Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 02:37 AM EDT

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 (i) 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 (i)) were used in the production of this report:

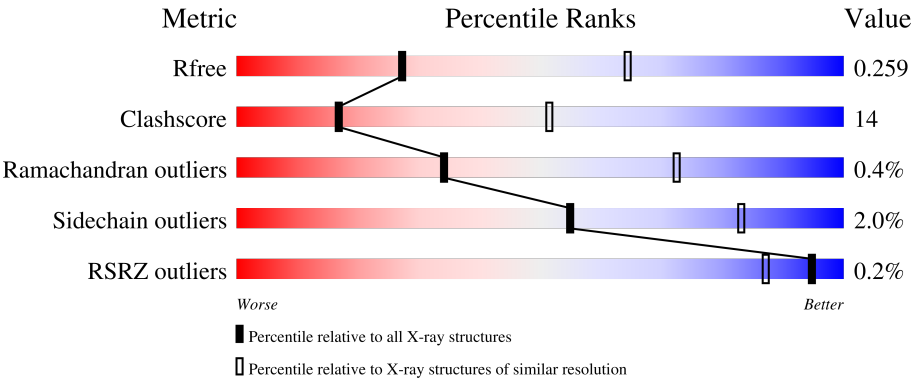
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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 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 <=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	% 69% 27%
1	B	582	74% 22%
1	C	582	75% 21%
1	D	582	70% 26%
1	E	582	73% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	582	
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 (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

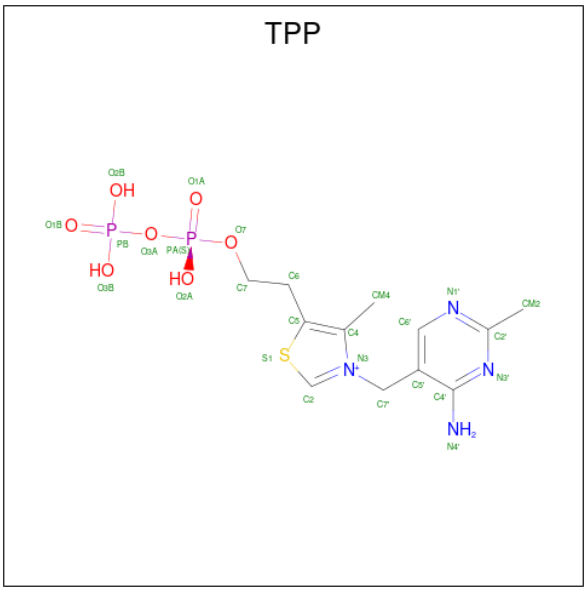
Continued from previous page...

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	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 4 is water.

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

Continued on next page...

Continued from previous page...

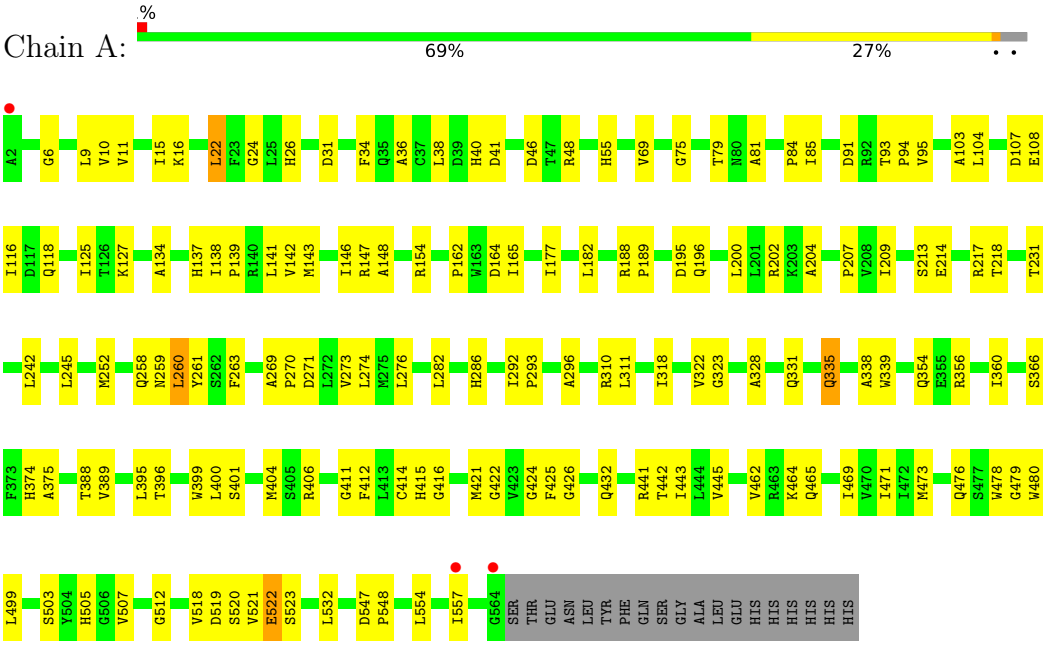
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	3	Total O 3 3	0	0

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.

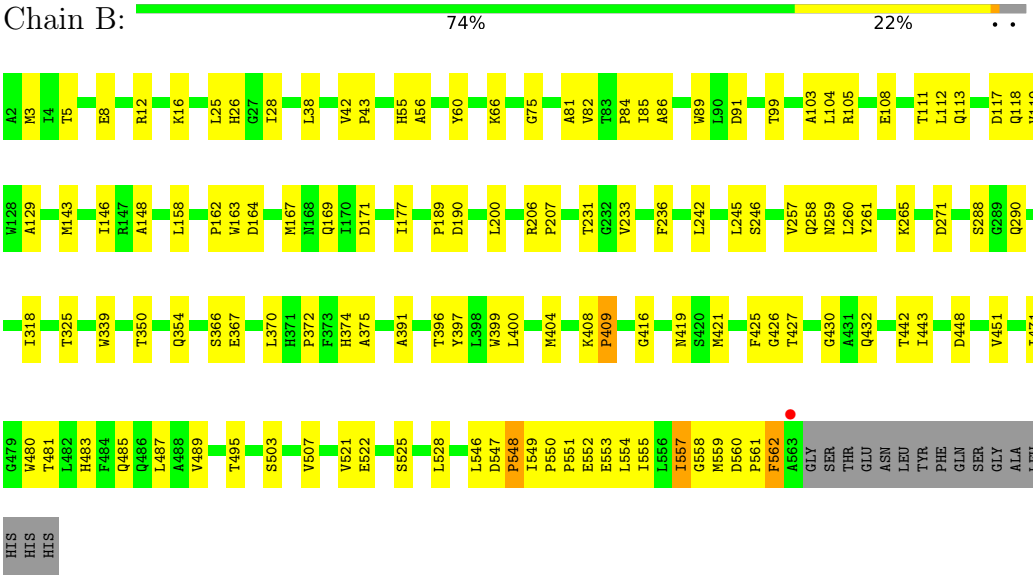
• Molecule 1: Formolase

Chain A:



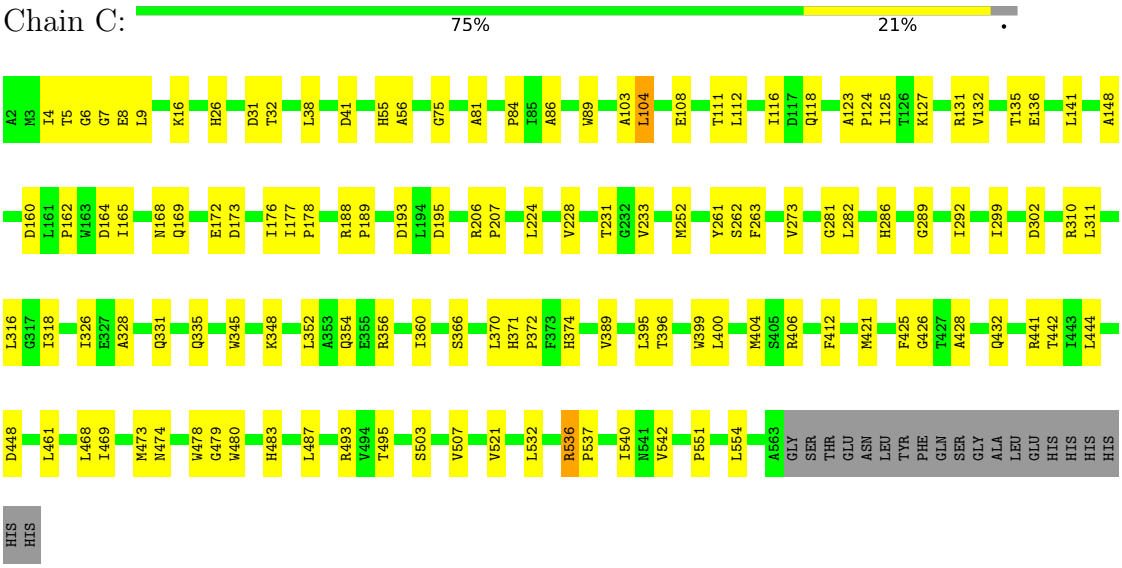
• Molecule 1: Formolase

Chain B:



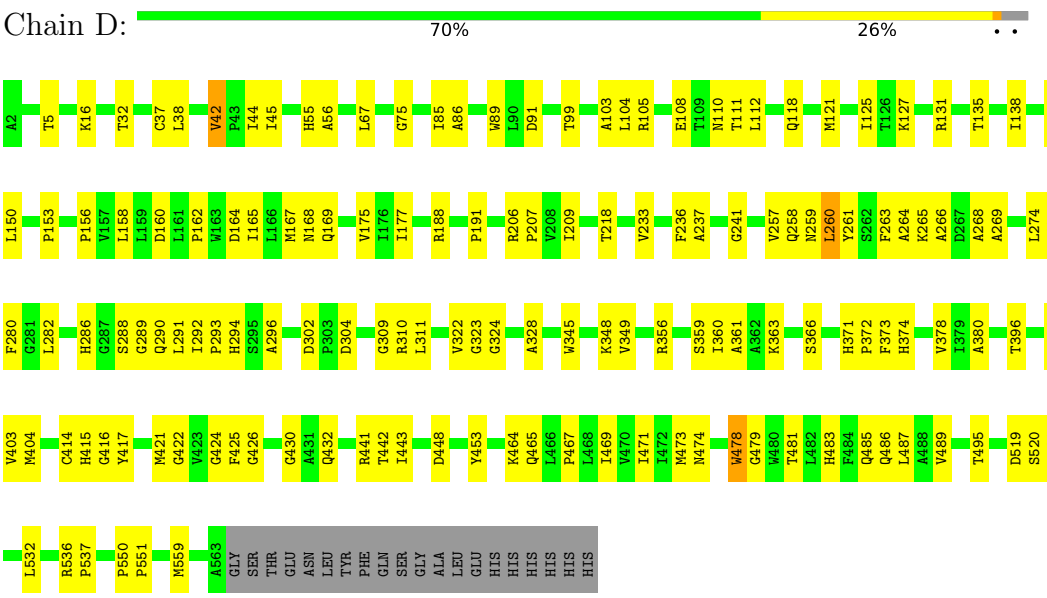
• Molecule 1: Formolase

Chain C:



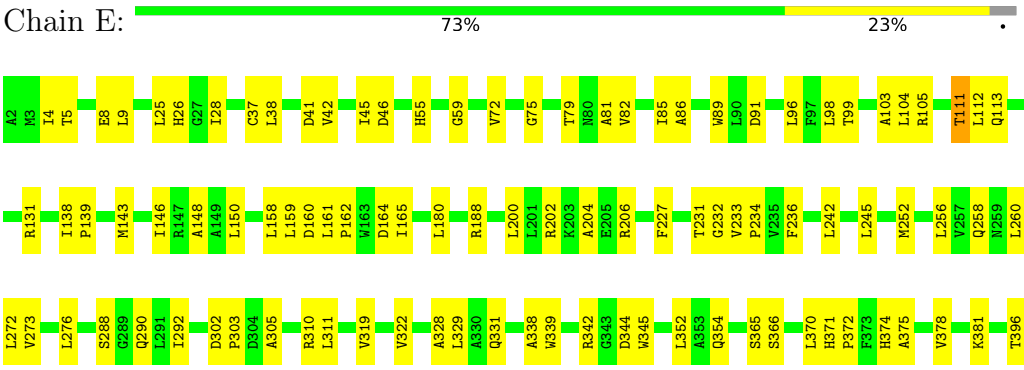
• Molecule 1: Formolase

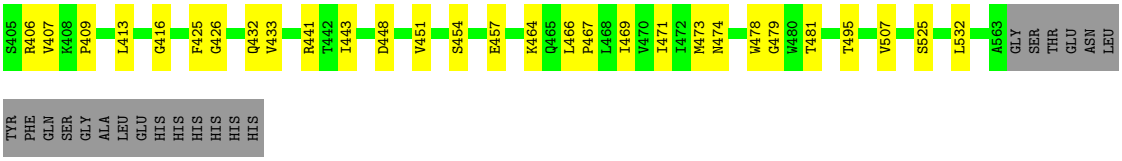
Chain D:



• Molecule 1: Formolase

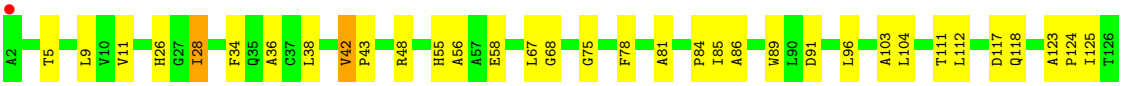
Chain E:

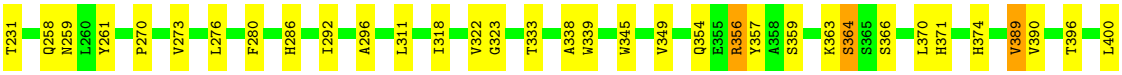




• Molecule 1: Formolase

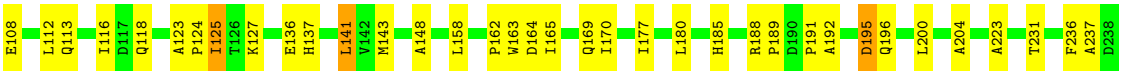
Chain F:

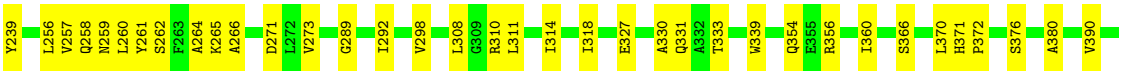


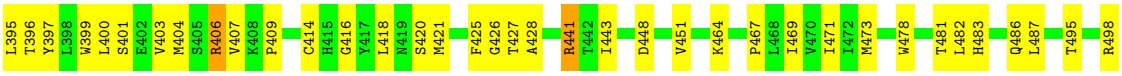


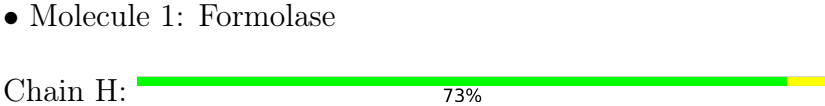
• Molecule 1: Formolase

Chain G:



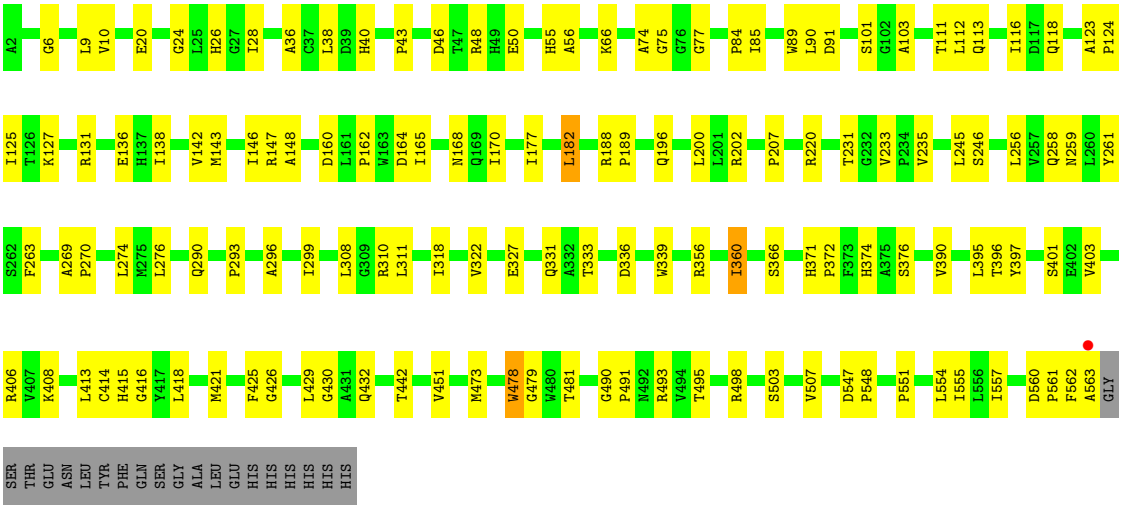






• Molecule 1: Formolase

Chain H:


A2 G6 L9 V10 E20 G24 L25 H26 G27 I28 A36 C37 L38 D39 H40 P43 D46 T47 R48 H49 E50 H55 A56 K66 A74 G75 G76 G77 P84 I85 W89 L90 D91 S101 G102 A103 T111 L112 Q113 I116 D117 Q118 A123 P124
I125 T126 K127 R131 E136 H137 I138 V142 M143 I146 R147 A148 D160 L161 P162 W163 D164 I165 N168 Q169 I170 I177 L182 R188 P189 Q196 L200 L201 R202 P207 R220 T231 G232 V233 P234 V235 L245 S246 L256 V257 Q258 N259 L260 Y261
S262 F263 A269 P270 L274 M275 L276 Q290 P293 A296 I299 L308 G309 R310 L311 I318 V322 E327 Q331 A332 T333 D336 W339 R356 I360 S366 H371 P372 F373 H374 A375 S376 V390 L395 T396 Y397 S401 E402 V403
R406 V407 K408 L413 C414 H415 G416 Y417 L418 M421 F425 G426 L429 G430 A431 Q432 T442 V451 M473 W478 G479 W480 T481 G490 P491 N492 R493 V494 T495 R498 S503 V507 D547 P548 P551 L554 I555 L556 I557 D560 P561 F562 A563 GLY
SER THR GLU ASN LEU TYR PHE GLN SER GLY ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	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 $< |L| >$, $< L^2 >$ 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	0.50	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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:4:ILE:HD11	1:E:8:GLU:HG3	1.61	0.82
1:E:425:PHE:HZ	1:E:451:VAL:CG2	1.90	0.82

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:91:ASP:OD1	1:A:416:GLY:HA3	1.91	0.70
1:A:462:VAL:CG2	1:A:512:GLY:O	2.39	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

Continued on next page...

Continued from previous page...

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:5:THR:HG22	1:G:169:GLN:HG2	1.80	0.64
1:G:55:HIS:HB2	1:G:426:GLY:HA3	1.79	0.64

Continued on next page...

Continued from previous page...

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:75:GLY:H	1:D:118:GLN:HE22	1.46	0.64
1:D:282:LEU:HD12	1:D:286:HIS:CE1	2.32	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:310:ARG:HH12	1:B:108:GLU:HG3	1.62	0.63
1:A:370:LEU:HD21	1:A:375:ALA:HB2	1.80	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:91:ASP:OD1	1:H:416:GLY:HA3	2.00	0.62
1:H:112:LEU:HD21	1:H:113:GLN:NE2	2.15	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:HN42	3:E:602:TPP:H2	1.65	0.62
1:F:104:LEU:HD12	1:F:165:ILE:HD11	1.83	0.61

Continued on next page...

Continued from previous page...

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:HG22	1:E:125:ILE:O	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:4:ILE:HG22	1:C:5:THR:N	2.16	0.60
1:C:108:GLU:HG3	1:D:310:ARG:NH2	2.17	0.60
1:C:370:LEU:CD1	1:C:521:VAL:HG22	2.32	0.60
1:D:292:ILE:HG13	1:D:292:ILE:O	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:127:LYS:CE	1:H:148:ALA:O	2.48	0.59
1:H:147:ARG:HG2	1:H:182:LEU:HD23	1.84	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

Continued on next page...

Continued from previous page...

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:28:ILE:HG23	1:H:481:THR:HG22	1.83	0.59
1:G:108:GLU:HG3	1:H:310:ARG:HH21	1.66	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:4:ILE:HG13	1:E:8:GLU:CB	2.33	0.57
1:E:441:ARG:HE	1:E:467:PRO:HB2	1.67	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:46:ASP:OD1	1:G:464:LYS:HE3	2.05	0.57
1:G:127:LYS:CE	1:G:148:ALA:O	2.53	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

Continued on next page...

Continued from previous page...

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:A:503:SER:HB2	1:A:505:HIS:CE1	2.41	0.56
1:C:299:ILE:HG23	1:C:316:LEU:HB3	1.87	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:55:HIS:HB2	1:A:426:GLY:HA3	1.88	0.56
1:A:137:HIS:O	1:A:141:LEU:HB2	2.06	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

Continued on next page...

Continued from previous page...

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:5:THR:O	1:G:8:GLU:N	2.40	0.54
1:G:407:VAL:O	1:G:409:PRO:HD3	2.07	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:258:GLN:NE2	1:D:401:SER:HB2	2.22	0.54
1:D:310:ARG:HG3	1:D:311:LEU:HG	1.88	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

Continued on next page...

Continued from previous page...

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: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:B:548:PRO:O	1:B:549:ILE:HG13	2.08	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:36:ALA:O	1:A:40:HIS:HD2	1.92	0.52
1:A:356:ARG:O	1:A:360:ILE:HG12	2.08	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:9:LEU:HD11	1:F:170:ILE:HD11	1.92	0.52
1:F:111:THR:HG22	1:F:112:LEU:H	1.73	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:93:THR:HG22	1:A:95:VAL:HG23	1.91	0.52
1:A:189:PRO:HB3	1:A:318:ILE:HG21	1.92	0.52
1:A:231:THR:OG1	1:A:233:VAL:HG22	2.09	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:81:ALA:O	1:C:84:PRO:HD2	2.11	0.51
1:C:231:THR:OG1	1:C:233:VAL:HG22	2.10	0.51

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:24:GLY:O	1:A:46:ASP:HA	2.11	0.49
1:A:270:PRO:O	1:A:296:ALA:HB2	2.12	0.49
1:B:75:GLY:H	1:B:118:GLN:NE2	2.10	0.49
1:B:103:ALA:HA	1:B:164:ASP:HB2	1.93	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

Continued on next page...

Continued from previous page...

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:75:GLY:H	1:A:118:GLN:HE22	1.61	0.48
1:A:547:ASP:N	1:A:548:PRO:CD	2.76	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:HD12	1:D:45:ILE:H	1.79	0.48
1:H:125:ILE:HD13	1:H:125:ILE:HA	1.57	0.48
1:A:286:HIS:NE2	1:B:111:THR:HG23	2.29	0.48
1:A:478:TRP:CE2	1:A:499:LEU:HD11	2.48	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

Continued on next page...

Continued from previous page...

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:81:ALA:C	1:A:84:PRO:HD2	2.33	0.47
1:A:479:GLY:N	3:A:602:TPP:O3B	2.39	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: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:HD13	1:G:125:ILE:HA	1.55	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: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:3:MET:HG2	1:G:170:ILE:C	2.34	0.47
1:G:298:VAL:HB	1:G:314:ILE:HG22	1.97	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

Continued on next page...

Continued from previous page...

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:4:ILE:HG12	1:E:8:GLU:CB	2.45	0.46
1:E:206:ARG:HG2	1:E:345:TRP:CE3	2.50	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

Continued on next page...

Continued from previous page...

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:443:ILE:HG23	1:G:471:ILE:CD1	2.46	0.46
1:G:469:ILE:H	1:G:469:ILE:HG13	1.50	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:C	1:B:25:LEU:HD23	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:HD2	1:H:220:ARG:HA	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:89:TRP:N	1:D:156:PRO:HG3	2.32	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:F:181:VAL:HG11	1:G:314:ILE:HG13	1.98	0.45
3:G:602:TPP:HN42	3:G:602:TPP:C2	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:99:THR:CG2	1:B:158:LEU:HD11	2.47	0.45
1:B:103:ALA:CA	1:B:164:ASP:HB2	2.46	0.45
3:C:602:TPP:H2	3:C:602:TPP:HN42	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

Continued on next page...

Continued from previous page...

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:5:THR:HG22	1:B:169:GLN:HG2	1.98	0.45
1:B:231:THR:HG22	1:B:339:TRP:CE2	2.52	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:HD2	1:F:48:ARG:HA	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:99:THR:HG21	1:E:158:LEU:HD11	1.98	0.45
1:E:407:VAL:O	1:E:409:PRO:HD3	2.17	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:99:THR:CG2	1:G:158:LEU:HD11	2.48	0.44
1:G:236:PHE:CE2	1:G:260:LEU:HD21	2.52	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: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:G:258:GLN:NE2	1:G:401:SER:HB2	2.33	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

Continued on next page...

Continued from previous page...

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:48:ARG:HA	1:H:48:ARG:HD2	1.75	0.44
1:H:164:ASP:O	1:H:168:ASN:HB2	2.17	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:C:104:LEU:HD13	1:C:162:PRO:CG	2.48	0.44
1:G:448:ASP:O	1:H:48:ARG:NH2	2.51	0.44
1:H:162:PRO:HG2	1:H:165:ILE:HD12	1.99	0.44
1:A:26:HIS:HD2	1:A:34:PHE:CD1	2.36	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:B:125:ILE:HG22	1:B:125:ILE:O	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:HA	1:A:331:GLN:NE2	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:46:ASP:OD1	1:E:464:LYS:HE3	2.17	0.43
1:E:273:VAL:HG21	1:E:292:ILE:HG23	2.00	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:O	1:B:528:LEU:HD12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ILE:HG22	1:B:555:ILE:O	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:9:LEU:HD11	1:G:170:ILE:HD11	1.99	0.43
1:G:93:THR:HG22	1:G:95:VAL:HG23	2.00	0.43
1:G:258:GLN:HE22	1:G:401:SER:CB	2.31	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:67:LEU:HG	1:F:68:GLY:N	2.34	0.43
1:F:203:LYS:HE3	1:F:203:LYS:HB2	1.76	0.43
1:H:136:GLU:CD	1:H:136:GLU:H	2.22	0.43
1:A:389:VAL:HG13	1:A:412:PHE:HD1	1.82	0.43
1:B:60:TYR:CZ	1:B:66:LYS:HE3	2.54	0.43
1:B:104:LEU:CD1	1:B:162:PRO:CG	2.96	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:103:ALA:CA	1:F:164:ASP:HB2	2.48	0.43
1:F:125:ILE:HA	1:F:125:ILE:HD13	1.63	0.43
1:A:26:HIS:NE2	1:A:31:ASP:OD1	2.52	0.43
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.74	0.43
1:D:421:MET:HG2	3:D:602:TPP:C6'	2.49	0.43
1:H:116:ILE:HD12	1:H:116:ILE:O	2.19	0.43
1:A:116:ILE:HG13	1:A:116:ILE:O	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:F:193:ASP:OD1	1:G:185:HIS:HD2	2.02	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:GLU:H	1:G:136:GLU:CD	2.22	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:O	1:E:265:LYS:CG	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:218:THR:OG1	1:A:323:GLY:HA3	2.19	0.42
1:A:274:LEU:HD21	1:A:276:LEU:HD21	2.01	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:25:LEU:HD22	3:F:602:TPP:HN41	1.85	0.42
1:E:202:ARG:HH12	1:E:338:ALA:C	2.22	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:425:PHE:CE1	1:B:451:VAL:HA	2.51	0.42
1:B:432:GLN:HE22	1:B:442:THR:H	1.68	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:81:ALA:C	1:G:84:PRO:HD2	2.39	0.42
1:G:237:ALA:O	1:G:256:LEU:HA	2.20	0.42
1:H:123:ALA:N	1:H:124:PRO:HD2	2.34	0.42
1:A:335:GLN:N	1:A:335:GLN:CD	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

Continued on next page...

Continued from previous page...

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:69:VAL:HG22	1:G:96:LEU:HB3	2.00	0.42
1:G:143:MET:HE1	1:G:180:LEU:HB2	2.02	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:4:ILE:CG2	1:C:8:GLU:HB3	2.50	0.41
1:C:135:THR:OG1	1:C:165:ILE:HG23	2.20	0.41
1:D:486:GLN:H	1:D:486:GLN:HG2	1.65	0.41
1:E:28:ILE:HG22	1:F:481:THR:HG22	2.02	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: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

Continued on next page...

Continued from previous page...

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:89:TRP:HB2	1:E:125:ILE:O	2.19	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: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:89:TRP:HB2	1:G:125:ILE:O	2.19	0.41
1:G:104:LEU:HD13	1:G:162:PRO:HG2	2.02	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:86:ALA:O	1:C:89:TRP:HB3	2.20	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:CD	1:C:136:GLU:H	2.24	0.41
1:C:195:ASP:O	1:C:195:ASP:OD1	2.39	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:231:THR:HG22	1:A:339:TRP:CE2	2.56	0.41
1:A:236:PHE:CZ	1:A:260:LEU:HD21	2.56	0.41
1:B:391:ALA:HB1	1:B:397:TYR:HB2	2.03	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:206:ARG:NH2	1:D:269:ALA:O	2.54	0.41
1:D:264:ALA:O	1:D:266:ALA:N	2.54	0.41
1:E:45:ILE:HD12	1:E:45:ILE:H	1.86	0.41
1:G:556:LEU:HD23	1:G:556:LEU:HA	1.98	0.41
1:H:6:GLY:O	1:H:10:VAL:HG23	2.20	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:42:VAL:HA	1:F:43:PRO:HD3	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:CYS:SG	1:F:415:HIS:N	2.91	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:56:ALA:HA	1:C:426:GLY:O	2.21	0.40
1:C:554:LEU:HD23	1:C:554:LEU:HA	1.84	0.40
1:G:376:SER:CB	1:G:403:VAL:HG21	2.50	0.40
1:A:94:PRO:HB3	1:A:154:ARG:HB3	2.04	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:B:258:GLN:OE1	1:B:552:GLU:OE2	2.39	0.40
1:B:478:TRP:HB3	3:B:602:TPP:H61	2.03	0.40
1:C:4:ILE:CG2	1:C:8:GLU:HB2	2.51	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: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:A:507:VAL:HG13	1:B:507:VAL:HG13	2.03	0.40
1:B:99:THR:HG22	1:B:158:LEU:HD11	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:HH11	1:H:498:ARG:CG	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:79:THR:HA	1:E:82:VAL:HG23	2.02	0.40
1:E:344:ASP:OD1	1:E:344:ASP:N	2.54	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:HA	1:G:464:LYS:HD3	1.82	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	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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Sometimes 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

Continued on next page...

Continued from previous page...

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	G	602	2	22,27,27	2.87	5 (22%)	29,40,40	2.13	10 (34%)
3	TPP	D	602	2	22,27,27	2.57	3 (13%)	29,40,40	2.12	9 (31%)
3	TPP	F	602	2	22,27,27	2.00	4 (18%)	29,40,40	1.98	11 (37%)
3	TPP	E	602	2	22,27,27	2.88	3 (13%)	29,40,40	1.81	10 (34%)
3	TPP	H	602	2	22,27,27	2.33	5 (22%)	29,40,40	2.15	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%)
3	TPP	B	602	2	22,27,27	2.18	4 (18%)	29,40,40	2.26	12 (41%)

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	G	602	2	-	2/16/17/17	0/2/2/2
3	TPP	D	602	2	-	5/16/17/17	0/2/2/2
3	TPP	F	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	H	602	2	-	4/16/17/17	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
3	TPP	B	602	2	-	4/16/17/17	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

Continued on next page...

Continued from previous page...

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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	B	602	TPP	C6'-C5'-C7'-N3
3	B	602	TPP	PA-O3A-PB-O3B
3	C	602	TPP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

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

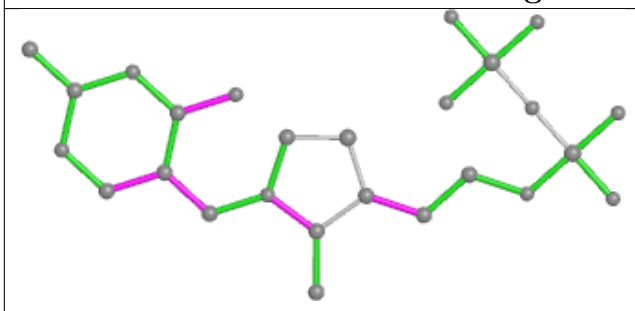
8 monomers are involved in 63 short contacts:

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

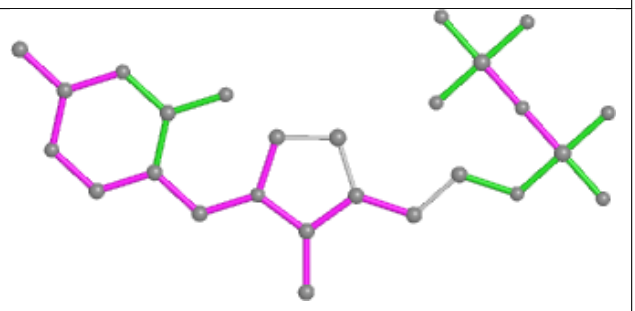
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

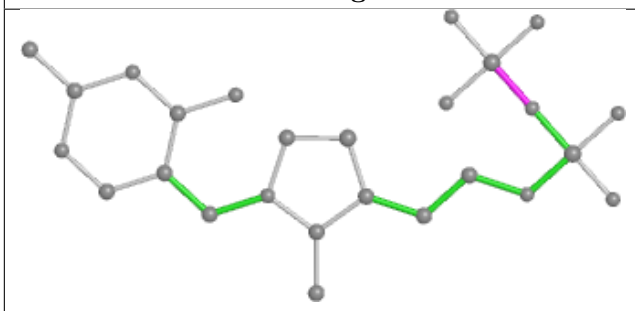
Ligand TPP G 602



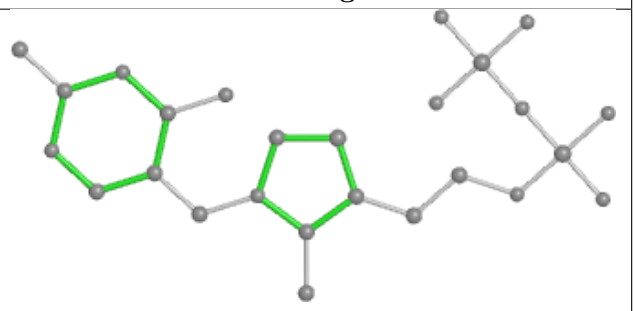
Bond lengths



Bond angles

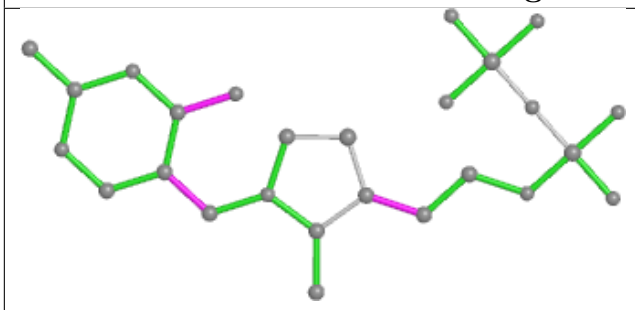


Torsions

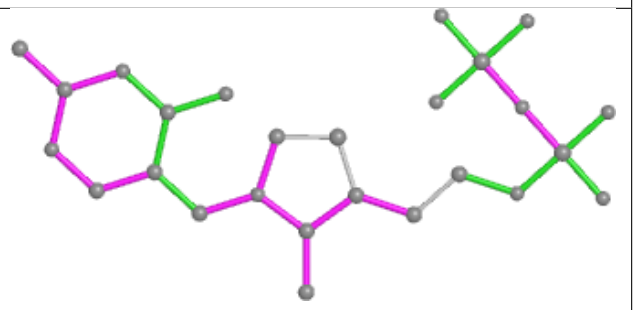


Rings

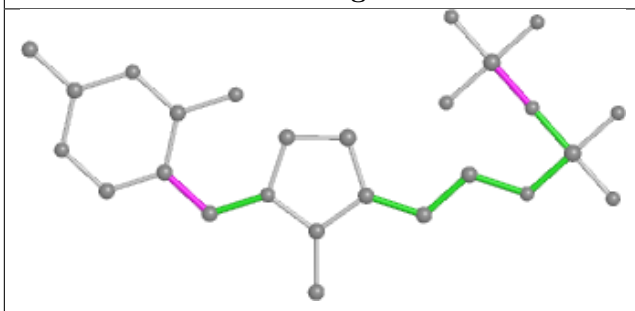
Ligand TPP D 602



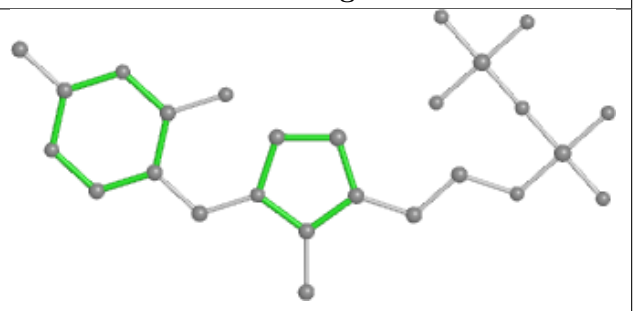
Bond lengths



Bond angles

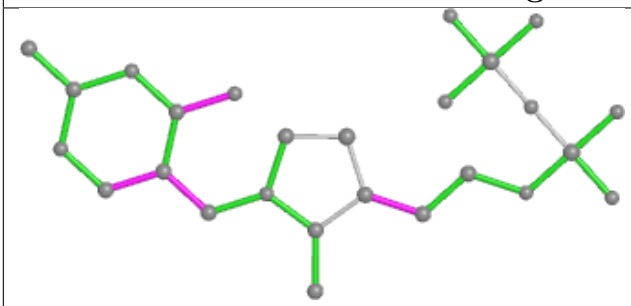


Torsions

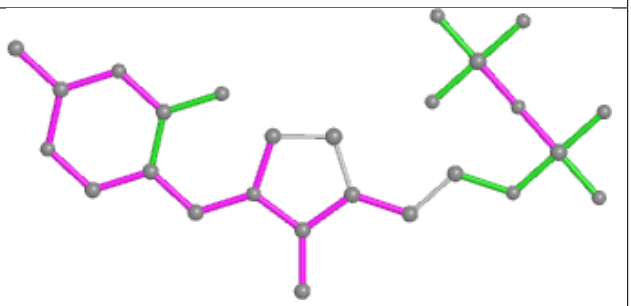


Rings

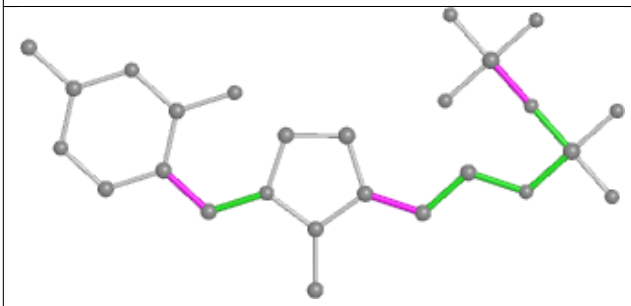
Ligand TPP F 602



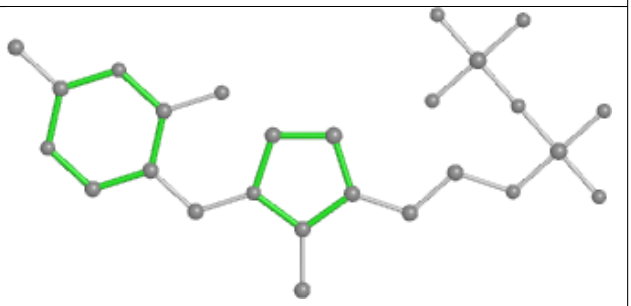
Bond lengths



Bond angles

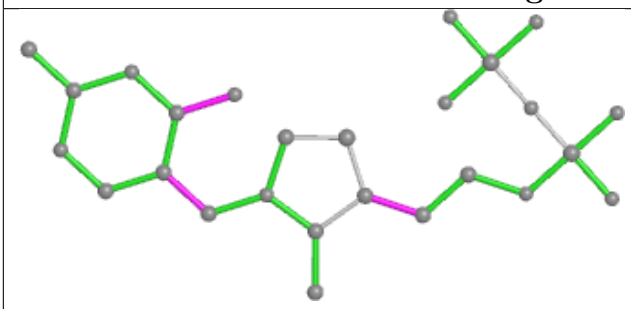


Torsions

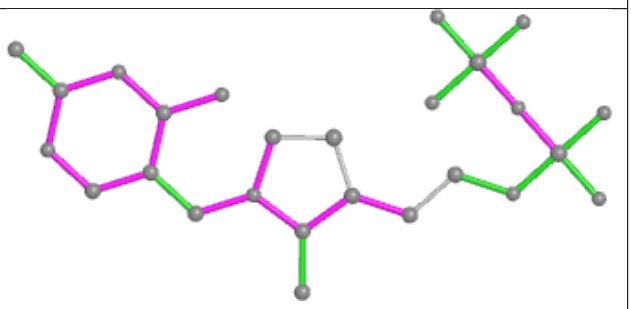


Rings

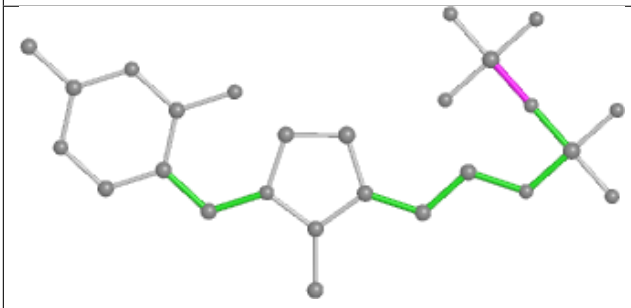
Ligand TPP E 602



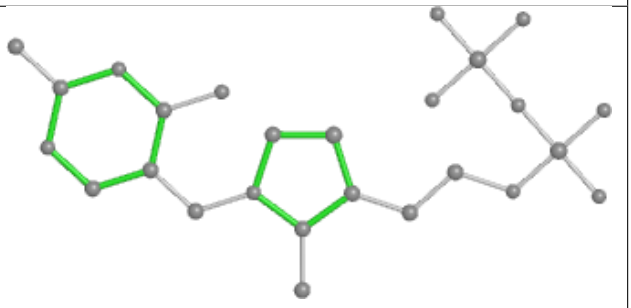
Bond lengths



Bond angles

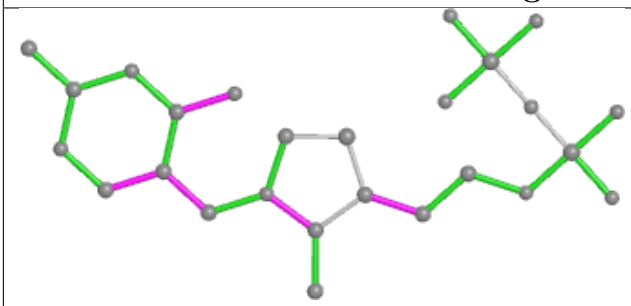


Torsions

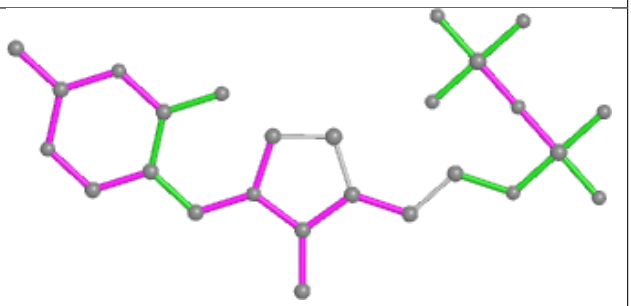


Rings

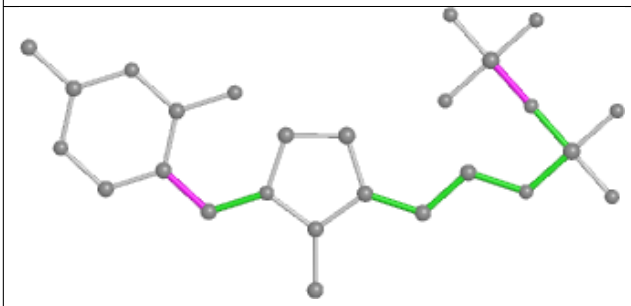
Ligand TPP H 602



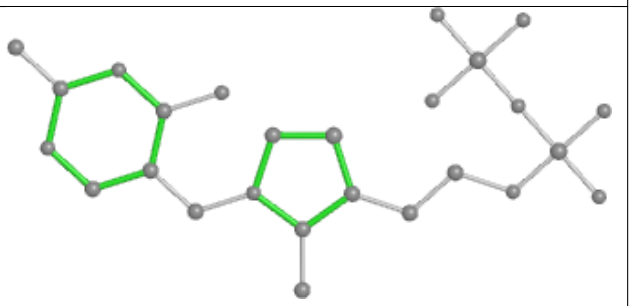
Bond lengths



Bond angles

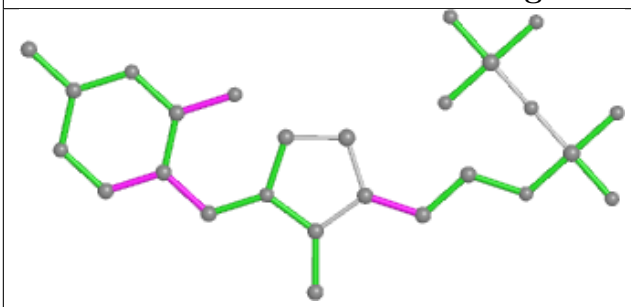


Torsions

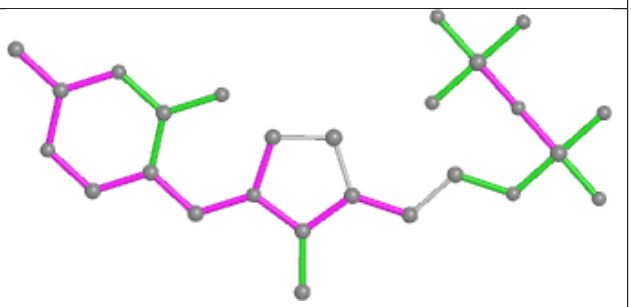


Rings

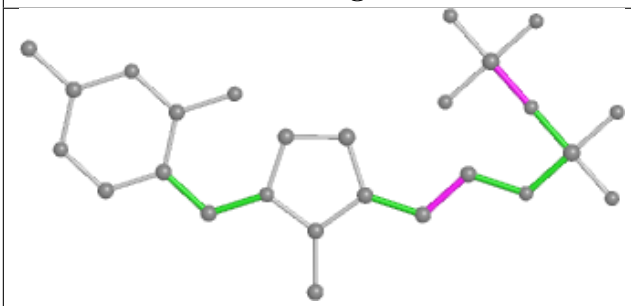
Ligand TPP C 602



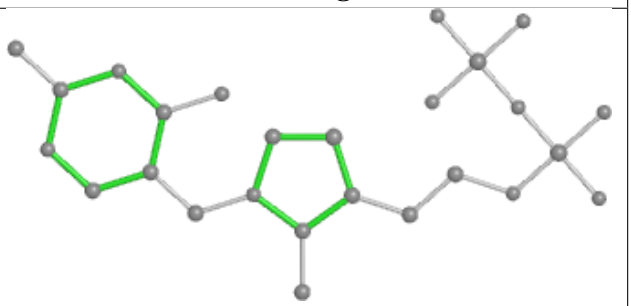
Bond lengths



Bond angles

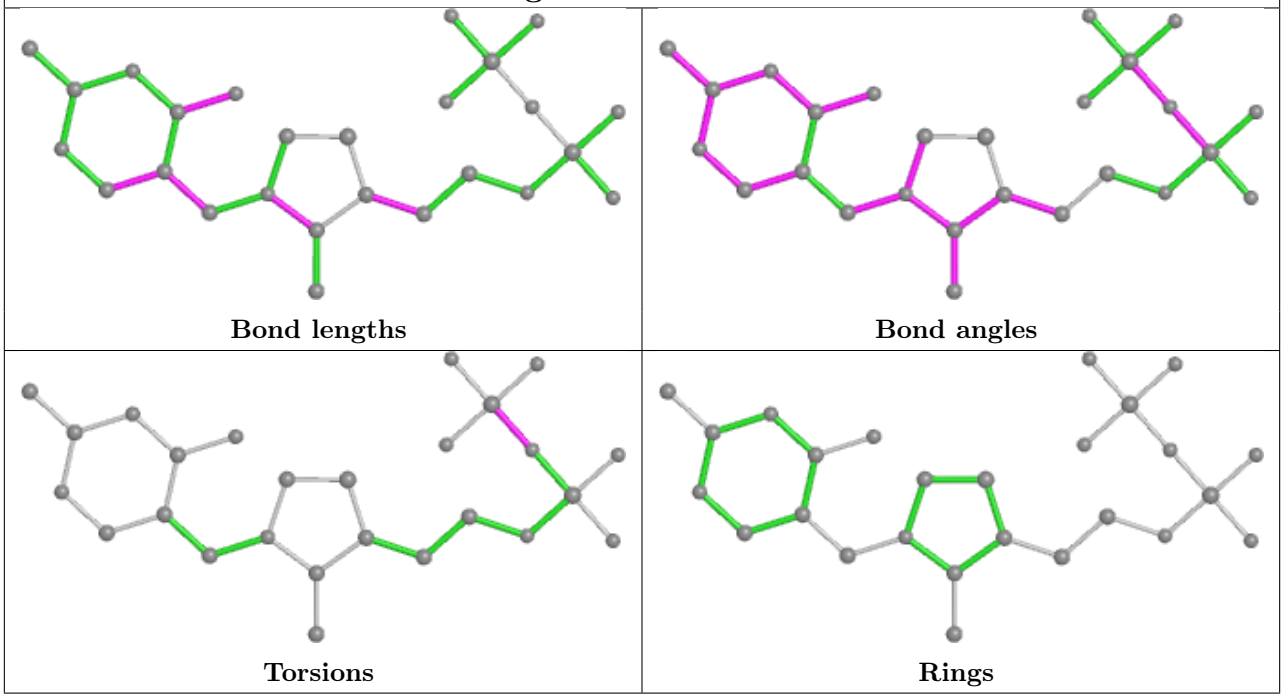


Torsions

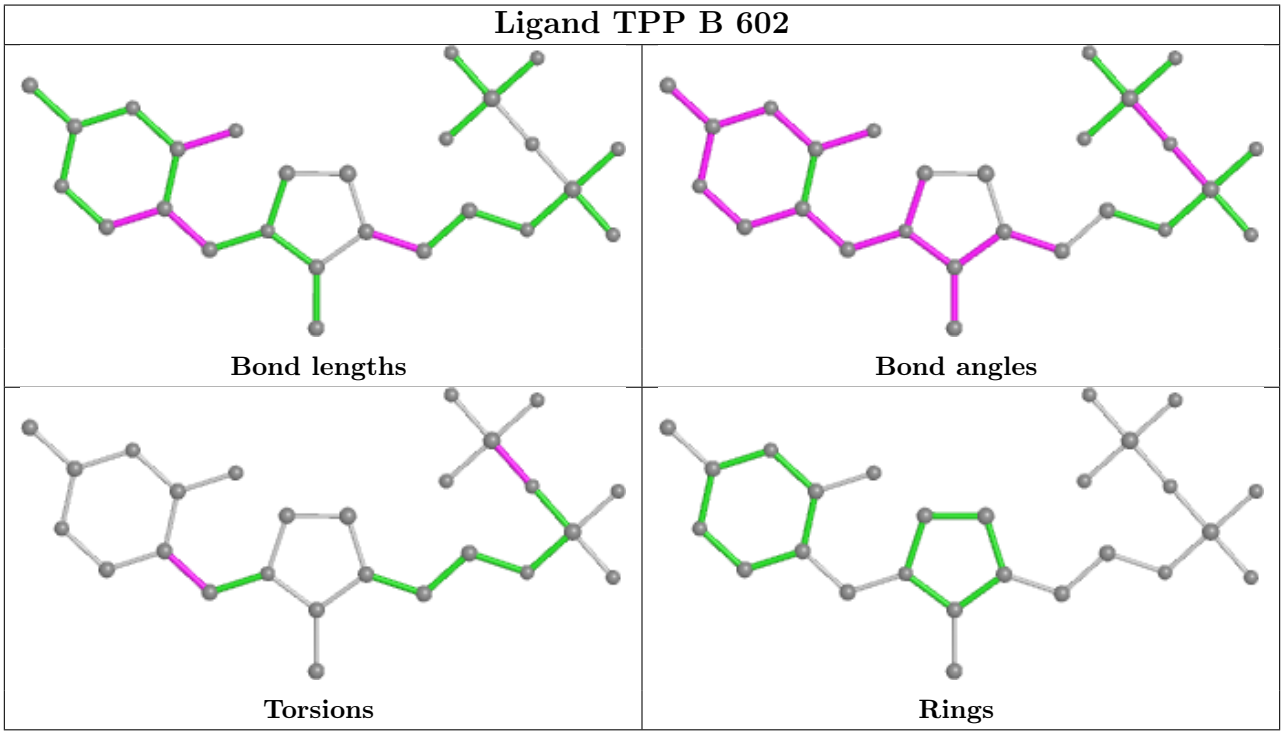


Rings

Ligand TPP A 602



Ligand TPP B 602



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, 95^{th} 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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

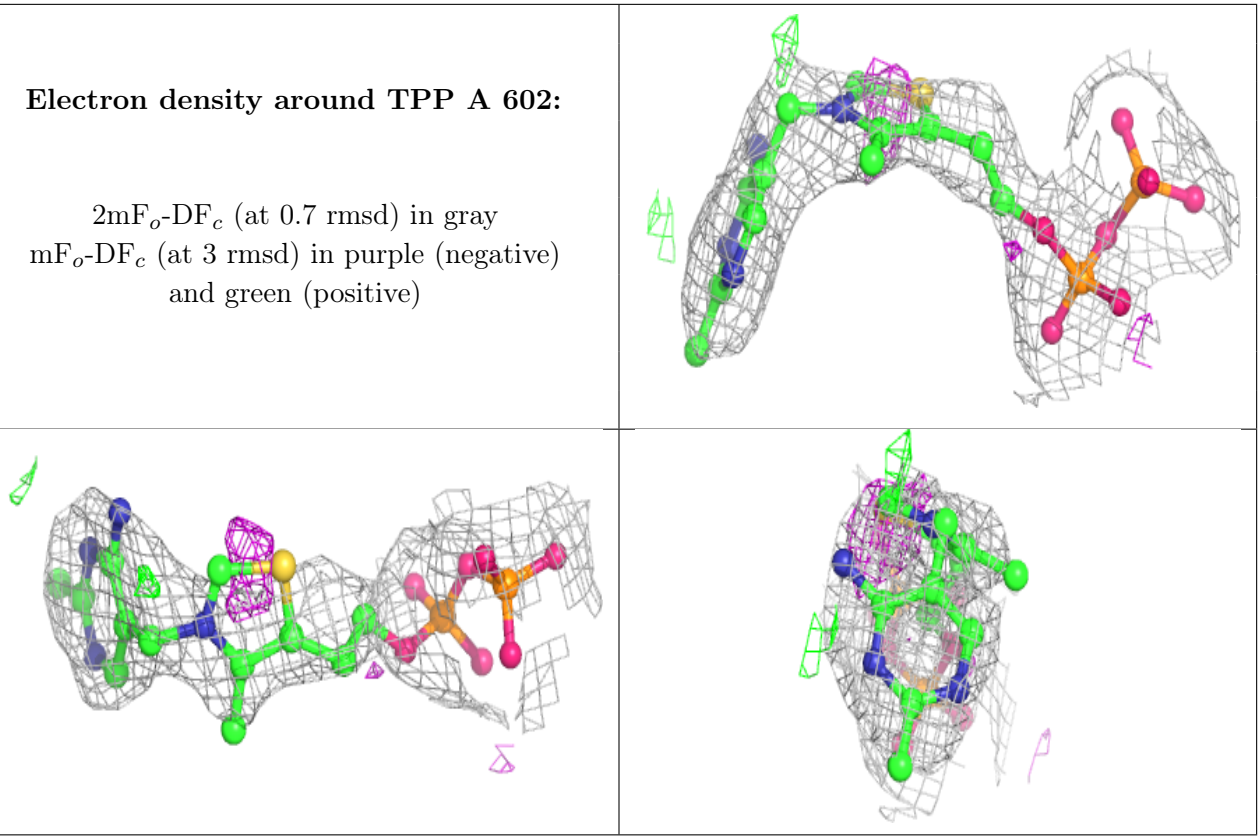
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	D	601	1/1	0.96	0.11	75,75,75,75	0
3	TPP	B	602	26/26	0.96	0.17	77,95,120,126	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
3	TPP	F	602	26/26	0.96	0.16	61,82,112,119	0
3	TPP	G	602	26/26	0.96	0.17	55,75,91,94	0
3	TPP	H	602	26/26	0.96	0.19	52,84,108,121	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	E	601	1/1	0.99	0.16	62,62,62,62	0
2	MG	F	601	1/1	0.99	0.10	45,45,45,45	0
2	MG	C	601	1/1	0.99	0.15	49,49,49,49	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.

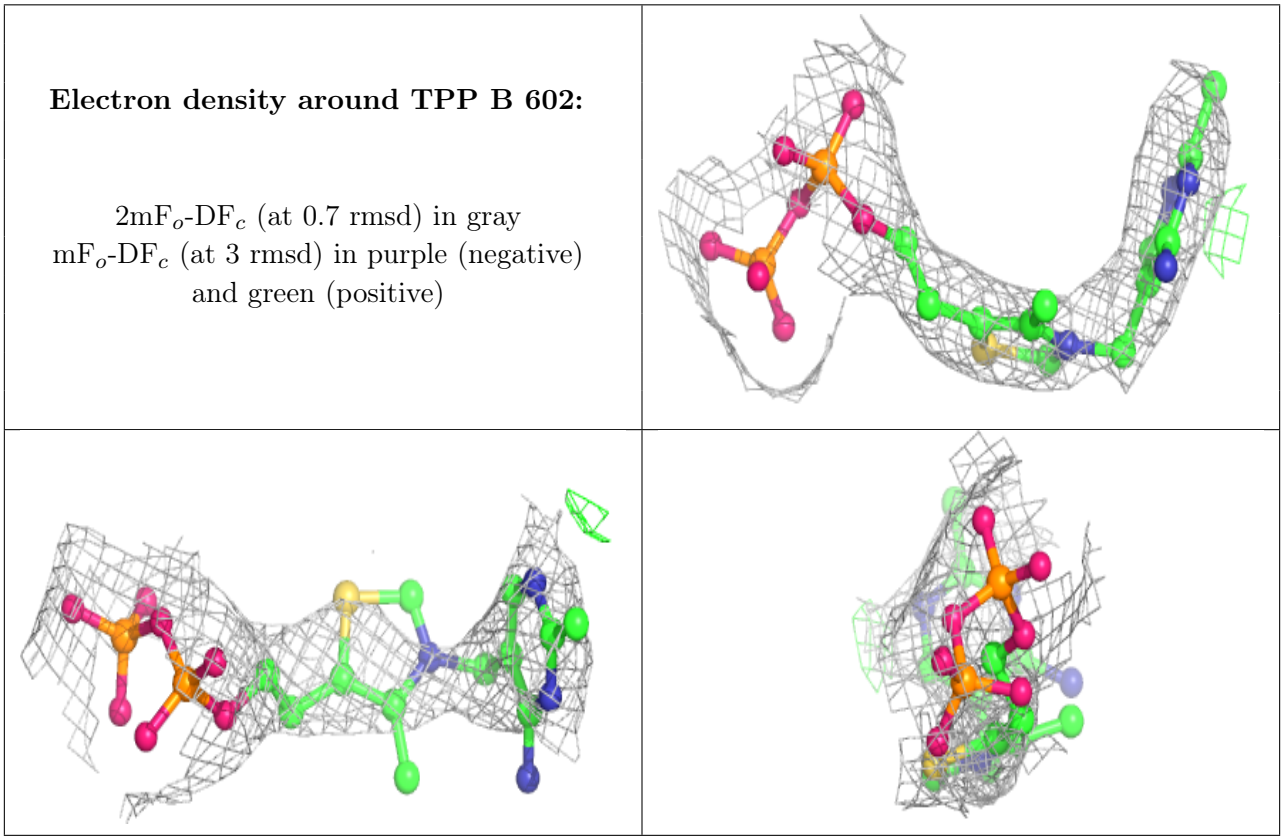
Electron density around TPP A 602:

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



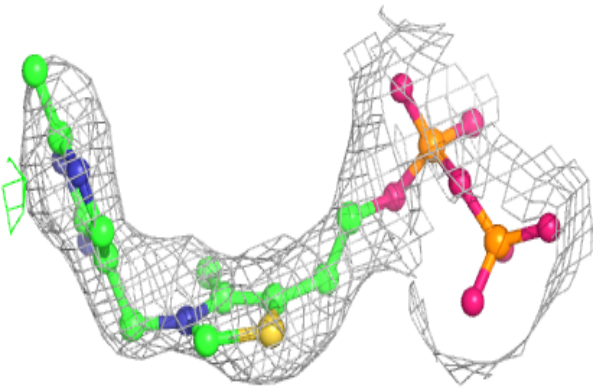
Electron density around TPP B 602:

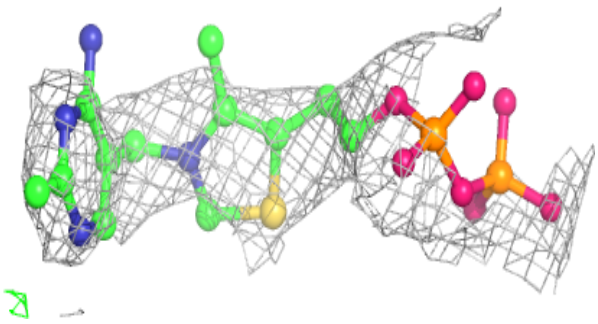
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

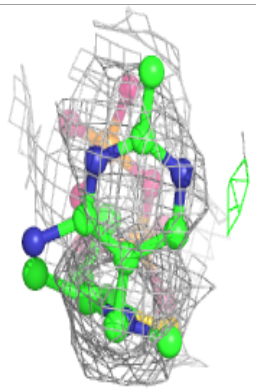


Electron density around TPP D 602:

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

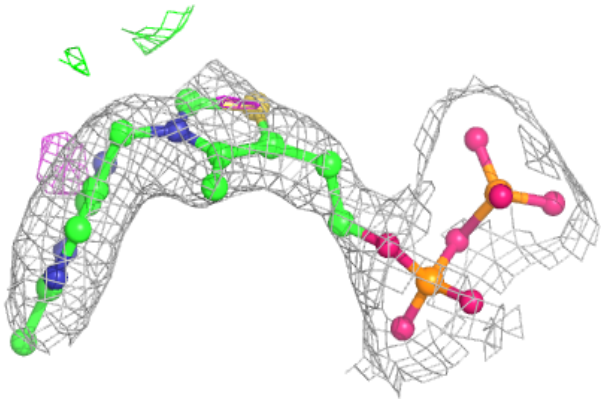


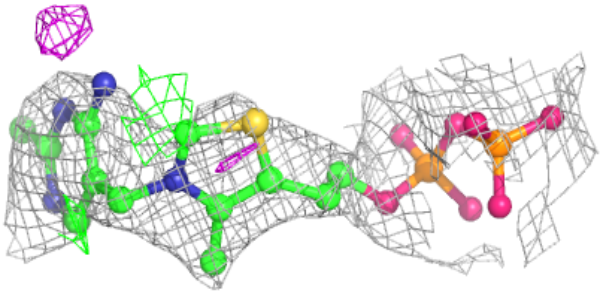


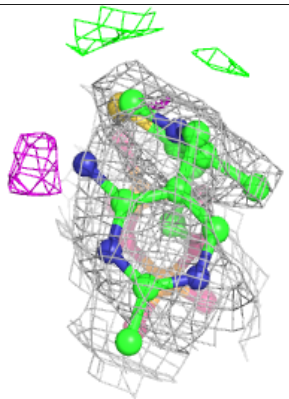


Electron density around TPP E 602:

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

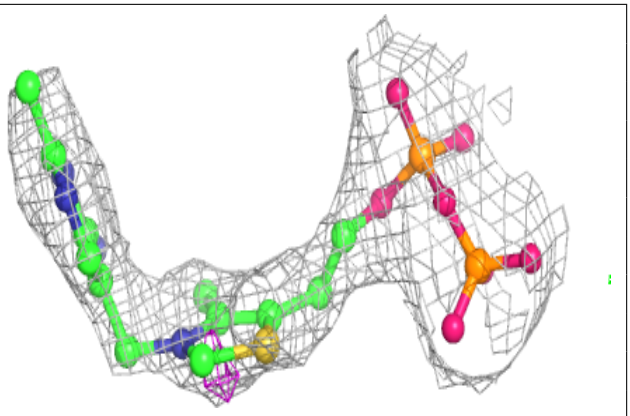


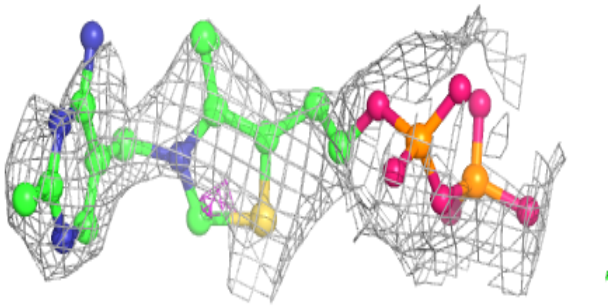


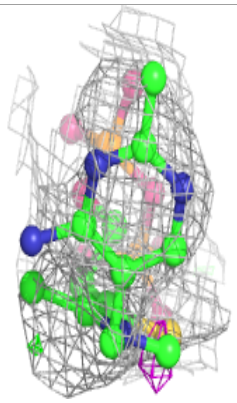


Electron density around TPP F 602:

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

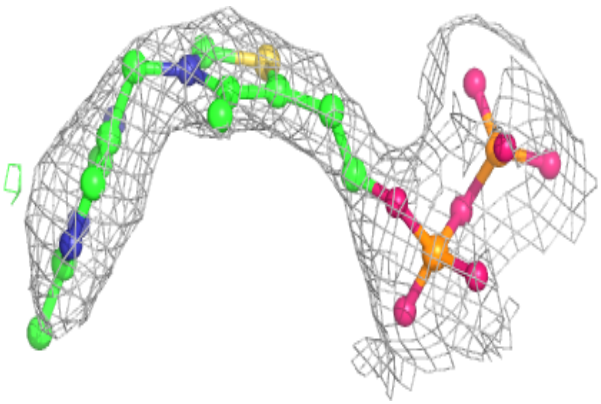


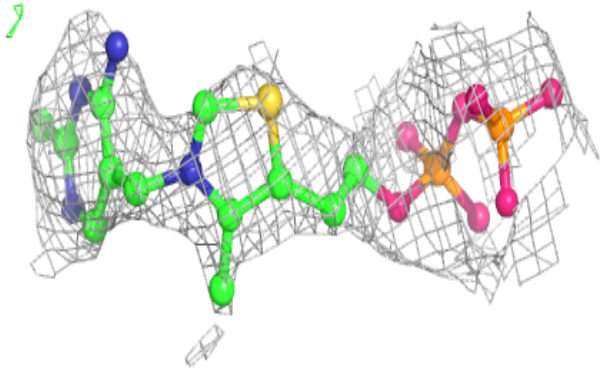


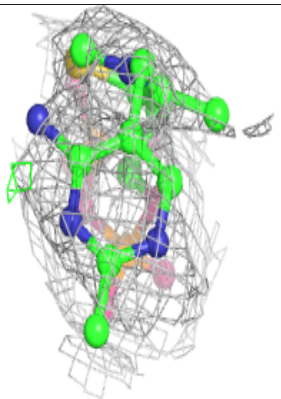


Electron density around TPP G 602:

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

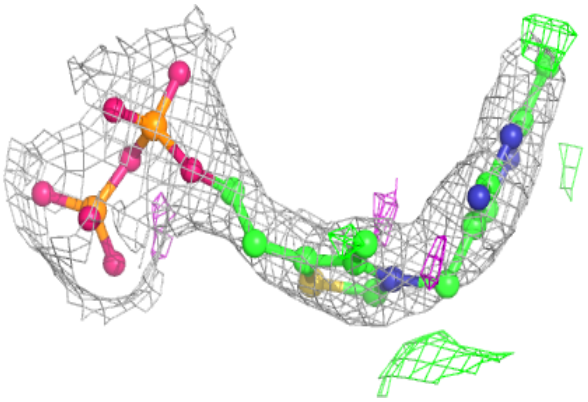


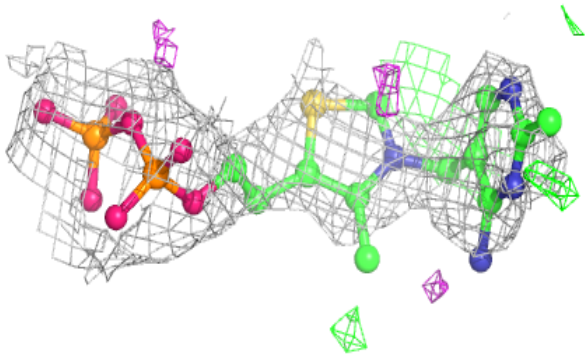


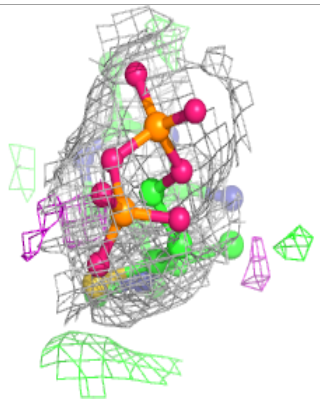


Electron density around TPP H 602:

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

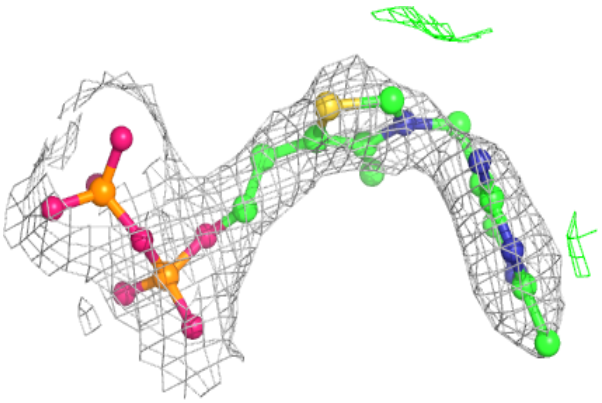


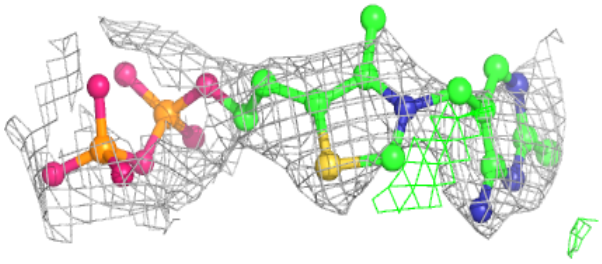


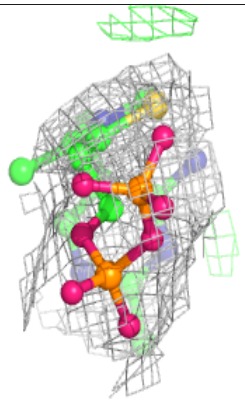


Electron density around TPP C 602:

$2mF_o$-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.