0/2/2/2
2	TPP	F	601	3	-	1/17/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	601	TPP	C5-C4	2.98	1.41	1.35
2	J	601	TPP	C5-C4	2.80	1.41	1.35
2	K	601	TPP	C5-C4	2.71	1.40	1.35
2	D	601	TPP	C5-C4	2.69	1.40	1.35
2	H	601	TPP	C5-C4	2.67	1.40	1.35
2	C	601	TPP	C5-C4	2.58	1.40	1.35
2	F	601	TPP	C5-C4	2.56	1.40	1.35
2	E	601	TPP	C5-C4	2.53	1.40	1.35
2	I	601	TPP	C5-C4	2.47	1.40	1.35
2	A	601	TPP	C5-C4	2.45	1.40	1.35
2	G	601	TPP	C5-C4	2.41	1.40	1.35
2	B	601	TPP	C5-S1	-2.40	1.66	1.72
2	G	601	TPP	C5-S1	-2.30	1.66	1.72
2	I	601	TPP	C5-S1	-2.21	1.67	1.72
2	E	601	TPP	C5-S1	-2.19	1.67	1.72
2	A	601	TPP	C5-S1	-2.19	1.67	1.72
2	C	601	TPP	C5-S1	-2.15	1.67	1.72
2	F	601	TPP	C5-S1	-2.15	1.67	1.72

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	601	TPP	C2-S1-C5	9.19	97.30	91.22
2	B	601	TPP	C2-S1-C5	8.61	96.92	91.22
2	K	601	TPP	C2-S1-C5	8.53	96.86	91.22
2	L	601	TPP	C2-S1-C5	8.31	96.72	91.22
2	I	601	TPP	C2-S1-C5	8.19	96.64	91.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	TPP	C2-S1-C5	8.08	96.57	91.22
2	C	601	TPP	C2-S1-C5	7.96	96.48	91.22
2	D	601	TPP	C2-S1-C5	7.94	96.48	91.22
2	E	601	TPP	C2-S1-C5	7.92	96.46	91.22
2	A	601	TPP	C2-S1-C5	7.90	96.45	91.22
2	G	601	TPP	C2-S1-C5	7.85	96.42	91.22
2	H	601	TPP	C2-S1-C5	5.91	95.13	91.22
2	J	601	TPP	C4-C5-S1	-2.54	106.59	110.56
2	K	601	TPP	C4-C5-S1	-2.29	106.99	110.56
2	B	601	TPP	S1-C2-N3	-2.26	109.43	112.30
2	J	601	TPP	S1-C2-N3	-2.26	109.43	112.30
2	D	601	TPP	C4-C5-S1	-2.20	107.13	110.56
2	L	601	TPP	C4-C5-S1	-2.15	107.20	110.56
2	B	601	TPP	C4-C5-S1	-2.02	107.41	110.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

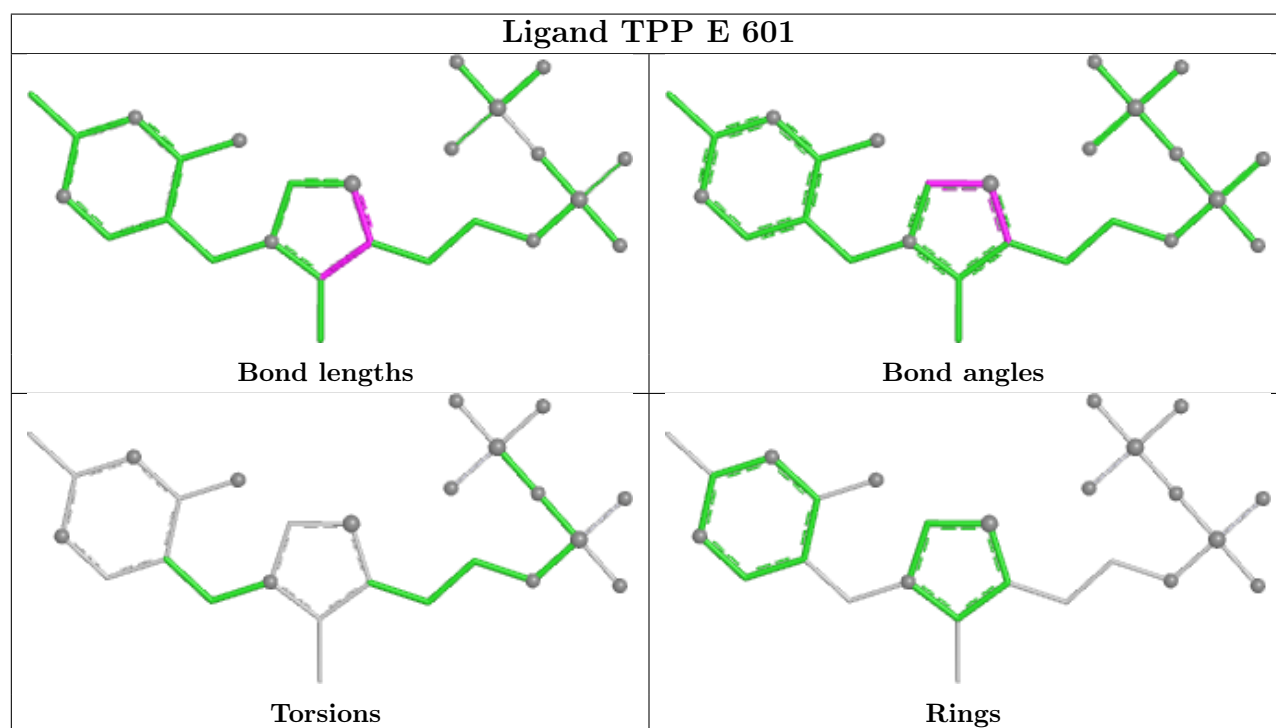
Mol	Chain	Res	Type	Atoms
2	C	601	TPP	PA-O3A-PB-O1B
2	D	601	TPP	PA-O3A-PB-O1B
2	F	601	TPP	PA-O3A-PB-O1B
2	G	601	TPP	C5-C6-C7-O7
2	I	601	TPP	C5-C6-C7-O7

There are no ring outliers.

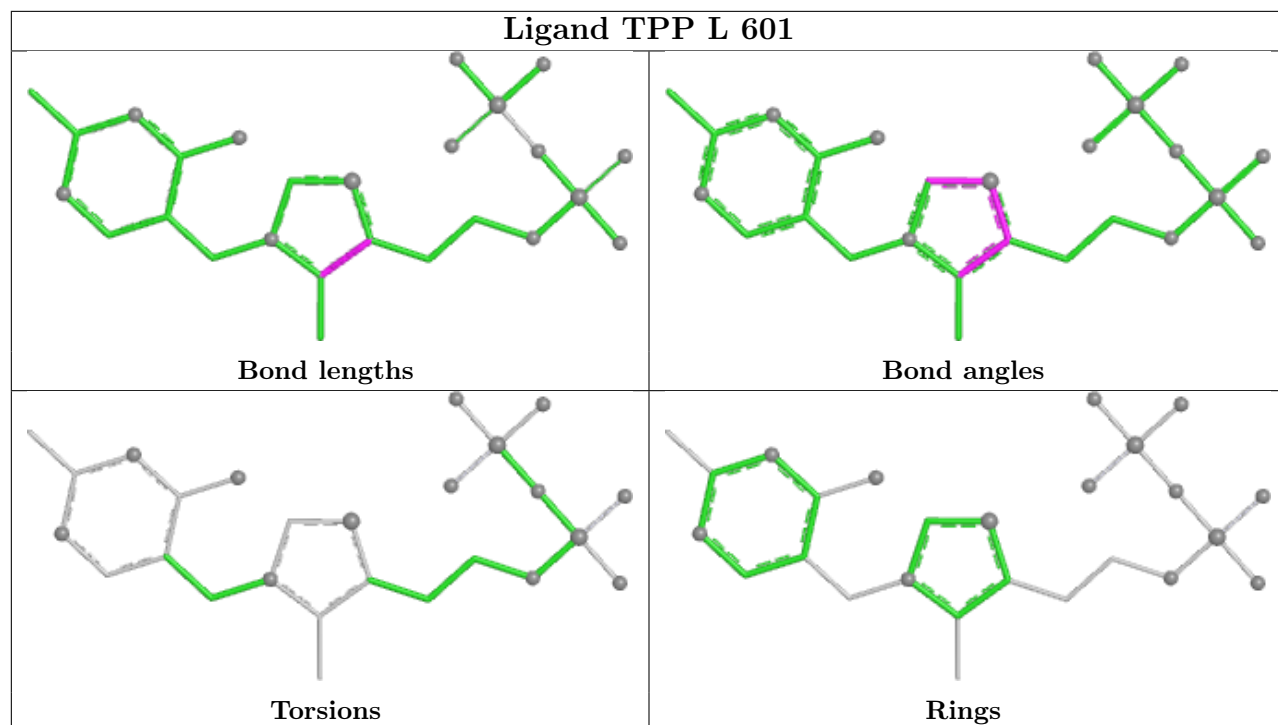
11 monomers are involved in 17 short contacts:

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

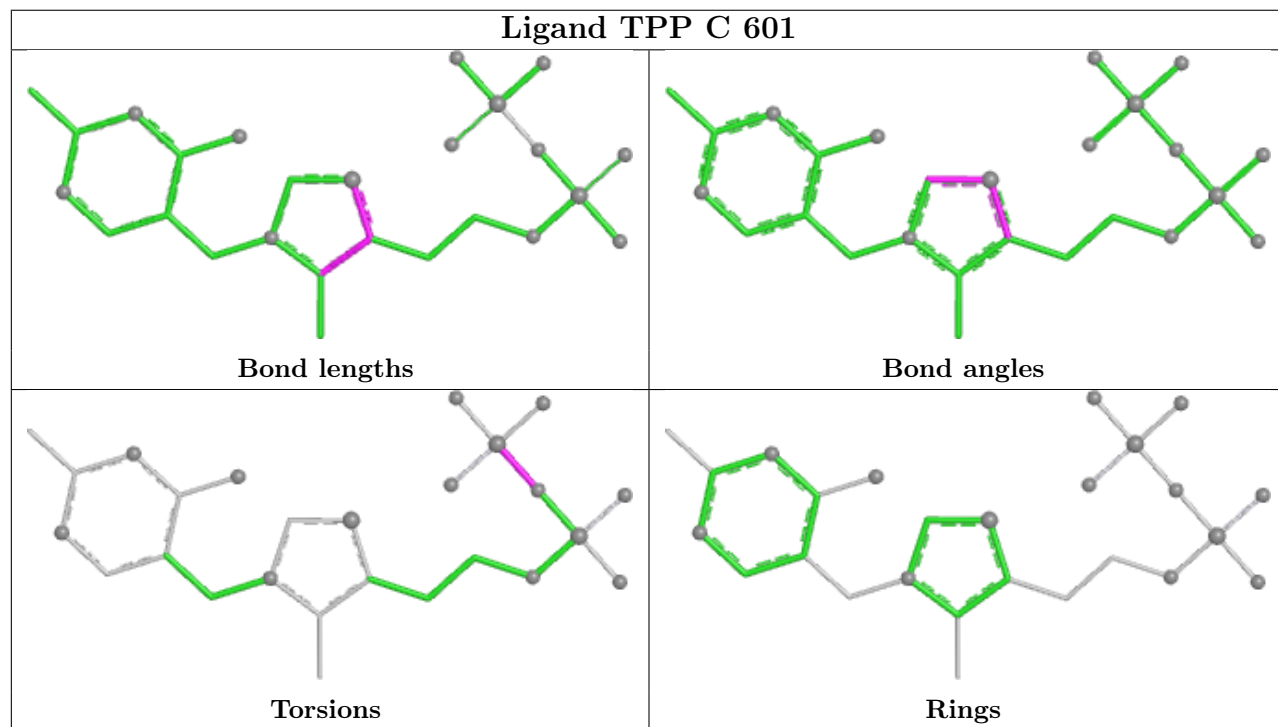
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



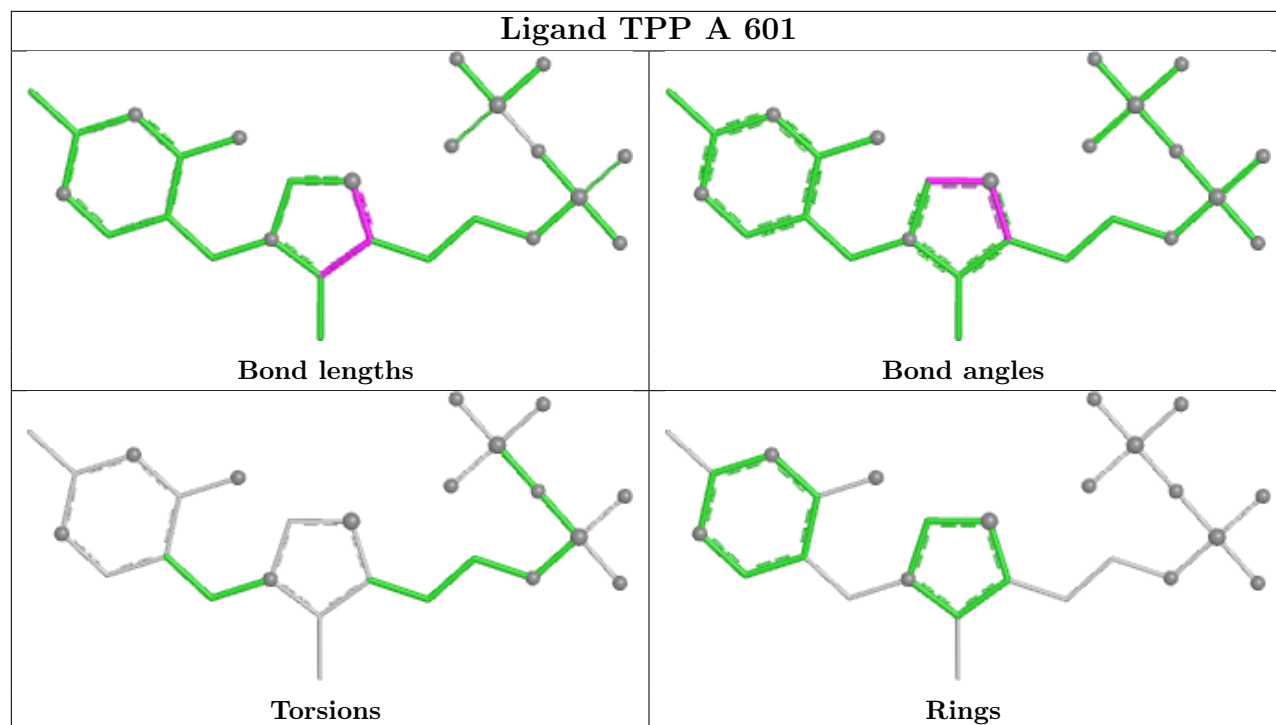
Ligand TPP L 601



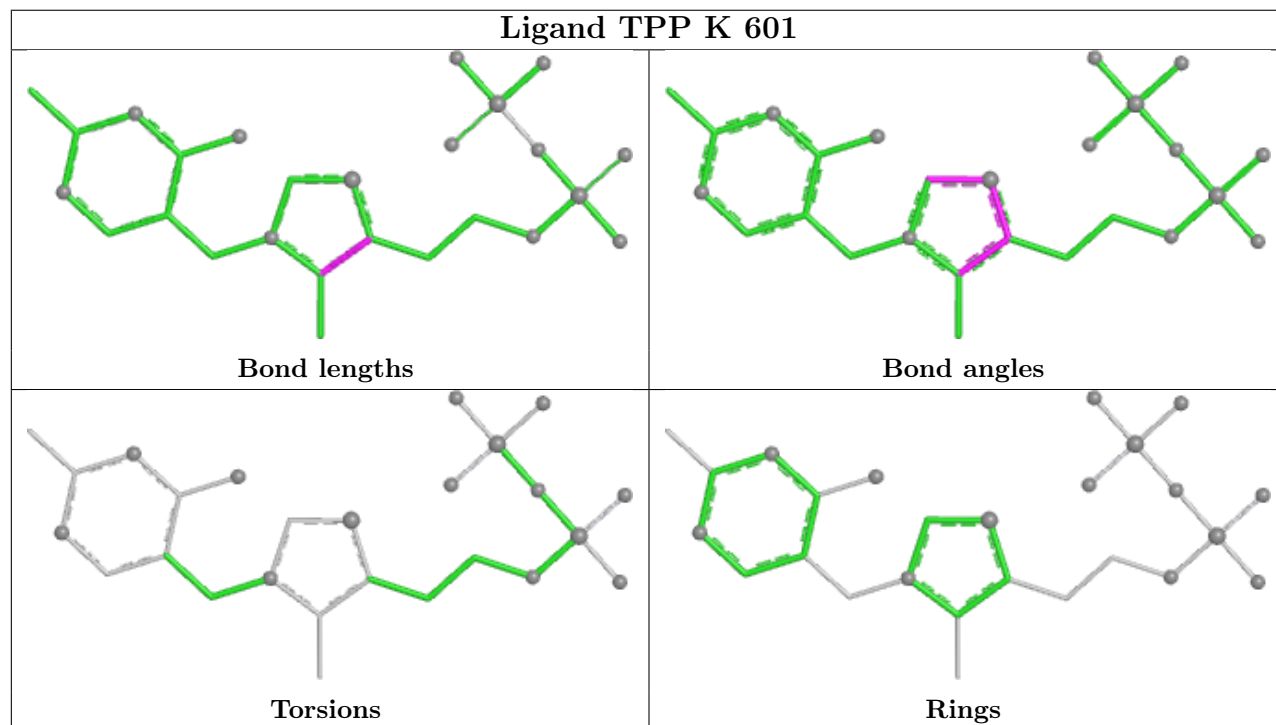
Ligand TPP C 601



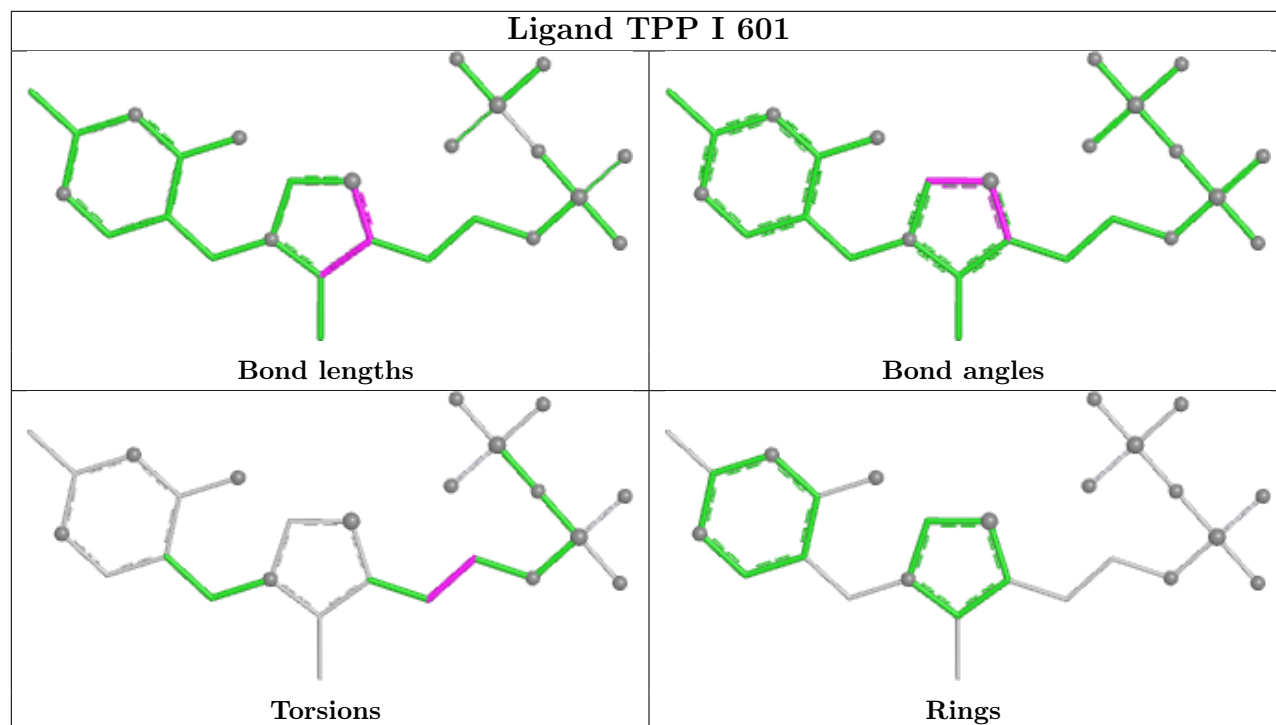
Ligand TPP A 601



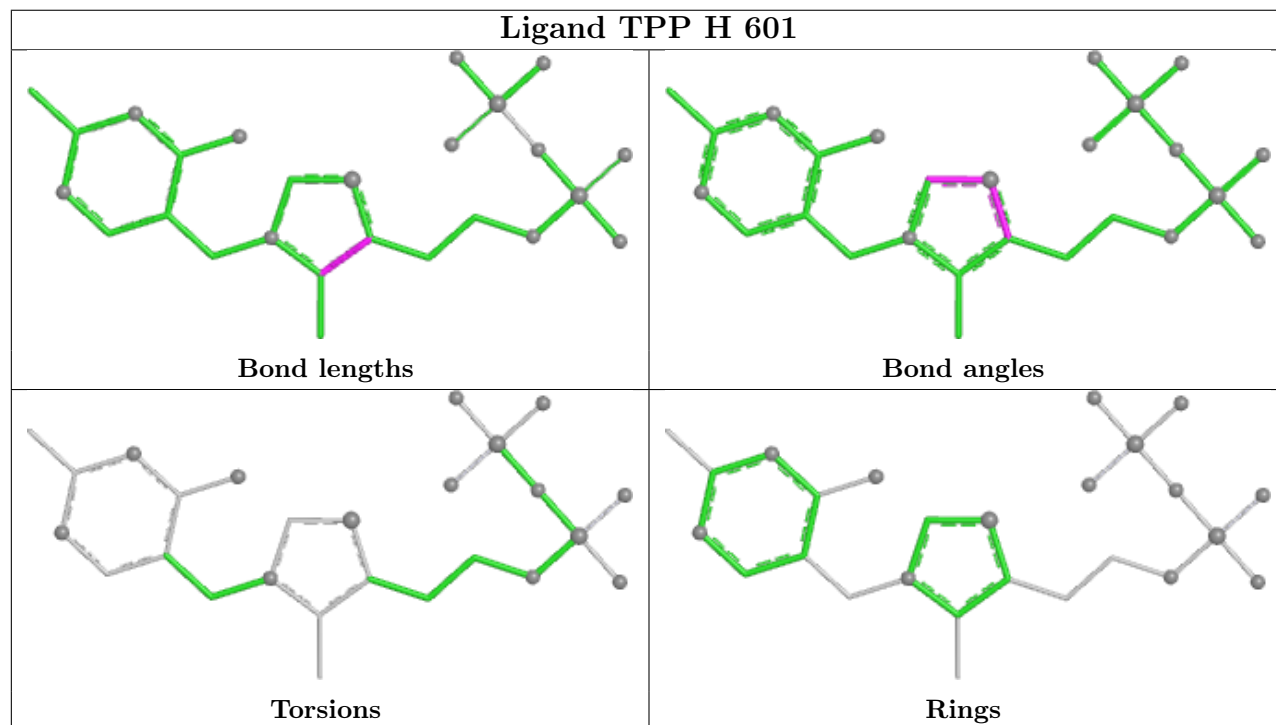
Ligand TPP K 601



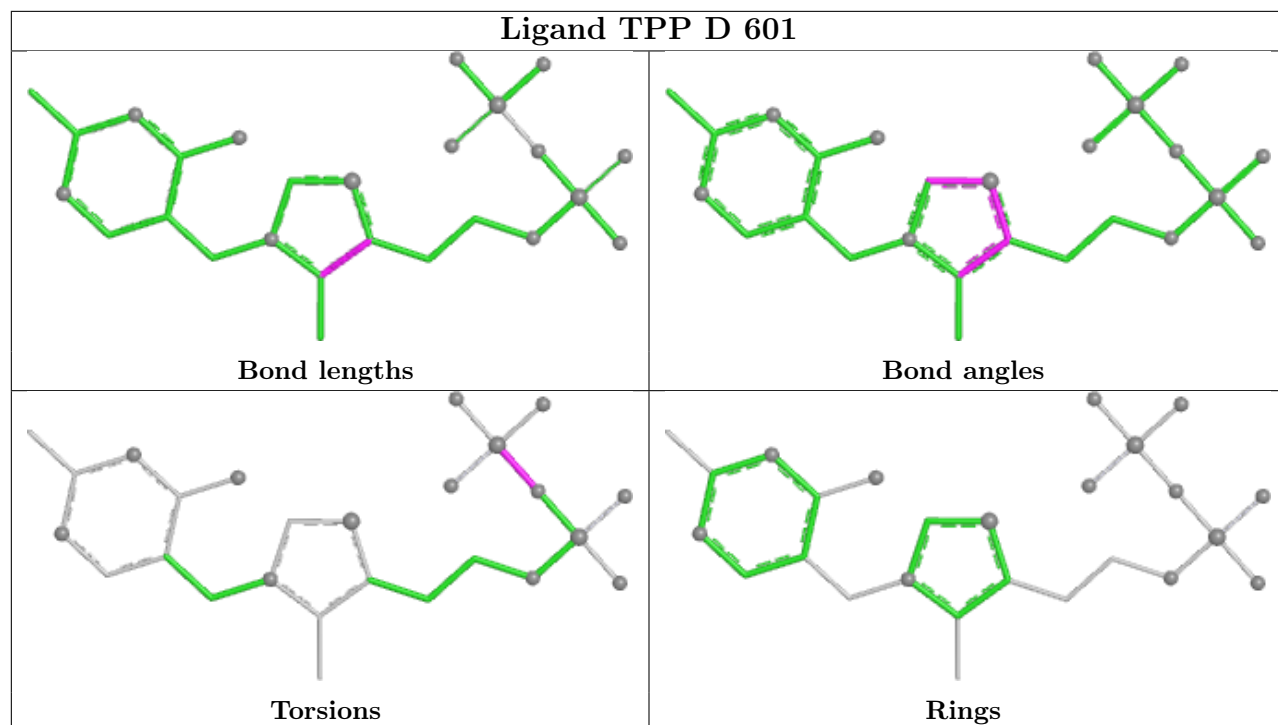
Ligand TPP I 601



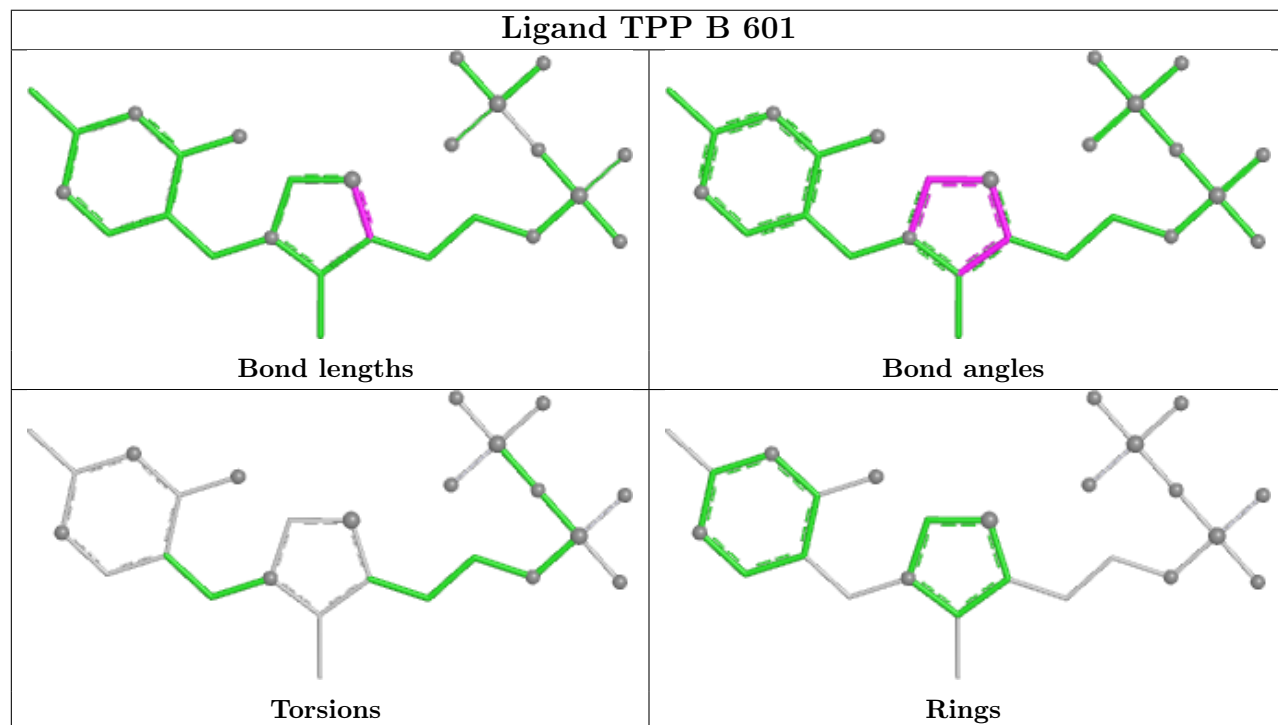
Ligand TPP H 601



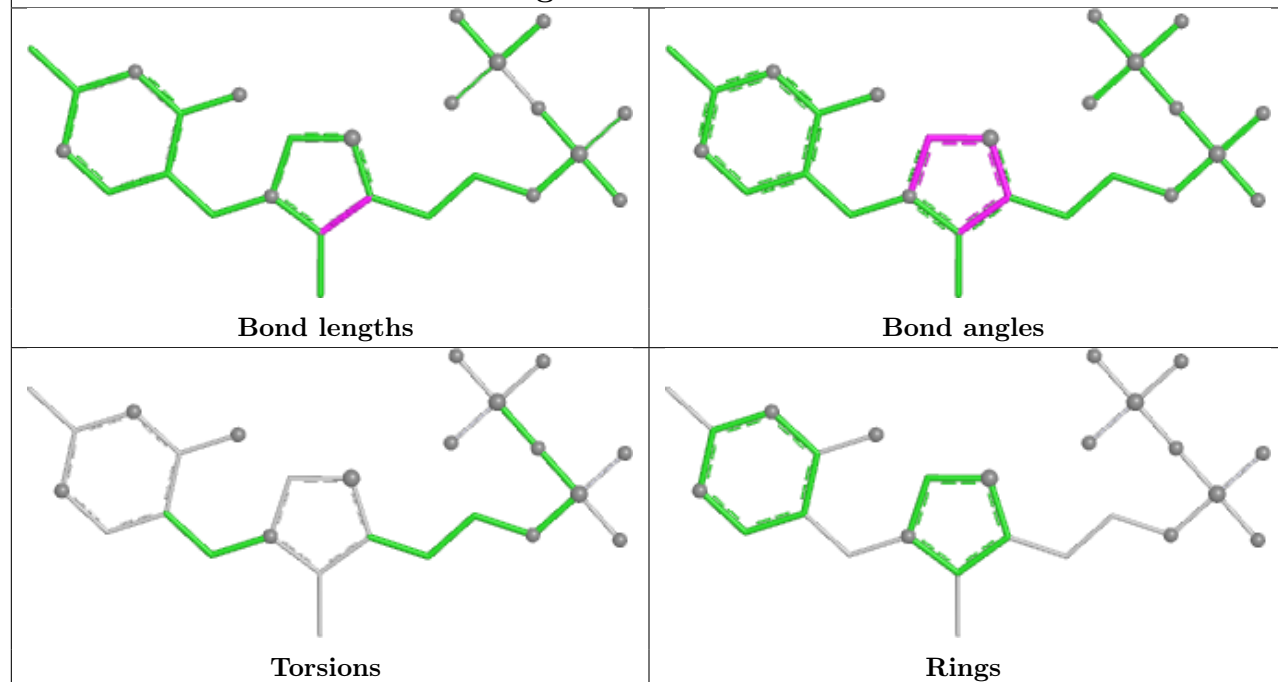
Ligand TPP D 601



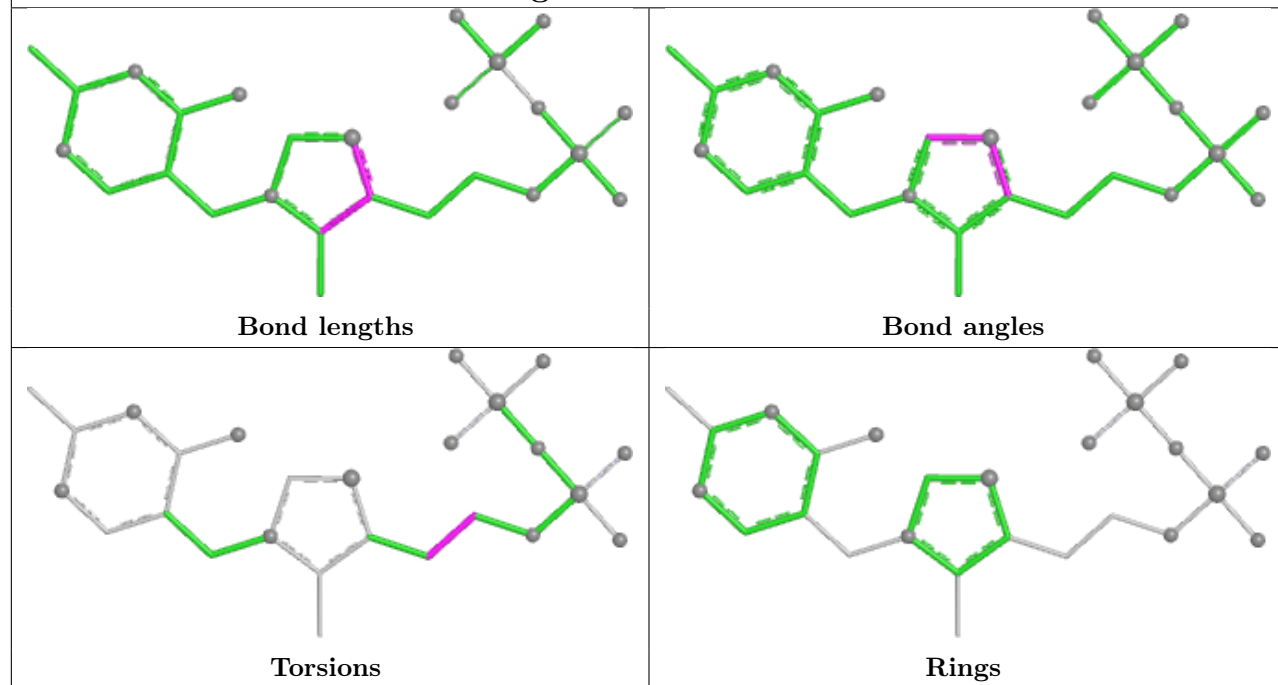
Ligand TPP B 601

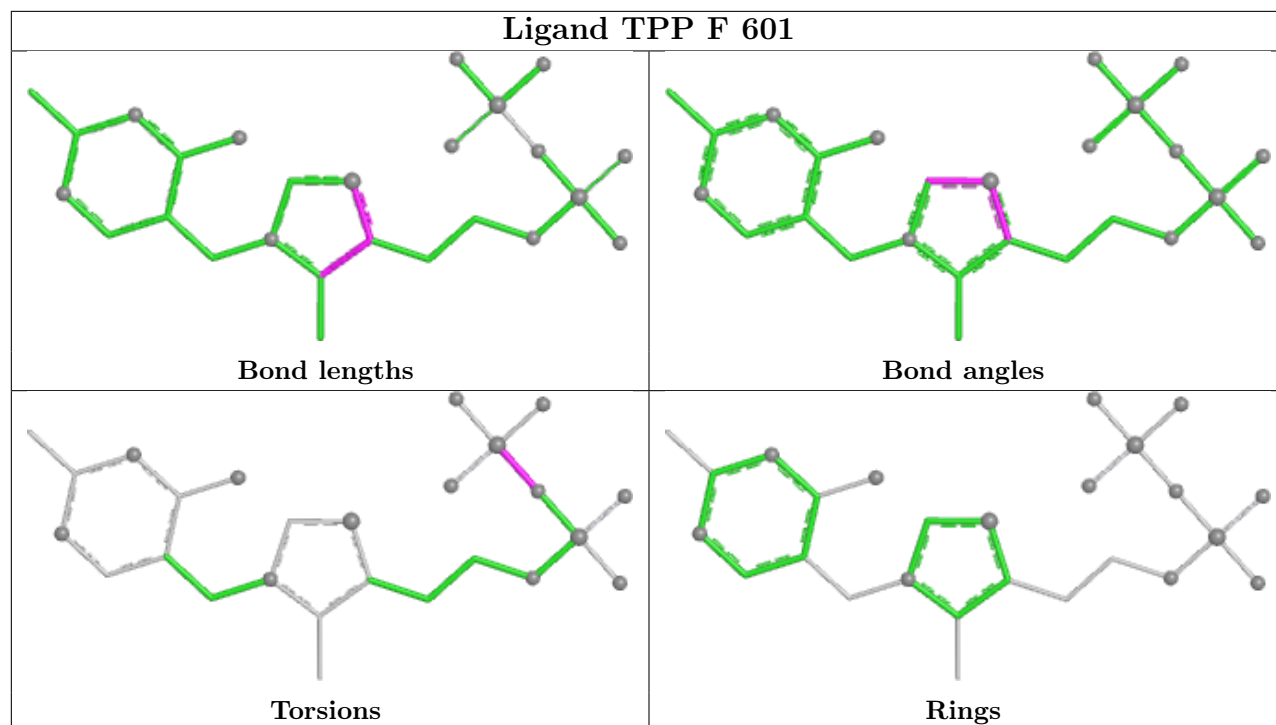


Ligand TPP J 601



Ligand TPP G 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/558 (99%)	-0.21	9 (1%) 70 68	20, 34, 52, 85	0
1	B	557/558 (99%)	-0.17	8 (1%) 73 71	20, 34, 54, 92	0
1	C	557/558 (99%)	-0.14	9 (1%) 70 68	23, 35, 56, 91	0
1	D	557/558 (99%)	-0.11	11 (1%) 65 61	23, 37, 57, 88	0
1	E	554/558 (99%)	0.09	12 (2%) 62 59	22, 39, 63, 93	0
1	F	554/558 (99%)	-0.05	8 (1%) 73 71	21, 39, 62, 86	0
1	G	557/558 (99%)	0.02	13 (2%) 61 57	24, 39, 61, 99	0
1	H	553/558 (99%)	0.13	7 (1%) 75 73	26, 42, 63, 92	0
1	I	552/558 (98%)	0.22	10 (1%) 67 65	27, 44, 68, 95	0
1	J	553/558 (99%)	0.01	14 (2%) 58 54	25, 39, 57, 89	0
1	K	550/558 (98%)	0.26	18 (3%) 49 44	25, 46, 70, 85	0
1	L	553/558 (99%)	0.29	12 (2%) 62 59	29, 49, 68, 89	0
All	All	6654/6696 (99%)	0.03	131 (1%) 65 61	20, 39, 63, 99	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	GLY	7.5
1	L	171	ASP	6.8
1	C	174	ALA	5.1
1	C	558	PHE	4.8
1	J	176	GLY	4.5
1	G	173	LEU	4.3
1	J	558	PHE	4.2
1	E	188	ALA	4.1
1	F	181	GLY	4.1
1	I	182	ALA	3.8
1	I	183	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	558	PHE	3.7
1	C	184	ALA	3.6
1	K	170	ASP	3.6
1	B	558	PHE	3.6
1	A	174	ALA	3.5
1	H	172	ALA	3.5
1	E	176	GLY	3.5
1	D	183	HIS	3.5
1	F	218	GLY	3.4
1	E	39	ARG	3.4
1	G	557	PRO	3.4
1	K	339	ASP	3.4
1	G	489	ARG	3.4
1	E	180	LEU	3.4
1	C	183	HIS	3.4
1	I	172	ALA	3.4
1	A	176	GLY	3.3
1	J	39	ARG	3.2
1	D	182	ALA	3.2
1	F	556	LYS	3.2
1	D	328	ARG	3.1
1	G	555	GLY	3.1
1	D	187	ALA	3.1
1	E	187	ALA	3.1
1	E	292	ASP	3.0
1	J	557	PRO	3.0
1	E	172	ALA	3.0
1	J	263	GLU	3.0
1	B	552	LEU	3.0
1	E	183	HIS	3.0
1	A	175	ASP	3.0
1	C	182	ALA	2.9
1	E	516	ASP	2.9
1	J	555	GLY	2.9
1	J	187	ALA	2.9
1	F	182	ALA	2.9
1	K	187	ALA	2.9
1	C	175	ASP	2.9
1	C	553	LEU	2.9
1	C	170	ASP	2.8
1	I	184	ALA	2.8
1	K	532	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	250	LEU	2.7
1	A	172	ALA	2.7
1	B	187	ALA	2.7
1	K	241	ALA	2.7
1	A	219	ASP	2.7
1	J	309	GLN	2.6
1	E	356	GLU	2.6
1	B	553	LEU	2.6
1	H	516	ASP	2.6
1	H	183	HIS	2.6
1	L	348	ARG	2.6
1	L	532	ARG	2.6
1	F	357	SER	2.6
1	K	512	ILE	2.6
1	B	556	LYS	2.6
1	K	188	ALA	2.6
1	G	219	ASP	2.5
1	I	219	ASP	2.5
1	I	177	VAL	2.5
1	D	516	ASP	2.5
1	G	175	ASP	2.5
1	J	171	ASP	2.5
1	C	173	LEU	2.5
1	F	266	ARG	2.5
1	K	175	ASP	2.5
1	B	188	ALA	2.5
1	E	226	ARG	2.4
1	K	183	HIS	2.4
1	H	494	ARG	2.4
1	I	130	ARG	2.4
1	I	187	ALA	2.4
1	L	180	LEU	2.3
1	I	176	GLY	2.3
1	H	246	ARG	2.3
1	F	172	ALA	2.3
1	G	188	ALA	2.3
1	L	552	LEU	2.3
1	J	177	VAL	2.3
1	B	554	GLY	2.3
1	G	177	VAL	2.3
1	D	185	LEU	2.3
1	D	172	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	187	ALA	2.3
1	D	184	ALA	2.2
1	G	174	ALA	2.2
1	L	523	THR	2.2
1	K	205	GLU	2.2
1	K	190	GLY	2.2
1	L	250	LEU	2.2
1	K	177	VAL	2.2
1	K	511	SER	2.2
1	B	174	ALA	2.1
1	K	174	ALA	2.1
1	K	265	GLU	2.1
1	J	437	PRO	2.1
1	A	170	ASP	2.1
1	K	488	ASP	2.1
1	K	516	ASP	2.1
1	F	558	PHE	2.1
1	J	182	ALA	2.1
1	A	173	LEU	2.1
1	L	553	LEU	2.1
1	D	171	ASP	2.1
1	J	178	GLU	2.1
1	L	11	ARG	2.1
1	I	546	PRO	2.1
1	A	188	ALA	2.1
1	G	172	ALA	2.1
1	L	263	GLU	2.1
1	D	174	ALA	2.0
1	H	553	LEU	2.0
1	L	177	VAL	2.0
1	K	340	ARG	2.0
1	E	263	GLU	2.0
1	A	216	THR	2.0
1	L	137	LEU	2.0
1	G	475	GLY	2.0
1	J	221	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

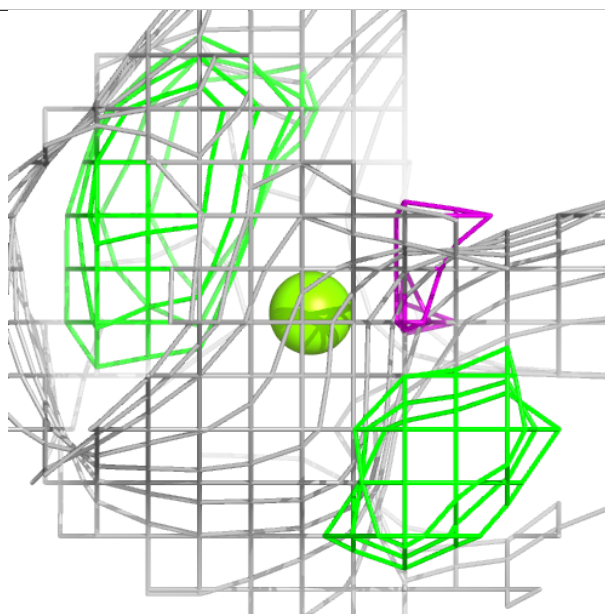
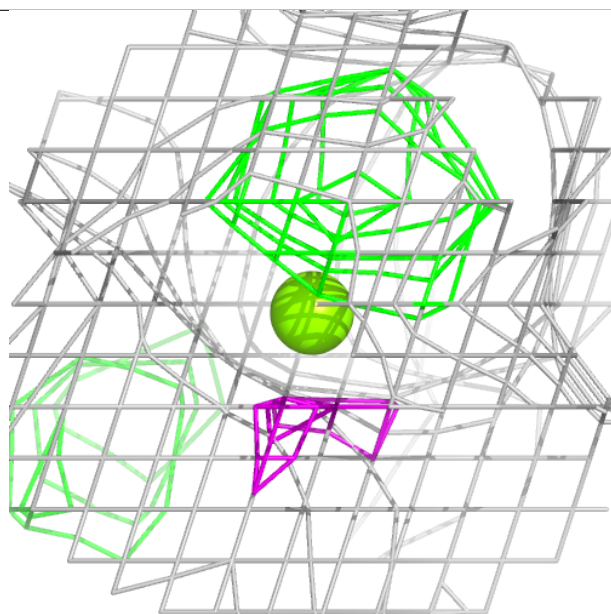
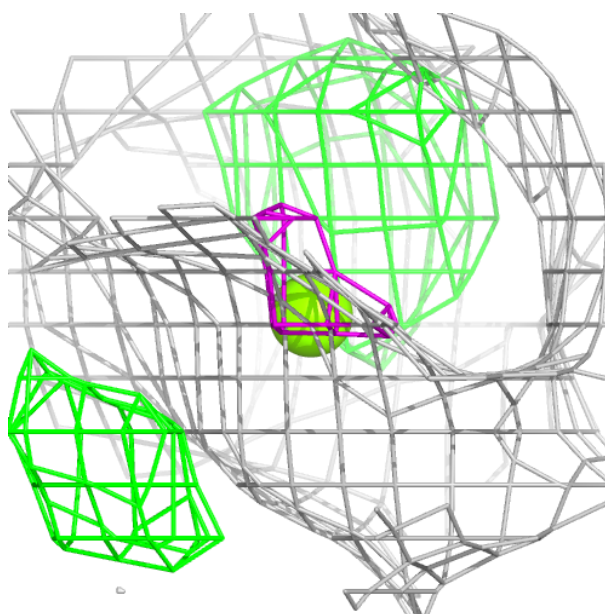
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	F	602	1/1	0.82	0.13	36,36,36,36	0
3	MG	E	602	1/1	0.83	0.18	70,70,70,70	0
3	MG	H	602	1/1	0.85	0.13	39,39,39,39	0
3	MG	J	602	1/1	0.90	0.09	39,39,39,39	0
3	MG	B	602	1/1	0.91	0.09	41,41,41,41	0
3	MG	D	602	1/1	0.91	0.10	38,38,38,38	0
3	MG	L	602	1/1	0.91	0.09	45,45,45,45	0
3	MG	I	602	1/1	0.93	0.07	42,42,42,42	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
2	TPP	E	601	26/26	0.95	0.09	22,37,45,96	0
2	TPP	L	601	26/26	0.95	0.09	29,45,55,56	0
3	MG	C	602	1/1	0.96	0.05	32,32,32,32	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	C	601	26/26	0.96	0.08	18,31,45,80	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
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
2	TPP	D	601	26/26	0.97	0.07	27,32,43,50	0
2	TPP	A	601	26/26	0.98	0.06	17,31,39,45	0
3	MG	K	602	1/1	0.99	0.05	42,42,42,42	0
3	MG	G	602	1/1	0.99	0.06	30,30,30,30	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.

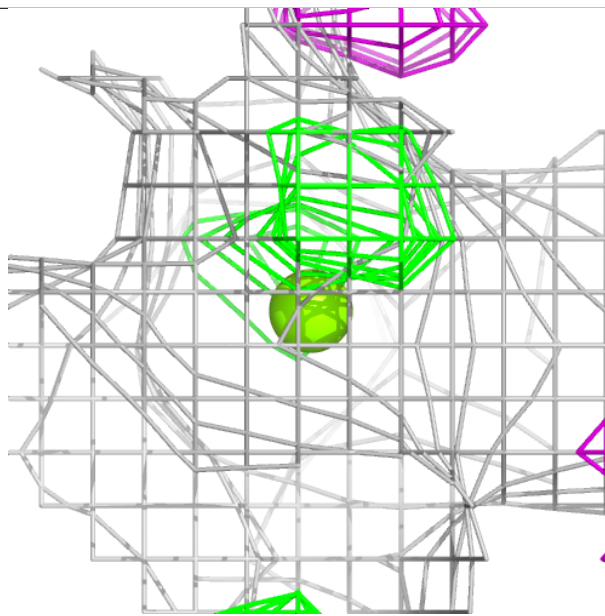
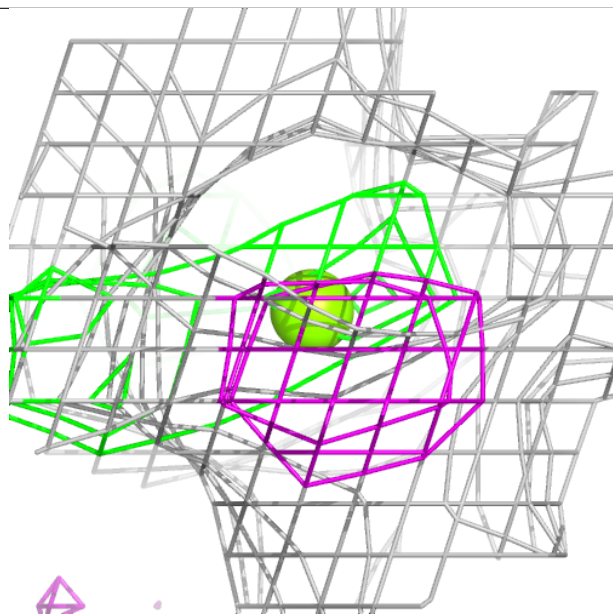
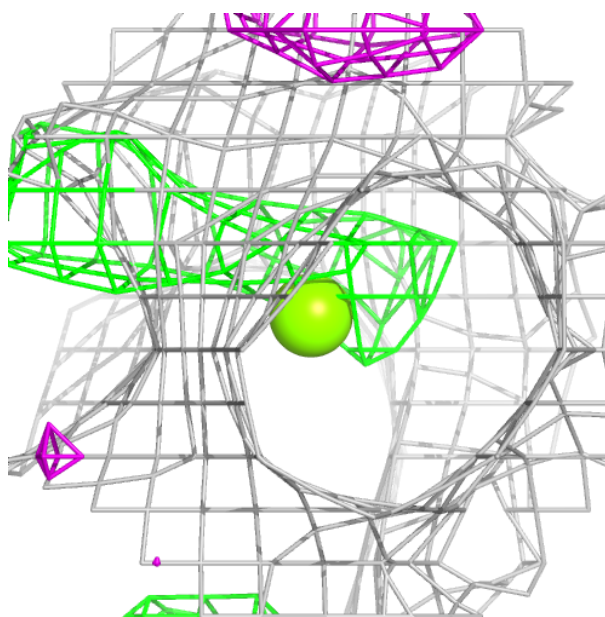
Electron density around MG F 602:

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



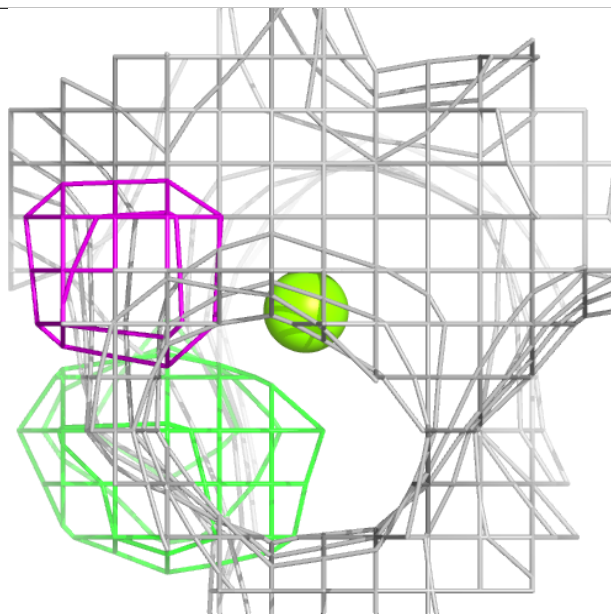
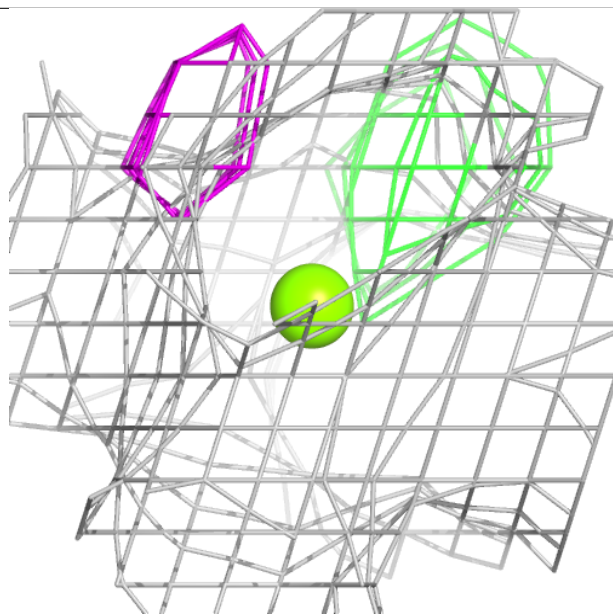
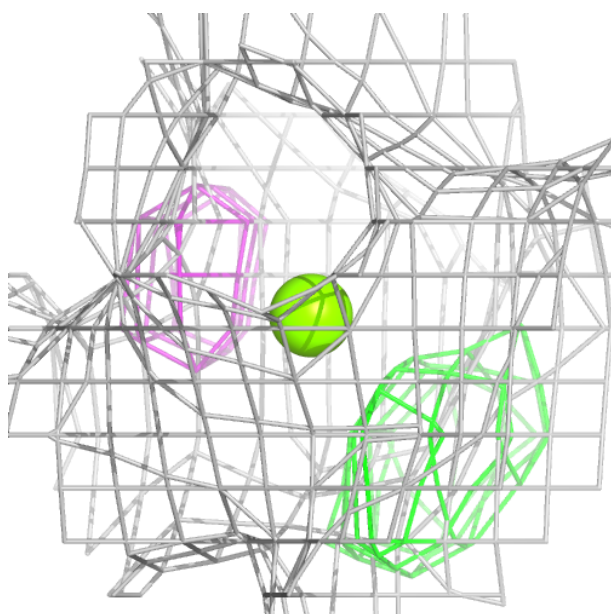
Electron density around MG E 602:

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



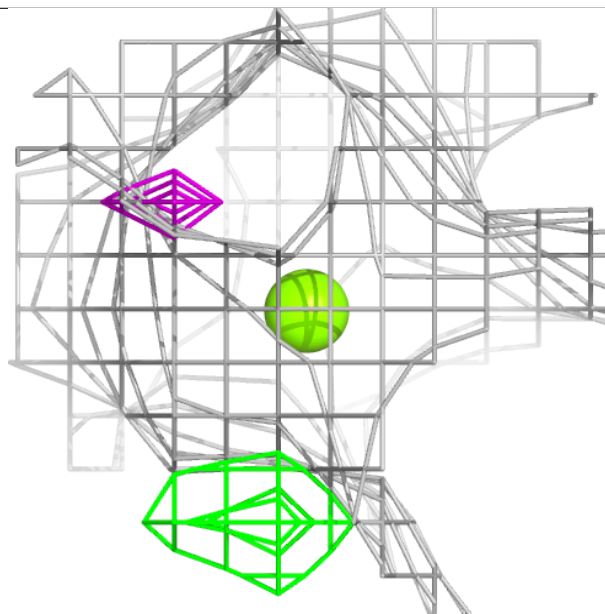
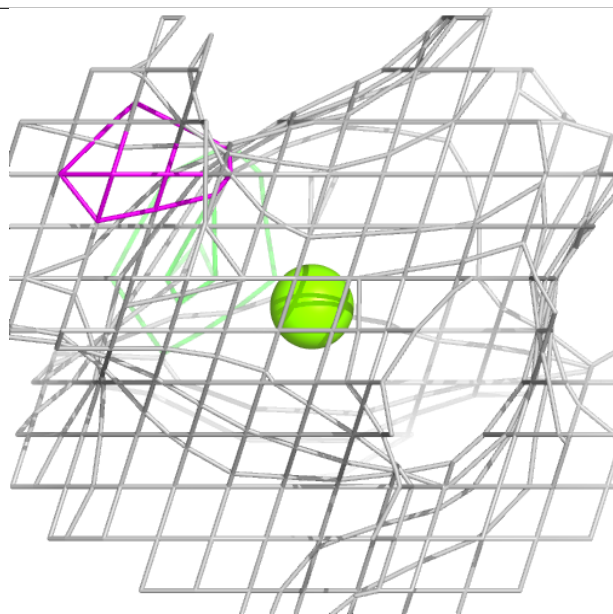
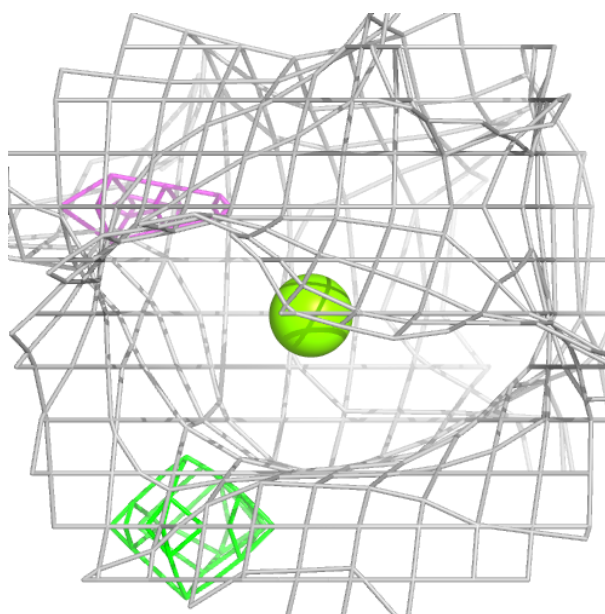
Electron density around MG H 602:

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



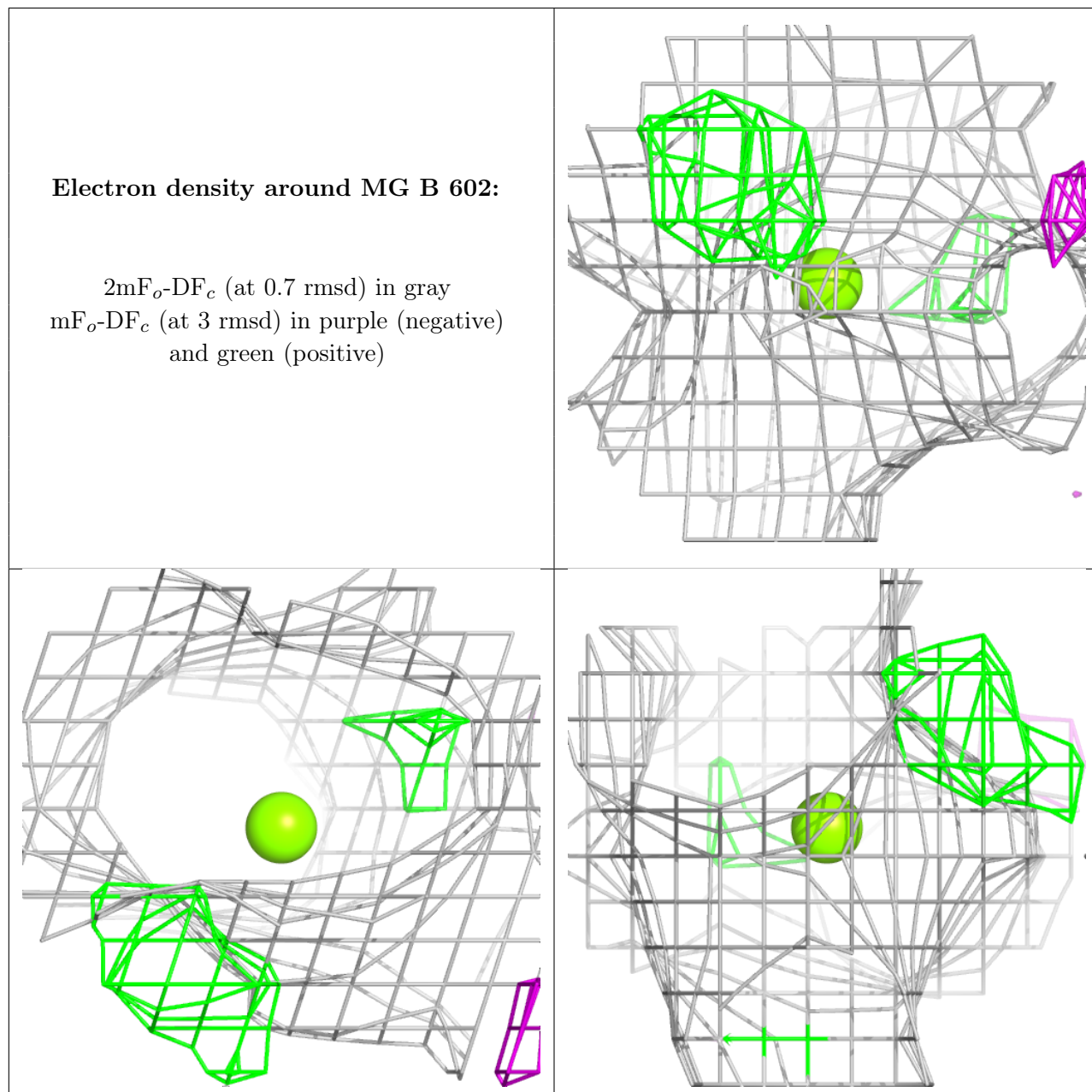
Electron density around MG J 602:

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



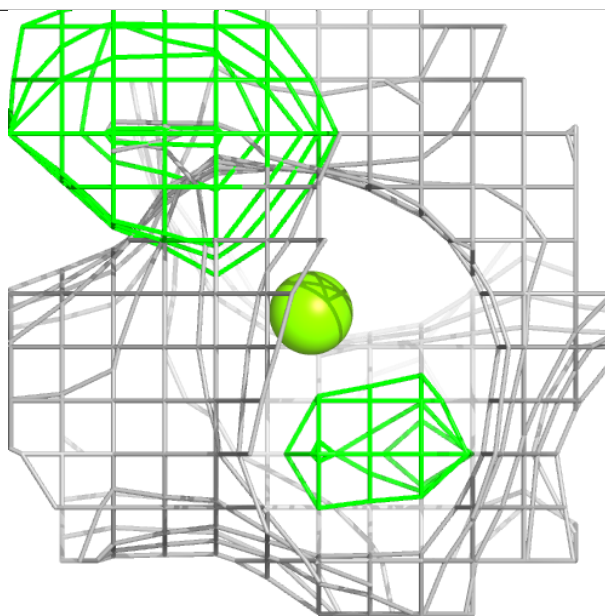
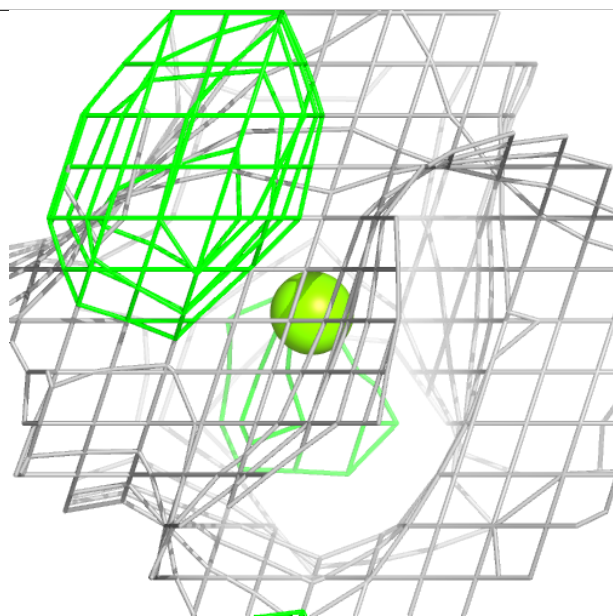
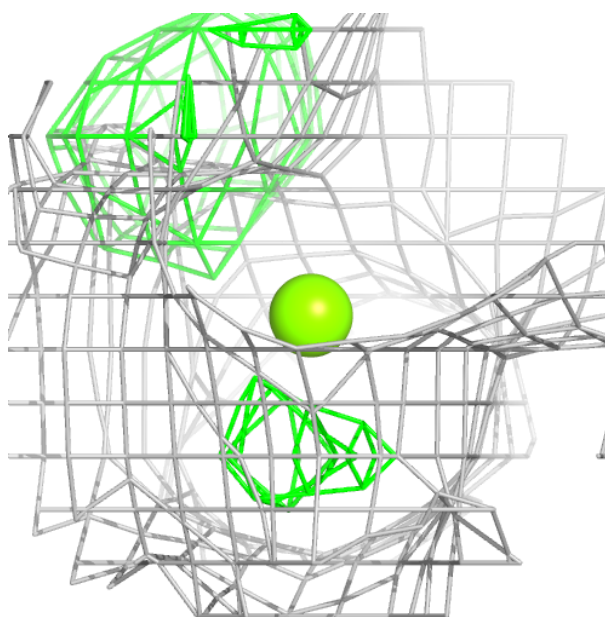
Electron density around MG B 602:

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and green (positive)



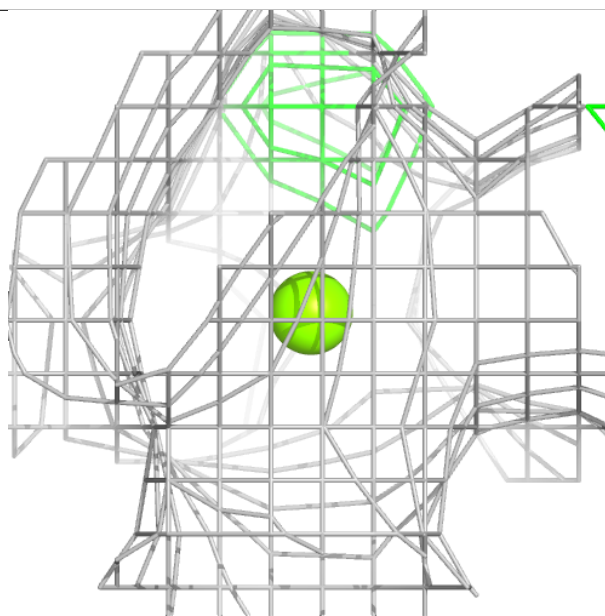
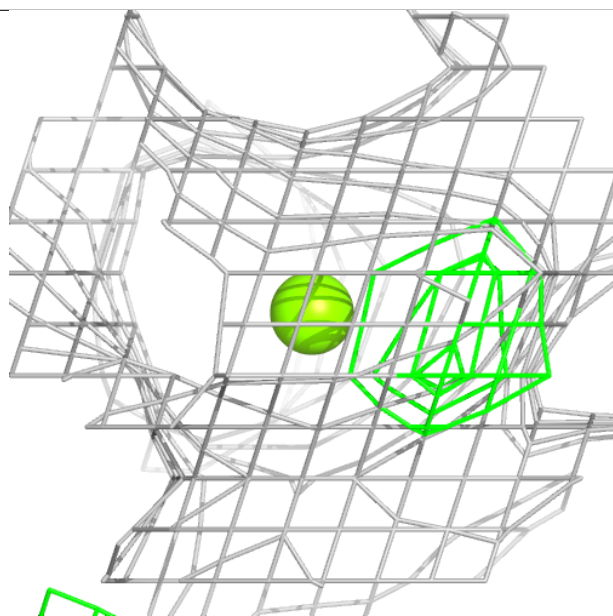
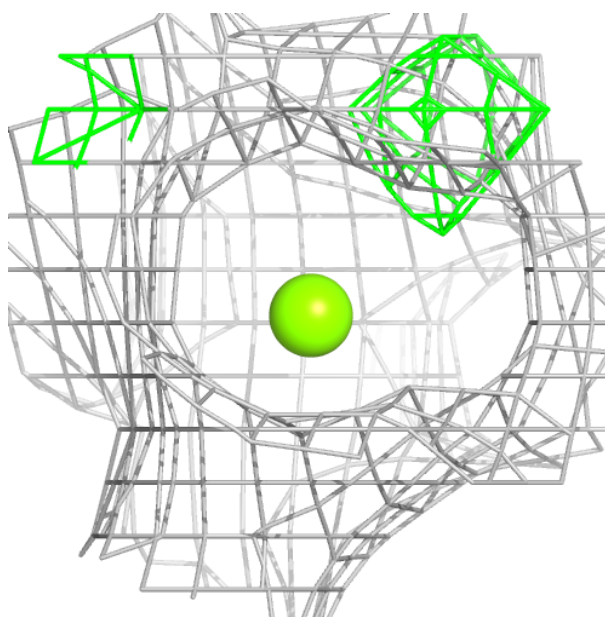
Electron density around MG D 602:

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



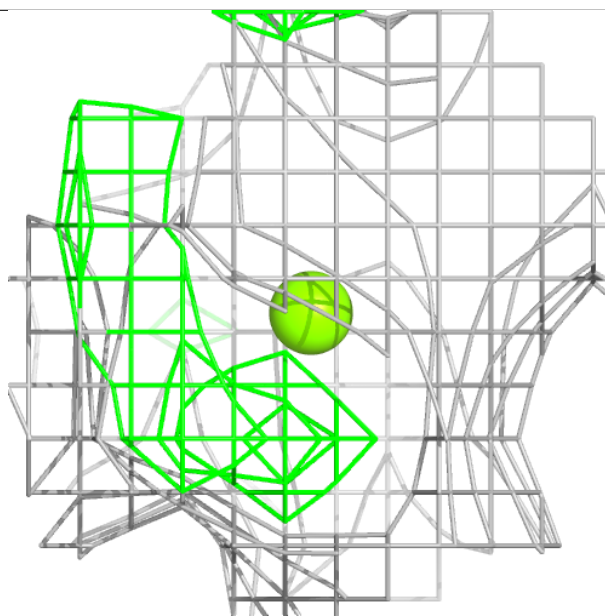
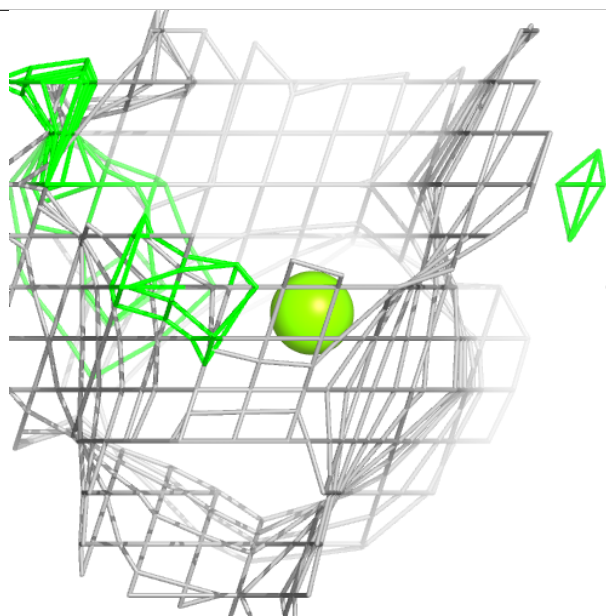
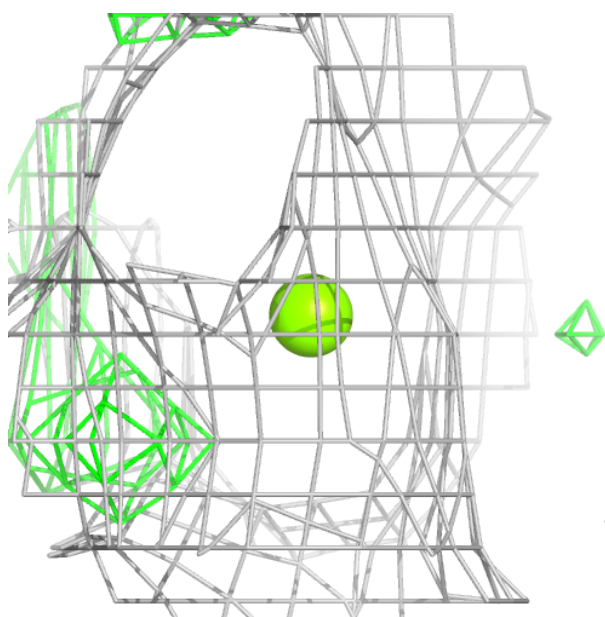
Electron density around MG L 602:

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



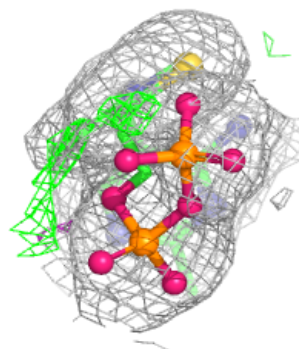
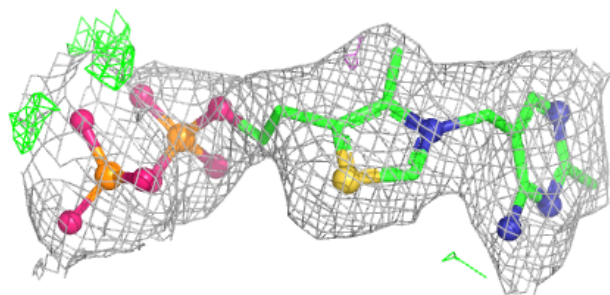
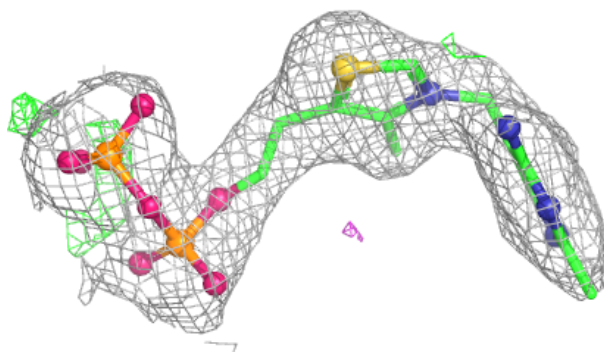
Electron density around MG I 602:

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

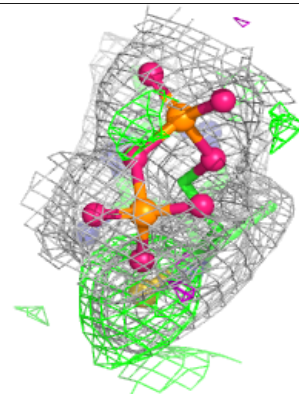
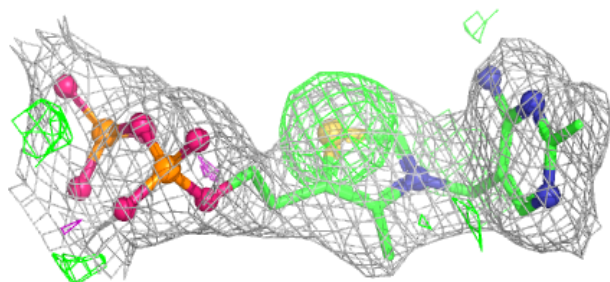
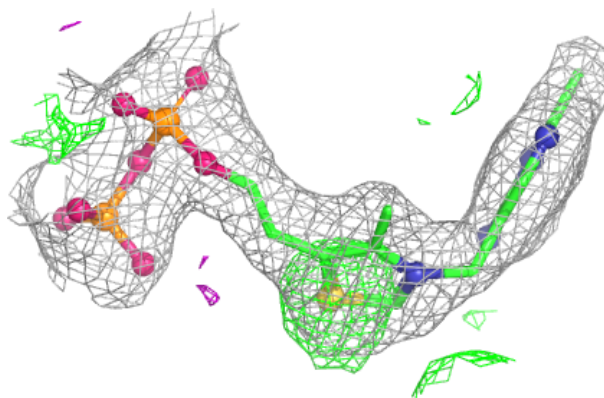


Electron density around TPP I 601:

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

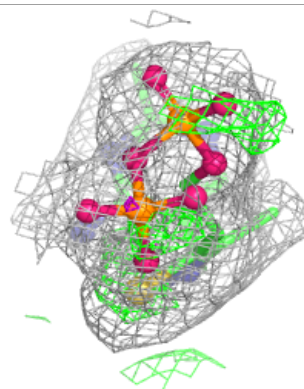
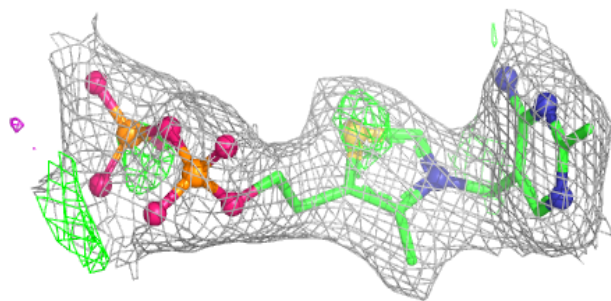
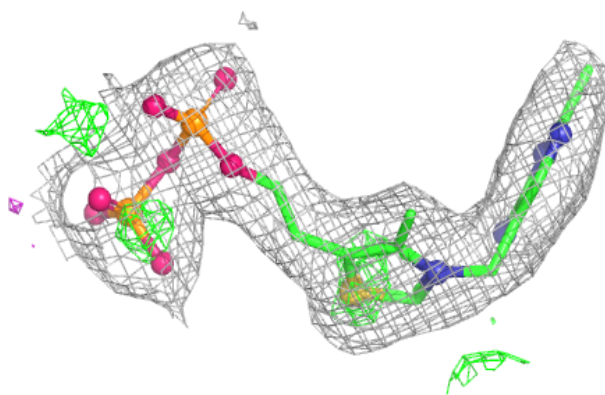
**Electron density around TPP B 601:**

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

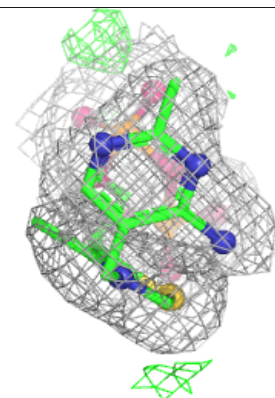
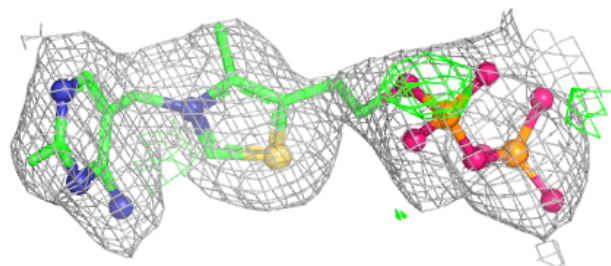
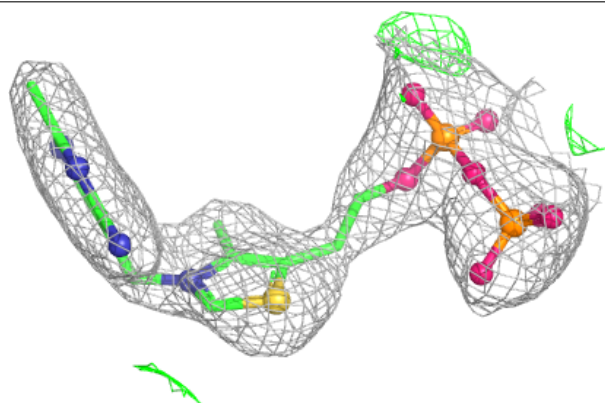


Electron density around TPP E 601:

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

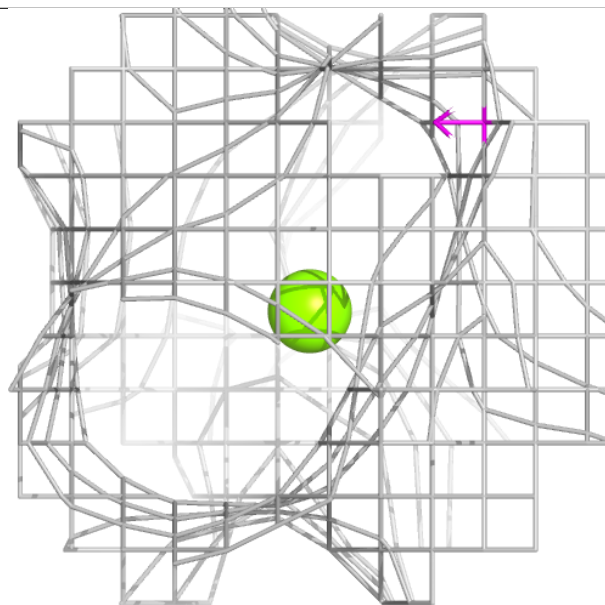
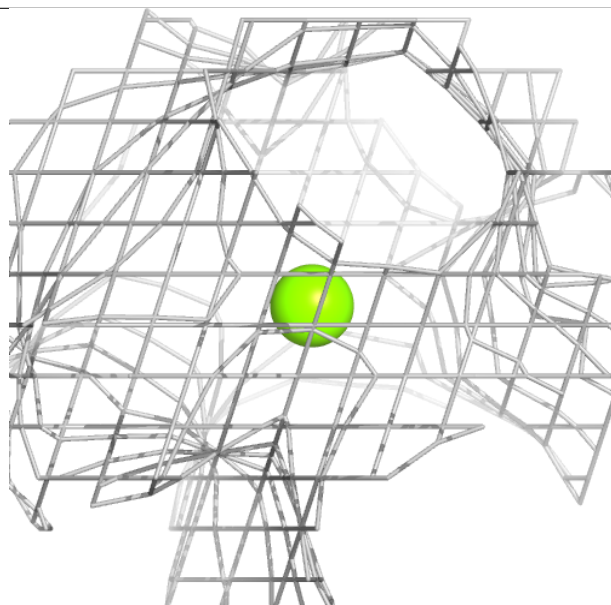
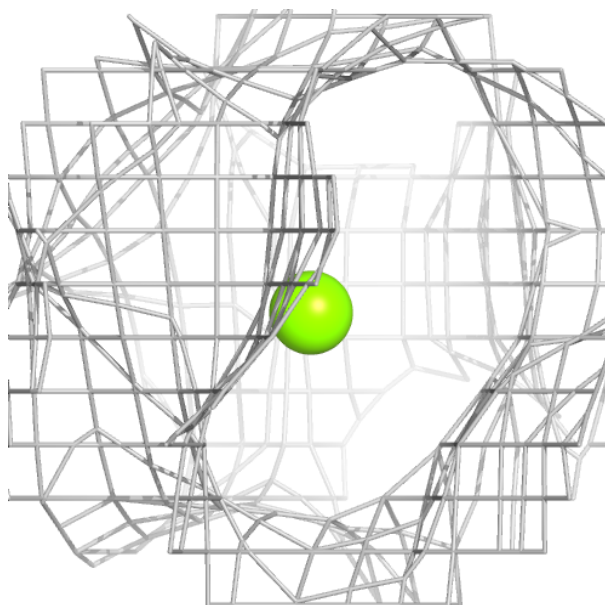
**Electron density around TPP L 601:**

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



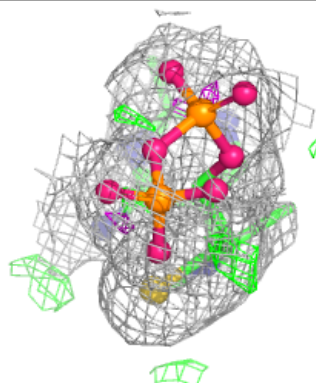
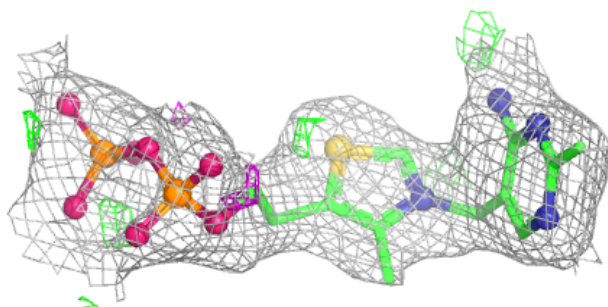
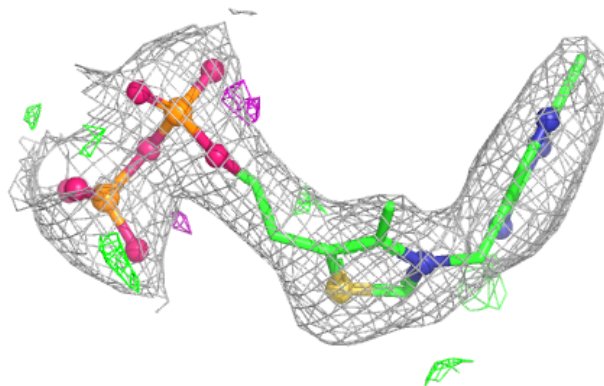
Electron density around MG C 602:

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



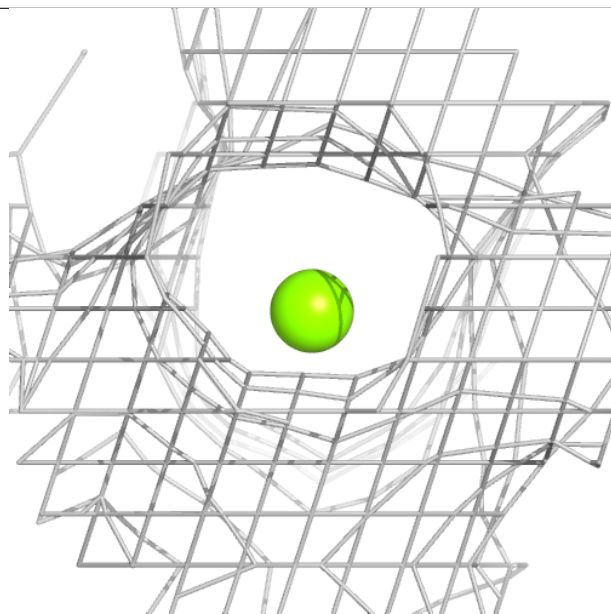
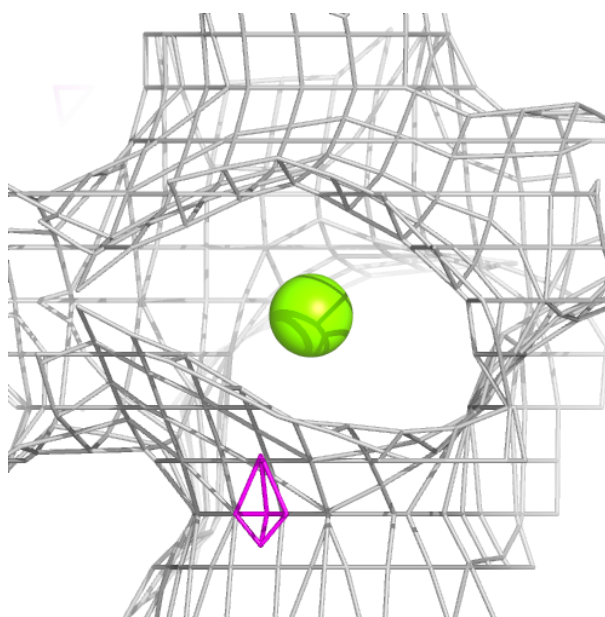
Electron density around TPP G 601:

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



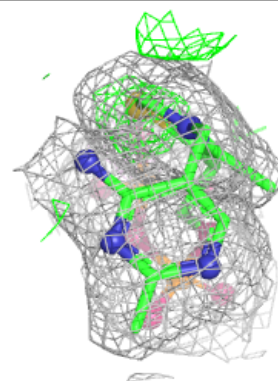
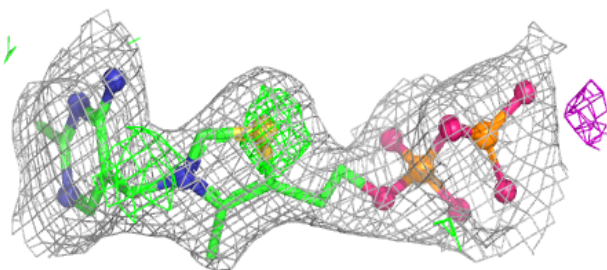
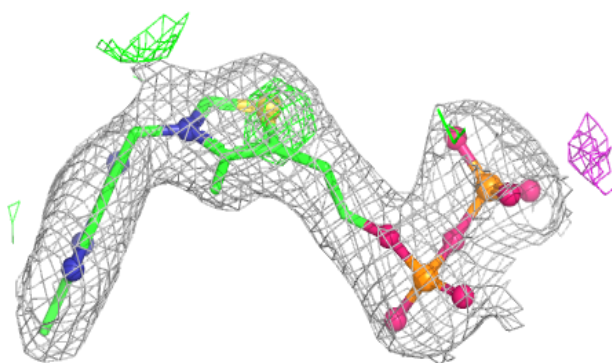
Electron density around MG A 602:

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

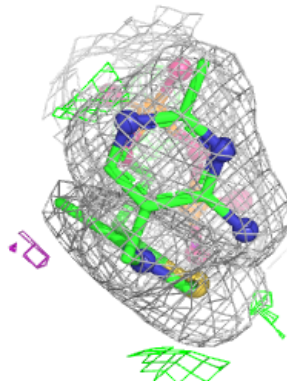
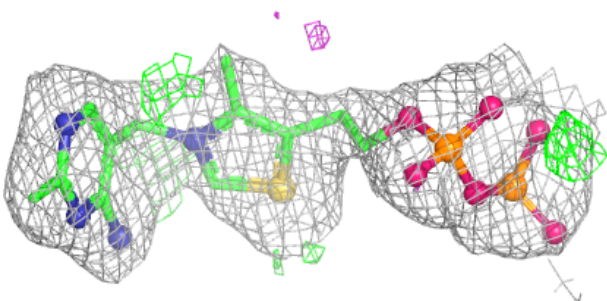
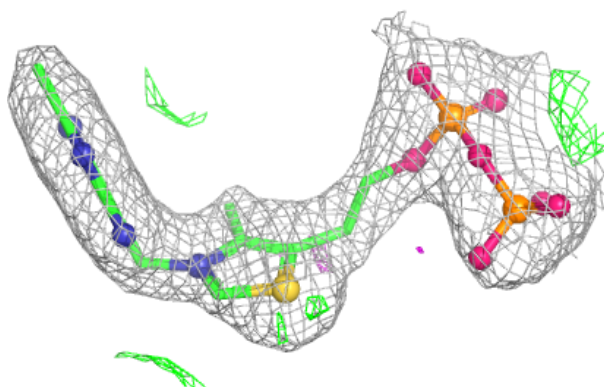


Electron density around TPP C 601:

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

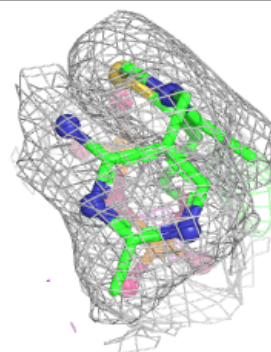
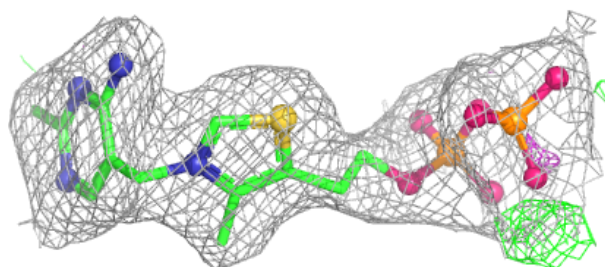
**Electron density around TPP H 601:**

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

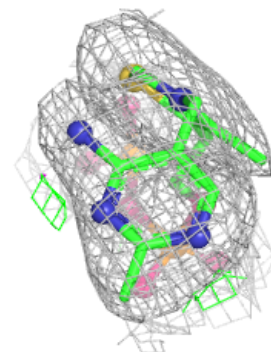
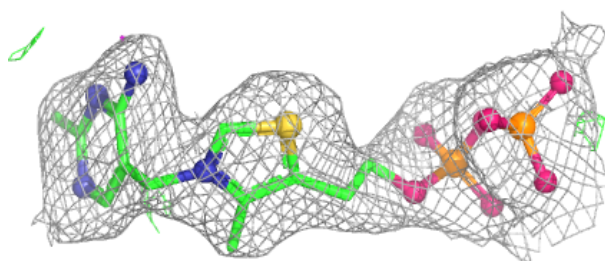
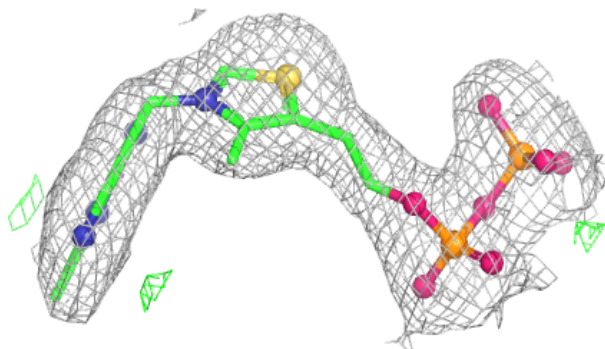


Electron density around TPP F 601:

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

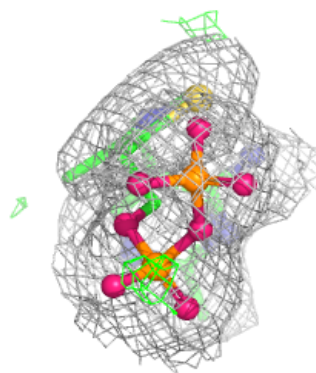
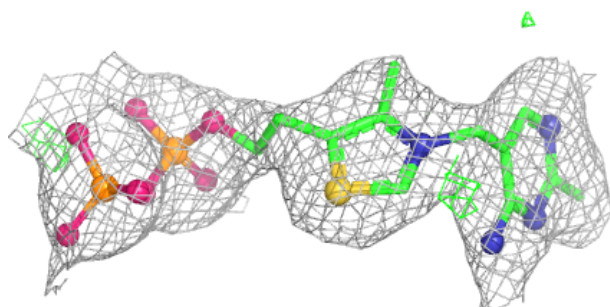
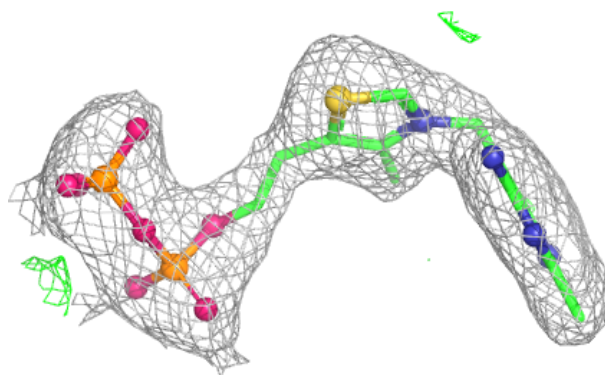
**Electron density around TPP J 601:**

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

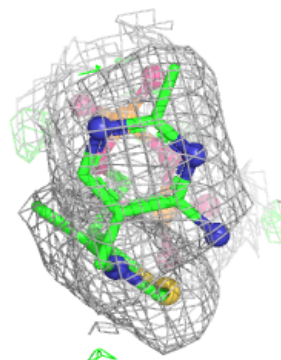
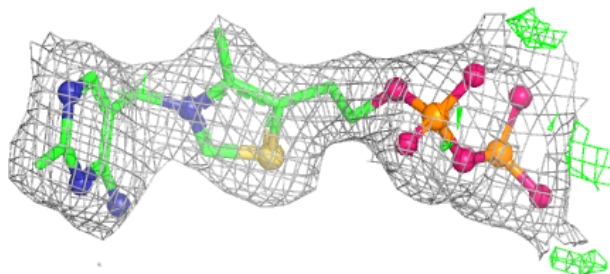
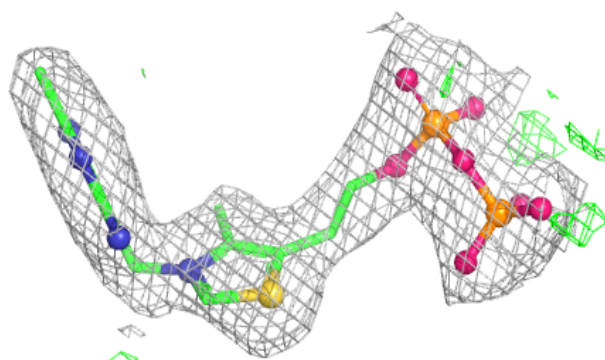


Electron density around TPP K 601:

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

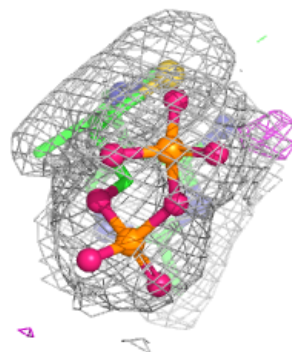
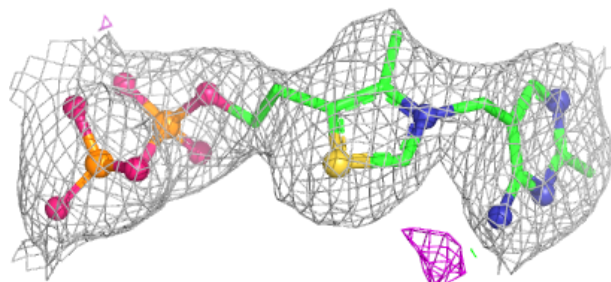
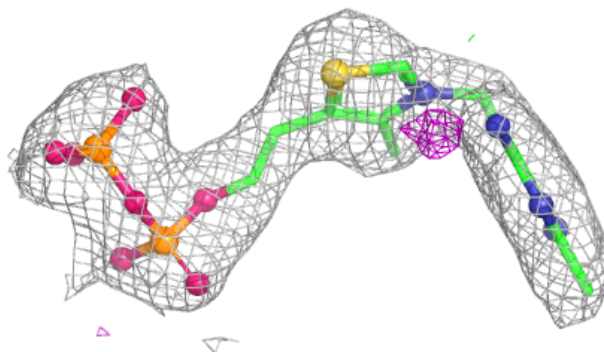
**Electron density around TPP D 601:**

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



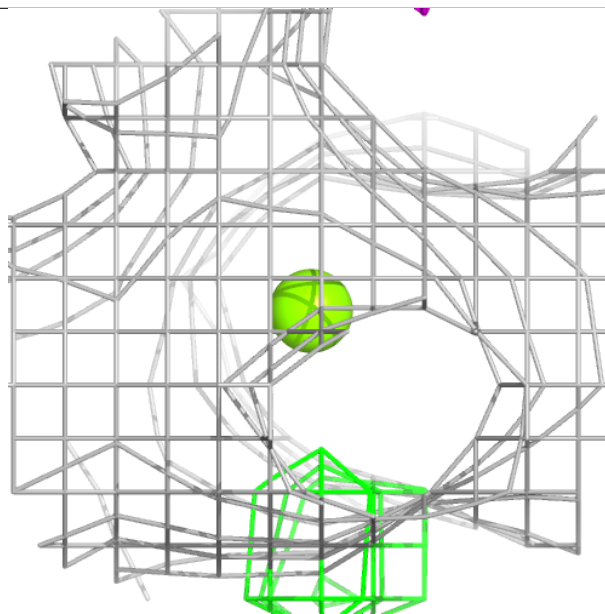
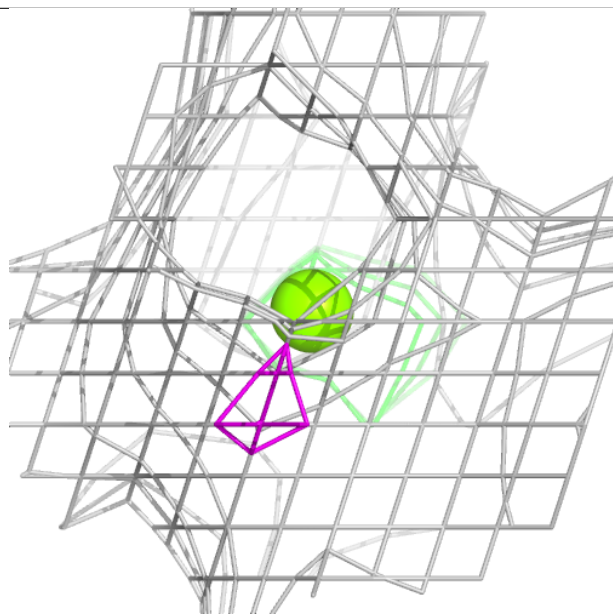
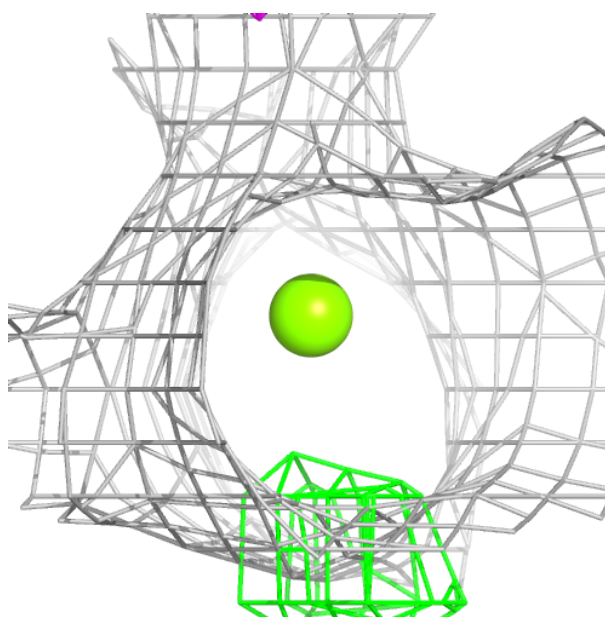
Electron density around TPP A 601:

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



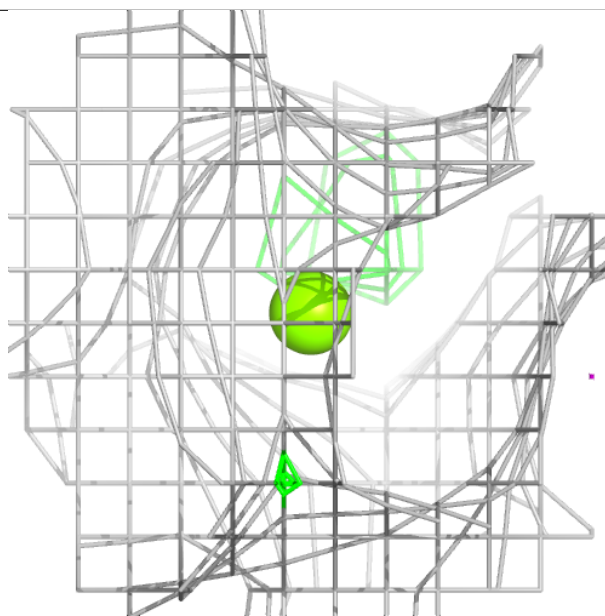
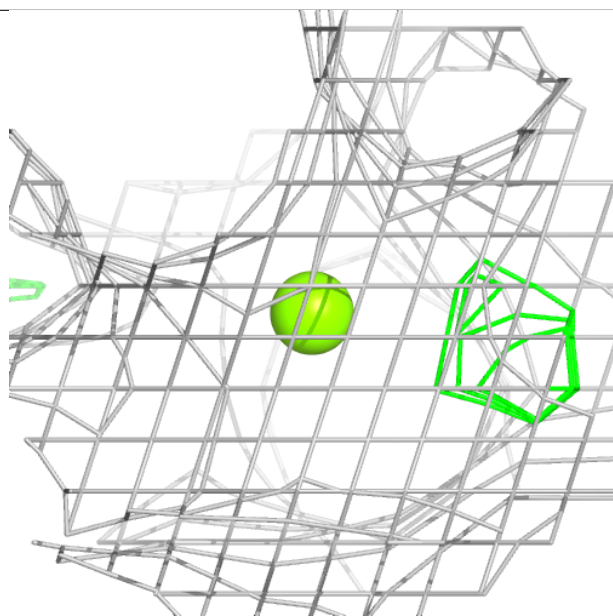
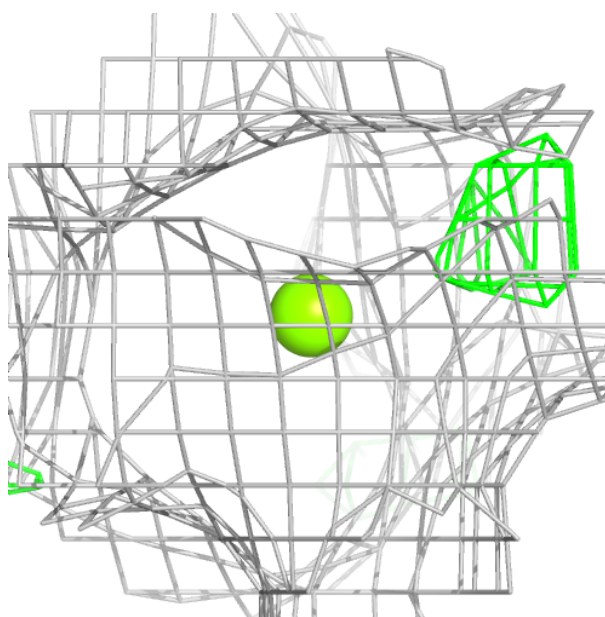
Electron density around MG K 602:

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



Electron density around MG 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.