



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 06:16 am BST

PDB ID : 4QPZ
Title : Crystal structure of the formolase FLS_v2 in space group P 21
Authors : Shen, B.W.; Siegel, J.B.; Stoddard, B.L.; Baker, D.
Deposited on : 2014-06-25
Resolution : 3.00 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 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

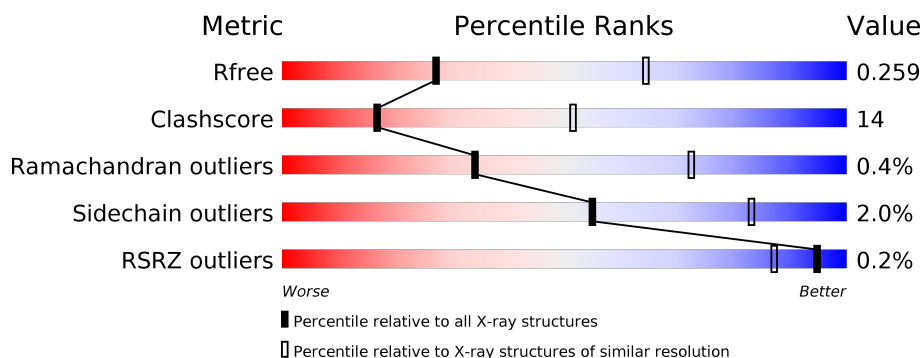
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	582	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>..</div> </div> </div>
1	B	582	<div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	C	582	<div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	D	582	<div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	E	582	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	F	582	<div> <div>%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	582	
1	H	582	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TPP	C	602	-	-	X	-
3	TPP	F	602	-	-	X	-
3	TPP	G	602	-	-	X	-
3	TPP	H	602	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33455 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 Formolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4157	2630	734	776	17			
1	B	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	C	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	D	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	E	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	F	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	G	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	H	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ILE	ALA	CONFLICT	UNP Q9F4L3
A	394	GLY	ALA	CONFLICT	UNP Q9F4L3
A	419	ASN	GLY	CONFLICT	UNP Q9F4L3
A	480	TRP	ALA	CONFLICT	UNP Q9F4L3
A	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
A	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
A	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
A	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
A	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
A	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
A	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
A	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
A	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
A	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
A	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
A	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
A	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
A	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	28	ILE	ALA	CONFLICT	UNP Q9F4L3
B	394	GLY	ALA	CONFLICT	UNP Q9F4L3
B	419	ASN	GLY	CONFLICT	UNP Q9F4L3
B	480	TRP	ALA	CONFLICT	UNP Q9F4L3
B	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
B	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
B	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
B	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
B	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
B	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
B	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
B	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
B	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
B	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
B	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
B	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
B	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
B	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
B	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	28	ILE	ALA	CONFLICT	UNP Q9F4L3
C	394	GLY	ALA	CONFLICT	UNP Q9F4L3
C	419	ASN	GLY	CONFLICT	UNP Q9F4L3
C	480	TRP	ALA	CONFLICT	UNP Q9F4L3
C	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
C	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
C	566	THR	-	EXPRESSION TAG	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
C	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
C	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
C	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
C	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
C	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
C	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
C	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
C	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
C	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
C	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
C	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	28	ILE	ALA	CONFLICT	UNP Q9F4L3
D	394	GLY	ALA	CONFLICT	UNP Q9F4L3
D	419	ASN	GLY	CONFLICT	UNP Q9F4L3
D	480	TRP	ALA	CONFLICT	UNP Q9F4L3
D	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
D	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
D	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
D	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
D	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
D	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
D	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
D	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
D	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
D	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
D	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
D	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
D	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
D	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
D	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	28	ILE	ALA	CONFLICT	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	394	GLY	ALA	CONFLICT	UNP Q9F4L3
E	419	ASN	GLY	CONFLICT	UNP Q9F4L3
E	480	TRP	ALA	CONFLICT	UNP Q9F4L3
E	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
E	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
E	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
E	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
E	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
E	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
E	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
E	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
E	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
E	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
E	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
E	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
E	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
E	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
E	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	28	ILE	ALA	CONFLICT	UNP Q9F4L3
F	394	GLY	ALA	CONFLICT	UNP Q9F4L3
F	419	ASN	GLY	CONFLICT	UNP Q9F4L3
F	480	TRP	ALA	CONFLICT	UNP Q9F4L3
F	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
F	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
F	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
F	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
F	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
F	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
F	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
F	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
F	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
F	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
F	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
F	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
F	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
F	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
F	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	28	ILE	ALA	CONFLICT	UNP Q9F4L3
G	394	GLY	ALA	CONFLICT	UNP Q9F4L3
G	419	ASN	GLY	CONFLICT	UNP Q9F4L3
G	480	TRP	ALA	CONFLICT	UNP Q9F4L3
G	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
G	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
G	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
G	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
G	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
G	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
G	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
G	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
G	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
G	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
G	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
G	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
G	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
G	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
G	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	28	ILE	ALA	CONFLICT	UNP Q9F4L3
H	394	GLY	ALA	CONFLICT	UNP Q9F4L3
H	419	ASN	GLY	CONFLICT	UNP Q9F4L3
H	480	TRP	ALA	CONFLICT	UNP Q9F4L3
H	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
H	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
H	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
H	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
H	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
H	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
H	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
H	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
H	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3

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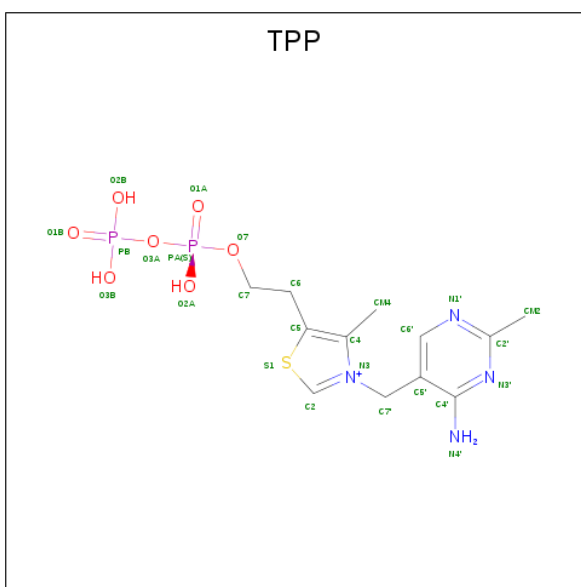
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Chain	Residue	Modelled	Actual	Comment	Reference
H	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
H	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
H	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
H	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
H	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
H	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0
4	D	2	Total O 2 2	0	0
4	E	3	Total O 3 3	0	0
4	F	2	Total O 2 2	0	0

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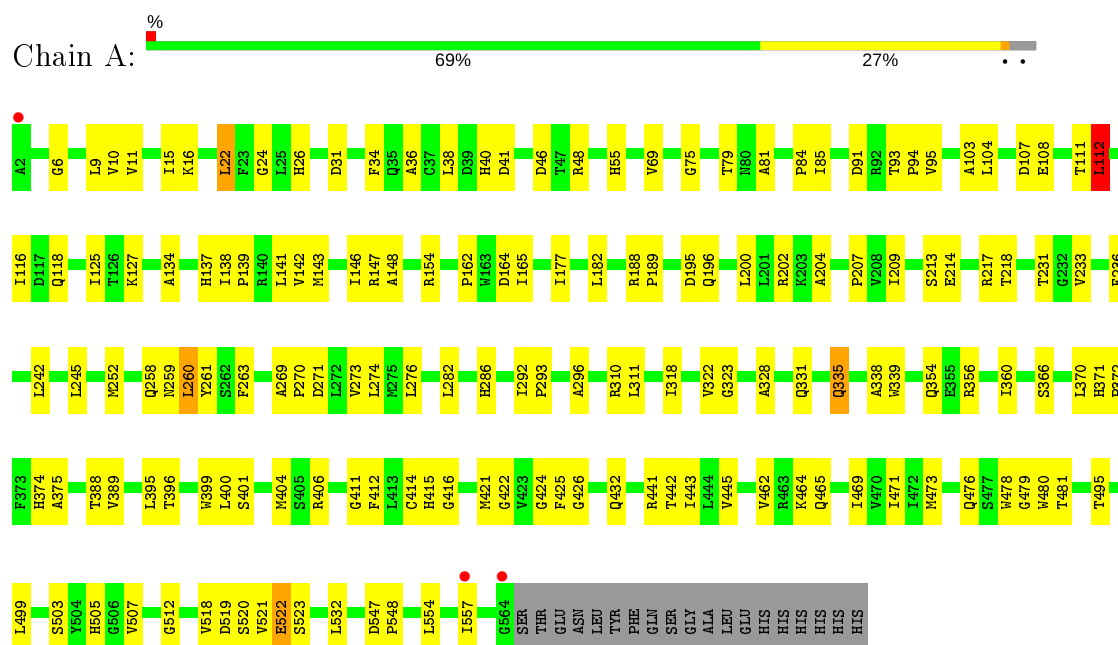
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	3	Total	O	0	0
			3	3		

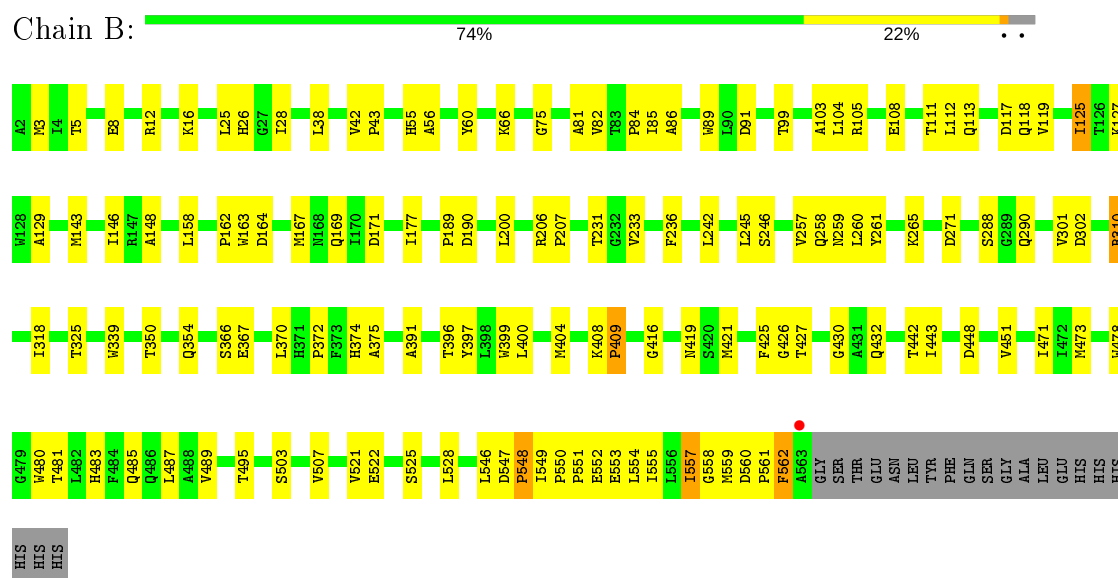
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

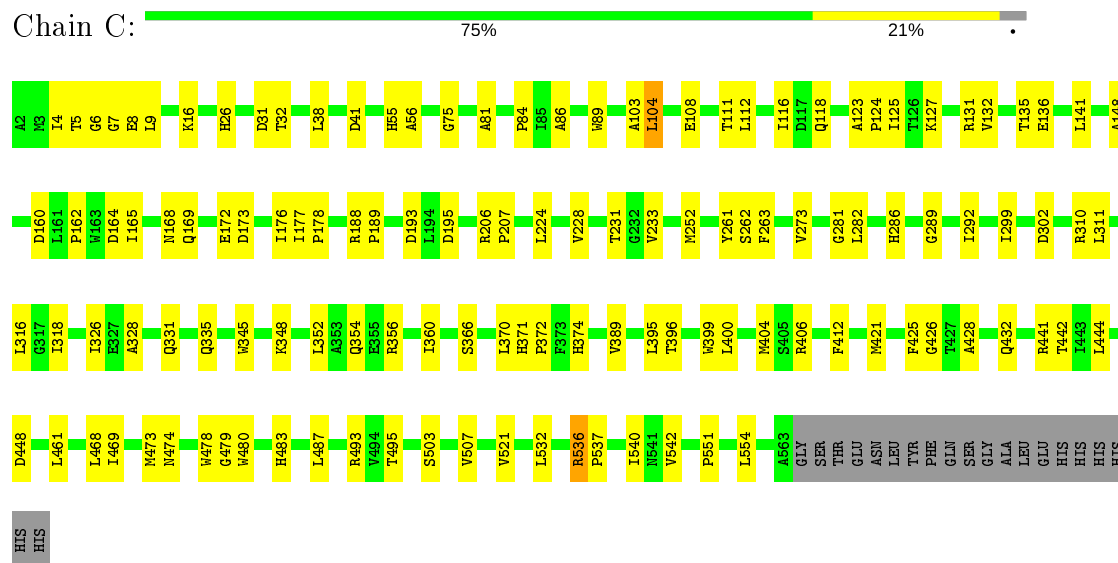
• Molecule 1: Formolase



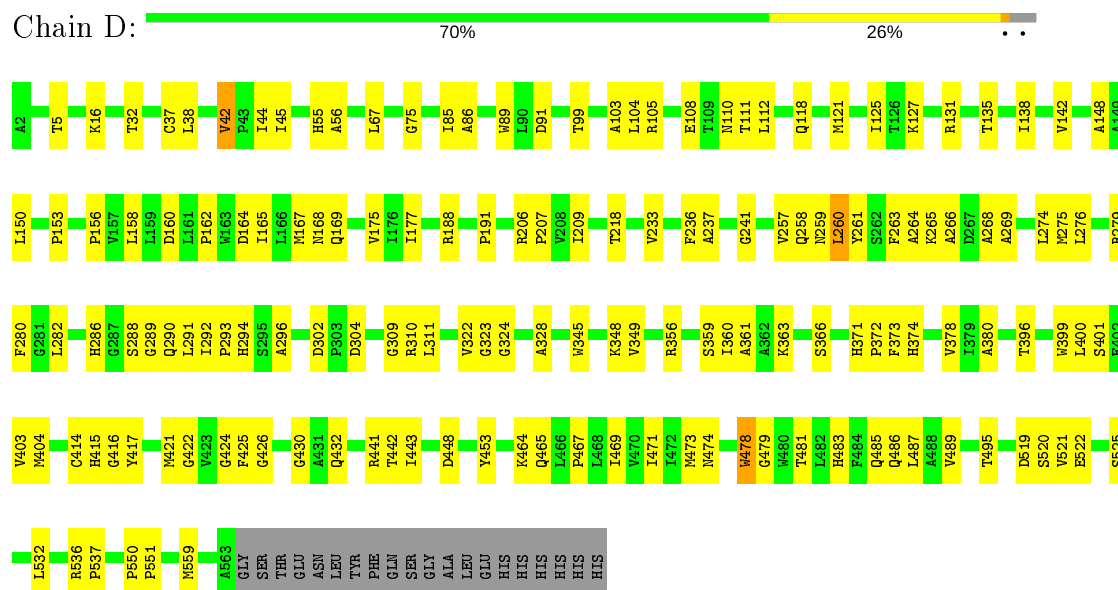
• Molecule 1: Formolase



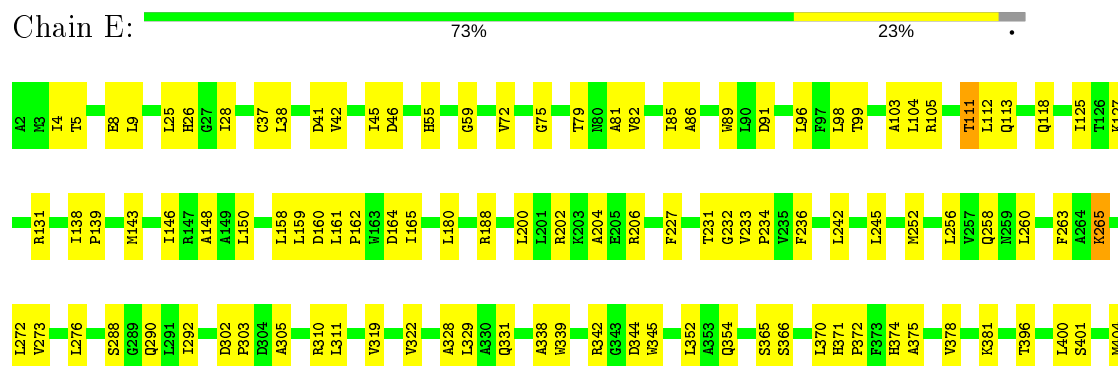
- Molecule 1: Formolase

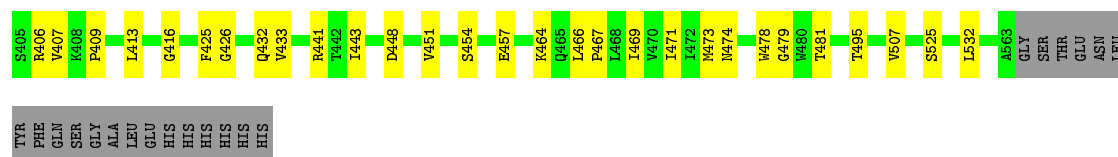


- Molecule 1: Formolase

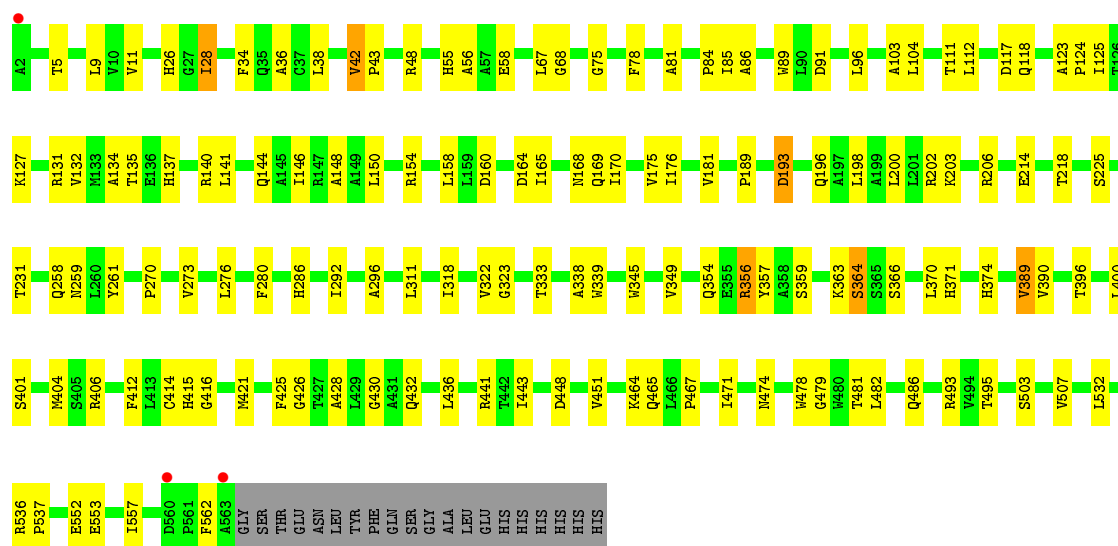
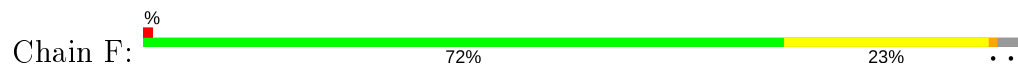


- Molecule 1: Formolase

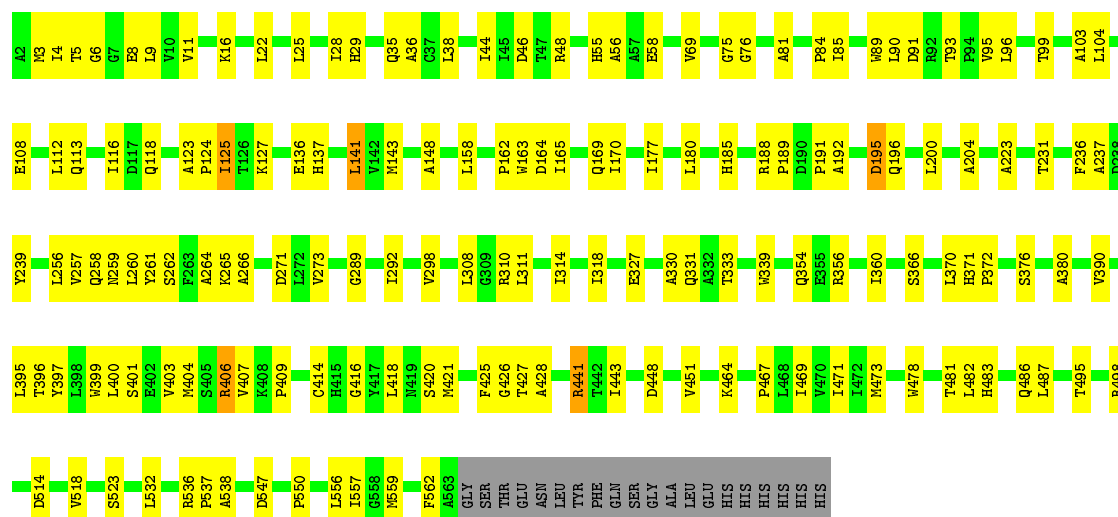




• Molecule 1: Formolase



• Molecule 1: Formolase



• Molecule 1: Formolase



SER	R406	S262	A2
THR	Y407	F263	I125
GLU	R408	A269	G6
ASN		P270	L9
LEU	L413	L274	V10
TYR	C414	E136	E20
PRO	H415	H137	G24
GLN	G416	L276	L25
SER	Y417	Q290	H26
GLY	L418	P283	G27
ALA		A296	I28
LEU	H421	I299	A36
GLU	F425	L308	C37
HIS	G426	G309	L38
HIS		R310	D89
HIS	L429	L311	H40
HIS	G430	I318	P43
HIS	A431	V322	D46
HIS	Q432	E327	T47
	T442	Q331	R48
	V451	A332	H49
		T333	E50
	M473	D336	H55
	W478	W339	A56
	G479	R356	K66
	H480	I360	A74
	T481	S366	G75
	G490	H371	G76
	P491	P372	G77
	N492	F373	P84
	R493	R374	I85
	Y494	A375	W89
	T495	S376	L90
		V390	D91
	R498	L395	S101
	S503	T396	G102
	V507	Y397	A103
	D547	S401	T111
	P548	E402	L112
	P551	V403	Q113
	L554	D560	I116
	I555	F561	D117
	L556	F562	Q118
	I557	A563	A123
		GLY	P124
			I126
			K127
			R131
			E136
			H137
			I138
			V142
			M143
			I146
			R147
			A148
			D160
			I161
			P162
			W163
			D164
			I165
			W168
			Q169
			I170
			I177
			L182
			R188
			P189
			Q196
			L200
			L201
			R202
			P207
			R220
			T231
			G232
			V233
			P234
			V235
			L245
			S246
			L256
			V257
			Q258
			N259
			L260
			A123
			P124

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.88Å 136.56Å 167.06Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	166.33 – 3.00 48.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.4 (166.33-3.00) 89.5 (48.91-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.208 , 0.257 0.212 , 0.259	Depositor DCC
R_{free} test set	4028 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	33455	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3419e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, TPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/4244	0.74	1/5789 (0.0%)
1	B	0.54	1/4240 (0.0%)	0.76	2/5784 (0.0%)
1	C	0.52	0/4240	0.77	0/5784
1	D	0.51	0/4240	0.74	0/5784
1	E	0.52	0/4240	0.76	1/5784 (0.0%)
1	F	0.51	0/4240	0.75	1/5784 (0.0%)
1	G	0.54	0/4240	0.76	1/5784 (0.0%)
1	H	0.53	0/4240	0.79	1/5784 (0.0%)
All	All	0.52	1/33924 (0.0%)	0.76	7/46277 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	PRO	N-CD	-5.57	1.40	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LEU	CA-CB-CG	6.85	131.05	115.30
1	B	117	ASP	CB-CG-OD1	6.44	124.10	118.30
1	E	159	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	H	429	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	F	96	LEU	CA-CB-CG	-5.19	103.36	115.30
1	B	125	ILE	CG1-CB-CG2	-5.16	100.06	111.40
1	G	125	ILE	CG1-CB-CG2	-5.06	100.27	111.40

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	4157	0	4143	141	0
1	B	4153	0	4140	115	0
1	C	4153	0	4140	109	0
1	D	4153	0	4140	138	0
1	E	4153	0	4140	121	0
1	F	4153	0	4140	116	0
1	G	4153	0	4140	131	0
1	H	4153	0	4140	112	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	26	0	16	8	0
3	B	26	0	16	7	0
3	C	26	0	16	9	0
3	D	26	0	16	6	0
3	E	26	0	16	5	0
3	F	26	0	16	9	0
3	G	26	0	16	10	0
3	H	26	0	16	9	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
All	All	33455	0	33251	941	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 14.

All (941) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:PHE:CZ	1:E:451:VAL:HG23	1.78	1.18
1:F:5:THR:HG22	1:F:169:GLN:HG2	1.27	1.13
1:F:196:GLN:O	1:F:200:LEU:HD13	1.50	1.11
1:G:38:LEU:HD13	1:H:495:THR:HG21	1.20	1.10
1:E:425:PHE:HZ	1:E:451:VAL:HG23	1.08	1.07
1:E:38:LEU:HD13	1:F:495:THR:HG21	1.33	1.06
1:A:147:ARG:HG2	1:A:182:LEU:HD23	1.33	1.05
1:F:425:PHE:CZ	1:F:451:VAL:HG23	1.96	0.99
1:B:111:THR:HG22	1:B:112:LEU:H	1.24	0.99
1:H:554:LEU:HD23	1:H:557:ILE:HD11	1.42	0.99
1:C:310:ARG:NH2	1:D:108:GLU:HG3	1.78	0.97
1:D:279:ARG:NH1	1:D:417:TYR:CE2	2.33	0.97
1:C:310:ARG:HH21	1:D:108:GLU:HG3	1.27	0.96
1:G:425:PHE:CZ	1:G:451:VAL:HG23	2.02	0.95
1:G:108:GLU:HG3	1:H:310:ARG:NH2	1.83	0.94
1:B:85:ILE:HG22	1:B:125:ILE:HG22	1.49	0.94
1:E:425:PHE:HE2	1:E:451:VAL:HA	1.32	0.94
1:H:421:MET:HE3	3:H:602:TPP:S1	2.08	0.94
1:A:554:LEU:HD23	1:A:557:ILE:HD11	1.49	0.93
1:C:38:LEU:HD13	1:D:495:THR:HG21	1.49	0.93
1:D:279:ARG:NH1	1:D:417:TYR:HE2	1.66	0.93
1:G:536:ARG:HB2	1:G:537:PRO:HD2	1.51	0.93
1:F:425:PHE:HZ	1:F:451:VAL:HG23	1.32	0.92
1:C:127:LYS:HE2	1:C:148:ALA:O	1.70	0.91
1:F:356:ARG:HD2	1:F:562:PHE:CZ	2.05	0.91
1:H:111:THR:HG22	1:H:112:LEU:H	1.32	0.90
1:H:421:MET:CE	3:H:602:TPP:S1	2.59	0.90
1:C:7:GLY:HA3	1:C:32:THR:HG22	1.54	0.90
1:H:127:LYS:HE2	1:H:148:ALA:O	1.72	0.89
1:C:4:ILE:HD11	1:C:172:GLU:HG2	1.55	0.87
1:F:258:GLN:HE22	1:F:401:SER:HB2	1.39	0.86
1:A:147:ARG:HG2	1:A:182:LEU:CD2	2.05	0.86
1:A:147:ARG:CG	1:A:182:LEU:HD23	2.05	0.85
1:G:557:ILE:HG23	1:G:559:MET:HG2	1.58	0.85
1:H:421:MET:HE2	3:H:602:TPP:C2	2.07	0.84
1:A:38:LEU:HD13	1:B:495:THR:HG21	1.60	0.83
1:B:425:PHE:CZ	1:B:451:VAL:HG23	2.14	0.83
1:A:258:GLN:HE22	1:A:401:SER:HB2	1.43	0.83
1:B:91:ASP:OD1	1:B:416:GLY:HA3	1.77	0.83
1:D:536:ARG:HB2	1:D:537:PRO:HD2	1.59	0.82
1:E:425:PHE:HZ	1:E:451:VAL:CG2	1.90	0.82
1:E:4:ILE:HD11	1:E:8:GLU:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ILE:HG22	1:F:125:ILE:HG22	1.59	0.82
1:A:38:LEU:HD13	1:B:495:THR:CG2	2.10	0.81
1:D:85:ILE:HG22	1:D:125:ILE:HG22	1.63	0.81
1:F:5:THR:HG22	1:F:169:GLN:CG	2.09	0.80
1:C:366:SER:HB2	1:C:374:HIS:HD2	1.46	0.80
1:D:5:THR:HG22	1:D:169:GLN:CG	2.11	0.80
1:A:462:VAL:HG21	1:A:512:GLY:O	1.80	0.80
1:D:67:LEU:HB2	1:D:150:LEU:HD21	1.63	0.80
1:D:37:CYS:CB	1:D:42:VAL:HG23	2.12	0.79
1:H:366:SER:HB2	1:H:374:HIS:CD2	2.16	0.79
1:H:111:THR:HG22	1:H:112:LEU:N	1.96	0.79
1:G:481:THR:HG22	1:H:28:ILE:HG23	1.64	0.79
1:F:132:VAL:HG22	1:F:141:LEU:HD23	1.65	0.79
1:E:127:LYS:HE2	1:E:148:ALA:O	1.83	0.78
1:A:495:THR:HG21	1:B:38:LEU:HD13	1.64	0.78
1:G:441:ARG:HE	1:G:467:PRO:HB2	1.48	0.78
1:F:425:PHE:HZ	1:F:451:VAL:CG2	1.96	0.78
1:H:196:GLN:O	1:H:200:LEU:HD13	1.82	0.78
1:F:91:ASP:OD1	1:F:416:GLY:HA3	1.84	0.78
1:C:441:ARG:HH12	1:C:469:ILE:HD11	1.49	0.77
1:G:38:LEU:HD13	1:H:495:THR:CG2	2.11	0.77
1:G:425:PHE:HZ	1:G:451:VAL:HG23	1.49	0.77
1:G:425:PHE:HZ	1:G:451:VAL:CG2	1.98	0.77
1:A:366:SER:OG	1:A:370:LEU:HA	1.85	0.77
1:E:112:LEU:HD23	1:E:113:GLN:HG3	1.66	0.76
1:D:279:ARG:CZ	1:D:417:TYR:HE2	1.97	0.76
1:C:111:THR:HG22	1:C:112:LEU:H	1.51	0.76
1:E:111:THR:HG22	1:E:112:LEU:H	1.48	0.76
1:B:111:THR:CG2	1:B:112:LEU:H	1.99	0.76
1:D:111:THR:HG22	1:D:112:LEU:H	1.50	0.76
1:E:4:ILE:HG13	1:E:8:GLU:HB2	1.66	0.76
1:E:103:ALA:HB1	1:E:164:ASP:HB2	1.68	0.75
1:C:366:SER:HB2	1:C:374:HIS:CD2	2.20	0.75
1:G:557:ILE:CG2	1:G:559:MET:HG2	2.16	0.75
1:D:37:CYS:HA	1:D:42:VAL:CG2	2.17	0.75
1:E:4:ILE:CD1	1:E:8:GLU:HG3	2.17	0.75
1:B:557:ILE:HD13	1:B:558:GLY:N	2.00	0.74
1:E:4:ILE:CG1	1:E:8:GLU:HG3	2.17	0.74
1:G:127:LYS:HE2	1:G:148:ALA:O	1.86	0.74
1:D:5:THR:HG22	1:D:169:GLN:HG2	1.68	0.74
1:G:85:ILE:HG22	1:G:125:ILE:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLY:HA3	1:C:32:THR:CG2	2.16	0.74
1:F:425:PHE:HE2	1:F:451:VAL:HA	1.53	0.73
1:F:441:ARG:HH12	1:F:532:LEU:HA	1.52	0.73
1:D:37:CYS:CA	1:D:42:VAL:HG23	2.19	0.72
1:B:111:THR:HG22	1:B:112:LEU:N	2.02	0.72
1:H:189:PRO:HB3	1:H:318:ILE:HG21	1.71	0.72
1:B:85:ILE:HG22	1:B:125:ILE:CG2	2.19	0.72
1:A:85:ILE:HG22	1:A:125:ILE:HG22	1.72	0.72
1:G:91:ASP:OD1	1:G:416:GLY:HA3	1.89	0.72
1:F:441:ARG:HE	1:F:467:PRO:HB2	1.54	0.72
1:F:196:GLN:O	1:F:200:LEU:CD1	2.34	0.72
1:B:557:ILE:CD1	1:B:559:MET:H	2.02	0.71
1:A:11:VAL:HG21	1:A:36:ALA:HB3	1.72	0.71
1:G:162:PRO:HG2	1:G:165:ILE:HD12	1.72	0.71
1:H:111:THR:CG2	1:H:112:LEU:H	2.04	0.71
1:H:396:THR:HG23	3:H:602:TPP:O1B	1.90	0.71
1:C:354:GLN:HE21	1:C:406:ARG:NH2	1.88	0.71
1:A:396:THR:HG23	3:A:602:TPP:O1B	1.90	0.71
1:G:425:PHE:CZ	1:G:451:VAL:CG2	2.72	0.70
1:A:310:ARG:NH1	1:B:108:GLU:HG3	2.06	0.70
1:A:462:VAL:CG2	1:A:512:GLY:O	2.39	0.70
1:A:91:ASP:OD1	1:A:416:GLY:HA3	1.91	0.70
1:A:310:ARG:HG3	1:A:311:LEU:HG	1.72	0.70
1:B:396:THR:HG23	3:B:602:TPP:O1B	1.92	0.70
1:D:188:ARG:HD3	1:D:328:ALA:HB2	1.73	0.70
1:G:536:ARG:HB2	1:G:537:PRO:CD	2.20	0.70
1:B:366:SER:HB2	1:B:374:HIS:CD2	2.27	0.70
1:E:495:THR:HG21	1:F:38:LEU:HD13	1.74	0.70
1:B:561:PRO:O	1:B:562:PHE:CD1	2.45	0.70
1:D:396:THR:HG21	1:D:473:MET:HB2	1.73	0.69
1:E:55:HIS:HB2	1:E:426:GLY:HA3	1.74	0.69
1:G:35:GLN:HB3	1:H:493:ARG:HH21	1.54	0.69
1:D:105:ARG:HG2	1:D:164:ASP:OD1	1.91	0.69
1:G:310:ARG:HG3	1:G:311:LEU:HG	1.73	0.69
1:H:103:ALA:HB1	1:H:164:ASP:HB2	1.74	0.69
1:A:127:LYS:CE	1:A:148:ALA:O	2.40	0.69
1:H:207:PRO:HG2	1:H:233:VAL:HG12	1.75	0.69
1:H:85:ILE:HG22	1:H:125:ILE:HG22	1.75	0.69
1:A:441:ARG:HH12	1:A:532:LEU:HA	1.57	0.69
1:B:557:ILE:HD13	1:B:559:MET:H	1.57	0.69
1:B:425:PHE:HZ	1:B:451:VAL:HG23	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PRO:HG2	1:B:233:VAL:HG12	1.75	0.68
1:E:425:PHE:CE2	1:E:451:VAL:HA	2.22	0.68
1:D:448:ASP:HB3	1:D:474:ASN:HA	1.76	0.68
1:A:354:GLN:HG2	1:A:406:ARG:HH21	1.58	0.68
1:E:396:THR:HG23	3:E:602:TPP:O1B	1.94	0.68
1:G:108:GLU:HG3	1:H:310:ARG:HH22	1.59	0.68
1:H:55:HIS:HB2	1:H:426:GLY:HA3	1.74	0.68
1:G:236:PHE:CZ	1:G:260:LEU:HD21	2.27	0.68
1:C:4:ILE:CD1	1:C:172:GLU:HG2	2.23	0.67
1:G:366:SER:HB2	1:G:370:LEU:HA	1.76	0.67
1:C:396:THR:HG23	3:C:602:TPP:O1B	1.94	0.67
1:A:354:GLN:HG2	1:A:406:ARG:NH2	2.09	0.67
1:D:127:LYS:HE2	1:D:148:ALA:O	1.94	0.67
1:E:265:LYS:O	1:E:265:LYS:HG3	1.92	0.67
1:C:86:ALA:HA	1:C:125:ILE:CG2	2.23	0.67
1:F:258:GLN:NE2	1:F:401:SER:HB2	2.09	0.67
1:A:111:THR:HG22	1:A:112:LEU:H	1.59	0.67
1:D:91:ASP:OD1	1:D:416:GLY:HA3	1.95	0.67
1:G:441:ARG:HH12	1:G:532:LEU:HA	1.59	0.67
1:D:396:THR:HG23	3:D:602:TPP:O1B	1.95	0.67
1:A:127:LYS:HE2	1:A:148:ALA:O	1.93	0.66
1:D:280:PHE:HE2	1:D:309:GLY:HA2	1.60	0.66
1:D:282:LEU:HD12	1:D:286:HIS:HE1	1.61	0.66
1:C:5:THR:HG22	1:C:169:GLN:HG2	1.78	0.66
1:H:89:TRP:HB2	1:H:125:ILE:O	1.96	0.66
1:G:400:LEU:O	1:G:404:MET:HG2	1.94	0.66
1:H:498:ARG:HG2	1:H:498:ARG:HH11	1.60	0.66
1:B:55:HIS:HB2	1:B:426:GLY:HA3	1.76	0.65
1:B:547:ASP:N	1:B:548:PRO:CD	2.59	0.65
1:E:86:ALA:HA	1:E:125:ILE:HG23	1.78	0.65
1:E:354:GLN:HE21	1:E:406:ARG:NH2	1.94	0.65
1:F:127:LYS:HE2	1:F:148:ALA:O	1.96	0.65
1:A:366:SER:HB2	1:A:374:HIS:CD2	2.31	0.65
3:E:602:TPP:HN42	3:E:602:TPP:C2	2.09	0.65
1:B:557:ILE:HD11	1:B:559:MET:HB2	1.79	0.65
1:D:258:GLN:HE22	1:D:401:SER:HB2	1.62	0.65
1:G:75:GLY:HA2	1:G:116:ILE:HD11	1.77	0.65
1:B:288:SER:OG	1:B:290:GLN:HG3	1.96	0.64
1:E:103:ALA:CB	1:E:164:ASP:HB2	2.26	0.64
1:G:55:HIS:HB2	1:G:426:GLY:HA3	1.79	0.64
1:G:5:THR:HG22	1:G:169:GLN:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASP:OD1	1:A:520:SER:N	2.30	0.64
1:A:441:ARG:HH12	1:A:469:ILE:HD11	1.63	0.64
1:C:6:GLY:HA2	1:C:9:LEU:HD12	1.78	0.64
1:H:395:LEU:N	3:H:602:TPP:O2B	2.26	0.64
1:H:554:LEU:HA	1:H:557:ILE:HD11	1.80	0.64
1:D:282:LEU:HD12	1:D:286:HIS:CE1	2.32	0.64
1:D:75:GLY:H	1:D:118:GLN:HE22	1.46	0.64
1:B:56:ALA:O	1:B:430:GLY:HA3	1.98	0.64
1:H:421:MET:HE2	3:H:602:TPP:S1	2.36	0.64
1:C:396:THR:HG21	1:C:473:MET:HB2	1.78	0.63
1:E:112:LEU:CD2	1:E:113:GLN:HG3	2.28	0.63
1:D:16:LYS:HE3	1:D:177:ILE:HD12	1.79	0.63
1:A:370:LEU:HD21	1:A:375:ALA:HB2	1.80	0.63
1:A:310:ARG:HH12	1:B:108:GLU:HG3	1.62	0.63
1:F:86:ALA:HA	1:F:125:ILE:HG23	1.79	0.63
1:A:481:THR:HG22	1:B:28:ILE:HG23	1.81	0.63
1:F:55:HIS:HB2	1:F:426:GLY:HA3	1.81	0.63
1:E:26:HIS:CE1	1:F:481:THR:HB	2.34	0.63
1:F:553:GLU:O	1:F:557:ILE:HG12	1.98	0.63
1:H:366:SER:HB2	1:H:374:HIS:HD2	1.62	0.63
1:C:441:ARG:HH11	1:C:532:LEU:HD23	1.63	0.63
1:A:11:VAL:O	1:A:15:ILE:HG13	1.99	0.63
1:A:137:HIS:HB3	1:A:141:LEU:HD13	1.81	0.63
1:G:38:LEU:CD1	1:H:495:THR:HG21	2.13	0.63
1:C:164:ASP:O	1:C:168:ASN:HB2	1.99	0.62
1:E:425:PHE:CE2	1:E:451:VAL:HG23	2.32	0.62
1:B:301:VAL:HG22	1:B:318:ILE:HB	1.81	0.62
1:B:551:PRO:O	1:B:555:ILE:HG13	1.99	0.62
1:H:112:LEU:HD21	1:H:113:GLN:NE2	2.15	0.62
1:H:91:ASP:OD1	1:H:416:GLY:HA3	2.00	0.62
1:H:333:THR:HG23	1:H:339:TRP:HE1	1.63	0.62
1:A:273:VAL:HG21	1:A:292:ILE:HG23	1.80	0.62
1:A:441:ARG:NH1	1:A:469:ILE:HD11	2.14	0.62
1:C:441:ARG:NH1	1:C:469:ILE:HD11	2.13	0.62
1:D:441:ARG:HH12	1:D:532:LEU:HA	1.65	0.62
1:A:432:GLN:NE2	1:A:442:THR:H	1.98	0.62
1:B:546:LEU:C	1:B:548:PRO:HD2	2.19	0.62
1:H:276:LEU:HB3	1:H:322:VAL:HG13	1.81	0.62
1:A:188:ARG:HD3	1:A:328:ALA:HB2	1.82	0.62
3:E:602:TPP:H2	3:E:602:TPP:HN42	1.65	0.62
1:F:104:LEU:HD12	1:F:165:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:PHE:CZ	1:B:260:LEU:HD21	2.35	0.61
1:E:433:VAL:HG22	1:E:466:LEU:HD21	1.83	0.61
1:B:547:ASP:N	1:B:548:PRO:HD2	2.15	0.61
1:E:4:ILE:HG12	1:E:8:GLU:HG3	1.82	0.61
1:E:425:PHE:CZ	1:E:451:VAL:CG2	2.68	0.61
1:E:507:VAL:HG13	1:F:507:VAL:HG13	1.81	0.61
1:E:479:GLY:N	3:E:602:TPP:O3B	2.26	0.61
1:D:366:SER:HB2	1:D:374:HIS:HD2	1.65	0.61
1:F:85:ILE:HG22	1:F:125:ILE:CG2	2.29	0.61
1:A:441:ARG:NH1	1:A:532:LEU:HA	2.16	0.61
1:E:125:ILE:O	1:E:125:ILE:HG22	2.00	0.61
1:G:16:LYS:HE3	1:G:177:ILE:HD12	1.83	0.60
1:H:479:GLY:N	3:H:602:TPP:O3B	2.33	0.60
1:A:138:ILE:HD11	1:A:165:ILE:HG22	1.84	0.60
1:B:127:LYS:CE	1:B:148:ALA:O	2.50	0.60
1:B:396:THR:CG2	1:B:473:MET:HB2	2.31	0.60
1:C:108:GLU:HG3	1:D:310:ARG:NH2	2.17	0.60
1:C:4:ILE:HG22	1:C:5:THR:N	2.16	0.60
1:C:370:LEU:CD1	1:C:521:VAL:HG22	2.32	0.60
1:D:292:ILE:O	1:D:292:ILE:HG13	2.00	0.60
1:G:103:ALA:HB1	1:G:164:ASP:HB2	1.84	0.60
1:A:134:ALA:HB3	1:A:137:HIS:CD2	2.37	0.60
1:C:38:LEU:HD13	1:D:495:THR:CG2	2.26	0.60
1:F:103:ALA:HA	1:F:164:ASP:HB2	1.83	0.60
1:D:37:CYS:HB3	1:D:42:VAL:HG23	1.82	0.60
1:D:85:ILE:HG22	1:D:125:ILE:CG2	2.32	0.59
1:D:356:ARG:O	1:D:360:ILE:HG12	2.02	0.59
1:B:425:PHE:HZ	1:B:451:VAL:CG2	2.16	0.59
1:G:421:MET:CE	3:G:602:TPP:S1	2.90	0.59
1:A:432:GLN:HE22	1:A:442:THR:H	1.48	0.59
1:H:425:PHE:CZ	1:H:451:VAL:HG23	2.37	0.59
1:E:188:ARG:HD3	1:E:328:ALA:HB2	1.85	0.59
1:F:356:ARG:HD2	1:F:562:PHE:HZ	1.58	0.59
1:G:354:GLN:HE21	1:G:406:ARG:HH22	1.50	0.59
1:H:147:ARG:HG2	1:H:182:LEU:HD23	1.84	0.59
1:H:127:LYS:CE	1:H:148:ALA:O	2.48	0.59
1:A:258:GLN:NE2	1:A:401:SER:HB2	2.14	0.59
1:E:258:GLN:HE22	1:E:401:SER:HB2	1.66	0.59
1:A:469:ILE:HD13	1:A:532:LEU:HD12	1.84	0.59
1:A:478:TRP:HB3	3:A:602:TPP:H61	1.84	0.59
1:C:103:ALA:HB1	1:C:164:ASP:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:GLY:H	1:G:118:GLN:HE22	1.50	0.59
1:E:111:THR:HG23	1:F:286:HIS:NE2	2.16	0.59
1:C:75:GLY:H	1:C:118:GLN:HE22	1.50	0.59
1:F:127:LYS:CE	1:F:148:ALA:O	2.51	0.59
1:G:108:GLU:HG3	1:H:310:ARG:HH21	1.66	0.59
1:G:28:ILE:HG23	1:H:481:THR:HG22	1.83	0.59
1:G:354:GLN:HE21	1:G:406:ARG:NH2	2.01	0.59
1:G:370:LEU:HD12	1:G:371:HIS:N	2.18	0.59
1:G:395:LEU:N	3:G:602:TPP:O2B	2.28	0.59
1:F:359:SER:O	1:F:363:LYS:HE3	2.03	0.58
3:G:602:TPP:H2	3:G:602:TPP:HN42	1.68	0.58
1:D:345:TRP:O	1:D:349:VAL:HG23	2.04	0.58
1:D:443:ILE:HG23	1:D:471:ILE:CD1	2.34	0.58
1:D:441:ARG:HE	1:D:467:PRO:HB2	1.67	0.58
1:D:55:HIS:HB2	1:D:426:GLY:HA3	1.84	0.58
1:D:441:ARG:HH12	1:D:469:ILE:HD11	1.68	0.58
1:G:90:LEU:HD12	1:G:418:LEU:HB2	1.85	0.58
1:G:421:MET:HE3	3:G:602:TPP:S1	2.43	0.58
1:A:142:VAL:O	1:A:146:ILE:HG12	2.03	0.58
1:E:441:ARG:HH12	1:E:532:LEU:HA	1.69	0.58
1:H:551:PRO:O	1:H:555:ILE:HG13	2.03	0.58
1:B:56:ALA:HA	1:B:426:GLY:O	2.04	0.58
1:D:359:SER:O	1:D:363:LYS:HG2	2.04	0.58
1:E:441:ARG:HE	1:E:467:PRO:HB2	1.67	0.57
1:E:4:ILE:HG13	1:E:8:GLU:CB	2.33	0.57
1:G:425:PHE:CE1	1:G:451:VAL:HG23	2.39	0.57
1:E:38:LEU:HD13	1:F:495:THR:CG2	2.21	0.57
1:F:432:GLN:O	1:F:436:LEU:HG	2.04	0.57
1:B:189:PRO:HG2	1:B:325:THR:HG23	1.85	0.57
1:B:425:PHE:HE1	1:B:451:VAL:HA	1.69	0.57
1:H:103:ALA:CB	1:H:164:ASP:HB2	2.34	0.57
1:C:495:THR:HG21	1:D:38:LEU:HD13	1.87	0.57
1:G:127:LYS:CE	1:G:148:ALA:O	2.53	0.57
1:G:46:ASP:OD1	1:G:464:LYS:HE3	2.05	0.57
1:C:123:ALA:N	1:C:124:PRO:HD2	2.20	0.57
1:F:189:PRO:HB3	1:F:318:ILE:HG21	1.87	0.57
1:E:9:LEU:HD22	1:E:139:PRO:HG3	1.85	0.57
1:H:498:ARG:HG2	1:H:498:ARG:NH1	2.16	0.57
1:A:207:PRO:HG2	1:A:233:VAL:HG12	1.86	0.57
1:D:479:GLY:N	3:D:602:TPP:O3B	2.35	0.57
1:E:4:ILE:CG1	1:E:8:GLU:CB	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:SER:HB2	1:F:371:HIS:H	1.70	0.57
1:G:396:THR:HG23	3:G:602:TPP:O1B	2.05	0.57
1:A:147:ARG:CG	1:A:182:LEU:CD2	2.76	0.57
1:E:75:GLY:H	1:E:118:GLN:HE22	1.51	0.57
1:E:99:THR:CG2	1:E:158:LEU:HD11	2.35	0.57
1:F:231:THR:HG22	1:F:339:TRP:CE2	2.39	0.57
1:A:366:SER:HB2	1:A:374:HIS:HD2	1.68	0.57
1:D:125:ILE:HG22	1:D:125:ILE:O	2.04	0.57
1:D:264:ALA:C	1:D:266:ALA:H	2.08	0.57
1:D:280:PHE:O	1:D:311:LEU:HD12	2.05	0.57
1:B:366:SER:OG	1:B:370:LEU:HA	2.05	0.56
1:C:356:ARG:O	1:C:360:ILE:HG12	2.05	0.56
1:F:75:GLY:H	1:F:118:GLN:HE22	1.53	0.56
1:C:299:ILE:HG23	1:C:316:LEU:HB3	1.87	0.56
1:A:503:SER:HB2	1:A:505:HIS:CE1	2.41	0.56
1:A:421:MET:HE3	3:A:602:TPP:S1	2.46	0.56
1:B:127:LYS:HE2	1:B:148:ALA:O	2.05	0.56
1:A:137:HIS:O	1:A:141:LEU:HB2	2.06	0.56
1:A:55:HIS:HB2	1:A:426:GLY:HA3	1.88	0.56
1:B:557:ILE:HD13	1:B:558:GLY:H	1.71	0.56
1:H:560:ASP:OD1	1:H:562:PHE:N	2.34	0.56
1:B:242:LEU:HD12	1:B:245:LEU:HD12	1.88	0.56
1:C:441:ARG:NH1	1:C:532:LEU:HD23	2.20	0.56
1:A:127:LYS:HE3	1:A:148:ALA:O	2.06	0.56
1:B:103:ALA:HB1	1:B:164:ASP:HB2	1.88	0.56
1:C:111:THR:HG22	1:C:112:LEU:N	2.21	0.56
1:H:142:VAL:O	1:H:146:ILE:HG12	2.06	0.56
1:H:143:MET:HE3	1:H:146:ILE:HG13	1.86	0.56
1:A:22:LEU:N	1:A:22:LEU:HD12	2.21	0.55
1:D:236:PHE:CZ	1:D:260:LEU:HD21	2.41	0.55
1:E:112:LEU:HD23	1:E:113:GLN:CG	2.34	0.55
1:A:202:ARG:NH1	1:A:338:ALA:O	2.38	0.55
1:E:260:LEU:HA	1:E:263:PHE:CD1	2.41	0.55
1:D:464:LYS:O	1:D:465:GLN:HB2	2.06	0.55
1:F:333:THR:HG23	1:F:339:TRP:HE1	1.70	0.55
1:C:441:ARG:HH12	1:C:532:LEU:HA	1.71	0.55
1:H:9:LEU:HD11	1:H:170:ILE:HD11	1.88	0.55
1:B:103:ALA:CB	1:B:164:ASP:HB2	2.35	0.55
1:E:370:LEU:HD21	1:E:375:ALA:HB2	1.88	0.55
1:B:366:SER:HB2	1:B:374:HIS:HD2	1.72	0.55
1:B:554:LEU:O	1:B:557:ILE:CD1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:VAL:HG13	1:D:522:GLU:N	2.22	0.55
1:E:91:ASP:OD1	1:E:416:GLY:HA3	2.06	0.55
1:G:28:ILE:CG2	1:H:481:THR:HG22	2.37	0.55
1:H:333:THR:HG23	1:H:339:TRP:NE1	2.21	0.55
1:B:503:SER:O	1:B:507:VAL:HG23	2.07	0.55
1:C:207:PRO:HG2	1:C:233:VAL:HG12	1.88	0.55
1:D:399:TRP:CE2	1:D:550:PRO:HG3	2.42	0.55
1:F:425:PHE:CE2	1:F:451:VAL:HA	2.38	0.55
1:F:536:ARG:HB2	1:F:537:PRO:HD2	1.88	0.55
1:G:425:PHE:HE1	1:G:451:VAL:HA	1.72	0.55
1:B:104:LEU:CD1	1:B:162:PRO:HG2	2.37	0.54
1:C:189:PRO:HB3	1:C:318:ILE:HG21	1.89	0.54
1:C:396:THR:CG2	1:C:473:MET:HB2	2.37	0.54
1:D:5:THR:HG22	1:D:169:GLN:HG3	1.89	0.54
1:G:4:ILE:HD11	1:G:9:LEU:CD2	2.37	0.54
1:D:218:THR:OG1	1:D:323:GLY:HA3	2.07	0.54
1:E:104:LEU:HD13	1:E:162:PRO:HG2	1.87	0.54
1:F:9:LEU:HD21	1:F:175:VAL:HG11	1.89	0.54
1:G:407:VAL:O	1:G:409:PRO:HD3	2.07	0.54
1:G:5:THR:O	1:G:8:GLU:N	2.40	0.54
1:A:147:ARG:CD	1:A:182:LEU:HD23	2.37	0.54
1:C:310:ARG:HG3	1:C:311:LEU:HG	1.89	0.54
1:E:310:ARG:HG3	1:E:311:LEU:HG	1.89	0.54
1:F:503:SER:O	1:F:507:VAL:HG23	2.07	0.54
1:C:483:HIS:O	1:C:487:LEU:HB2	2.07	0.54
1:F:425:PHE:CZ	1:F:451:VAL:CG2	2.75	0.54
1:G:76:GLY:HA3	3:H:602:TPP:HM23	1.90	0.54
1:F:154:ARG:NH1	1:F:214:GLU:OE1	2.41	0.54
1:D:310:ARG:HG3	1:D:311:LEU:HG	1.88	0.54
1:D:258:GLN:NE2	1:D:401:SER:HB2	2.22	0.54
1:D:441:ARG:NH1	1:D:469:ILE:HD11	2.23	0.54
1:A:143:MET:HE3	1:A:146:ILE:HG13	1.89	0.53
1:C:366:SER:OG	1:C:370:LEU:HA	2.09	0.53
1:E:204:ALA:HB2	1:E:272:LEU:HD13	1.90	0.53
1:F:137:HIS:HB3	1:F:141:LEU:HD22	1.89	0.53
1:F:482:LEU:O	1:F:486:GLN:HG2	2.09	0.53
1:H:55:HIS:CE1	1:H:84:PRO:HG3	2.43	0.53
1:D:289:GLY:HA2	1:D:292:ILE:O	2.08	0.53
1:B:3:MET:HG2	1:B:171:ASP:HA	1.91	0.53
1:B:400:LEU:O	1:B:404:MET:HG2	2.08	0.53
1:E:112:LEU:HD21	1:E:113:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLY:H	1:C:118:GLN:NE2	2.07	0.53
1:F:400:LEU:O	1:F:404:MET:HG2	2.09	0.53
1:F:478:TRP:HE3	3:F:602:TPP:H61	1.74	0.53
1:B:548:PRO:O	1:B:549:ILE:HG13	2.08	0.53
1:A:79:THR:HB	1:B:82:VAL:HG12	1.91	0.53
1:B:86:ALA:HA	1:B:125:ILE:HG23	1.91	0.53
1:C:55:HIS:HB2	1:C:426:GLY:HA3	1.91	0.53
1:F:366:SER:HB2	1:F:370:LEU:HA	1.90	0.53
1:B:112:LEU:HD21	1:B:113:GLN:NE2	2.24	0.53
1:E:354:GLN:HE21	1:E:406:ARG:HH22	1.57	0.53
1:H:56:ALA:HA	1:H:426:GLY:O	2.09	0.53
1:E:4:ILE:CG1	1:E:8:GLU:CG	2.87	0.53
1:G:421:MET:HE2	3:G:602:TPP:C2	2.39	0.52
1:A:6:GLY:HA2	1:A:9:LEU:HD12	1.90	0.52
1:D:400:LEU:O	1:D:404:MET:HG2	2.10	0.52
1:B:89:TRP:HB2	1:B:125:ILE:O	2.09	0.52
1:D:138:ILE:O	1:D:142:VAL:HG23	2.08	0.52
1:A:356:ARG:O	1:A:360:ILE:HG12	2.08	0.52
1:A:36:ALA:O	1:A:40:HIS:HD2	1.92	0.52
1:B:419:ASN:HD21	1:B:480:TRP:HZ3	1.57	0.52
1:F:158:LEU:C	1:F:158:LEU:HD23	2.30	0.52
1:F:280:PHE:HB3	1:F:311:LEU:HD12	1.92	0.52
1:G:264:ALA:C	1:G:266:ALA:H	2.13	0.52
1:A:400:LEU:O	1:A:404:MET:HG2	2.10	0.52
1:C:389:VAL:HG13	1:C:412:PHE:HD1	1.74	0.52
1:F:396:THR:HG23	3:F:602:TPP:O1B	2.09	0.52
1:F:111:THR:HG22	1:F:112:LEU:H	1.73	0.52
1:F:9:LEU:HD11	1:F:170:ILE:HD11	1.92	0.52
1:A:138:ILE:HB	1:A:139:PRO:HD3	1.90	0.52
1:A:518:VAL:HB	1:A:523:SER:HB3	1.91	0.52
1:F:276:LEU:HB3	1:F:322:VAL:HG13	1.92	0.52
1:A:154:ARG:NH1	1:A:214:GLU:OE1	2.43	0.52
1:H:116:ILE:HD12	1:H:118:GLN:HG2	1.92	0.52
1:A:231:THR:OG1	1:A:233:VAL:HG22	2.09	0.52
1:A:189:PRO:HB3	1:A:318:ILE:HG21	1.92	0.52
1:A:93:THR:HG22	1:A:95:VAL:HG23	1.91	0.52
1:D:378:VAL:HG13	1:D:525:SER:HB3	1.93	0.52
1:E:98:LEU:HD22	1:E:161:LEU:HD11	1.92	0.51
1:G:258:GLN:HE22	1:G:401:SER:HB2	1.73	0.51
1:C:231:THR:OG1	1:C:233:VAL:HG22	2.10	0.51
1:C:81:ALA:O	1:C:84:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:TRP:HE3	3:D:602:TPP:H61	1.74	0.51
1:F:111:THR:HG22	1:F:112:LEU:N	2.26	0.51
1:F:345:TRP:O	1:F:349:VAL:HG23	2.10	0.51
1:H:562:PHE:O	1:H:563:ALA:HB2	2.11	0.51
1:C:26:HIS:NE2	1:C:31:ASP:OD1	2.42	0.51
1:D:32:THR:HG21	1:D:167:MET:HA	1.92	0.51
1:G:11:VAL:HG21	1:G:36:ALA:HB3	1.92	0.51
1:G:231:THR:HG22	1:G:339:TRP:CE2	2.45	0.51
1:A:16:LYS:HE3	1:A:177:ILE:HG22	1.93	0.51
1:C:540:ILE:HG22	1:C:542:VAL:HG22	1.92	0.51
1:G:75:GLY:H	1:G:118:GLN:NE2	2.09	0.51
1:E:4:ILE:HG12	1:E:8:GLU:CG	2.39	0.51
3:G:602:TPP:HM43	1:H:26:HIS:O	2.10	0.51
1:H:425:PHE:CZ	1:H:451:VAL:CG2	2.93	0.51
1:D:125:ILE:CG2	1:D:125:ILE:O	2.59	0.51
1:H:75:GLY:H	1:H:118:GLN:HE22	1.58	0.51
1:A:400:LEU:HD21	1:A:445:VAL:HG21	1.92	0.51
1:D:237:ALA:HB1	1:D:241:GLY:HA3	1.92	0.51
1:E:236:PHE:CZ	1:E:260:LEU:HD21	2.46	0.51
1:F:364:SER:HB3	1:F:371:HIS:CE1	2.45	0.51
1:A:26:HIS:O	3:B:602:TPP:HM43	2.11	0.51
1:B:163:TRP:CD1	1:B:167:MET:HG3	2.46	0.51
1:D:75:GLY:H	1:D:118:GLN:NE2	2.09	0.51
1:D:153:PRO:HG3	1:D:304:ASP:HB2	1.91	0.51
1:E:85:ILE:HG22	1:E:125:ILE:HG22	1.93	0.51
1:B:246:SER:HA	1:B:408:LYS:HD2	1.93	0.51
1:E:37:CYS:SG	1:E:42:VAL:HG23	2.50	0.51
1:F:123:ALA:N	1:F:124:PRO:HD2	2.26	0.51
1:F:356:ARG:NH2	1:F:552:GLU:OE2	2.42	0.51
1:B:421:MET:HE3	3:B:602:TPP:S1	2.50	0.51
1:C:281:GLY:HA3	1:D:110:ASN:HB2	1.93	0.51
1:D:432:GLN:HE22	1:D:442:THR:H	1.58	0.50
1:H:188:ARG:HH22	1:H:331:GLN:HG3	1.76	0.50
1:F:75:GLY:H	1:F:118:GLN:NE2	2.08	0.50
1:H:274:LEU:HD12	1:H:299:ILE:HB	1.93	0.50
1:D:453:TYR:CE1	1:D:478:TRP:HH2	2.30	0.50
1:E:258:GLN:NE2	1:E:401:SER:HB2	2.27	0.50
1:D:422:GLY:C	1:D:424:GLY:H	2.14	0.50
3:F:602:TPP:N4'	3:F:602:TPP:HM42	2.27	0.50
1:H:261:TYR:C	1:H:263:PHE:H	2.14	0.50
1:F:258:GLN:HE22	1:F:401:SER:CB	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:ILE:HD11	1:G:9:LEU:HD21	1.93	0.50
1:D:268:ALA:HB2	1:D:348:LYS:NZ	2.26	0.50
1:A:464:LYS:O	1:A:465:GLN:HB2	2.11	0.50
1:H:390:VAL:HG22	1:H:413:LEU:HB2	1.94	0.50
1:C:503:SER:O	1:C:507:VAL:HG23	2.12	0.50
1:D:485:GLN:O	1:D:489:VAL:HB	2.11	0.50
1:B:143:MET:HE3	1:B:146:ILE:HD12	1.94	0.49
1:D:257:VAL:HG22	1:D:291:LEU:HD13	1.93	0.49
1:A:396:THR:HG21	1:A:473:MET:HB2	1.93	0.49
1:B:127:LYS:HE3	1:B:148:ALA:O	2.11	0.49
1:C:228:VAL:HG12	1:C:252:MET:SD	2.52	0.49
1:E:441:ARG:NH1	1:E:469:ILE:HD11	2.27	0.49
1:G:478:TRP:HB3	3:G:602:TPP:H61	1.93	0.49
1:A:388:THR:HG23	1:A:411:GLY:HA3	1.95	0.49
1:A:480:TRP:HB3	3:A:602:TPP:S1	2.52	0.49
1:B:370:LEU:HD21	1:B:375:ALA:HB2	1.94	0.49
1:C:421:MET:HE3	3:C:602:TPP:S1	2.52	0.49
1:D:399:TRP:NE1	1:D:550:PRO:HG3	2.28	0.49
1:A:270:PRO:O	1:A:296:ALA:HB2	2.12	0.49
1:A:24:GLY:O	1:A:46:ASP:HA	2.11	0.49
1:B:103:ALA:HA	1:B:164:ASP:HB2	1.93	0.49
1:B:75:GLY:H	1:B:118:GLN:NE2	2.10	0.49
1:C:348:LYS:HE3	1:C:352:LEU:HD11	1.95	0.49
1:F:206:ARG:HG2	1:F:345:TRP:CE3	2.46	0.49
1:D:519:ASP:OD1	1:D:520:SER:N	2.45	0.49
1:E:143:MET:HE3	1:E:146:ILE:HG13	1.94	0.49
1:E:481:THR:HG22	1:F:28:ILE:HG23	1.93	0.49
1:F:478:TRP:HB3	3:F:602:TPP:H61	1.94	0.49
1:G:380:ALA:HB2	1:G:403:VAL:CG1	2.42	0.49
1:H:24:GLY:O	1:H:46:ASP:HA	2.12	0.49
1:H:554:LEU:HD23	1:H:557:ILE:CD1	2.29	0.49
1:B:443:ILE:HG23	1:B:471:ILE:CD1	2.42	0.49
1:D:138:ILE:HD11	1:D:165:ILE:HG22	1.93	0.49
1:G:356:ARG:O	1:G:360:ILE:HG12	2.13	0.49
1:B:421:MET:HE2	3:B:602:TPP:C2	2.43	0.49
1:F:134:ALA:HB3	1:F:137:HIS:CD2	2.48	0.49
1:G:192:ALA:O	1:G:196:GLN:HG3	2.12	0.49
1:H:356:ARG:O	1:H:360:ILE:HG12	2.12	0.49
1:D:103:ALA:HA	1:D:164:ASP:HB2	1.95	0.49
1:D:104:LEU:HD22	1:D:165:ILE:HD11	1.95	0.49
1:G:390:VAL:HG21	1:G:428:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:THR:HG21	1:B:473:MET:HB2	1.93	0.49
1:E:454:SER:HB3	1:E:457:GLU:HG2	1.94	0.49
1:H:432:GLN:HE22	1:H:442:THR:H	1.61	0.49
1:A:103:ALA:HA	1:A:164:ASP:HB2	1.94	0.49
1:B:16:LYS:HE3	1:B:177:ILE:HD12	1.95	0.49
1:D:37:CYS:SG	1:D:44:ILE:HD11	2.53	0.49
1:A:547:ASP:N	1:A:548:PRO:CD	2.76	0.48
1:A:75:GLY:H	1:A:118:GLN:HE22	1.61	0.48
1:C:273:VAL:HG21	1:C:292:ILE:HG23	1.95	0.48
1:C:360:ILE:HD12	1:C:551:PRO:HG2	1.95	0.48
1:F:56:ALA:O	1:F:430:GLY:HA3	2.13	0.48
1:F:421:MET:HE3	3:F:602:TPP:S1	2.53	0.48
1:G:196:GLN:O	1:G:200:LEU:HD13	2.13	0.48
1:F:443:ILE:CG2	1:F:471:ILE:HD12	2.43	0.48
1:A:125:ILE:HG22	1:A:125:ILE:O	2.12	0.48
1:F:86:ALA:O	1:F:89:TRP:HB3	2.12	0.48
1:A:521:VAL:HG13	1:A:522:GLU:N	2.27	0.48
1:D:361:ALA:HA	1:D:373:PHE:CE2	2.49	0.48
1:E:232:GLY:HA2	1:E:252:MET:CE	2.43	0.48
1:G:55:HIS:HB3	1:G:427:THR:HG23	1.95	0.48
1:H:425:PHE:HZ	1:H:451:VAL:CG2	2.27	0.48
1:A:242:LEU:HD12	1:A:245:LEU:HD12	1.95	0.48
1:C:495:THR:CG2	1:D:38:LEU:HD13	2.42	0.48
1:H:371:HIS:CG	1:H:372:PRO:HD2	2.49	0.48
1:A:196:GLN:O	1:A:200:LEU:HD13	2.14	0.48
1:B:483:HIS:O	1:B:487:LEU:HB2	2.14	0.48
1:B:485:GLN:O	1:B:489:VAL:HB	2.14	0.48
1:D:56:ALA:O	1:D:430:GLY:HA3	2.14	0.48
1:H:270:PRO:O	1:H:296:ALA:HB2	2.13	0.48
1:A:371:HIS:CG	1:A:372:PRO:HD2	2.49	0.48
1:D:45:ILE:H	1:D:45:ILE:HD12	1.79	0.48
1:H:125:ILE:HA	1:H:125:ILE:HD13	1.57	0.48
1:A:478:TRP:CE2	1:A:499:LEU:HD11	2.48	0.48
1:A:286:HIS:NE2	1:B:111:THR:HG23	2.29	0.48
1:B:557:ILE:HD11	1:B:559:MET:H	1.79	0.48
1:D:188:ARG:HG2	1:D:324:GLY:O	2.14	0.48
1:E:425:PHE:HE2	1:E:451:VAL:CA	2.16	0.48
1:C:441:ARG:NH1	1:C:532:LEU:HA	2.29	0.47
1:E:143:MET:HE1	1:E:180:LEU:HB2	1.96	0.47
1:F:11:VAL:HG21	1:F:36:ALA:HB3	1.94	0.47
1:F:390:VAL:HG21	1:F:428:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:THR:HG21	1:G:473:MET:HB2	1.95	0.47
1:H:547:ASP:N	1:H:548:PRO:CD	2.77	0.47
1:C:478:TRP:HB3	3:C:602:TPP:H61	1.95	0.47
1:D:259:ASN:C	1:D:261:TYR:H	2.16	0.47
1:A:9:LEU:HD22	1:A:139:PRO:HG3	1.96	0.47
1:C:125:ILE:HD12	1:C:125:ILE:HG23	1.46	0.47
1:D:125:ILE:HD13	1:D:125:ILE:HA	1.59	0.47
1:D:536:ARG:CB	1:D:537:PRO:HD2	2.35	0.47
1:E:111:THR:CG2	1:E:112:LEU:H	2.24	0.47
1:A:26:HIS:ND1	1:B:481:THR:HB	2.30	0.47
1:A:479:GLY:N	3:A:602:TPP:O3B	2.39	0.47
1:A:81:ALA:C	1:A:84:PRO:HD2	2.33	0.47
1:C:125:ILE:HD11	1:D:121:MET:CE	2.44	0.47
1:A:495:THR:CG2	1:B:38:LEU:HD13	2.40	0.47
1:E:86:ALA:HA	1:E:125:ILE:CG2	2.43	0.47
1:F:131:ARG:HA	1:F:160:ASP:HB3	1.96	0.47
1:G:103:ALA:CB	1:G:164:ASP:HB2	2.44	0.47
1:C:26:HIS:ND1	1:D:481:THR:HB	2.30	0.47
1:G:137:HIS:HB3	1:G:141:LEU:HD22	1.95	0.47
1:H:231:THR:HG22	1:H:339:TRP:CE2	2.50	0.47
1:D:275:MET:SD	1:D:280:PHE:CE1	3.08	0.47
1:D:293:PRO:HG2	1:D:296:ALA:HB2	1.96	0.47
1:D:360:ILE:HD12	1:D:551:PRO:HG3	1.95	0.47
1:F:366:SER:HB3	1:F:374:HIS:HD2	1.80	0.47
1:G:125:ILE:HA	1:G:125:ILE:HD13	1.55	0.47
1:B:259:ASN:C	1:B:261:TYR:H	2.17	0.47
1:D:37:CYS:SG	1:D:42:VAL:CG2	3.02	0.47
1:D:453:TYR:HE1	1:D:478:TRP:HH2	1.61	0.47
1:E:400:LEU:O	1:E:404:MET:HG2	2.14	0.47
1:G:298:VAL:HB	1:G:314:ILE:HG22	1.97	0.47
1:G:3:MET:HG2	1:G:170:ILE:C	2.34	0.47
1:G:420:SER:OG	3:G:602:TPP:HM21	2.15	0.47
1:C:108:GLU:HG3	1:D:310:ARG:HH22	1.79	0.47
1:D:258:GLN:HE22	1:D:401:SER:CB	2.26	0.47
1:F:104:LEU:CD1	1:F:165:ILE:HD11	2.44	0.47
1:G:123:ALA:HB3	1:G:124:PRO:HD3	1.97	0.47
1:A:414:CYS:SG	1:A:415:HIS:N	2.87	0.47
1:B:75:GLY:H	1:B:118:GLN:HE22	1.62	0.47
1:B:81:ALA:O	1:B:84:PRO:HD2	2.15	0.47
1:A:259:ASN:C	1:A:261:TYR:H	2.17	0.46
1:C:370:LEU:HD11	1:C:521:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:TRP:HA	1:D:156:PRO:CD	2.44	0.46
1:D:89:TRP:HA	1:D:156:PRO:HD3	1.97	0.46
1:E:104:LEU:HD13	1:E:162:PRO:CG	2.46	0.46
1:G:482:LEU:O	1:G:486:GLN:HG2	2.15	0.46
1:B:350:THR:O	1:B:354:GLN:HB2	2.14	0.46
1:B:478:TRP:HE3	3:B:602:TPP:H61	1.79	0.46
1:D:421:MET:HE3	3:D:602:TPP:S1	2.55	0.46
1:E:206:ARG:HG2	1:E:345:TRP:CE3	2.50	0.46
1:E:4:ILE:HG12	1:E:8:GLU:CB	2.45	0.46
1:H:396:THR:HG21	1:H:473:MET:HB2	1.97	0.46
1:A:207:PRO:CG	1:A:233:VAL:HG12	2.45	0.46
1:C:206:ARG:HG2	1:C:345:TRP:CE3	2.51	0.46
1:E:202:ARG:NH1	1:E:338:ALA:O	2.49	0.46
1:F:164:ASP:O	1:F:168:ASN:HB2	2.15	0.46
1:F:202:ARG:HH12	1:F:338:ALA:C	2.18	0.46
1:A:213:SER:O	1:A:217:ARG:HG2	2.16	0.46
1:B:483:HIS:HE1	1:B:548:PRO:O	1.98	0.46
1:E:112:LEU:HD21	1:E:113:GLN:HE21	1.77	0.46
1:A:111:THR:HG22	1:A:112:LEU:N	2.28	0.46
1:C:536:ARG:HA	1:C:537:PRO:HD2	1.68	0.46
1:D:280:PHE:CE2	1:D:309:GLY:HA2	2.45	0.46
1:E:366:SER:HB2	1:E:374:HIS:CD2	2.51	0.46
1:E:396:THR:HG21	1:E:473:MET:HB2	1.97	0.46
1:F:366:SER:CB	1:F:371:HIS:H	2.28	0.46
1:F:448:ASP:HB3	1:F:474:ASN:HA	1.98	0.46
1:G:189:PRO:HB3	1:G:318:ILE:HG21	1.96	0.46
1:A:6:GLY:O	1:A:10:VAL:HG23	2.15	0.46
1:F:443:ILE:HG23	1:F:471:ILE:HD12	1.98	0.46
1:C:132:VAL:HG22	1:C:141:LEU:HD23	1.97	0.46
1:D:380:ALA:HB2	1:D:403:VAL:HG11	1.98	0.46
1:E:4:ILE:HG13	1:E:5:THR:N	2.30	0.46
1:F:146:ILE:HG22	1:F:150:LEU:HD12	1.97	0.46
1:F:357:TYR:CE2	1:F:406:ARG:HD2	2.51	0.46
1:G:498:ARG:HG2	1:G:498:ARG:HH11	1.81	0.46
1:H:258:GLN:HE22	1:H:401:SER:HB2	1.81	0.46
1:H:554:LEU:HA	1:H:557:ILE:CD1	2.45	0.46
1:B:119:VAL:HG13	1:B:129:ALA:CB	2.46	0.46
1:C:479:GLY:N	3:C:602:TPP:O3B	2.40	0.46
1:D:443:ILE:HG23	1:D:471:ILE:HD13	1.97	0.46
1:E:146:ILE:HG22	1:E:150:LEU:HD12	1.97	0.46
1:A:138:ILE:O	1:A:142:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:THR:HG23	1:F:339:TRP:NE1	2.31	0.46
1:G:469:ILE:HG13	1:G:469:ILE:H	1.50	0.46
1:G:443:ILE:HG23	1:G:471:ILE:CD1	2.46	0.46
1:H:425:PHE:CE1	1:H:451:VAL:HG23	2.51	0.46
1:H:555:ILE:HD11	1:H:561:PRO:HG3	1.98	0.46
1:B:25:LEU:HD23	1:B:25:LEU:C	2.37	0.45
1:C:478:TRP:CE3	3:C:602:TPP:HM41	2.52	0.45
1:E:233:VAL:HG12	1:E:234:PRO:O	2.16	0.45
1:A:469:ILE:CD1	1:A:532:LEU:HD12	2.45	0.45
1:B:396:THR:HG22	1:B:473:MET:HB2	1.98	0.45
1:B:547:ASP:O	1:B:548:PRO:O	2.34	0.45
1:D:264:ALA:C	1:D:266:ALA:N	2.69	0.45
1:E:28:ILE:CG2	1:F:481:THR:HG22	2.45	0.45
1:G:514:ASP:HB2	1:G:538:ALA:HB2	1.98	0.45
1:H:220:ARG:HA	1:H:220:ARG:HD2	1.72	0.45
1:H:256:LEU:HB3	1:H:258:GLN:HG2	1.98	0.45
1:A:478:TRP:NE1	1:A:499:LEU:HD11	2.31	0.45
1:C:124:PRO:HG2	1:C:125:ILE:HG12	1.97	0.45
1:E:143:MET:CE	1:E:180:LEU:HB2	2.46	0.45
1:H:75:GLY:H	1:H:118:GLN:NE2	2.14	0.45
1:C:4:ILE:CG2	1:C:8:GLU:CB	2.94	0.45
1:D:207:PRO:HG2	1:D:233:VAL:HG12	1.97	0.45
1:D:483:HIS:O	1:D:487:LEU:HB2	2.15	0.45
1:D:89:TRP:N	1:D:156:PRO:HG3	2.32	0.45
1:F:181:VAL:HG11	1:G:314:ILE:HG13	1.98	0.45
3:G:602:TPP:C2	3:G:602:TPP:HN42	2.29	0.45
1:H:50:GLU:HG2	1:H:77:GLY:O	2.16	0.45
1:A:75:GLY:H	1:A:118:GLN:NE2	2.14	0.45
1:D:131:ARG:HE	1:D:162:PRO:HG3	1.81	0.45
1:D:260:LEU:HA	1:D:263:PHE:CD1	2.52	0.45
1:H:503:SER:O	1:H:507:VAL:HG23	2.16	0.45
1:D:131:ARG:HA	1:D:160:ASP:HB3	1.98	0.45
1:G:112:LEU:HD12	1:G:113:GLN:HG3	1.99	0.45
1:H:490:GLY:HA2	1:H:491:PRO:HD2	1.79	0.45
1:B:103:ALA:CA	1:B:164:ASP:HB2	2.46	0.45
1:B:99:THR:CG2	1:B:158:LEU:HD11	2.47	0.45
3:C:602:TPP:HN42	3:C:602:TPP:H2	1.81	0.45
1:D:414:CYS:SG	1:D:415:HIS:N	2.87	0.45
1:E:131:ARG:HA	1:E:160:ASP:HB3	1.99	0.45
1:E:371:HIS:CG	1:E:372:PRO:HD2	2.52	0.45
1:G:204:ALA:HA	1:G:271:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:THR:CG2	1:G:473:MET:HB2	2.46	0.45
1:H:414:CYS:SG	1:H:415:HIS:N	2.89	0.45
1:E:138:ILE:HD11	1:E:165:ILE:HG22	1.97	0.45
1:F:359:SER:O	1:F:363:LYS:HG3	2.17	0.45
1:F:421:MET:CE	3:F:602:TPP:S1	3.05	0.45
1:H:138:ILE:HD11	1:H:165:ILE:HG22	1.99	0.45
1:A:276:LEU:HB3	1:A:322:VAL:HG13	1.98	0.45
1:B:231:THR:HG22	1:B:339:TRP:CE2	2.52	0.45
1:B:5:THR:HG22	1:B:169:GLN:HG2	1.98	0.45
1:D:37:CYS:SG	1:D:42:VAL:HG21	2.57	0.45
1:E:303:PRO:O	1:E:319:VAL:HG13	2.17	0.45
1:F:48:ARG:HA	1:F:48:ARG:HD2	1.75	0.45
1:G:239:TYR:HB3	1:G:414:CYS:HB3	1.99	0.45
1:C:81:ALA:C	1:C:84:PRO:HD2	2.37	0.45
1:E:407:VAL:O	1:E:409:PRO:HD3	2.17	0.45
1:E:99:THR:HG21	1:E:158:LEU:HD11	1.98	0.45
1:F:464:LYS:O	1:F:465:GLN:HB2	2.16	0.45
1:A:547:ASP:N	1:A:548:PRO:HD3	2.31	0.44
1:B:104:LEU:HD11	1:B:162:PRO:HG2	1.99	0.44
1:D:89:TRP:HB2	1:D:125:ILE:O	2.16	0.44
1:G:518:VAL:HB	1:G:523:SER:CB	2.47	0.44
1:A:81:ALA:O	1:A:84:PRO:HD2	2.16	0.44
1:C:448:ASP:HB3	1:C:474:ASN:HA	1.98	0.44
1:E:366:SER:HB2	1:E:374:HIS:HD2	1.82	0.44
1:G:236:PHE:CE2	1:G:260:LEU:HD21	2.52	0.44
1:G:99:THR:CG2	1:G:158:LEU:HD11	2.48	0.44
1:H:246:SER:O	1:H:408:LYS:HD2	2.16	0.44
1:D:5:THR:CG2	1:D:169:GLN:HG2	2.41	0.44
1:D:16:LYS:HE3	1:D:177:ILE:CD1	2.47	0.44
1:G:48:ARG:HD2	1:G:48:ARG:HA	1.74	0.44
1:G:495:THR:HG21	1:H:38:LEU:HD13	2.00	0.44
1:H:90:LEU:HD12	1:H:418:LEU:HB2	2.00	0.44
1:A:396:THR:CG2	1:A:473:MET:HB2	2.48	0.44
1:B:8:GLU:O	1:B:12:ARG:HG3	2.18	0.44
1:H:360:ILE:HD12	1:H:551:PRO:HG2	1.99	0.44
1:G:258:GLN:NE2	1:G:401:SER:HB2	2.33	0.44
1:G:55:HIS:O	1:G:58:GLU:HB2	2.17	0.44
1:G:56:ALA:HA	1:G:426:GLY:O	2.17	0.44
1:H:188:ARG:NH1	1:H:327:GLU:HB3	2.32	0.44
1:H:310:ARG:HG3	1:H:311:LEU:HG	1.98	0.44
1:E:232:GLY:O	1:E:342:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ALA:HA	1:F:426:GLY:O	2.17	0.44
1:C:289:GLY:HA2	1:C:292:ILE:O	2.18	0.44
1:E:242:LEU:HD12	1:E:245:LEU:HD12	2.00	0.44
1:G:104:LEU:HD13	1:G:162:PRO:CG	2.47	0.44
1:G:264:ALA:O	1:G:266:ALA:N	2.51	0.44
1:H:164:ASP:O	1:H:168:ASN:HB2	2.17	0.44
1:H:48:ARG:HD2	1:H:48:ARG:HA	1.75	0.44
1:C:104:LEU:HD13	1:C:162:PRO:CG	2.48	0.44
1:C:16:LYS:HE3	1:C:177:ILE:HD12	1.98	0.44
1:C:26:HIS:O	3:D:602:TPP:HM43	2.17	0.44
1:C:86:ALA:HA	1:C:125:ILE:HG21	1.99	0.44
1:H:162:PRO:HG2	1:H:165:ILE:HD12	1.99	0.44
1:G:448:ASP:O	1:H:48:ARG:NH2	2.51	0.44
1:A:138:ILE:N	1:A:139:PRO:CD	2.81	0.44
1:A:143:MET:CE	1:A:146:ILE:HG13	2.47	0.44
1:A:26:HIS:HD2	1:A:34:PHE:CD1	2.36	0.44
1:B:125:ILE:O	1:B:125:ILE:HG22	2.17	0.44
1:B:521:VAL:HG13	1:B:522:GLU:N	2.32	0.44
1:D:396:THR:CG2	1:D:473:MET:HB2	2.46	0.44
1:F:479:GLY:N	3:F:602:TPP:O3B	2.35	0.44
1:G:188:ARG:NH1	1:G:327:GLU:HB3	2.33	0.44
1:G:289:GLY:HA2	1:G:292:ILE:O	2.18	0.44
1:G:518:VAL:HB	1:G:523:SER:HB2	2.00	0.44
1:H:20:GLU:O	1:H:43:PRO:HD2	2.18	0.44
1:A:331:GLN:NE2	1:A:331:GLN:HA	2.33	0.43
1:B:425:PHE:CZ	1:B:451:VAL:CG2	2.90	0.43
1:D:164:ASP:O	1:D:168:ASN:HB2	2.18	0.43
1:E:276:LEU:HB3	1:E:322:VAL:HG13	1.99	0.43
1:H:376:SER:HB3	1:H:403:VAL:HG21	2.00	0.43
1:C:372:PRO:HB2	1:C:399:TRP:CD1	2.54	0.43
1:C:421:MET:CE	3:C:602:TPP:S1	3.06	0.43
1:E:305:ALA:HB2	1:E:319:VAL:HG21	2.01	0.43
1:E:443:ILE:HG23	1:E:471:ILE:CD1	2.47	0.43
1:G:22:LEU:HB2	1:G:44:ILE:HG12	2.00	0.43
1:H:6:GLY:HA2	1:H:9:LEU:HD12	2.00	0.43
1:E:273:VAL:HG21	1:E:292:ILE:HG23	2.00	0.43
1:E:46:ASP:OD1	1:E:464:LYS:HE3	2.17	0.43
1:F:198:LEU:HD22	1:F:339:TRP:HZ2	1.83	0.43
1:H:56:ALA:O	1:H:430:GLY:HA3	2.18	0.43
1:B:42:VAL:HA	1:B:43:PRO:HD3	1.81	0.43
1:B:528:LEU:HD12	1:B:528:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ILE:O	1:B:555:ILE:HG22	2.18	0.43
1:C:176:ILE:O	1:C:178:PRO:HD3	2.18	0.43
1:C:395:LEU:N	3:C:602:TPP:O2B	2.33	0.43
1:E:75:GLY:H	1:E:118:GLN:NE2	2.16	0.43
1:F:273:VAL:HG21	1:F:292:ILE:HG23	2.00	0.43
1:G:258:GLN:HE22	1:G:401:SER:CB	2.31	0.43
1:G:93:THR:HG22	1:G:95:VAL:HG23	2.00	0.43
1:G:9:LEU:HD11	1:G:170:ILE:HD11	1.99	0.43
1:A:209:ILE:HG23	1:A:274:LEU:HD23	2.00	0.43
1:A:282:LEU:HA	1:A:286:HIS:CE1	2.52	0.43
1:B:560:ASP:OD1	1:B:562:PHE:N	2.51	0.43
1:C:480:TRP:HB3	3:C:602:TPP:S1	2.59	0.43
1:E:378:VAL:HG13	1:E:525:SER:HB3	2.00	0.43
1:E:400:LEU:HG	1:E:404:MET:HG2	2.01	0.43
1:F:203:LYS:HB2	1:F:203:LYS:HE3	1.76	0.43
1:F:67:LEU:HG	1:F:68:GLY:N	2.34	0.43
1:H:136:GLU:H	1:H:136:GLU:CD	2.22	0.43
1:A:389:VAL:HG13	1:A:412:PHE:HD1	1.82	0.43
1:B:104:LEU:CD1	1:B:162:PRO:CG	2.96	0.43
1:B:60:TYR:CZ	1:B:66:LYS:HE3	2.54	0.43
1:C:26:HIS:CE1	1:D:481:THR:HB	2.53	0.43
1:C:188:ARG:HD3	1:C:328:ALA:HB2	1.99	0.43
1:D:288:SER:O	1:D:294:HIS:HE1	2.01	0.43
1:H:235:VAL:HG12	1:H:245:LEU:HD21	2.01	0.43
1:A:104:LEU:HD13	1:A:162:PRO:CG	2.48	0.43
1:A:518:VAL:HG11	1:A:523:SER:O	2.18	0.43
1:C:461:LEU:HD21	1:C:468:LEU:HD23	2.00	0.43
1:E:4:ILE:HG13	1:E:5:THR:H	1.83	0.43
1:E:59:GLY:HA2	1:E:413:LEU:HD21	2.00	0.43
1:F:78:PHE:CD2	1:F:118:GLN:HG2	2.54	0.43
1:B:55:HIS:HB3	1:B:427:THR:HG23	2.01	0.43
1:F:125:ILE:HD13	1:F:125:ILE:HA	1.63	0.43
1:F:103:ALA:CA	1:F:164:ASP:HB2	2.48	0.43
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.74	0.43
1:A:26:HIS:NE2	1:A:31:ASP:OD1	2.52	0.43
1:D:421:MET:HG2	3:D:602:TPP:C6'	2.49	0.43
1:H:116:ILE:O	1:H:116:ILE:HD12	2.19	0.43
1:A:116:ILE:O	1:A:116:ILE:HG13	2.19	0.43
1:D:5:THR:HA	1:D:168:ASN:O	2.18	0.43
1:D:257:VAL:O	1:D:291:LEU:HD22	2.18	0.43
1:G:136:GLU:CD	1:G:136:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ASP:OD1	1:G:185:HIS:HD2	2.02	0.43
1:A:214:GLU:HB2	1:A:322:VAL:HG21	2.01	0.42
1:B:421:MET:CE	3:B:602:TPP:S1	3.07	0.42
1:C:224:LEU:HD13	1:C:326:ILE:HD13	2.01	0.42
1:E:99:THR:HG22	1:E:158:LEU:HD11	2.01	0.42
1:E:242:LEU:HD13	1:E:256:LEU:HD23	2.01	0.42
1:E:265:LYS:CG	1:E:265:LYS:O	2.64	0.42
1:E:443:ILE:HG23	1:E:471:ILE:HD13	2.01	0.42
1:F:140:ARG:O	1:F:144:GLN:HB2	2.18	0.42
1:G:333:THR:HG23	1:G:339:TRP:HE1	1.83	0.42
1:A:274:LEU:HD21	1:A:276:LEU:HD21	2.01	0.42
1:A:218:THR:OG1	1:A:323:GLY:HA3	2.19	0.42
1:B:372:PRO:HB2	1:B:399:TRP:CD1	2.54	0.42
1:C:282:LEU:HA	1:C:286:HIS:CE1	2.54	0.42
1:C:371:HIS:CG	1:C:372:PRO:HD2	2.54	0.42
1:E:231:THR:HG22	1:E:339:TRP:CE2	2.54	0.42
1:E:396:THR:CG2	1:E:473:MET:HB2	2.49	0.42
3:E:602:TPP:C2	3:E:602:TPP:N4'	2.81	0.42
1:G:81:ALA:O	1:G:85:ILE:HG13	2.20	0.42
1:H:432:GLN:NE2	1:H:442:THR:H	2.16	0.42
1:D:99:THR:CG2	1:D:158:LEU:HD11	2.49	0.42
1:E:202:ARG:HH12	1:E:338:ALA:C	2.22	0.42
1:E:25:LEU:HD22	3:F:602:TPP:HN41	1.85	0.42
1:F:482:LEU:O	1:F:482:LEU:HD23	2.18	0.42
1:G:264:ALA:C	1:G:266:ALA:N	2.73	0.42
1:B:432:GLN:HE22	1:B:442:THR:H	1.68	0.42
1:B:425:PHE:CE1	1:B:451:VAL:HA	2.51	0.42
1:C:370:LEU:HD12	1:C:521:VAL:HG22	2.01	0.42
1:G:376:SER:HB3	1:G:403:VAL:HG21	2.00	0.42
1:G:399:TRP:CE2	1:G:550:PRO:HG3	2.54	0.42
1:A:48:ARG:HD2	1:A:48:ARG:HA	1.68	0.42
1:B:125:ILE:HG23	1:B:125:ILE:HD12	1.79	0.42
1:C:261:TYR:C	1:C:263:PHE:H	2.23	0.42
1:E:96:LEU:HD12	1:E:96:LEU:HA	1.77	0.42
1:G:237:ALA:O	1:G:256:LEU:HA	2.20	0.42
1:G:81:ALA:C	1:G:84:PRO:HD2	2.39	0.42
1:H:123:ALA:N	1:H:124:PRO:HD2	2.34	0.42
1:A:335:GLN:CD	1:A:335:GLN:N	2.73	0.42
1:C:331:GLN:NE2	1:C:331:GLN:HA	2.33	0.42
1:E:432:GLN:HE22	1:E:441:ARG:HG3	1.84	0.42
1:G:259:ASN:C	1:G:261:TYR:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:PRO:HD2	1:B:553:GLU:OE1	2.19	0.42
1:C:75:GLY:HA2	1:C:116:ILE:HD11	2.01	0.42
1:F:421:MET:HE2	3:F:602:TPP:C2	2.50	0.42
1:G:143:MET:HE1	1:G:180:LEU:HB2	2.02	0.42
1:G:69:VAL:HG22	1:G:96:LEU:HB3	2.00	0.42
1:D:380:ALA:HB2	1:D:403:VAL:CG1	2.49	0.42
1:A:261:TYR:C	1:A:263:PHE:H	2.24	0.42
1:A:421:MET:CE	3:A:602:TPP:S1	3.06	0.42
1:D:209:ILE:HG12	1:D:274:LEU:HD23	2.01	0.42
1:H:202:ARG:HH22	1:H:336:ASP:HB3	1.85	0.42
1:A:370:LEU:CD2	1:A:375:ALA:HB2	2.47	0.42
1:D:276:LEU:HB3	1:D:322:VAL:HG13	2.02	0.42
1:D:371:HIS:CG	1:D:372:PRO:HD2	2.55	0.42
1:D:453:TYR:HE1	1:D:478:TRP:CH2	2.37	0.42
1:E:72:VAL:HG11	1:E:81:ALA:HB2	2.02	0.42
1:G:125:ILE:HD12	1:G:125:ILE:HG23	1.79	0.42
1:G:236:PHE:CE1	1:G:260:LEU:HD21	2.54	0.42
1:A:188:ARG:CZ	1:D:191:PRO:HD2	2.50	0.41
1:D:86:ALA:HA	1:D:125:ILE:HG23	2.01	0.41
1:G:223:ALA:O	1:G:330:ALA:HB2	2.20	0.41
1:G:483:HIS:O	1:G:487:LEU:HB2	2.20	0.41
1:A:48:ARG:NH2	1:B:448:ASP:O	2.53	0.41
1:B:206:ARG:H	1:B:271:ASP:HB3	1.85	0.41
1:C:135:THR:OG1	1:C:165:ILE:HG23	2.20	0.41
1:C:4:ILE:CG2	1:C:8:GLU:HB3	2.50	0.41
1:D:486:GLN:HG2	1:D:486:GLN:H	1.65	0.41
1:F:123:ALA:N	1:F:124:PRO:CD	2.83	0.41
1:F:425:PHE:CE2	1:F:451:VAL:HG23	2.50	0.41
1:E:28:ILE:HG22	1:F:481:THR:HG22	2.02	0.41
1:G:137:HIS:O	1:G:141:LEU:HB2	2.20	0.41
1:H:207:PRO:HG2	1:H:233:VAL:CG1	2.48	0.41
1:A:269:ALA:HB1	1:A:293:PRO:HG3	2.02	0.41
1:A:395:LEU:N	3:A:602:TPP:O2B	2.42	0.41
1:C:428:ALA:HB2	1:C:444:LEU:HD13	2.02	0.41
1:D:111:THR:HG22	1:D:112:LEU:N	2.27	0.41
1:D:432:GLN:NE2	1:D:442:THR:H	2.16	0.41
1:E:227:PHE:CE1	1:E:329:LEU:HB3	2.55	0.41
1:G:162:PRO:CG	1:G:165:ILE:HD12	2.47	0.41
1:C:4:ILE:HG23	1:C:8:GLU:CB	2.50	0.41
1:E:258:GLN:HE22	1:E:401:SER:CB	2.32	0.41
1:F:135:THR:OG1	1:F:165:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:HIS:CG	1:G:372:PRO:HD2	2.56	0.41
1:C:354:GLN:HE21	1:C:406:ARG:HH22	1.66	0.41
1:D:135:THR:HG23	1:D:138:ILE:HD12	2.02	0.41
1:E:105:ARG:HG2	1:E:164:ASP:OD1	2.20	0.41
1:E:441:ARG:HH12	1:E:469:ILE:HD11	1.85	0.41
1:E:89:TRP:HB2	1:E:125:ILE:O	2.19	0.41
1:H:478:TRP:HB3	3:H:602:TPP:H61	2.02	0.41
1:A:16:LYS:HE3	1:A:177:ILE:CG2	2.51	0.41
3:A:602:TPP:HM43	1:B:26:HIS:O	2.20	0.41
1:C:360:ILE:HD12	1:C:551:PRO:CG	2.50	0.41
1:G:498:ARG:HG2	1:G:498:ARG:NH1	2.35	0.41
1:C:131:ARG:HA	1:C:160:ASP:HB3	2.01	0.41
1:F:259:ASN:C	1:F:261:TYR:H	2.23	0.41
1:G:104:LEU:HD13	1:G:162:PRO:HG2	2.02	0.41
1:G:89:TRP:HB2	1:G:125:ILE:O	2.19	0.41
1:H:36:ALA:O	1:H:40:HIS:HD2	2.03	0.41
1:A:103:ALA:CA	1:A:164:ASP:HB2	2.50	0.41
1:C:116:ILE:O	1:C:116:ILE:HG13	2.20	0.41
1:C:123:ALA:N	1:C:124:PRO:CD	2.83	0.41
1:C:136:GLU:H	1:C:136:GLU:CD	2.24	0.41
1:C:195:ASP:O	1:C:195:ASP:OD1	2.39	0.41
1:C:86:ALA:O	1:C:89:TRP:HB3	2.20	0.41
1:F:26:HIS:HD2	1:F:34:PHE:CD2	2.38	0.41
1:F:81:ALA:O	1:F:84:PRO:HD2	2.20	0.41
1:H:269:ALA:HB1	1:H:293:PRO:HG3	2.02	0.41
1:A:236:PHE:CZ	1:A:260:LEU:HD21	2.56	0.41
1:A:231:THR:HG22	1:A:339:TRP:CE2	2.56	0.41
1:B:408:LYS:HA	1:B:409:PRO:HD3	1.82	0.41
1:C:432:GLN:HE22	1:C:442:THR:H	1.68	0.41
1:D:103:ALA:CA	1:D:164:ASP:HB2	2.50	0.41
1:D:264:ALA:O	1:D:266:ALA:N	2.54	0.41
1:D:206:ARG:NH2	1:D:269:ALA:O	2.54	0.41
1:E:45:ILE:HD12	1:E:45:ILE:H	1.86	0.41
1:G:556:LEU:HA	1:G:556:LEU:HD23	1.98	0.41
1:H:6:GLY:O	1:H:10:VAL:HG23	2.20	0.41
1:B:391:ALA:HB1	1:B:397:TYR:HB2	2.03	0.41
1:H:259:ASN:C	1:H:261:TYR:H	2.25	0.41
1:E:125:ILE:O	1:E:125:ILE:CG2	2.67	0.41
1:E:288:SER:OG	1:E:290:GLN:HG3	2.21	0.41
1:E:448:ASP:HB3	1:E:474:ASN:HA	2.03	0.41
1:F:414:CYS:SG	1:F:415:HIS:N	2.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:VAL:HA	1:F:43:PRO:HD3	1.88	0.41
1:G:29:HIS:HD2	1:G:163:TRP:HB2	1.86	0.41
1:G:191:PRO:O	1:G:195:ASP:HB2	2.21	0.41
1:G:256:LEU:C	1:G:258:GLN:H	2.24	0.41
1:H:131:ARG:HA	1:H:160:ASP:HB3	2.02	0.41
1:A:372:PRO:HB2	1:A:399:TRP:CD1	2.56	0.40
1:C:554:LEU:HA	1:C:554:LEU:HD23	1.84	0.40
1:C:56:ALA:HA	1:C:426:GLY:O	2.21	0.40
1:G:376:SER:CB	1:G:403:VAL:HG21	2.50	0.40
1:A:443:ILE:HG23	1:A:471:ILE:CD1	2.51	0.40
1:A:462:VAL:HG22	1:A:512:GLY:O	2.21	0.40
1:A:94:PRO:HB3	1:A:154:ARG:HB3	2.04	0.40
1:B:478:TRP:HB3	3:B:602:TPP:H61	2.03	0.40
1:B:258:GLN:OE1	1:B:552:GLU:OE2	2.39	0.40
1:C:4:ILE:CG1	1:C:172:GLU:HG2	2.51	0.40
1:C:400:LEU:O	1:C:404:MET:HG2	2.22	0.40
1:C:4:ILE:CG2	1:C:8:GLU:HB2	2.51	0.40
1:D:103:ALA:HB1	1:D:164:ASP:HB2	2.02	0.40
1:F:55:HIS:O	1:F:58:GLU:HB2	2.22	0.40
1:H:74:ALA:CB	1:H:101:SER:HA	2.52	0.40
1:F:218:THR:OG1	1:F:323:GLY:HA3	2.22	0.40
1:G:273:VAL:HB	1:G:298:VAL:HG13	2.03	0.40
1:H:308:LEU:HD23	1:H:308:LEU:HA	1.92	0.40
1:A:204:ALA:HA	1:A:271:ASP:OD2	2.22	0.40
1:B:99:THR:HG22	1:B:158:LEU:HD11	2.03	0.40
1:A:507:VAL:HG13	1:B:507:VAL:HG13	2.03	0.40
1:D:280:PHE:CE1	1:D:292:ILE:HD13	2.56	0.40
1:G:46:ASP:OD1	1:G:464:LYS:CE	2.67	0.40
1:H:498:ARG:CG	1:H:498:ARG:HH11	2.28	0.40
1:A:104:LEU:O	1:A:107:ASP:HB2	2.22	0.40
1:A:108:GLU:HG3	1:B:310:ARG:NH1	2.37	0.40
1:A:422:GLY:C	1:A:424:GLY:H	2.25	0.40
1:E:344:ASP:N	1:E:344:ASP:OD1	2.54	0.40
1:E:79:THR:HA	1:E:82:VAL:HG23	2.02	0.40
1:F:127:LYS:HE3	1:F:148:ALA:O	2.21	0.40
1:F:270:PRO:O	1:F:296:ALA:HB2	2.20	0.40
1:F:389:VAL:HG13	1:F:412:PHE:HD1	1.86	0.40
1:G:464:LYS:HD3	1:G:464:LYS:HA	1.82	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	561/582 (96%)	524 (93%)	35 (6%)	2 (0%)	34	72
1	B	560/582 (96%)	522 (93%)	35 (6%)	3 (0%)	29	68
1	C	560/582 (96%)	529 (94%)	29 (5%)	2 (0%)	34	72
1	D	560/582 (96%)	517 (92%)	39 (7%)	4 (1%)	22	60
1	E	560/582 (96%)	532 (95%)	27 (5%)	1 (0%)	47	82
1	F	560/582 (96%)	531 (95%)	28 (5%)	1 (0%)	47	82
1	G	560/582 (96%)	528 (94%)	27 (5%)	5 (1%)	17	55
1	H	560/582 (96%)	530 (95%)	29 (5%)	1 (0%)	47	82
All	All	4481/4656 (96%)	4213 (94%)	249 (6%)	19 (0%)	34	72

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	PRO
1	C	41	ASP
1	D	265	LYS
1	D	290	GLN
1	F	117	ASP
1	G	265	LYS
1	D	478	TRP
1	E	478	TRP
1	G	6	GLY
1	H	478	TRP
1	A	260	LEU
1	B	562	PHE
1	D	260	LEU
1	G	308	LEU
1	A	41	ASP
1	G	262	SER
1	C	262	SER

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Mol	Chain	Res	Type
1	B	257	VAL
1	G	257	VAL

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	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	B	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	C	421/438 (96%)	413 (98%)	8 (2%)	57	84
1	D	421/438 (96%)	416 (99%)	5 (1%)	71	90
1	E	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	F	421/438 (96%)	411 (98%)	10 (2%)	49	79
1	G	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	H	421/438 (96%)	414 (98%)	7 (2%)	60	85
All	All	3368/3504 (96%)	3302 (98%)	66 (2%)	55	83

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	69	VAL
1	A	112	LEU
1	A	195	ASP
1	A	252	MET
1	A	335	GLN
1	A	425	PHE
1	A	476	GLN
1	A	522	GLU
1	B	105	ARG
1	B	190	ASP
1	B	200	LEU
1	B	265	LYS

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Mol	Chain	Res	Type
1	B	302	ASP
1	B	310	ARG
1	B	367	GLU
1	B	525	SER
1	B	557	ILE
1	C	104	LEU
1	C	173	ASP
1	C	193	ASP
1	C	302	ASP
1	C	335	GLN
1	C	425	PHE
1	C	493	ARG
1	C	536	ARG
1	D	42	VAL
1	D	175	VAL
1	D	302	ASP
1	D	425	PHE
1	D	559	MET
1	E	41	ASP
1	E	111	THR
1	E	200	LEU
1	E	265	LYS
1	E	302	ASP
1	E	331	GLN
1	E	352	LEU
1	E	365	SER
1	E	381	LYS
1	F	28	ILE
1	F	42	VAL
1	F	176	ILE
1	F	193	ASP
1	F	225	SER
1	F	354	GLN
1	F	356	ARG
1	F	364	SER
1	F	389	VAL
1	F	493	ARG
1	G	25	LEU
1	G	141	LEU
1	G	195	ASP
1	G	331	GLN
1	G	397	TYR

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Mol	Chain	Res	Type
1	G	406	ARG
1	G	441	ARG
1	G	547	ASP
1	G	562	PHE
1	H	66	LYS
1	H	177	ILE
1	H	182	LEU
1	H	290	GLN
1	H	360	ILE
1	H	397	TYR
1	H	406	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	40	HIS
1	A	118	GLN
1	A	258	GLN
1	A	331	GLN
1	A	374	HIS
1	A	419	ASN
1	A	432	GLN
1	A	476	GLN
1	B	113	GLN
1	B	118	GLN
1	B	294	HIS
1	B	374	HIS
1	B	419	ASN
1	B	432	GLN
1	C	118	GLN
1	C	312	GLN
1	C	331	GLN
1	C	354	GLN
1	C	415	HIS
1	C	419	ASN
1	C	432	GLN
1	C	476	GLN
1	D	118	GLN
1	D	258	GLN
1	D	286	HIS
1	D	294	HIS

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Mol	Chain	Res	Type
1	D	354	GLN
1	D	432	GLN
1	E	113	GLN
1	E	118	GLN
1	E	258	GLN
1	E	354	GLN
1	E	432	GLN
1	F	118	GLN
1	F	137	HIS
1	F	258	GLN
1	F	312	GLN
1	F	374	HIS
1	F	432	GLN
1	F	476	GLN
1	G	29	HIS
1	G	118	GLN
1	G	185	HIS
1	G	258	GLN
1	G	354	GLN
1	G	432	GLN
1	H	40	HIS
1	H	55	HIS
1	H	113	GLN
1	H	118	GLN
1	H	258	GLN
1	H	354	GLN
1	H	419	ASN
1	H	432	GLN
1	H	465	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	H	602	2	22,27,27	2.33	5 (22%)	29,40,40	2.15	10 (34%)
3	TPP	G	602	2	22,27,27	2.87	5 (22%)	29,40,40	2.13	10 (34%)
3	TPP	F	602	2	22,27,27	2.00	4 (18%)	29,40,40	1.98	11 (37%)
3	TPP	D	602	2	22,27,27	2.57	3 (13%)	29,40,40	2.12	9 (31%)
3	TPP	B	602	2	22,27,27	2.18	4 (18%)	29,40,40	2.26	12 (41%)
3	TPP	E	602	2	22,27,27	2.88	3 (13%)	29,40,40	1.81	10 (34%)
3	TPP	C	602	2	22,27,27	2.39	4 (18%)	29,40,40	1.81	9 (31%)
3	TPP	A	602	2	22,27,27	2.38	5 (22%)	29,40,40	2.17	10 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	H	602	2	-	4/16/17/17	0/2/2/2
3	TPP	G	602	2	-	2/16/17/17	0/2/2/2
3	TPP	F	602	2	-	4/16/17/17	0/2/2/2
3	TPP	D	602	2	-	5/16/17/17	0/2/2/2
3	TPP	B	602	2	-	4/16/17/17	0/2/2/2
3	TPP	E	602	2	-	2/16/17/17	0/2/2/2
3	TPP	C	602	2	-	4/16/17/17	0/2/2/2
3	TPP	A	602	2	-	3/16/17/17	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	TPP	C6-C5	12.27	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	TPP	C6-C5	11.90	1.56	1.50
3	D	602	TPP	C6-C5	10.65	1.55	1.50
3	C	602	TPP	C6-C5	9.02	1.54	1.50
3	A	602	TPP	C6-C5	8.81	1.54	1.50
3	H	602	TPP	C6-C5	8.72	1.54	1.50
3	B	602	TPP	C6-C5	8.35	1.54	1.50
3	F	602	TPP	C6-C5	7.00	1.54	1.50
3	C	602	TPP	C7'-C5'	3.81	1.59	1.51
3	B	602	TPP	C4'-N4'	3.43	1.42	1.34
3	F	602	TPP	C7'-C5'	3.42	1.58	1.51
3	A	602	TPP	C7'-C5'	3.40	1.58	1.51
3	A	602	TPP	C4'-N4'	3.34	1.42	1.34
3	D	602	TPP	C4'-N4'	3.26	1.42	1.34
3	H	602	TPP	C7'-C5'	3.20	1.57	1.51
3	F	602	TPP	C4'-N4'	3.19	1.42	1.34
3	H	602	TPP	C4'-N4'	3.14	1.42	1.34
3	G	602	TPP	C7'-C5'	3.09	1.57	1.51
3	C	602	TPP	C4'-N4'	3.01	1.41	1.34
3	E	602	TPP	C4'-N4'	2.76	1.41	1.34
3	G	602	TPP	C4'-N4'	2.74	1.41	1.34
3	H	602	TPP	C6'-C5'	2.68	1.43	1.37
3	G	602	TPP	C4-N3	2.67	1.42	1.39
3	B	602	TPP	C7'-C5'	2.54	1.56	1.51
3	F	602	TPP	C6'-C5'	2.51	1.43	1.37
3	A	602	TPP	C4-N3	2.50	1.41	1.39
3	A	602	TPP	C6'-C5'	2.43	1.42	1.37
3	E	602	TPP	C7'-C5'	2.35	1.56	1.51
3	H	602	TPP	C4-N3	2.32	1.41	1.39
3	B	602	TPP	C6'-C5'	2.31	1.42	1.37
3	C	602	TPP	C6'-C5'	2.31	1.42	1.37
3	G	602	TPP	C6'-C5'	2.15	1.42	1.37
3	D	602	TPP	C7'-C5'	2.00	1.55	1.51

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	TPP	C6-C5-C4	6.33	132.51	127.43
3	G	602	TPP	C6-C5-C4	6.19	132.40	127.43
3	B	602	TPP	C6-C5-C4	6.18	132.40	127.43
3	D	602	TPP	C6-C5-C4	5.53	131.88	127.43
3	H	602	TPP	C6-C5-C4	4.63	131.15	127.43
3	H	602	TPP	CM2-C2'-N1'	4.34	121.91	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	TPP	C6'-N1'-C2'	4.26	123.22	115.96
3	B	602	TPP	PA-O3A-PB	-4.23	118.32	132.83
3	H	602	TPP	PA-O3A-PB	-3.96	119.23	132.83
3	A	602	TPP	C6'-N1'-C2'	3.94	122.67	115.96
3	D	602	TPP	C6'-N1'-C2'	3.86	122.52	115.96
3	F	602	TPP	CM2-C2'-N1'	3.76	121.27	117.14
3	G	602	TPP	PA-O3A-PB	-3.69	120.16	132.83
3	F	602	TPP	C6-C5-C4	3.67	130.38	127.43
3	G	602	TPP	C6'-N1'-C2'	3.65	122.17	115.96
3	F	602	TPP	PA-O3A-PB	-3.64	120.32	132.83
3	D	602	TPP	C5'-C6'-N1'	-3.59	117.83	123.82
3	D	602	TPP	PA-O3A-PB	-3.51	120.77	132.83
3	E	602	TPP	C6'-N1'-C2'	3.49	121.91	115.96
3	D	602	TPP	C7'-N3-C2	-3.43	119.16	125.35
3	C	602	TPP	PA-O3A-PB	-3.40	121.17	132.83
3	A	602	TPP	C7'-N3-C2	-3.35	119.30	125.35
3	A	602	TPP	PA-O3A-PB	-3.35	121.33	132.83
3	F	602	TPP	C6'-N1'-C2'	3.34	121.64	115.96
3	H	602	TPP	C6'-N1'-C2'	3.31	121.59	115.96
3	B	602	TPP	C6'-N1'-C2'	3.24	121.47	115.96
3	B	602	TPP	C7'-N3-C2	-3.20	119.56	125.35
3	H	602	TPP	C7'-N3-C2	-3.20	119.57	125.35
3	D	602	TPP	CM2-C2'-N1'	3.17	120.62	117.14
3	B	602	TPP	C5'-C7'-N3	-3.15	108.03	113.28
3	G	602	TPP	C7'-N3-C2	-3.12	119.71	125.35
3	A	602	TPP	C5-C4-N3	3.09	113.76	107.57
3	G	602	TPP	C5-C4-N3	3.09	113.75	107.57
3	C	602	TPP	N1'-C2'-N3'	-3.07	120.25	125.54
3	E	602	TPP	PA-O3A-PB	-3.07	122.30	132.83
3	H	602	TPP	N1'-C2'-N3'	-3.05	120.28	125.54
3	H	602	TPP	C5-C4-N3	3.04	113.65	107.57
3	A	602	TPP	C5'-C6'-N1'	-3.03	118.77	123.82
3	G	602	TPP	C5'-C6'-N1'	-3.00	118.82	123.82
3	F	602	TPP	N1'-C2'-N3'	-2.99	120.39	125.54
3	G	602	TPP	CM2-C2'-N1'	2.99	120.42	117.14
3	D	602	TPP	C5-C4-N3	2.98	113.54	107.57
3	B	602	TPP	C5-C4-N3	2.95	113.47	107.57
3	H	602	TPP	C2'-N3'-C4'	2.95	122.67	118.08
3	F	602	TPP	C2'-N3'-C4'	2.88	122.57	118.08
3	H	602	TPP	CM4-C4-C5	-2.86	121.35	127.60
3	F	602	TPP	C7'-N3-C2	-2.84	120.22	125.35
3	E	602	TPP	C5-C4-N3	2.81	113.20	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	602	TPP	N4'-C4'-N3'	2.81	121.01	117.03
3	E	602	TPP	C6-C5-C4	2.79	129.67	127.43
3	E	602	TPP	N1'-C2'-N3'	-2.78	120.76	125.54
3	C	602	TPP	C7'-N3-C2	-2.76	120.36	125.35
3	E	602	TPP	C7'-N3-C2	-2.76	120.36	125.35
3	F	602	TPP	C5-C4-N3	2.74	113.06	107.57
3	B	602	TPP	C5'-C6'-N1'	-2.72	119.29	123.82
3	B	602	TPP	C2'-N3'-C4'	2.69	122.28	118.08
3	E	602	TPP	C5'-C6'-N1'	-2.67	119.36	123.82
3	C	602	TPP	C5'-C6'-N1'	-2.66	119.40	123.82
3	F	602	TPP	C5'-C7'-N3	-2.65	108.87	113.28
3	B	602	TPP	N4'-C4'-N3'	2.60	120.70	117.03
3	G	602	TPP	N1'-C2'-N3'	-2.59	121.08	125.54
3	B	602	TPP	CM2-C2'-N1'	2.56	119.95	117.14
3	B	602	TPP	N1'-C2'-N3'	-2.56	121.14	125.54
3	G	602	TPP	C5'-C7'-N3	-2.50	109.11	113.28
3	A	602	TPP	N1'-C2'-N3'	-2.48	121.28	125.54
3	C	602	TPP	C6-C5-C4	2.44	129.39	127.43
3	A	602	TPP	CM4-C4-C5	-2.40	122.35	127.60
3	C	602	TPP	C5-C4-N3	2.39	112.35	107.57
3	G	602	TPP	CM4-C4-C5	-2.38	122.39	127.60
3	D	602	TPP	N1'-C2'-N3'	-2.33	121.53	125.54
3	D	602	TPP	CM4-C4-C5	-2.33	122.52	127.60
3	C	602	TPP	CM2-C2'-N3'	2.33	120.78	117.15
3	A	602	TPP	N4'-C4'-N3'	2.32	120.31	117.03
3	F	602	TPP	CM4-C4-C5	-2.30	122.56	127.60
3	H	602	TPP	C5'-C6'-N1'	-2.26	120.05	123.82
3	E	602	TPP	C5'-C4'-N4'	-2.25	119.00	122.19
3	C	602	TPP	C5'-C7'-N3	-2.21	109.60	113.28
3	B	602	TPP	CM4-C4-C5	-2.19	122.82	127.60
3	E	602	TPP	C2'-N3'-C4'	2.18	121.47	118.08
3	A	602	TPP	CM2-C2'-N1'	2.17	119.52	117.14
3	F	602	TPP	C5'-C6'-N1'	-2.06	120.38	123.82

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	TPP	PA-O3A-PB-O3B
3	F	602	TPP	C6'-C5'-C7'-N3
3	F	602	TPP	PA-O3A-PB-O3B
3	D	602	TPP	C6'-C5'-C7'-N3

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Mol	Chain	Res	Type	Atoms
3	D	602	TPP	PA-O3A-PB-O3B
3	E	602	TPP	PA-O3A-PB-O3B
3	H	602	TPP	C6'-C5'-C7'-N3
3	H	602	TPP	PA-O3A-PB-O3B
3	B	602	TPP	C6'-C5'-C7'-N3
3	B	602	TPP	PA-O3A-PB-O3B
3	C	602	TPP	PA-O3A-PB-O3B
3	G	602	TPP	PA-O3A-PB-O3B
3	D	602	TPP	C4'-C5'-C7'-N3
3	B	602	TPP	C4'-C5'-C7'-N3
3	C	602	TPP	C5-C6-C7-O7
3	F	602	TPP	C4-C5-C6-C7
3	D	602	TPP	PA-O3A-PB-O1B
3	C	602	TPP	PA-O3A-PB-O1B
3	A	602	TPP	PA-O3A-PB-O2B
3	F	602	TPP	PA-O3A-PB-O2B
3	D	602	TPP	PA-O3A-PB-O2B
3	E	602	TPP	PA-O3A-PB-O2B
3	H	602	TPP	PA-O3A-PB-O2B
3	B	602	TPP	PA-O3A-PB-O2B
3	C	602	TPP	PA-O3A-PB-O2B
3	G	602	TPP	PA-O3A-PB-O2B
3	A	602	TPP	PA-O3A-PB-O1B
3	H	602	TPP	PA-O3A-PB-O1B

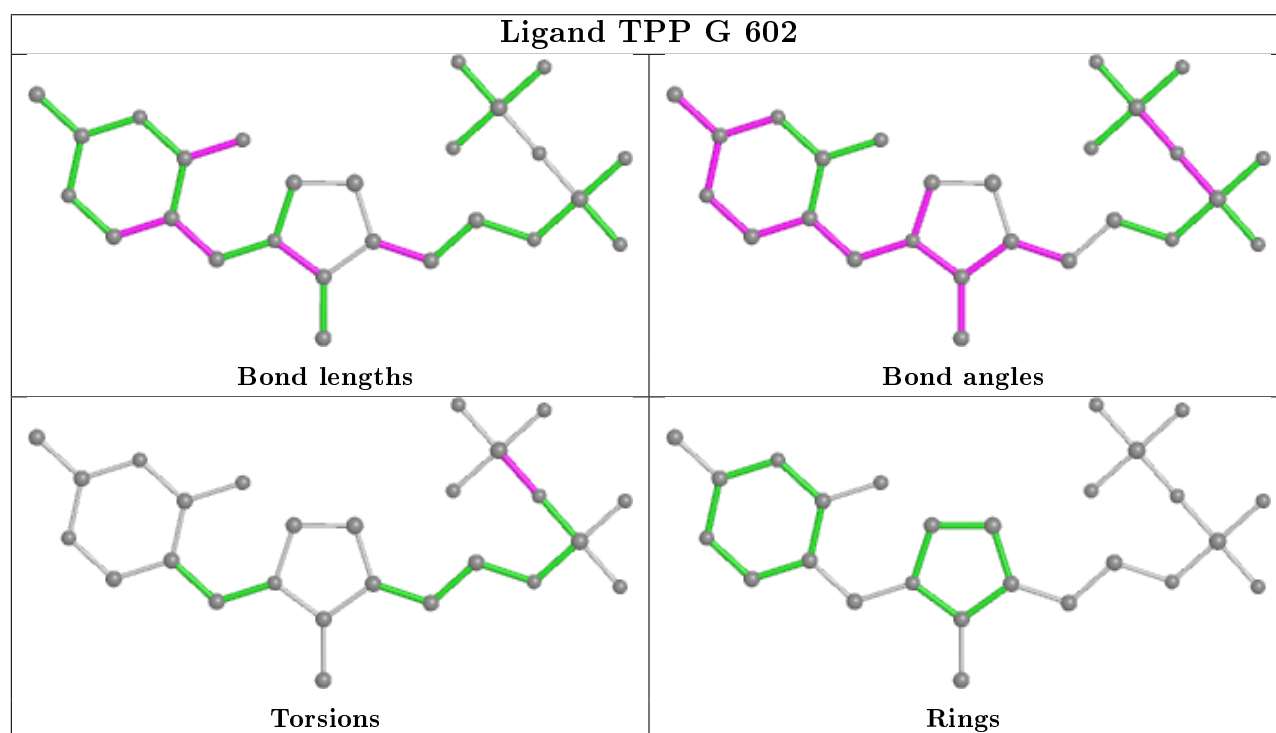
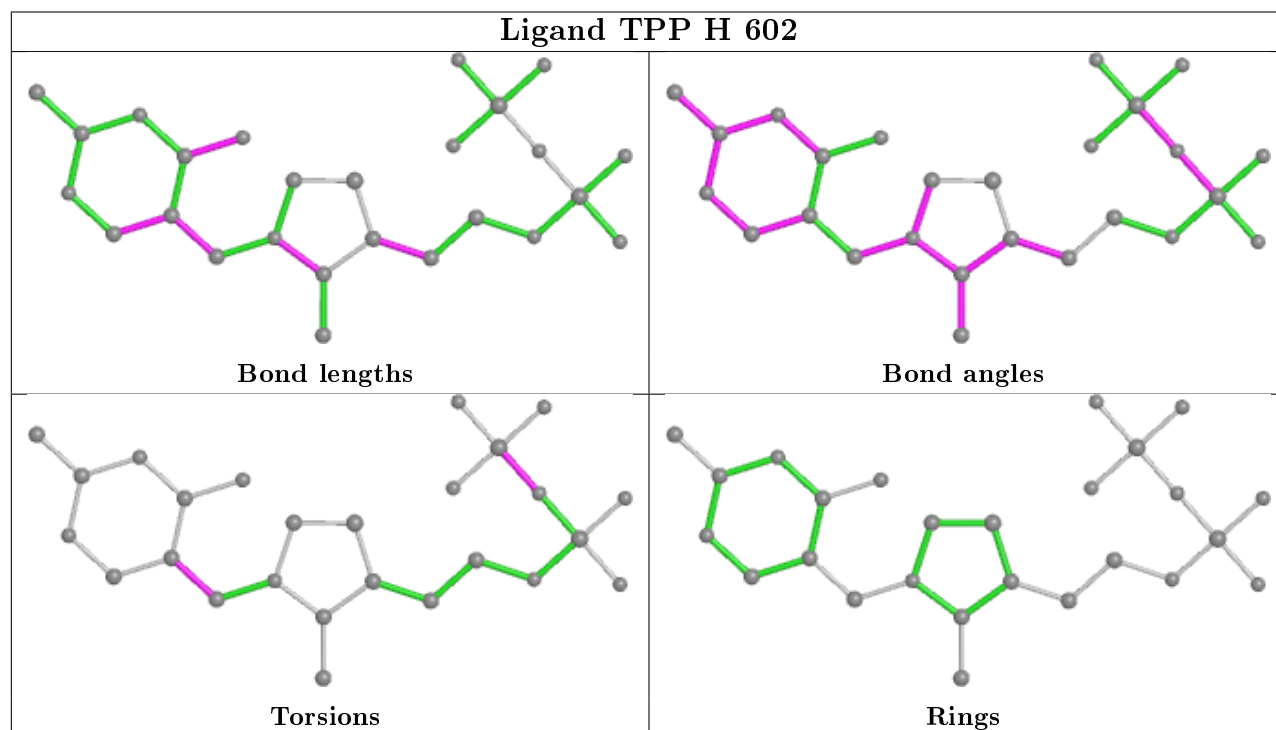
There are no ring outliers.

8 monomers are involved in 63 short contacts:

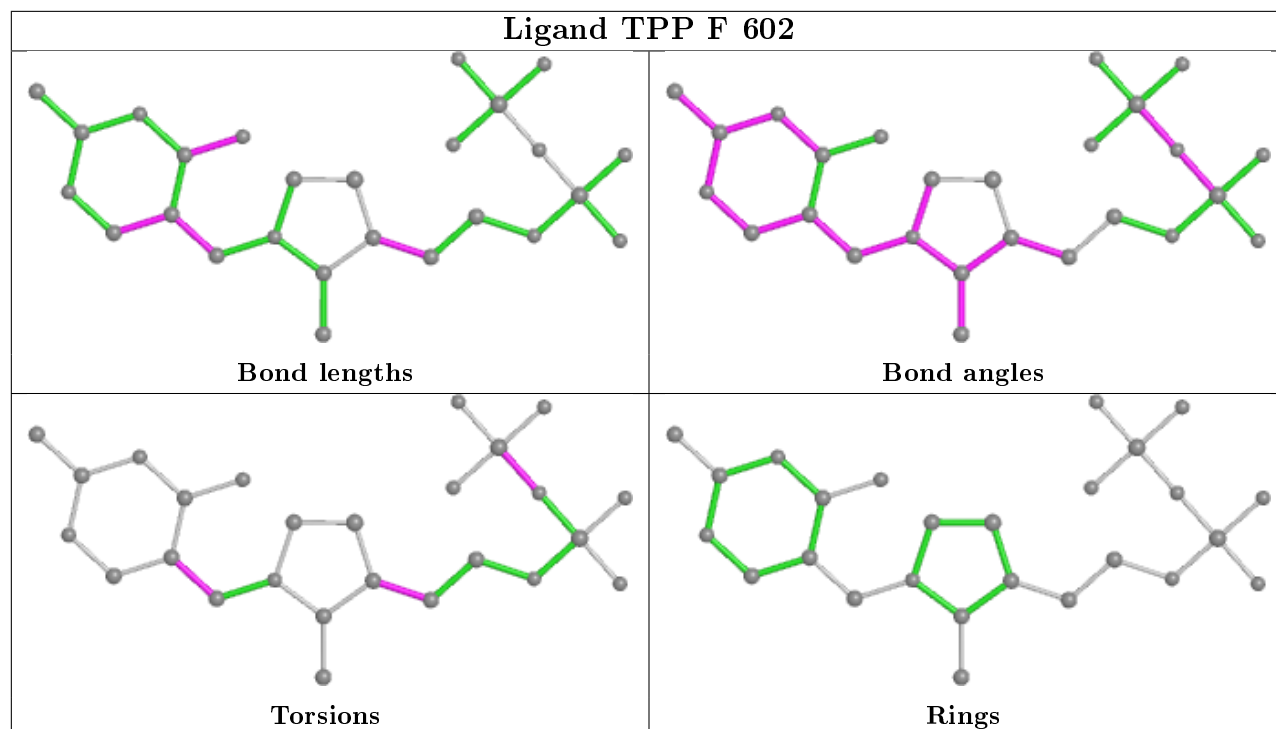
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	602	TPP	9	0
3	G	602	TPP	10	0
3	F	602	TPP	9	0
3	D	602	TPP	6	0
3	B	602	TPP	7	0
3	E	602	TPP	5	0
3	C	602	TPP	9	0
3	A	602	TPP	8	0

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

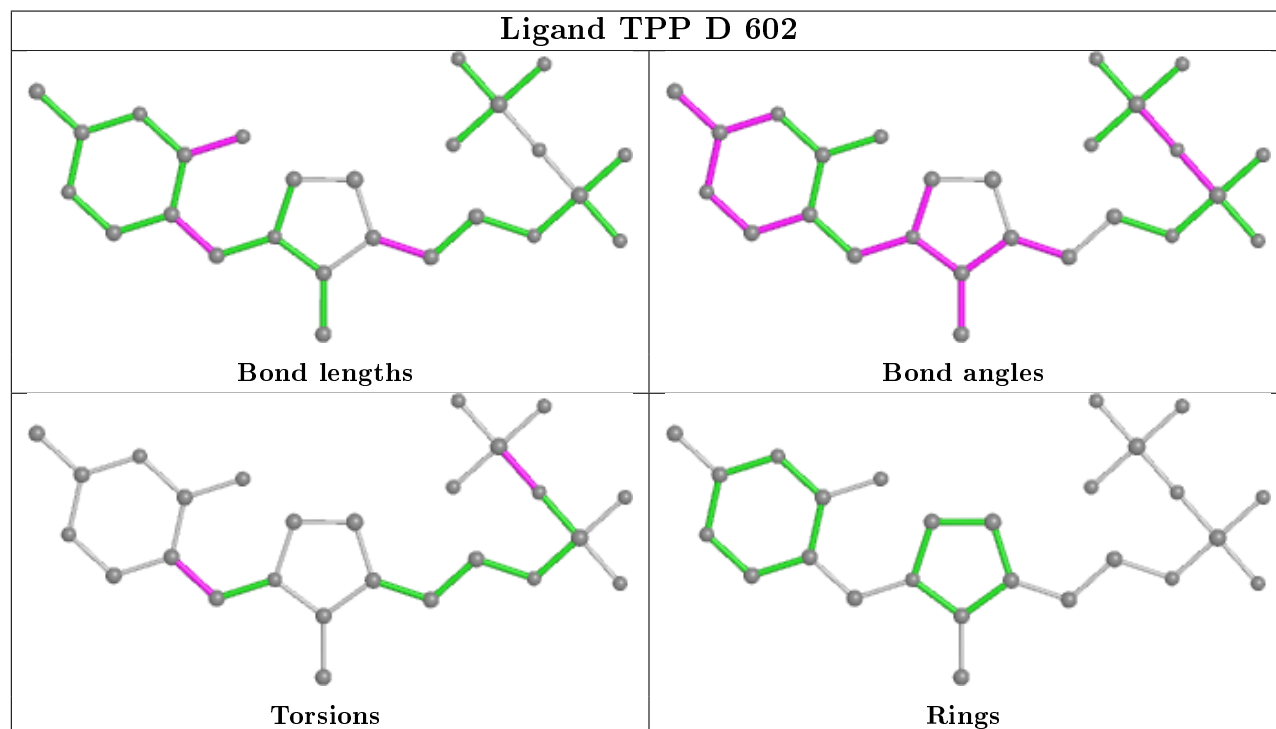
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



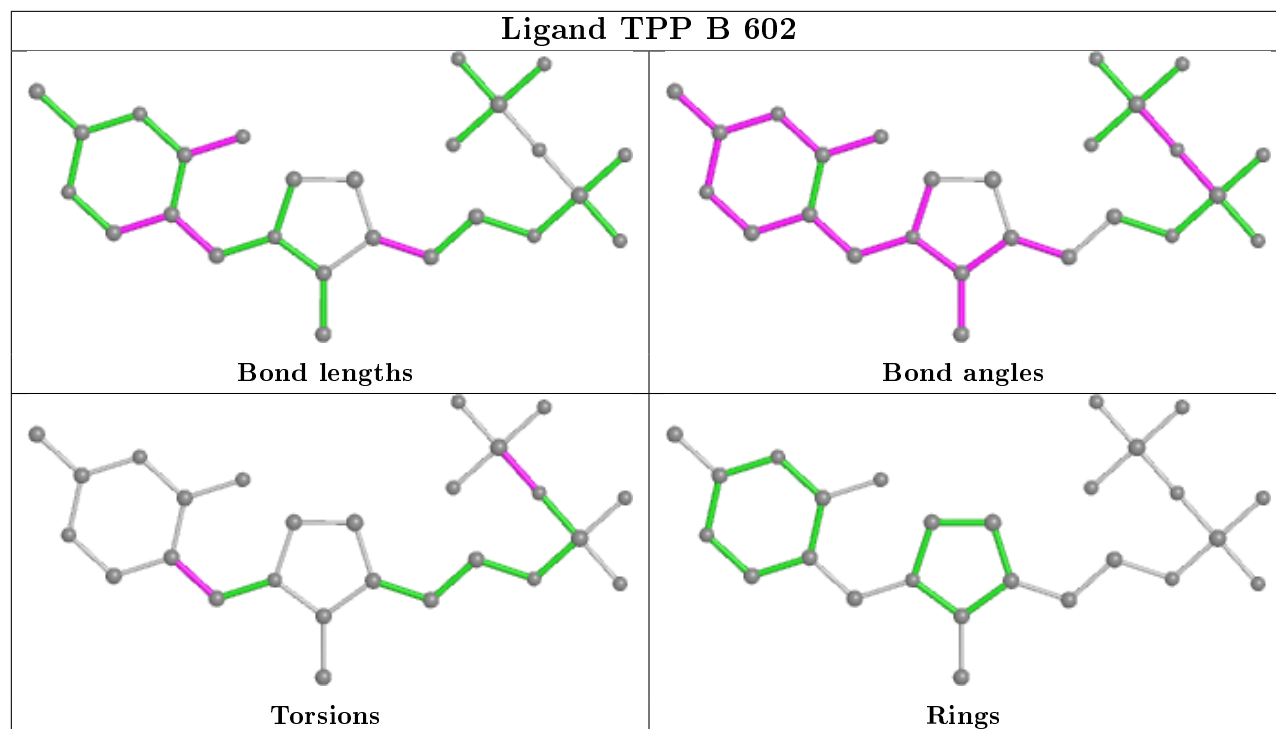
Ligand TPP F 602



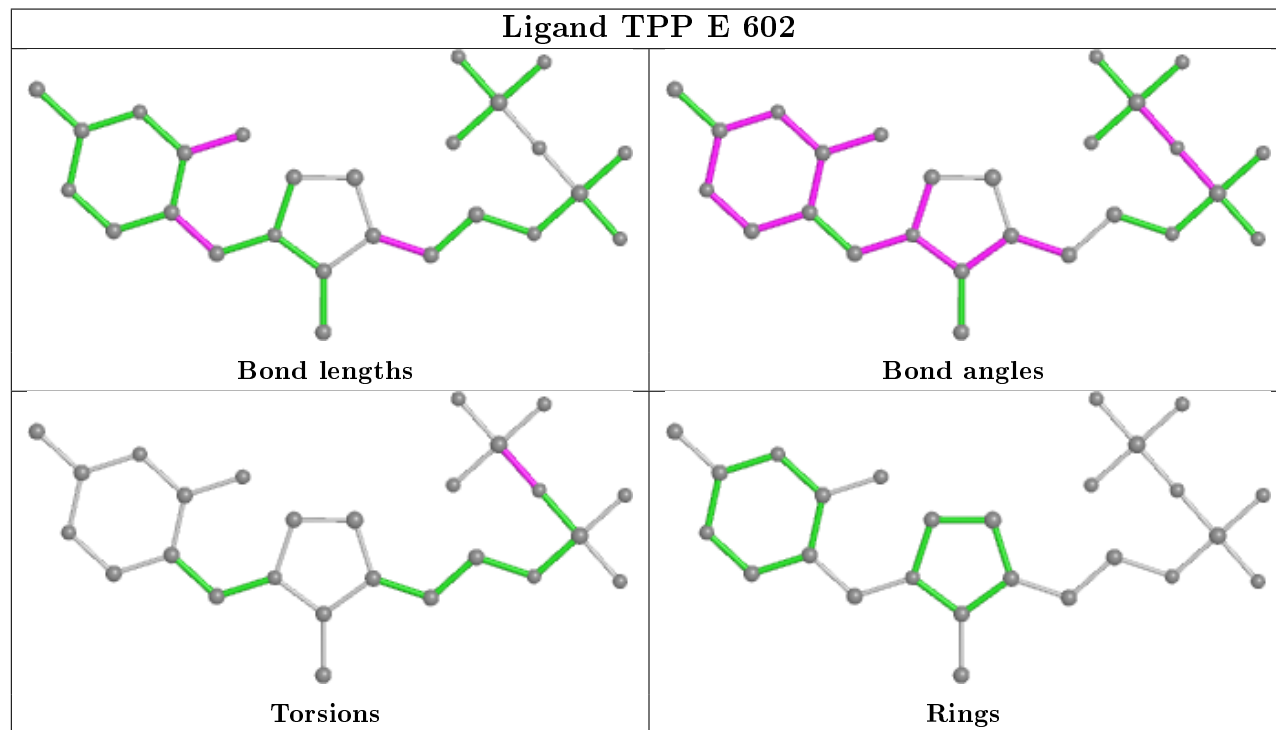
Ligand TPP D 602

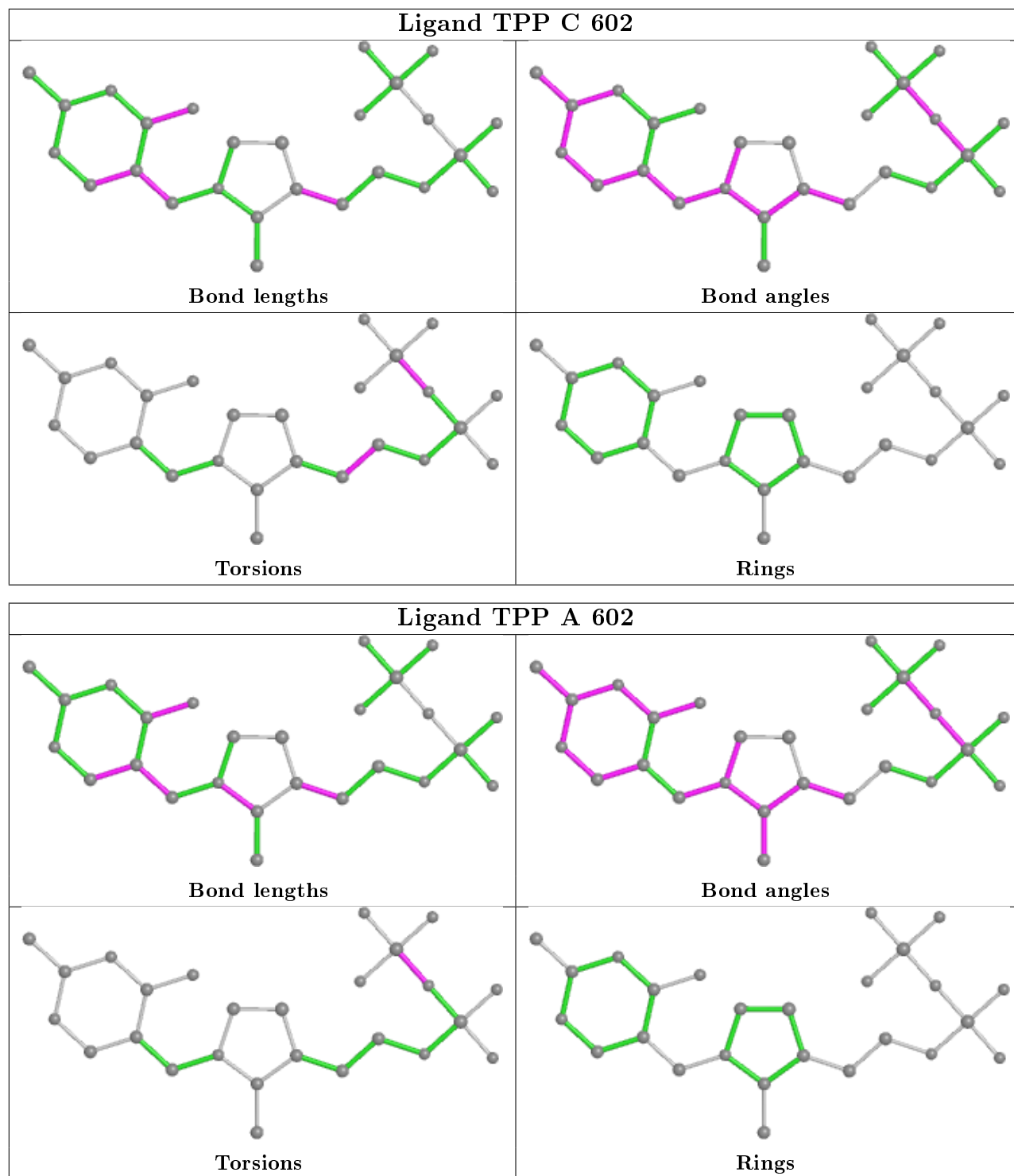


Ligand TPP B 602



Ligand TPP E 602





5.7 Other polymers ⓘ

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	563/582 (96%)	-0.46	3 (0%) 91 75	31, 65, 89, 116	0
1	B	562/582 (96%)	-0.50	1 (0%) 95 87	28, 64, 110, 146	0
1	C	562/582 (96%)	-0.51	0 100 100	30, 60, 88, 116	0
1	D	562/582 (96%)	-0.47	0 100 100	32, 72, 112, 132	0
1	E	562/582 (96%)	-0.45	0 100 100	31, 69, 115, 149	0
1	F	562/582 (96%)	-0.42	3 (0%) 91 75	32, 66, 97, 136	0
1	G	562/582 (96%)	-0.48	0 100 100	22, 64, 116, 144	0
1	H	562/582 (96%)	-0.48	1 (0%) 95 87	26, 58, 97, 130	0
All	All	4497/4656 (96%)	-0.47	8 (0%) 95 87	22, 64, 107, 149	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	563	ALA	3.2
1	F	563	ALA	3.0
1	A	2	ALA	2.6
1	A	564	GLY	2.5
1	B	563	ALA	2.4
1	F	2	ALA	2.3
1	A	557	ILE	2.2
1	F	560	ASP	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

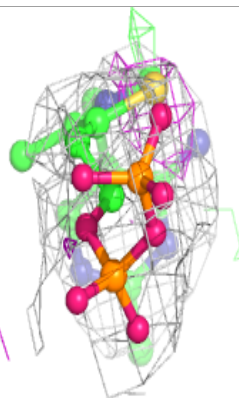
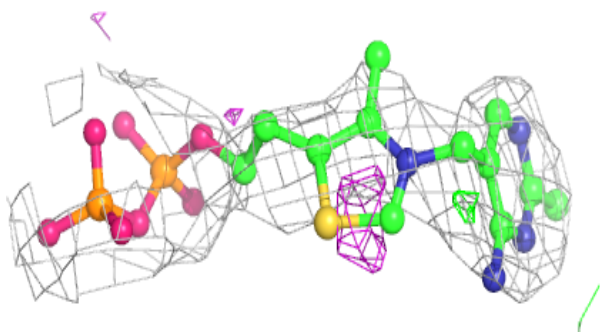
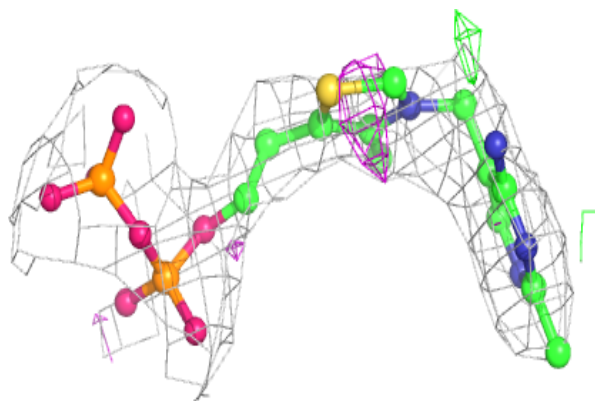
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	601	1/1	0.94	0.21	56,56,56,56	0
3	TPP	A	602	26/26	0.95	0.19	55,71,98,114	0
3	TPP	D	602	26/26	0.96	0.18	73,92,112,123	0
3	TPP	E	602	26/26	0.96	0.17	66,73,93,100	0
2	MG	D	601	1/1	0.96	0.11	75,75,75,75	0
3	TPP	H	602	26/26	0.96	0.19	52,84,108,121	0
3	TPP	F	602	26/26	0.96	0.16	61,82,112,119	0
3	TPP	B	602	26/26	0.96	0.17	77,95,120,126	0
3	TPP	G	602	26/26	0.96	0.17	55,75,91,94	0
3	TPP	C	602	26/26	0.97	0.16	60,80,103,108	0
2	MG	H	601	1/1	0.97	0.14	43,43,43,43	0
2	MG	G	601	1/1	0.98	0.16	36,36,36,36	0
2	MG	B	601	1/1	0.98	0.12	68,68,68,68	0
2	MG	C	601	1/1	0.99	0.15	49,49,49,49	0
2	MG	F	601	1/1	0.99	0.10	45,45,45,45	0
2	MG	E	601	1/1	0.99	0.16	62,62,62,62	0

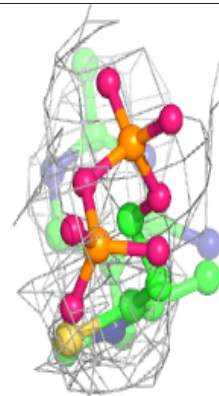
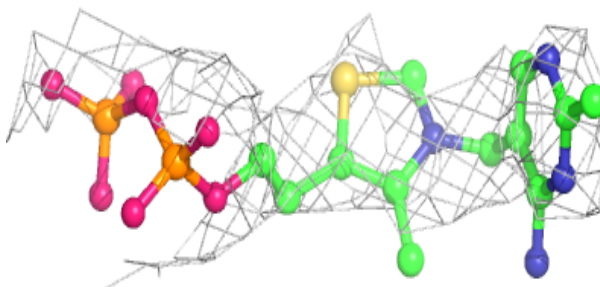
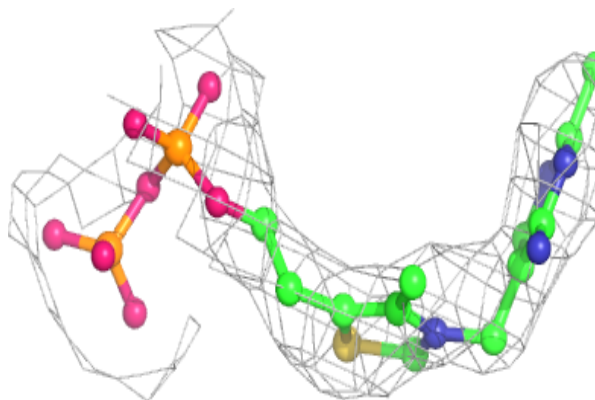
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP 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)

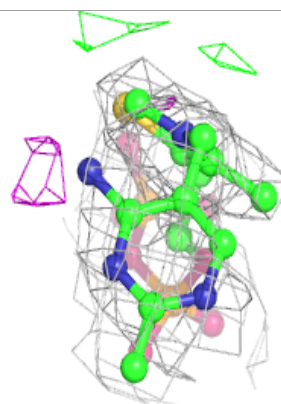
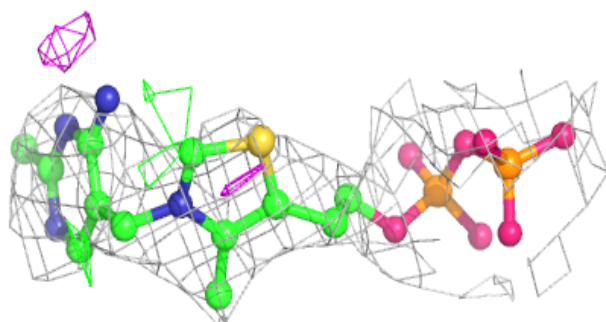
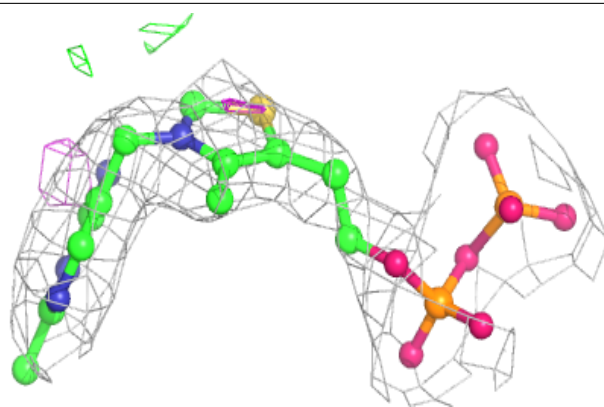
**Electron density around TPP D 602:**

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

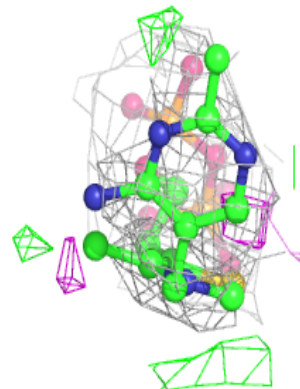
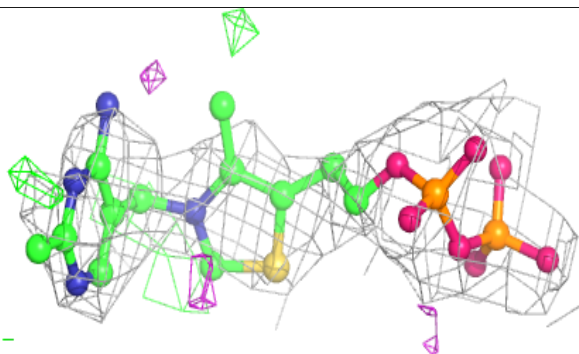
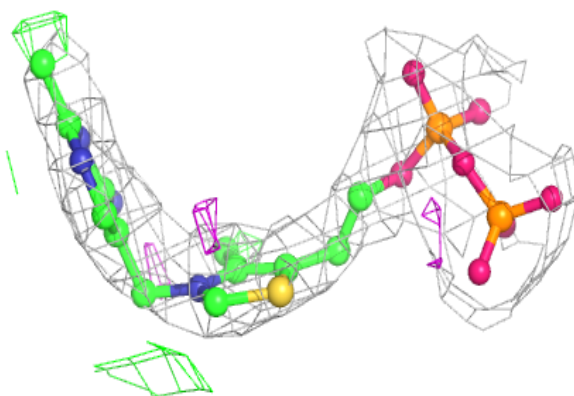


Electron density around TPP E 602:

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

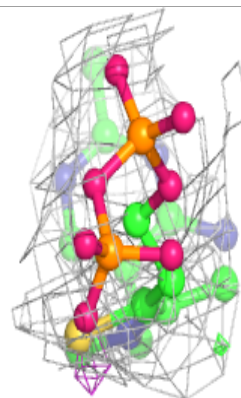
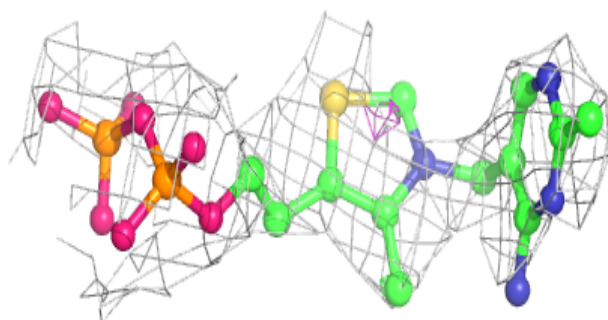
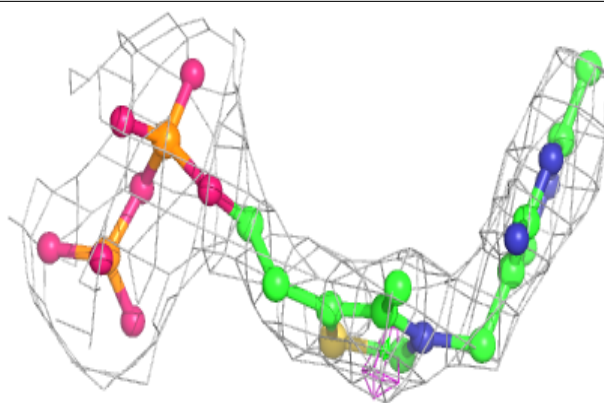
**Electron density around TPP H 602:**

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

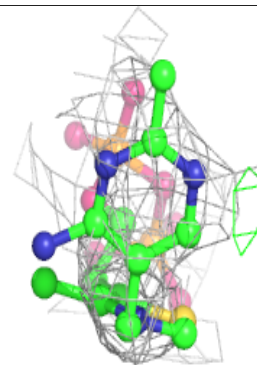
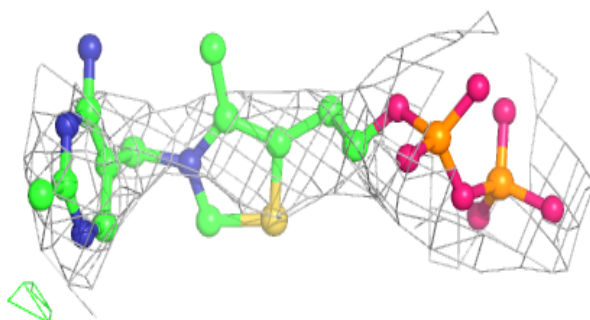
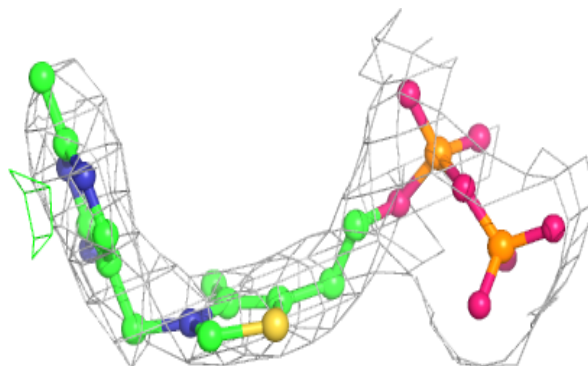


Electron density around TPP F 602:

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

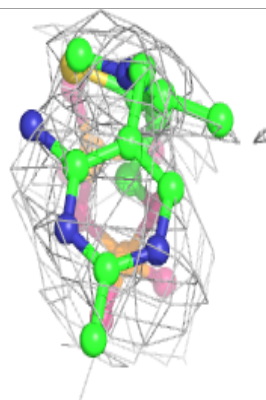
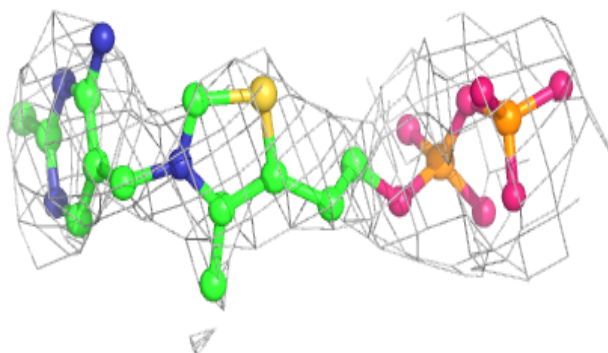
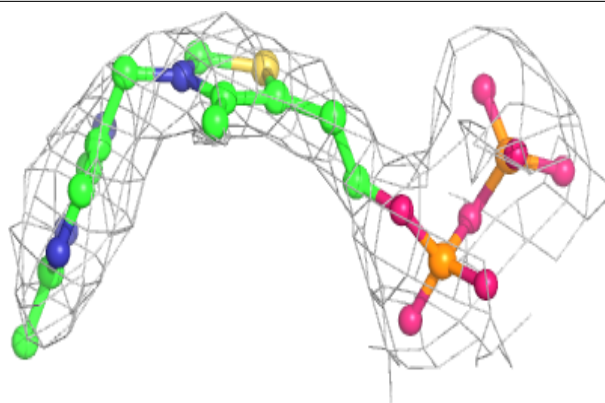
**Electron density around TPP B 602:**

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

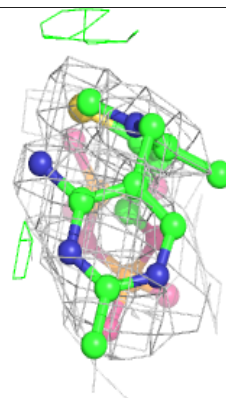
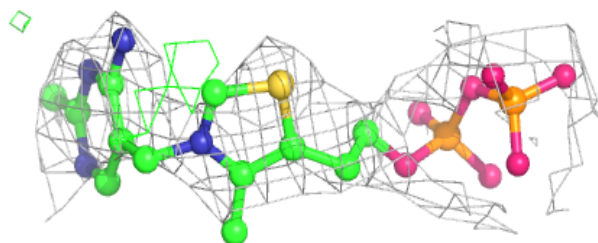
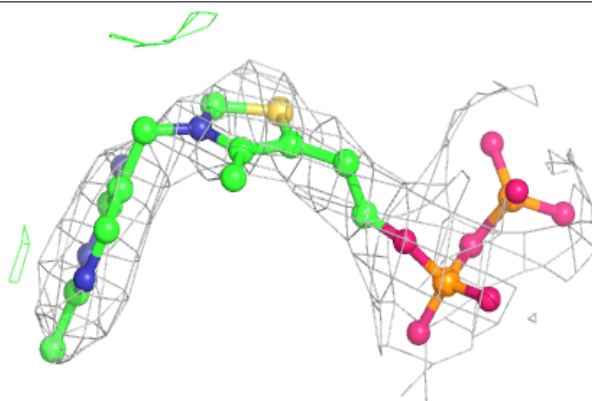


Electron density around TPP G 602:

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

**Electron density around TPP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.