



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:20 pm BST

PDB ID : 3MBO  
Title : Crystal Structure of the Glycosyltransferase BaBshA bound with UDP and L-malate  
Authors : Wallace, B.D.; Claiborne, A.; Redinbo, M.R.  
Deposited on : 2010-03-25  
Resolution : 3.31 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

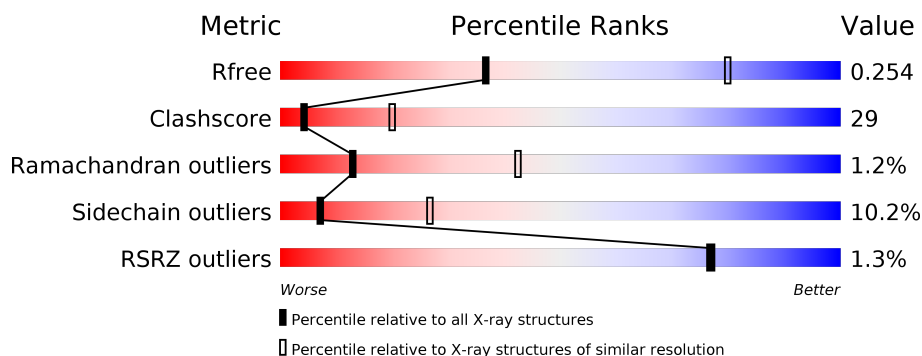
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	414	<div> <div>51%</div> <div>30%</div> <div>7%</div> <div>10%</div> </div>
1	B	414	<div> <div>50%</div> <div>30%</div> <div>7%</div> <div>11%</div> </div>
1	C	414	<div> <div>52%</div> <div>28%</div> <div>9%</div> <div>10%</div> </div>
1	D	414	<div> <div>52%</div> <div>29%</div> <div>7%</div> <div>11%</div> </div>
1	E	414	<div> <div>54%</div> <div>28%</div> <div>8%</div> <div>9%</div> </div>
1	F	414	<div> <div>51%</div> <div>29%</div> <div>7%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	414	
1	H	414	

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	GOL	A	384	-	-	-	X
3	GOL	A	387	-	-	-	X
3	GOL	B	382	-	-	-	X
3	GOL	D	382	-	-	-	X
3	GOL	D	383	-	-	-	X
3	GOL	E	385	-	-	X	X
3	GOL	E	386	-	-	-	X
3	GOL	F	383	-	-	X	X
5	MG	E	388	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23880 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 Glycosyltransferase, group 1 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2923	1865	491	554	13			
1	B	369	Total	C	N	O	S	0	0	0
			2907	1852	489	553	13			
1	C	373	Total	C	N	O	S	0	0	0
			2929	1870	493	553	13			
1	D	369	Total	C	N	O	S	0	0	0
			2903	1850	489	551	13			
1	E	375	Total	C	N	O	S	0	0	0
			2959	1886	500	560	13			
1	F	369	Total	C	N	O	S	0	0	0
			2919	1860	492	554	13			
1	G	365	Total	C	N	O	S	0	0	0
			2881	1834	486	548	13			
1	H	369	Total	C	N	O	S	0	0	0
			2907	1852	490	552	13			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
A	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
A	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
A	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
A	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
A	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
A	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7
A	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
A	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
A	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
A	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
A	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
A	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
A	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
A	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7
A	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
A	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
A	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
A	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
A	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
A	-11	SER	-	EXPRESSION TAG	UNP Q81ST7
A	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
A	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
A	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7
A	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
A	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
A	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
A	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
A	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
A	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7
A	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
A	0	SER	-	EXPRESSION TAG	UNP Q81ST7
B	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
B	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
B	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
B	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
B	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
B	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
B	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7
B	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
B	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
B	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
B	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
B	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
B	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7
B	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
B	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
B	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7
B	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
B	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
B	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
B	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
B	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
B	-11	SER	-	EXPRESSION TAG	UNP Q81ST7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
B	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
B	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7
B	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
B	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
B	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
B	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
B	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
B	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7
B	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
B	0	SER	-	EXPRESSION TAG	UNP Q81ST7
C	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
C	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
C	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
C	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
C	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
C	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
C	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7
C	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
C	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
C	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
C	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
C	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
C	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7
C	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
C	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
C	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7
C	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
C	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
C	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
C	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
C	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
C	-11	SER	-	EXPRESSION TAG	UNP Q81ST7
C	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
C	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
C	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7
C	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
C	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
C	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
C	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
C	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
C	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
C	0	SER	-	EXPRESSION TAG	UNP Q81ST7
D	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
D	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
D	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
D	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
D	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
D	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
D	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7
D	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
D	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
D	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
D	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
D	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
D	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7
D	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
D	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
D	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7
D	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
D	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
D	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
D	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
D	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
D	-11	SER	-	EXPRESSION TAG	UNP Q81ST7
D	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
D	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
D	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7
D	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
D	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
D	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
D	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
D	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
D	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7
D	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
D	0	SER	-	EXPRESSION TAG	UNP Q81ST7
E	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
E	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
E	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
E	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
E	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
E	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
E	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
E	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
E	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
E	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
E	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
E	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7
E	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
E	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
E	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7
E	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
E	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
E	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
E	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
E	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
E	-11	SER	-	EXPRESSION TAG	UNP Q81ST7
E	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
E	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
E	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7
E	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
E	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
E	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
E	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
E	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
E	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7
E	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
E	0	SER	-	EXPRESSION TAG	UNP Q81ST7
F	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
F	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
F	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
F	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
F	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
F	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
F	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7
F	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
F	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
F	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
F	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
F	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
F	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7
F	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
F	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
F	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7

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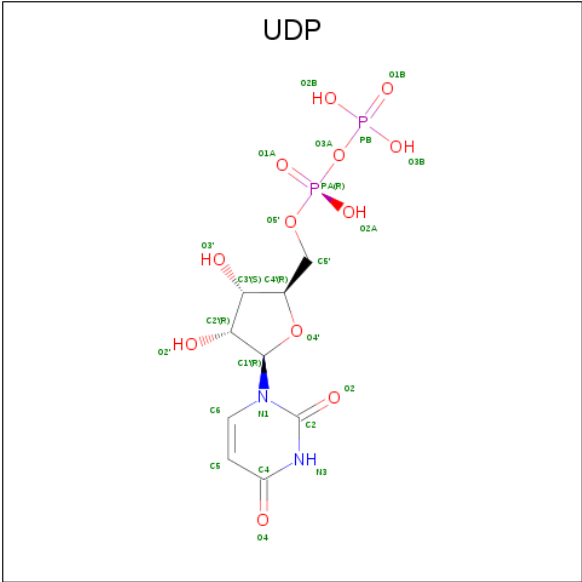
Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
F	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
F	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
F	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
F	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
F	-11	SER	-	EXPRESSION TAG	UNP Q81ST7
F	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
F	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
F	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7
F	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
F	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
F	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
F	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
F	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
F	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7
F	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
F	0	SER	-	EXPRESSION TAG	UNP Q81ST7
G	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
G	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
G	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
G	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
G	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
G	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
G	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7
G	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
G	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
G	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
G	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
G	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
G	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7
G	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
G	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
G	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7
G	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
G	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
G	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
G	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
G	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
G	-11	SER	-	EXPRESSION TAG	UNP Q81ST7
G	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
G	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
G	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7

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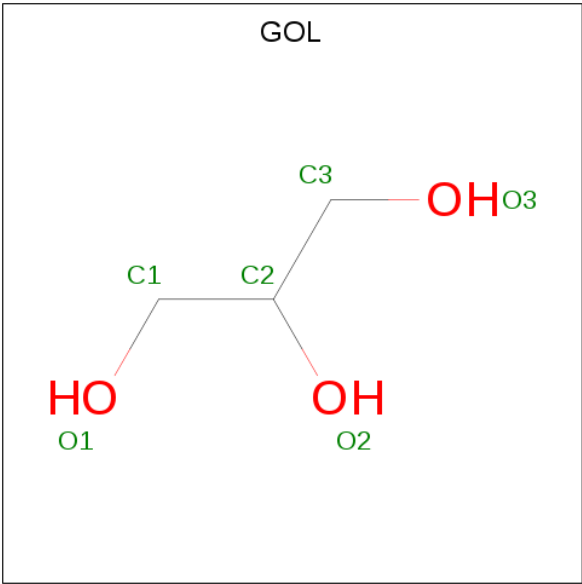
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
G	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
G	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
G	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
G	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
G	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7
G	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
G	0	SER	-	EXPRESSION TAG	UNP Q81ST7
H	-32	MET	-	EXPRESSION TAG	UNP Q81ST7
H	-31	GLY	-	EXPRESSION TAG	UNP Q81ST7
H	-30	SER	-	EXPRESSION TAG	UNP Q81ST7
H	-29	HIS	-	EXPRESSION TAG	UNP Q81ST7
H	-28	HIS	-	EXPRESSION TAG	UNP Q81ST7
H	-27	HIS	-	EXPRESSION TAG	UNP Q81ST7
H	-26	HIS	-	EXPRESSION TAG	UNP Q81ST7
H	-25	HIS	-	EXPRESSION TAG	UNP Q81ST7
H	-24	HIS	-	EXPRESSION TAG	UNP Q81ST7
H	-23	SER	-	EXPRESSION TAG	UNP Q81ST7
H	-22	SER	-	EXPRESSION TAG	UNP Q81ST7
H	-21	GLY	-	EXPRESSION TAG	UNP Q81ST7
H	-20	LEU	-	EXPRESSION TAG	UNP Q81ST7
H	-19	VAL	-	EXPRESSION TAG	UNP Q81ST7
H	-18	PRO	-	EXPRESSION TAG	UNP Q81ST7
H	-17	ARG	-	EXPRESSION TAG	UNP Q81ST7
H	-16	GLY	-	EXPRESSION TAG	UNP Q81ST7
H	-15	SER	-	EXPRESSION TAG	UNP Q81ST7
H	-14	HIS	-	EXPRESSION TAG	UNP Q81ST7
H	-13	MET	-	EXPRESSION TAG	UNP Q81ST7
H	-12	ALA	-	EXPRESSION TAG	UNP Q81ST7
H	-11	SER	-	EXPRESSION TAG	UNP Q81ST7
H	-10	MET	-	EXPRESSION TAG	UNP Q81ST7
H	-9	THR	-	EXPRESSION TAG	UNP Q81ST7
H	-8	GLY	-	EXPRESSION TAG	UNP Q81ST7
H	-7	GLY	-	EXPRESSION TAG	UNP Q81ST7
H	-6	GLN	-	EXPRESSION TAG	UNP Q81ST7
H	-5	GLN	-	EXPRESSION TAG	UNP Q81ST7
H	-4	MET	-	EXPRESSION TAG	UNP Q81ST7
H	-3	GLY	-	EXPRESSION TAG	UNP Q81ST7
H	-2	ARG	-	EXPRESSION TAG	UNP Q81ST7
H	-1	GLY	-	EXPRESSION TAG	UNP Q81ST7
H	0	SER	-	EXPRESSION TAG	UNP Q81ST7

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



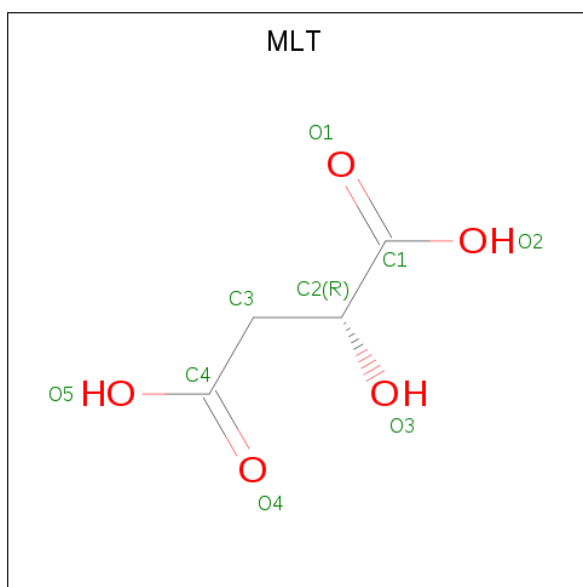
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	H	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		
4	C	1	Total	C	O	0	0
			9	4	5		
4	E	1	Total	C	O	0	0
			9	4	5		
4	H	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	30	Total	O	0	0
			30	30		
6	C	37	Total	O	0	0
			37	37		

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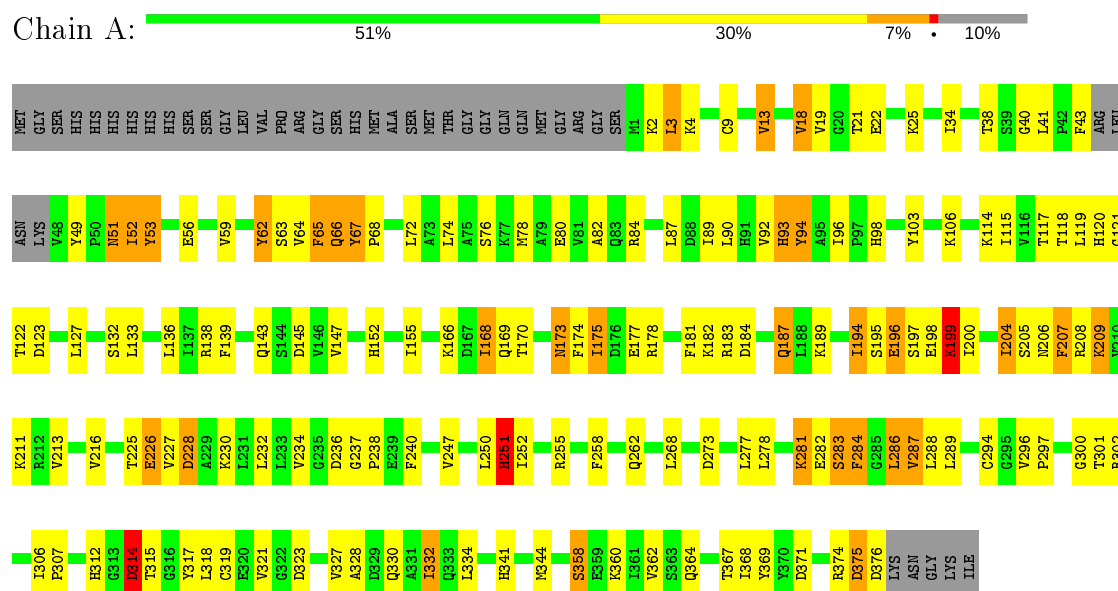
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	37	Total 37	O 37	0	0
6	E	41	Total 41	O 41	0	0
6	F	32	Total 32	O 32	0	0
6	G	33	Total 33	O 33	0	0
6	H	46	Total 46	O 46	0	0

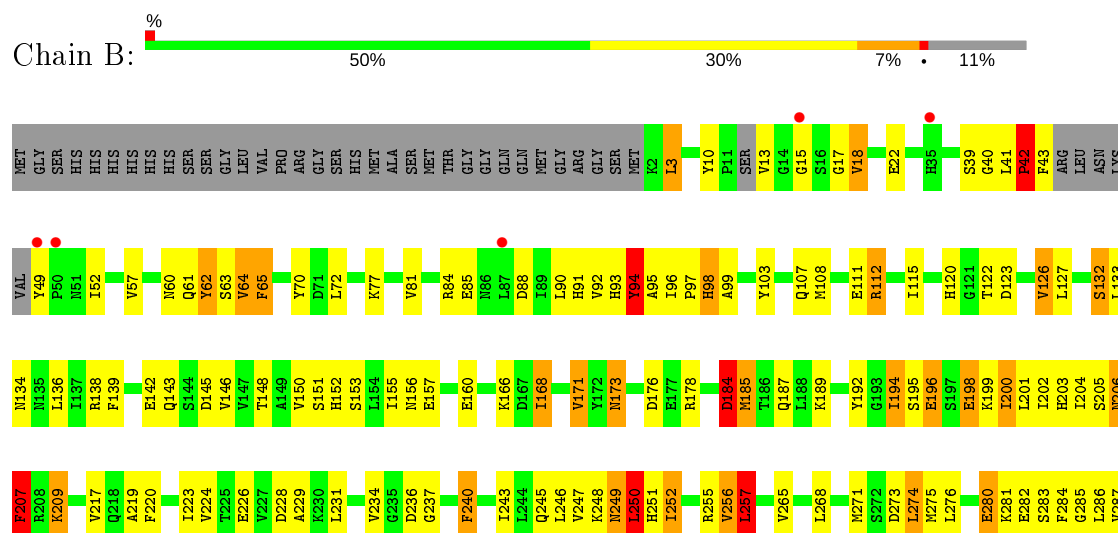
### 3 Residue-property plots

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

- Molecule 1: Glycosyltransferase, group 1 family

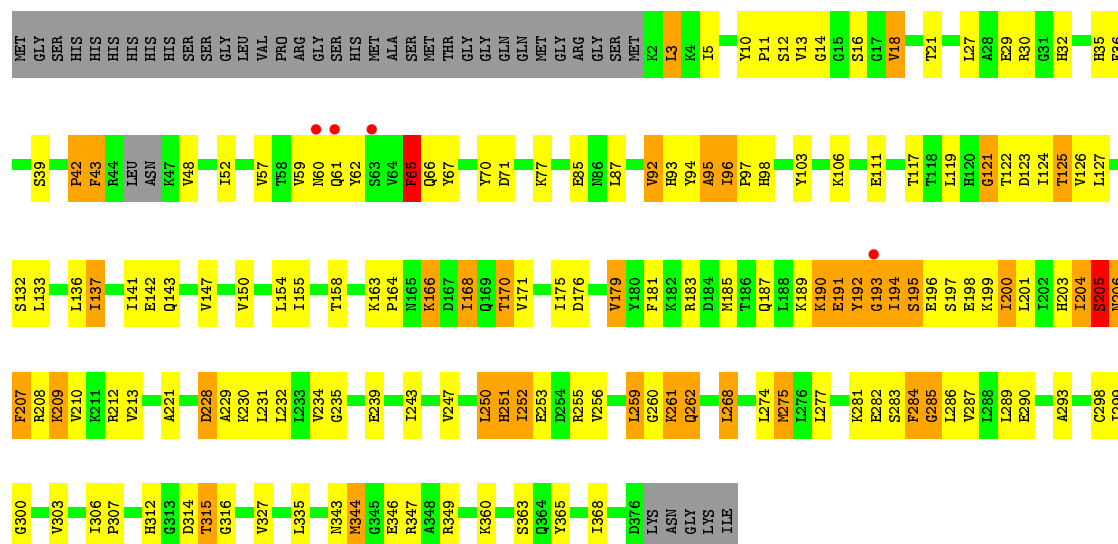


- Molecule 1: Glycosyltransferase, group 1 family

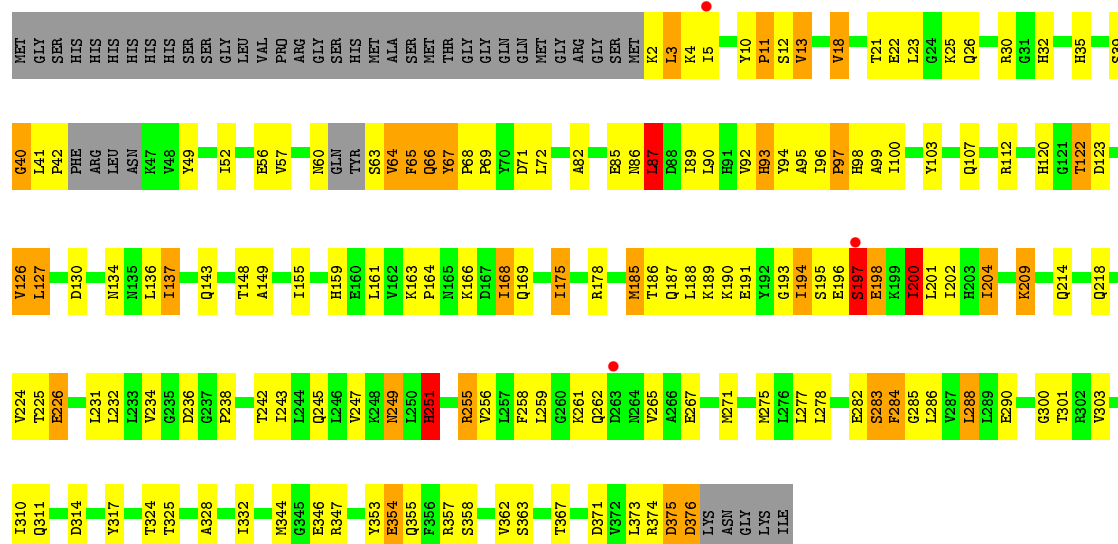




• Molecule 1: Glycosyltransferase, group 1 family

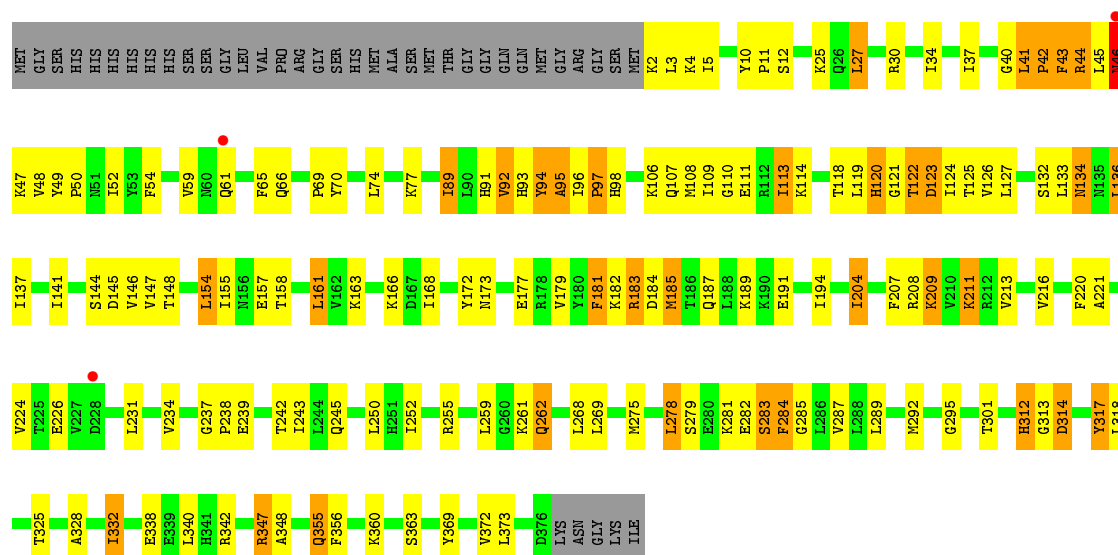


• Molecule 1: Glycosyltransferase, group 1 family

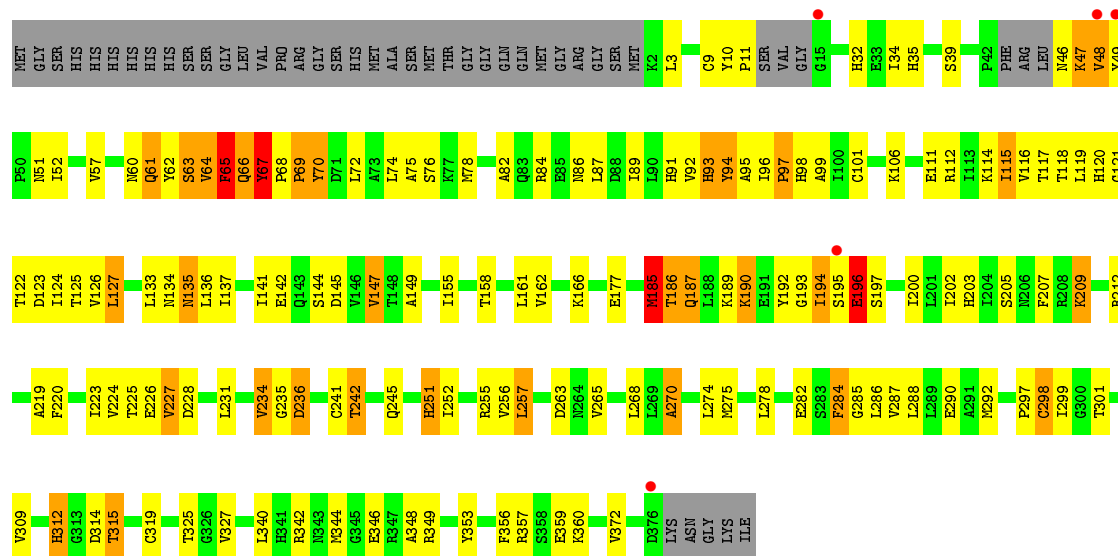


• Molecule 1: Glycosyltransferase, group 1 family

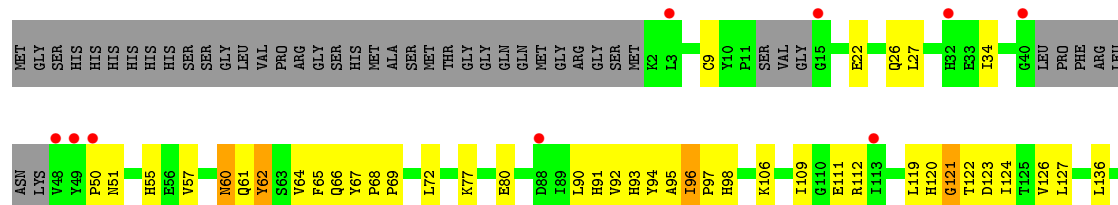


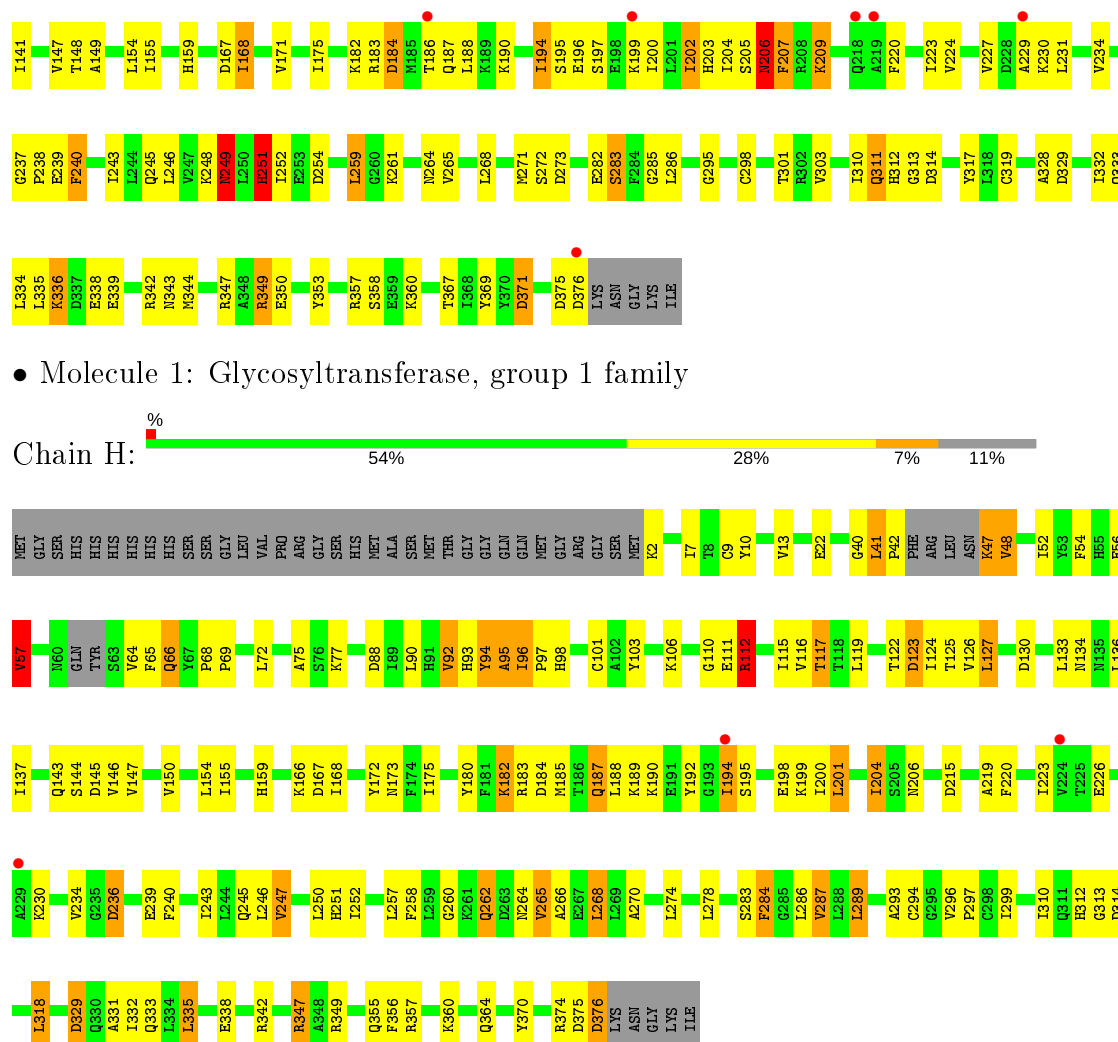


• Molecule 1: Glycosyltransferase, group 1 family



• Molecule 1: Glycosyltransferase, group 1 family





- Molecule 1: Glycosyltransferase, group 1 family

Chain H: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.27Å 226.27Å 75.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 3.31 48.22 – 3.31	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.22-3.31) 99.2 (48.22-3.31)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.228 , 0.257 0.225 , 0.254	Depositor DCC
$R_{free}$ test set	2907 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 66.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23880	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.51	2/2974 (0.1%)	0.89	20/4027 (0.5%)
1	B	0.43	0/2956	0.94	31/4000 (0.8%)
1	C	0.50	0/2980	0.91	29/4034 (0.7%)
1	D	0.47	0/2951	0.86	17/3991 (0.4%)
1	E	0.50	0/3011	0.92	21/4075 (0.5%)
1	F	0.45	0/2968	0.96	32/4014 (0.8%)
1	G	0.41	0/2929	0.87	19/3961 (0.5%)
1	H	0.44	0/2955	0.85	14/3996 (0.4%)
All	All	0.46	2/23724 (0.0%)	0.90	183/32098 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	CYS	CB-SG	-8.43	1.68	1.82
1	A	68	PRO	N-CD	5.51	1.55	1.47

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	TYR	C-N-CD	-13.48	90.94	120.60
1	B	256	VAL	CB-CA-C	-13.21	86.30	111.40
1	D	12	SER	N-CA-CB	-11.99	92.52	110.50
1	F	285	GLY	N-CA-C	-11.73	83.78	113.10
1	E	284	PHE	N-CA-C	-11.66	79.53	111.00
1	G	207	PHE	N-CA-CB	-11.56	89.79	110.60
1	C	66	GLN	N-CA-CB	-11.27	90.31	110.60
1	F	284	PHE	N-CA-C	-11.09	81.07	111.00
1	F	234	VAL	N-CA-C	11.08	140.92	111.00
1	H	182	LYS	N-CA-C	-10.71	82.09	111.00
1	C	251	HIS	CB-CA-C	-10.40	89.61	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	127	LEU	CB-CA-C	-10.30	90.62	110.20
1	B	207	PHE	N-CA-CB	-10.05	92.51	110.60
1	B	206	ASN	N-CA-C	-9.74	84.69	111.00
1	E	46	ASN	N-CA-CB	-9.66	93.22	110.60
1	F	135	ASN	CB-CA-C	-9.63	91.14	110.40
1	H	66	GLN	N-CA-CB	-9.57	93.37	110.60
1	D	126	VAL	N-CA-C	9.10	135.57	111.00
1	D	40	GLY	N-CA-C	8.97	135.52	113.10
1	C	65	PHE	N-CA-C	-8.96	86.81	111.00
1	D	126	VAL	CB-CA-C	-8.95	94.40	111.40
1	E	278	LEU	N-CA-C	-8.64	87.67	111.00
1	A	195	SER	CB-CA-C	-8.63	93.71	110.10
1	E	285	GLY	N-CA-C	-8.60	91.61	113.10
1	C	42	PRO	N-CA-C	-8.46	90.11	112.10
1	A	375	ASP	CB-CA-C	-8.41	93.58	110.40
1	D	93	HIS	N-CA-C	8.41	133.70	111.00
1	G	248	LYS	CB-CA-C	8.41	127.21	110.40
1	G	251	HIS	CB-CA-C	-8.24	93.93	110.40
1	A	376	ASP	N-CA-CB	8.22	125.40	110.60
1	F	63	SER	N-CA-C	-8.18	88.92	111.00
1	H	246	LEU	N-CA-CB	-8.14	94.12	110.40
1	A	93	HIS	N-CA-C	8.08	132.81	111.00
1	G	249	ASN	N-CA-CB	-8.07	96.08	110.60
1	C	314	ASP	N-CA-C	7.91	132.36	111.00
1	H	195	SER	N-CA-CB	-7.89	98.66	110.50
1	B	185	MET	N-CA-CB	7.84	124.71	110.60
1	C	261	LYS	N-CA-C	7.84	132.16	111.00
1	C	259	LEU	CB-CA-C	-7.81	95.37	110.20
1	D	197	SER	N-CA-C	-7.79	89.96	111.00
1	G	303	VAL	N-CA-CB	-7.72	94.51	111.50
1	F	121	GLY	N-CA-C	7.65	132.23	113.10
1	E	284	PHE	CB-CA-C	-7.59	95.22	110.40
1	G	283	SER	N-CA-C	-7.59	90.51	111.00
1	F	251	HIS	CB-CA-C	-7.57	95.25	110.40
1	H	112	ARG	CB-CA-C	-7.56	95.27	110.40
1	A	281	LYS	N-CA-C	-7.50	90.76	111.00
1	A	94	TYR	N-CA-C	-7.47	90.82	111.00
1	B	132	SER	CB-CA-C	7.43	124.21	110.10
1	F	315	THR	N-CA-CB	7.36	124.28	110.30
1	D	11	PRO	N-CA-C	-7.36	92.98	112.10
1	A	132	SER	CB-CA-C	7.33	124.03	110.10
1	C	252	ILE	N-CA-C	-7.29	91.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	93	HIS	N-CA-C	7.21	130.47	111.00
1	B	42	PRO	CB-CA-C	-7.19	94.02	112.00
1	B	374	ARG	N-CA-C	7.12	130.23	111.00
1	G	109	ILE	CB-CA-C	-7.08	97.43	111.60
1	E	61	GLN	N-CA-C	-7.06	91.94	111.00
1	F	314	ASP	CB-CA-C	-7.06	96.28	110.40
1	F	70	TYR	N-CA-C	-7.05	91.96	111.00
1	A	281	LYS	CB-CA-C	7.04	124.48	110.40
1	B	280	GLU	CB-CA-C	6.97	124.34	110.40
1	D	251	HIS	CB-CA-C	-6.97	96.46	110.40
1	F	312	HIS	N-CA-C	6.93	129.70	111.00
1	A	196	GLU	N-CA-C	-6.87	92.45	111.00
1	F	67	TYR	N-CA-C	-6.82	92.59	111.00
1	G	199	LYS	N-CA-C	6.81	129.39	111.00
1	G	51	ASN	N-CA-CB	6.74	122.74	110.60
1	B	43	PHE	N-CA-CB	6.71	122.68	110.60
1	E	279	SER	N-CA-C	-6.70	92.90	111.00
1	B	120	HIS	CB-CA-C	6.69	123.78	110.40
1	G	50	PRO	N-CA-C	6.67	129.46	112.10
1	E	313	GLY	N-CA-C	6.62	129.64	113.10
1	F	234	VAL	CB-CA-C	-6.61	98.84	111.40
1	E	185	MET	N-CA-C	-6.61	93.16	111.00
1	H	195	SER	CB-CA-C	-6.54	97.68	110.10
1	B	184	ASP	CB-CA-C	-6.52	97.35	110.40
1	D	12	SER	N-CA-C	6.52	128.60	111.00
1	A	314	ASP	CB-CA-C	-6.52	97.37	110.40
1	E	279	SER	N-CA-CB	6.51	120.27	110.50
1	H	194	ILE	N-CA-C	6.51	128.59	111.00
1	B	184	ASP	N-CA-C	-6.49	93.48	111.00
1	C	65	PHE	CB-CA-C	-6.48	97.45	110.40
1	F	136	LEU	N-CA-C	-6.43	93.64	111.00
1	C	194	ILE	N-CA-C	-6.40	93.71	111.00
1	B	257	LEU	N-CA-CB	-6.39	97.62	110.40
1	C	250	LEU	CB-CA-C	6.37	122.31	110.20
1	F	127	LEU	N-CA-C	6.35	128.14	111.00
1	E	226	GLU	N-CA-CB	-6.34	99.19	110.60
1	H	312	HIS	CB-CA-C	6.31	123.02	110.40
1	C	121	GLY	N-CA-C	6.30	128.85	113.10
1	B	64	VAL	CB-CA-C	-6.27	99.49	111.40
1	D	226	GLU	N-CA-CB	-6.24	99.37	110.60
1	F	314	ASP	N-CA-C	6.23	127.82	111.00
1	A	51	ASN	N-CA-C	6.23	127.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	LEU	N-CA-C	-6.20	94.25	111.00
1	F	185	MET	CB-CA-C	-6.19	98.02	110.40
1	F	312	HIS	CB-CA-C	-6.17	98.06	110.40
1	C	194	ILE	CB-CA-C	-6.17	99.26	111.60
1	C	60	ASN	N-CA-C	6.15	127.61	111.00
1	A	13	VAL	N-CA-C	6.14	127.58	111.00
1	C	207	PHE	N-CA-C	6.14	127.58	111.00
1	D	67	TYR	N-CA-C	-6.13	94.43	111.00
1	G	51	ASN	N-CA-C	-6.13	94.46	111.00
1	C	193	GLY	N-CA-C	-6.12	97.79	113.10
1	F	94	TYR	N-CA-C	-6.11	94.51	111.00
1	C	285	GLY	N-CA-C	6.06	128.26	113.10
1	B	43	PHE	N-CA-C	-6.05	94.66	111.00
1	H	65	PHE	N-CA-C	6.05	127.34	111.00
1	C	132	SER	CB-CA-C	6.02	121.54	110.10
1	H	182	LYS	CB-CA-C	-5.95	98.50	110.40
1	B	194	ILE	N-CA-C	5.93	127.01	111.00
1	F	252	ILE	N-CA-CB	5.91	124.38	110.80
1	F	136	LEU	N-CA-CB	5.88	122.16	110.40
1	A	133	LEU	N-CA-CB	-5.88	98.64	110.40
1	H	199	LYS	N-CA-C	5.87	126.84	111.00
1	F	263	ASP	N-CA-C	5.86	126.83	111.00
1	A	226	GLU	N-CA-C	5.82	126.72	111.00
1	E	312	HIS	CB-CA-C	5.82	122.05	110.40
1	B	281	LYS	N-CA-CB	-5.82	100.12	110.60
1	D	11	PRO	CB-CA-C	-5.79	97.53	112.00
1	B	65	PHE	N-CA-C	-5.77	95.42	111.00
1	G	121	GLY	N-CA-C	5.75	127.48	113.10
1	B	303	VAL	N-CA-CB	5.70	124.05	111.50
1	E	120	HIS	N-CA-C	-5.70	95.60	111.00
1	E	110	GLY	N-CA-C	5.70	127.35	113.10
1	C	48	VAL	N-CA-C	5.70	126.38	111.00
1	E	95	ALA	N-CA-C	5.69	126.36	111.00
1	C	30	ARG	CB-CA-C	-5.67	99.06	110.40
1	F	196	GLU	N-CA-C	5.64	126.23	111.00
1	D	94	TYR	N-CA-CB	-5.64	100.46	110.60
1	A	315	THR	N-CA-CB	5.59	120.92	110.30
1	G	336	LYS	CB-CA-C	-5.59	99.22	110.40
1	B	302	ARG	N-CA-C	-5.59	95.91	111.00
1	E	43	PHE	CB-CA-C	-5.56	99.27	110.40
1	G	202	ILE	CB-CA-C	-5.56	100.47	111.60
1	B	229	ALA	N-CA-CB	5.51	117.82	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	ILE	N-CA-C	5.51	125.87	111.00
1	C	314	ASP	N-CA-CB	-5.46	100.77	110.60
1	B	200	ILE	N-CA-C	5.45	125.71	111.00
1	B	196	GLU	N-CA-C	-5.45	96.30	111.00
1	C	284	PHE	CB-CA-C	-5.43	99.53	110.40
1	F	270	ALA	CB-CA-C	5.42	118.23	110.10
1	B	120	HIS	N-CA-C	-5.40	96.42	111.00
1	F	186	THR	N-CA-CB	-5.39	100.06	110.30
1	B	133	LEU	N-CA-CB	-5.39	99.62	110.40
1	E	48	VAL	CB-CA-C	5.38	121.62	111.40
1	D	194	ILE	N-CA-CB	-5.37	98.45	110.80
1	E	312	HIS	N-CA-C	-5.37	96.50	111.00
1	C	195	SER	CB-CA-C	-5.36	99.91	110.10
1	H	57	VAL	N-CA-C	5.35	125.45	111.00
1	H	64	VAL	N-CA-C	-5.35	96.55	111.00
1	C	207	PHE	N-CA-CB	-5.34	100.99	110.60
1	B	322	GLY	N-CA-C	5.33	126.42	113.10
1	D	314	ASP	N-CA-C	5.32	125.35	111.00
1	F	84	ARG	CB-CA-C	-5.32	99.77	110.40
1	H	313	GLY	N-CA-C	5.31	126.38	113.10
1	F	236	ASP	N-CA-CB	-5.31	101.04	110.60
1	A	251	HIS	CB-CA-C	-5.31	99.79	110.40
1	C	315	THR	N-CA-C	-5.30	96.68	111.00
1	G	9	CYS	CB-CA-C	-5.30	99.80	110.40
1	G	194	ILE	N-CA-C	5.30	125.30	111.00
1	E	211	LYS	CB-CA-C	5.29	120.98	110.40
1	E	208	ARG	N-CA-CB	5.29	120.12	110.60
1	A	166	LYS	N-CA-CB	-5.28	101.10	110.60
1	C	95	ALA	N-CA-C	5.26	125.20	111.00
1	F	65	PHE	N-CA-C	5.23	125.12	111.00
1	C	133	LEU	N-CA-CB	-5.22	99.97	110.40
1	G	375	ASP	CB-CA-C	-5.21	99.98	110.40
1	A	199	LYS	N-CA-C	5.20	125.04	111.00
1	C	195	SER	N-CA-CB	-5.18	102.73	110.50
1	C	29	GLU	CB-CA-C	-5.18	100.04	110.40
1	F	64	VAL	N-CA-C	5.17	124.96	111.00
1	B	257	LEU	CA-CB-CG	5.09	127.01	115.30
1	E	48	VAL	N-CA-C	-5.09	97.26	111.00
1	G	252	ILE	N-CA-CB	5.09	122.50	110.80
1	A	183	ARG	N-CA-C	-5.04	97.39	111.00
1	F	227	VAL	CB-CA-C	-5.04	101.82	111.40
1	B	321	VAL	CB-CA-C	5.03	120.96	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	VAL	N-CA-C	-5.01	97.46	111.00
1	D	200	ILE	N-CA-CB	-5.01	99.27	110.80
1	G	206	ASN	N-CA-C	-5.01	97.47	111.00
1	B	18	VAL	CB-CA-C	5.01	120.91	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2923	0	2932	207	0
1	B	2907	0	2916	200	0
1	C	2929	0	2940	171	0
1	D	2903	0	2929	169	0
1	E	2959	0	2977	194	0
1	F	2919	0	2941	189	0
1	G	2881	0	2885	170	0
1	H	2907	0	2934	155	0
2	A	25	0	11	0	0
2	C	25	0	11	2	0
2	E	25	0	11	2	0
2	H	25	0	11	2	0
3	A	30	0	40	6	0
3	B	12	0	16	1	0
3	C	12	0	16	1	0
3	D	18	0	24	3	0
3	E	24	0	32	7	0
3	F	24	0	32	8	0
3	H	6	0	8	1	0
4	A	9	0	4	0	0
4	C	9	0	4	1	0
4	E	9	0	4	0	0
4	H	9	0	4	1	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	32	0	0	7	0
6	B	30	0	0	4	0
6	C	37	0	0	5	0
6	D	37	0	0	13	0
6	E	41	0	0	9	0
6	F	32	0	0	3	0
6	G	33	0	0	5	0
6	H	46	0	0	10	0
All	All	23880	0	23682	1386	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 29.

All (1386) 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:A:66:GLN:HB3	1:A:67:TYR:CE2	1.38	1.59
1:E:245:GLN:CG	1:H:245:GLN:HE22	1.20	1.54
1:C:96:ILE:HG22	1:C:97:PRO:CD	1.38	1.48
1:E:42:PRO:HD2	1:E:43:PHE:CD2	1.45	1.47
1:E:245:GLN:HG3	1:H:245:GLN:NE2	1.16	1.46
1:B:196:GLU:HG2	1:B:198:GLU:CG	1.46	1.42
1:A:34:ILE:O	1:A:52:ILE:CG2	1.67	1.40
1:F:47:LYS:HD3	1:F:48:VAL:N	1.36	1.39
1:B:63:SER:O	1:B:64:VAL:CG1	1.68	1.38
1:A:63:SER:HA	1:A:65:PHE:CE2	1.60	1.35
1:G:62:TYR:CE2	1:G:65:PHE:HE1	1.44	1.34
1:E:42:PRO:CD	1:E:43:PHE:HD2	1.41	1.33
1:F:234:VAL:O	1:F:234:VAL:CG1	1.74	1.31
1:D:251:HIS:CD2	1:D:251:HIS:O	1.83	1.31
1:B:94:TYR:OH	1:B:122:THR:CB	1.79	1.29
1:A:96:ILE:HG13	1:A:127:LEU:CD1	1.63	1.27
1:A:96:ILE:HB	6:A:393:HOH:O	1.29	1.26
1:E:120:HIS:HB2	6:E:396:HOH:O	1.15	1.26
1:F:251:HIS:CD2	1:F:251:HIS:O	1.89	1.26
1:B:280:GLU:O	1:B:303:VAL:HG11	1.31	1.25
1:G:203:HIS:O	1:G:204:ILE:HG22	1.30	1.24
1:G:194:ILE:HG13	6:G:395:HOH:O	1.07	1.24
1:B:62:TYR:HB2	1:B:65:PHE:CG	1.71	1.23
1:A:34:ILE:HB	1:A:52:ILE:CG2	1.69	1.22
1:D:60:ASN:OD1	1:D:64:VAL:CG1	1.87	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:HIS:O	1:G:251:HIS:CG	1.82	1.21
1:G:62:TYR:CD2	1:G:65:PHE:CE1	2.30	1.19
1:G:62:TYR:CG	1:G:65:PHE:CE1	2.30	1.19
1:B:63:SER:O	1:B:64:VAL:HG12	1.04	1.19
1:G:62:TYR:CD1	1:G:65:PHE:CE1	2.30	1.18
1:G:62:TYR:CE1	1:G:65:PHE:CZ	2.30	1.18
1:E:12:SER:OG	1:E:42:PRO:O	1.61	1.18
1:C:206:ASN:OD1	1:C:207:PHE:N	1.72	1.18
1:A:34:ILE:C	1:A:52:ILE:HG22	1.64	1.18
1:E:96:ILE:HD11	1:E:137:ILE:CG1	1.72	1.18
1:F:190:LYS:O	1:F:193:GLY:HA2	1.42	1.18
1:G:62:TYR:CD2	1:G:65:PHE:HE1	1.60	1.17
1:F:284:PHE:O	3:F:385:GOL:O2	1.60	1.17
1:E:96:ILE:CD1	1:E:137:ILE:HG13	1.75	1.16
1:G:206:ASN:OD1	1:G:207:PHE:N	1.78	1.16
1:B:314:ASP:OD2	1:B:347:ARG:CB	1.93	1.16
1:C:96:ILE:CG2	1:C:97:PRO:HD3	1.75	1.16
1:E:11:PRO:CA	1:E:42:PRO:HB3	1.75	1.15
1:A:63:SER:CA	1:A:65:PHE:CE2	2.29	1.15
1:G:62:TYR:CZ	1:G:65:PHE:HE1	1.63	1.15
1:G:194:ILE:HD12	1:G:271:MET:CE	1.76	1.15
1:E:207:PHE:O	1:E:238:PRO:HD2	1.48	1.14
1:G:314:ASP:O	1:G:344:MET:HG2	1.46	1.14
1:G:62:TYR:CE2	1:G:65:PHE:CE1	2.35	1.13
1:B:196:GLU:CG	1:B:198:GLU:HG3	1.78	1.13
1:D:93:HIS:O	1:D:120:HIS:HD2	1.32	1.13
1:E:41:LEU:H	1:E:41:LEU:HD22	0.97	1.13
1:A:66:GLN:CB	1:A:67:TYR:CE2	2.30	1.13
1:G:62:TYR:CE1	1:G:65:PHE:CE1	2.35	1.13
1:F:251:HIS:O	1:F:251:HIS:CG	2.00	1.12
1:A:34:ILE:HB	1:A:52:ILE:HG23	1.21	1.12
1:A:96:ILE:CB	6:A:393:HOH:O	1.88	1.11
1:F:194:ILE:N	1:F:194:ILE:HD12	1.60	1.11
1:F:47:LYS:CE	1:F:48:VAL:HG23	1.80	1.10
1:G:62:TYR:CZ	1:G:65:PHE:CE1	2.37	1.10
1:D:60:ASN:OD1	1:D:64:VAL:HB	1.51	1.10
1:G:64:VAL:HG11	1:H:10:TYR:HE2	1.17	1.10
1:G:95:ALA:HB2	1:G:123:ASP:OD2	1.50	1.10
1:F:47:LYS:HE3	1:F:48:VAL:HG23	1.31	1.10
1:B:62:TYR:HB2	1:B:65:PHE:CB	1.80	1.10
1:C:96:ILE:CG2	1:C:97:PRO:CD	2.29	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HG22	1:B:64:VAL:O	1.47	1.09
1:E:312:HIS:O	6:E:426:HOH:O	1.71	1.09
1:F:234:VAL:O	1:F:234:VAL:HG12	1.38	1.09
1:E:282:GLU:OE2	1:E:284:PHE:O	1.68	1.09
1:B:314:ASP:OD2	1:B:347:ARG:HG3	1.53	1.08
1:E:40:GLY:C	1:E:41:LEU:HD13	1.73	1.08
1:D:60:ASN:OD1	1:D:64:VAL:CB	2.00	1.08
1:A:204:ILE:O	1:A:205:SER:OG	1.70	1.08
1:F:193:GLY:C	1:F:194:ILE:HD12	1.74	1.08
1:B:314:ASP:OD2	1:B:347:ARG:CG	2.02	1.07
1:A:63:SER:C	1:A:65:PHE:HD2	1.58	1.07
1:B:94:TYR:OH	1:B:122:THR:HB	0.89	1.06
1:C:206:ASN:ND2	1:C:208:ARG:HG3	1.67	1.06
1:A:96:ILE:CG2	6:A:393:HOH:O	2.00	1.06
1:A:96:ILE:HG13	1:A:127:LEU:HD12	1.33	1.06
1:B:256:VAL:O	1:B:256:VAL:CG1	1.88	1.06
1:G:194:ILE:HG22	1:G:194:ILE:O	1.54	1.06
1:A:34:ILE:O	1:A:52:ILE:HG22	0.89	1.05
1:F:65:PHE:HD1	1:F:65:PHE:N	1.54	1.05
1:G:194:ILE:HD12	1:G:271:MET:HE2	1.30	1.05
1:E:134:ASN:HD22	1:E:134:ASN:C	1.55	1.05
1:G:122:THR:O	1:G:126:VAL:HG22	1.56	1.05
1:B:252:ILE:H	1:B:252:ILE:HD12	1.22	1.04
1:B:196:GLU:OE1	1:B:255:ARG:NH2	1.89	1.04
1:D:41:LEU:H	1:D:42:PRO:HD2	1.17	1.04
1:C:204:ILE:O	1:C:205:SER:HB2	1.50	1.04
1:C:260:GLY:C	1:C:261:LYS:HG2	1.76	1.04
1:E:41:LEU:HD22	1:E:41:LEU:N	1.65	1.04
1:H:375:ASP:O	1:H:376:ASP:HB2	1.53	1.04
1:B:62:TYR:CB	1:B:65:PHE:CB	2.36	1.03
1:D:86:ASN:O	1:D:87:LEU:HB2	1.49	1.03
1:E:44:ARG:HG3	1:E:44:ARG:O	1.54	1.03
1:B:252:ILE:O	1:B:252:ILE:HD13	1.56	1.03
1:G:203:HIS:O	1:G:204:ILE:CG2	2.05	1.03
1:A:62:TYR:HD1	1:A:62:TYR:O	1.42	1.03
1:G:61:GLN:HE21	1:H:127:LEU:HD12	1.24	1.02
1:E:108:MET:CE	1:F:135:ASN:O	2.05	1.02
1:D:93:HIS:O	1:D:120:HIS:CD2	2.11	1.02
1:H:40:GLY:HA2	1:H:54:PHE:HZ	1.24	1.02
1:B:196:GLU:CG	1:B:198:GLU:CG	2.33	1.02
1:A:63:SER:C	1:A:65:PHE:CD2	2.33	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HB2	1:C:190:LYS:NZ	1.76	1.01
1:G:62:TYR:O	1:G:62:TYR:HD1	1.40	1.01
1:B:256:VAL:HG12	1:B:256:VAL:O	1.20	1.01
1:E:11:PRO:HA	1:E:42:PRO:CB	1.90	1.01
1:C:13:VAL:HG12	1:C:13:VAL:O	1.59	1.01
1:B:41:LEU:CB	1:C:190:LYS:NZ	2.24	1.00
1:G:64:VAL:HG11	1:H:10:TYR:CE2	1.95	1.00
1:F:47:LYS:CD	1:F:48:VAL:H	1.75	1.00
1:C:206:ASN:HD21	1:C:208:ARG:HG3	0.83	1.00
1:D:65:PHE:CD2	1:D:66:GLN:N	2.30	1.00
1:G:66:GLN:NE2	1:G:67:TYR:CD1	2.30	0.99
1:B:63:SER:C	1:B:64:VAL:HG12	1.77	0.99
1:A:251:HIS:CG	1:A:251:HIS:O	2.15	0.99
1:F:225:THR:O	1:F:226:GLU:HB2	1.62	0.99
1:C:262:GLN:H	1:C:262:GLN:NE2	1.61	0.99
1:E:182:LYS:HB2	3:E:385:GOL:O1	1.63	0.98
1:A:34:ILE:CB	1:A:52:ILE:CG2	2.41	0.98
1:E:181:PHE:CE1	1:E:183:ARG:NH2	2.30	0.98
1:F:234:VAL:O	1:F:234:VAL:HG13	1.61	0.98
1:G:249:ASN:H	1:G:249:ASN:HD22	0.99	0.98
1:A:66:GLN:HE21	1:A:66:GLN:CA	1.76	0.98
1:E:121:GLY:HA2	1:E:154:LEU:HD21	1.43	0.98
1:B:194:ILE:HG22	1:B:194:ILE:O	1.60	0.98
1:A:63:SER:HA	1:A:65:PHE:HE2	0.84	0.97
1:B:41:LEU:CB	1:C:190:LYS:HZ1	1.77	0.97
1:A:13:VAL:O	1:A:13:VAL:HG12	1.59	0.97
1:G:282:GLU:OE2	1:G:285:GLY:HA2	1.64	0.97
1:G:251:HIS:CD2	1:G:251:HIS:O	2.17	0.97
1:B:246:LEU:O	1:B:250:LEU:HB2	1.64	0.97
1:E:41:LEU:HD13	1:E:41:LEU:N	1.78	0.97
1:A:286:LEU:O	1:A:288:LEU:N	1.98	0.97
1:A:66:GLN:HB3	1:A:67:TYR:CD2	1.99	0.97
1:F:190:LYS:O	1:F:193:GLY:CA	2.12	0.96
1:A:96:ILE:HG13	1:A:127:LEU:HD13	1.48	0.96
1:C:206:ASN:HD21	1:C:208:ARG:CG	1.77	0.96
1:G:62:TYR:CD1	1:G:65:PHE:CZ	2.53	0.96
1:B:314:ASP:OD2	1:B:347:ARG:HB2	1.66	0.95
1:E:137:ILE:H	1:E:137:ILE:HD12	1.31	0.95
1:F:49:TYR:CD2	3:F:383:GOL:O1	2.19	0.95
1:A:52:ILE:N	1:A:52:ILE:HD13	1.80	0.95
1:A:63:SER:CA	1:A:65:PHE:HE2	1.73	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ILE:HD11	1:E:137:ILE:HG13	0.96	0.95
1:G:95:ALA:CB	1:G:123:ASP:OD2	2.13	0.95
1:A:76:SER:OG	1:B:132:SER:O	1.84	0.94
1:G:66:GLN:NE2	1:G:67:TYR:CE1	2.35	0.94
1:A:59:VAL:O	1:A:62:TYR:CE2	2.20	0.94
1:E:45:LEU:O	1:E:47:LYS:N	2.01	0.94
1:A:66:GLN:HA	1:A:66:GLN:HE21	1.33	0.94
1:F:47:LYS:CD	1:F:48:VAL:N	2.30	0.94
1:G:282:GLU:HG3	1:G:283:SER:O	1.68	0.94
1:C:96:ILE:CG2	1:C:97:PRO:N	2.30	0.93
1:C:262:GLN:N	1:C:262:GLN:HE21	1.67	0.93
1:C:262:GLN:N	1:C:262:GLN:NE2	2.17	0.93
1:E:11:PRO:HA	1:E:42:PRO:HB3	0.95	0.93
1:E:252:ILE:O	1:E:252:ILE:HD12	1.69	0.92
1:A:66:GLN:OE1	1:B:10:TYR:CE1	2.23	0.92
1:D:82:ALA:O	1:D:86:ASN:O	1.87	0.92
1:A:66:GLN:HB3	1:A:67:TYR:CZ	2.04	0.91
1:C:262:GLN:H	1:C:262:GLN:HE21	0.93	0.91
1:G:62:TYR:CE1	1:G:65:PHE:HZ	1.84	0.91
1:E:41:LEU:HA	1:E:43:PHE:HE2	1.35	0.91
1:B:63:SER:O	1:B:64:VAL:HG13	1.70	0.90
1:E:211:LYS:O	1:E:278:LEU:O	1.90	0.89
1:D:251:HIS:CG	1:D:251:HIS:O	2.19	0.89
1:B:196:GLU:O	1:B:198:GLU:HG3	1.72	0.89
1:A:65:PHE:N	1:A:65:PHE:CD2	2.39	0.89
1:F:194:ILE:N	1:F:194:ILE:CD1	2.29	0.89
1:A:63:SER:CA	1:A:65:PHE:CD2	2.57	0.88
1:F:134:ASN:HD21	1:F:162:VAL:HA	1.38	0.88
1:F:78:MET:HE1	1:F:101:CYS:HB3	1.52	0.88
1:G:209:LYS:H	1:G:209:LYS:HD2	1.38	0.88
1:E:108:MET:HE1	1:F:135:ASN:O	1.73	0.88
1:H:57:VAL:HG23	1:H:57:VAL:O	1.71	0.88
1:C:260:GLY:C	1:C:261:LYS:CG	2.42	0.88
1:C:96:ILE:O	6:C:392:HOH:O	1.91	0.88
1:D:41:LEU:N	1:D:42:PRO:HD2	1.89	0.88
1:G:314:ASP:O	1:G:344:MET:CG	2.20	0.88
1:A:66:GLN:OE1	1:B:10:TYR:CD1	2.27	0.87
1:A:18:VAL:HG12	1:A:43:PHE:HZ	1.39	0.87
1:B:62:TYR:CB	1:B:65:PHE:CG	2.58	0.87
1:B:257:LEU:H	1:B:257:LEU:HD13	1.40	0.87
1:C:192:TYR:O	1:C:193:GLY:C	2.13	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:GLU:CG	6:D:421:HOH:O	2.22	0.87
1:F:190:LYS:C	1:F:193:GLY:H	1.77	0.87
1:B:94:TYR:HH	1:B:122:THR:HB	1.38	0.87
1:H:133:LEU:O	1:H:137:ILE:HD12	1.74	0.87
1:A:121:GLY:HA3	3:A:386:GOL:H32	1.56	0.87
1:A:194:ILE:HG23	1:A:194:ILE:O	1.73	0.86
1:A:66:GLN:C	1:A:67:TYR:CG	2.48	0.86
1:B:196:GLU:HG2	1:B:198:GLU:HG2	1.55	0.86
1:E:245:GLN:CG	1:H:245:GLN:NE2	1.98	0.86
1:G:249:ASN:H	1:G:249:ASN:ND2	1.74	0.86
1:G:203:HIS:C	1:G:204:ILE:HG22	1.96	0.86
1:E:43:PHE:CD1	1:E:43:PHE:O	2.29	0.85
1:D:251:HIS:HD2	1:D:251:HIS:O	1.55	0.85
1:E:207:PHE:O	1:E:238:PRO:CD	2.23	0.85
1:F:49:TYR:HD2	3:F:383:GOL:HO1	1.23	0.85
1:F:62:TYR:O	1:F:62:TYR:CD1	2.30	0.85
1:A:62:TYR:O	1:A:65:PHE:CZ	2.30	0.85
1:G:186:THR:O	1:G:190:LYS:HE2	1.74	0.85
1:A:52:ILE:O	1:A:53:TYR:CD1	2.29	0.85
1:G:62:TYR:O	1:G:62:TYR:CD1	2.29	0.85
1:A:66:GLN:O	1:A:67:TYR:CD1	2.30	0.85
1:A:62:TYR:O	1:A:65:PHE:CE2	2.30	0.85
1:H:40:GLY:HA2	1:H:54:PHE:CZ	2.09	0.85
1:A:52:ILE:O	1:A:53:TYR:CG	2.30	0.85
1:E:42:PRO:CD	1:E:43:PHE:CD2	2.30	0.85
1:D:60:ASN:OD1	1:D:64:VAL:HG11	1.77	0.84
1:F:196:GLU:H	1:F:196:GLU:CD	1.80	0.84
1:E:10:TYR:HE1	1:E:98:HIS:HE2	1.24	0.84
1:E:108:MET:HE3	1:F:135:ASN:O	1.74	0.84
1:B:62:TYR:HB3	1:B:65:PHE:HB2	1.57	0.84
1:H:204:ILE:HB	1:H:234:VAL:HB	1.60	0.84
1:B:322:GLY:O	6:B:399:HOH:O	1.95	0.84
1:B:196:GLU:CD	1:B:255:ARG:HH21	1.80	0.83
1:G:207:PHE:O	1:G:238:PRO:HD2	1.77	0.83
1:H:194:ILE:O	1:H:194:ILE:CG1	2.24	0.83
1:G:194:ILE:HD12	1:G:271:MET:HE1	1.60	0.83
1:E:134:ASN:ND2	1:E:134:ASN:C	2.29	0.83
1:D:63:SER:O	1:D:64:VAL:HG13	1.79	0.83
1:C:96:ILE:HG22	1:C:97:PRO:HD3	0.83	0.83
1:D:190:LYS:O	1:D:193:GLY:N	2.10	0.83
1:B:201:LEU:HD23	1:B:276:LEU:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:HG22	1:C:97:PRO:N	1.89	0.83
1:F:275:MET:HB3	1:F:298:CYS:HB3	1.58	0.83
1:C:198:GLU:HB2	1:C:200:ILE:CD1	2.08	0.83
1:C:14:GLY:O	1:C:18:VAL:CG1	2.27	0.82
1:A:286:LEU:HD12	1:A:286:LEU:H	1.45	0.82
1:G:204:ILE:HA	1:G:234:VAL:HB	1.62	0.82
1:F:47:LYS:HD3	1:F:48:VAL:H	0.83	0.82
1:F:66:GLN:O	1:F:67:TYR:HB2	1.80	0.82
1:B:284:PHE:O	6:B:393:HOH:O	1.97	0.82
1:B:94:TYR:CZ	1:B:122:THR:HB	2.13	0.81
1:F:220:PHE:O	1:F:224:VAL:HG12	1.79	0.81
1:B:62:TYR:HB2	1:B:65:PHE:CD2	2.14	0.81
1:A:184:ASP:HB3	1:D:261:LYS:HE3	1.60	0.81
1:A:13:VAL:O	1:A:13:VAL:CG1	2.27	0.81
1:B:41:LEU:HB3	1:C:190:LYS:HZ1	1.43	0.81
1:B:196:GLU:HG2	1:B:198:GLU:HG3	0.82	0.81
1:B:62:TYR:CB	1:B:65:PHE:HB2	2.08	0.81
1:E:41:LEU:H	1:E:41:LEU:CD2	1.86	0.81
1:E:41:LEU:HA	1:E:43:PHE:CE2	2.15	0.81
1:B:41:LEU:HB3	1:C:190:LYS:NZ	1.93	0.81
1:E:42:PRO:HB2	6:E:413:HOH:O	1.81	0.81
1:G:207:PHE:HD1	1:G:207:PHE:O	1.64	0.81
1:G:91:HIS:HD1	1:G:369:TYR:HE1	1.28	0.81
1:H:329:ASP:HA	1:H:332:ILE:HG12	1.63	0.81
1:H:194:ILE:O	1:H:194:ILE:HD12	1.81	0.81
1:D:189:LYS:O	1:D:194:ILE:HG22	1.81	0.80
1:C:196:GLU:HG3	1:C:197:SER:HA	1.60	0.80
1:H:374:ARG:O	1:H:375:ASP:HB2	1.82	0.80
1:C:260:GLY:O	1:C:261:LYS:CG	2.30	0.80
1:G:353:TYR:O	1:G:357:ARG:NH1	2.14	0.80
1:A:227:VAL:O	1:A:228:ASP:OD1	2.00	0.80
1:A:62:TYR:CD1	1:A:65:PHE:CE1	2.70	0.80
1:B:252:ILE:N	1:B:252:ILE:HD12	1.92	0.80
1:B:252:ILE:CD1	1:B:252:ILE:O	2.30	0.80
1:D:283:SER:O	1:D:284:PHE:HB2	1.80	0.80
1:D:65:PHE:O	1:D:66:GLN:CG	2.30	0.80
1:F:192:TYR:O	1:F:194:ILE:CD1	2.30	0.80
1:D:186:THR:O	1:D:186:THR:HG22	1.80	0.80
1:H:194:ILE:O	1:H:194:ILE:HG13	1.80	0.80
1:G:57:VAL:HG12	1:G:57:VAL:O	1.81	0.80
1:C:199:LYS:O	1:C:229:ALA:HB1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLN:O	1:A:67:TYR:CG	2.35	0.80
1:B:41:LEU:HB2	1:C:190:LYS:HZ2	1.46	0.80
1:H:94:TYR:O	1:H:95:ALA:CB	2.29	0.80
1:C:13:VAL:CG1	1:C:13:VAL:O	2.29	0.79
1:C:10:TYR:OH	1:C:97:PRO:HG3	1.82	0.79
1:G:95:ALA:HB3	1:G:123:ASP:HB2	1.63	0.79
1:A:66:GLN:NE2	1:A:66:GLN:N	2.30	0.79
1:B:280:GLU:O	1:B:303:VAL:CG1	2.23	0.79
1:C:198:GLU:HG2	1:C:198:GLU:O	1.81	0.79
1:A:62:TYR:O	1:A:62:TYR:CD1	2.32	0.79
1:B:194:ILE:O	1:B:194:ILE:CG2	2.29	0.79
1:G:207:PHE:CD1	1:G:207:PHE:O	2.36	0.79
1:E:59:VAL:O	1:E:59:VAL:HG23	1.81	0.79
1:F:66:GLN:O	1:F:67:TYR:CB	2.30	0.79
1:H:194:ILE:O	1:H:194:ILE:CD1	2.31	0.79
1:B:207:PHE:HB2	1:B:237:GLY:HA3	1.63	0.78
1:D:60:ASN:OD1	1:D:64:VAL:HG12	1.82	0.78
1:H:147:VAL:HB	1:H:168:ILE:HG22	1.65	0.78
1:F:190:LYS:C	1:F:193:GLY:HA2	2.04	0.78
1:H:338:GLU:O	1:H:342:ARG:HD3	1.83	0.78
1:D:64:VAL:O	1:D:64:VAL:CG2	2.30	0.78
1:E:91:HIS:CE1	1:E:118:THR:HG23	2.18	0.78
1:F:34:ILE:HB	1:F:52:ILE:HG22	1.64	0.78
1:E:66:GLN:HE22	1:H:187:GLN:HE22	1.32	0.78
1:F:47:LYS:HE3	1:F:48:VAL:CG2	2.12	0.78
1:A:283:SER:O	1:A:284:PHE:HB2	1.84	0.78
1:D:65:PHE:O	1:D:66:GLN:CB	2.30	0.78
1:A:66:GLN:NE2	1:A:66:GLN:CA	2.46	0.78
1:C:14:GLY:O	1:C:18:VAL:HG12	1.82	0.78
1:C:363:SER:HB3	3:C:384:GOL:H32	1.64	0.78
1:G:66:GLN:NE2	1:G:67:TYR:HD1	1.79	0.78
1:A:96:ILE:CG1	1:A:127:LEU:CD1	2.55	0.77
1:B:62:TYR:HB2	1:B:65:PHE:HB3	1.67	0.77
1:H:122:THR:O	1:H:124:ILE:N	2.18	0.77
1:F:185:MET:O	1:F:189:LYS:HG3	1.83	0.77
1:B:64:VAL:O	1:B:64:VAL:CG2	2.22	0.77
1:E:41:LEU:CB	1:E:43:PHE:CE2	2.67	0.77
1:A:286:LEU:O	1:A:289:LEU:N	2.17	0.77
1:A:66:GLN:HE21	1:A:66:GLN:N	1.81	0.77
1:B:196:GLU:CG	1:B:198:GLU:HG2	2.11	0.77
1:G:149:ALA:HB2	1:G:168:ILE:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:H	1:D:42:PRO:CD	1.96	0.76
1:F:47:LYS:O	1:F:49:TYR:CD2	2.39	0.76
1:H:204:ILE:HD11	2:H:382:UDP:H2'	1.67	0.76
1:D:196:GLU:O	1:D:198:GLU:CG	2.34	0.76
1:D:202:ILE:HG23	1:D:275:MET:HG3	1.68	0.76
1:F:93:HIS:O	1:F:118:THR:O	2.02	0.76
1:G:62:TYR:CD2	1:G:65:PHE:CD1	2.73	0.76
1:B:41:LEU:CB	1:C:190:LYS:HZ2	1.99	0.76
1:C:94:TYR:O	1:C:94:TYR:CG	2.38	0.76
1:E:209:LYS:H	1:E:209:LYS:HD2	1.50	0.76
1:G:342:ARG:HE	1:G:342:ARG:HA	1.50	0.76
1:E:262:GLN:O	2:E:382:UDP:O4	2.03	0.76
1:B:196:GLU:O	1:B:198:GLU:CG	2.34	0.75
1:A:206:ASN:HB3	1:A:211:LYS:HG3	1.66	0.75
1:F:49:TYR:HD2	3:F:383:GOL:O1	1.60	0.75
1:C:57:VAL:HG12	1:C:77:LYS:HG2	1.67	0.75
1:E:42:PRO:CD	1:E:43:PHE:H	1.98	0.75
1:G:64:VAL:CG1	1:H:10:TYR:HE2	1.98	0.75
1:E:185:MET:O	1:E:189:LYS:HG3	1.85	0.75
1:E:41:LEU:CA	1:E:43:PHE:HE2	1.99	0.75
1:C:260:GLY:O	1:C:261:LYS:HG3	1.87	0.75
1:E:224:VAL:HG21	1:E:255:ARG:HD3	1.68	0.75
1:G:61:GLN:OE1	1:H:130:ASP:OD1	2.05	0.75
1:B:92:VAL:CG1	1:B:98:HIS:HB2	2.17	0.74
1:F:49:TYR:HB2	1:F:52:ILE:HD11	1.70	0.74
1:G:66:GLN:CD	1:G:67:TYR:CE1	2.61	0.74
1:E:11:PRO:C	1:E:42:PRO:HB3	2.08	0.74
1:B:198:GLU:O	1:B:228:ASP:O	2.06	0.74
1:H:22:GLU:HG3	6:H:393:HOH:O	1.88	0.74
1:C:16:SER:HB2	1:C:94:TYR:HB2	1.69	0.73
1:D:65:PHE:C	1:D:66:GLN:HG3	2.07	0.73
1:F:96:ILE:HD13	1:F:137:ILE:HG13	1.69	0.73
1:G:282:GLU:OE2	1:G:285:GLY:CA	2.36	0.73
1:A:194:ILE:CG2	1:A:194:ILE:O	2.34	0.73
1:A:66:GLN:C	1:A:67:TYR:CD2	2.62	0.73
1:B:62:TYR:CB	1:B:65:PHE:HB3	2.17	0.73
1:E:42:PRO:HD2	1:E:43:PHE:H	1.53	0.73
1:F:66:GLN:H	1:F:66:GLN:CD	1.89	0.73
1:E:245:GLN:HG2	1:H:245:GLN:HE22	1.46	0.73
1:F:190:LYS:C	1:F:193:GLY:N	2.42	0.73
1:B:314:ASP:O	1:B:344:MET:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:LYS:CD	1:F:48:VAL:HG23	2.19	0.72
1:F:49:TYR:HB2	1:F:52:ILE:CG1	2.19	0.72
1:B:150:VAL:HA	1:B:171:VAL:O	1.88	0.72
1:G:204:ILE:HG23	1:G:204:ILE:O	1.88	0.72
1:D:86:ASN:O	1:D:87:LEU:CB	2.34	0.72
1:E:204:ILE:HD11	2:E:382:UDP:O2	1.90	0.72
1:G:194:ILE:O	1:G:194:ILE:CG2	2.30	0.72
1:A:64:VAL:HG12	1:B:13:VAL:HG22	1.71	0.72
1:E:41:LEU:HB3	1:E:43:PHE:CE2	2.24	0.72
1:H:94:TYR:O	1:H:95:ALA:HB2	1.88	0.72
1:D:185:MET:O	1:D:188:LEU:HD23	1.89	0.72
1:D:175:ILE:HD11	1:D:290:GLU:HG3	1.72	0.72
1:G:339:GLU:O	1:G:343:ASN:HB2	1.90	0.72
1:B:374:ARG:O	1:B:374:ARG:HG3	1.90	0.71
1:D:189:LYS:NZ	1:D:198:GLU:OE1	2.20	0.71
1:B:196:GLU:OE1	1:B:255:ARG:CZ	2.37	0.71
1:C:106:LYS:HE2	1:C:111:GLU:HG2	1.72	0.71
1:D:282:GLU:HG3	1:D:284:PHE:H	1.54	0.71
1:C:136:LEU:HD21	1:D:72:LEU:HB3	1.72	0.71
1:D:198:GLU:HG3	6:D:421:HOH:O	1.89	0.71
1:D:65:PHE:O	1:D:66:GLN:HG3	1.90	0.71
1:F:189:LYS:HB3	1:F:195:SER:OG	1.90	0.71
1:F:69:PRO:HG2	1:F:69:PRO:O	1.90	0.71
1:G:194:ILE:O	6:G:401:HOH:O	2.07	0.71
1:A:286:LEU:O	1:A:287:VAL:C	2.28	0.71
1:B:357:ARG:HB2	1:B:360:LYS:HB2	1.72	0.71
1:E:245:GLN:HG3	1:H:245:GLN:HE22	0.56	0.71
1:D:64:VAL:HG22	1:D:64:VAL:O	1.90	0.71
1:A:152:HIS:NE2	1:A:170:THR:HG21	2.05	0.71
1:A:96:ILE:CG1	1:A:127:LEU:HD13	2.18	0.70
1:D:375:ASP:C	1:D:376:ASP:CG	2.49	0.70
1:D:65:PHE:HD2	1:D:66:GLN:H	1.37	0.70
1:B:247:VAL:O	1:B:250:LEU:O	2.09	0.70
1:F:207:PHE:CE1	1:F:235:GLY:O	2.44	0.70
1:E:44:ARG:CG	1:E:44:ARG:O	2.36	0.70
1:G:207:PHE:CD1	1:G:237:GLY:HA3	2.27	0.70
1:A:227:VAL:HG12	1:A:227:VAL:O	1.91	0.70
1:D:375:ASP:O	1:D:376:ASP:CG	2.29	0.70
1:E:173:ASN:HB2	1:E:284:PHE:CE1	2.26	0.70
1:D:375:ASP:C	1:D:376:ASP:OD2	2.30	0.70
1:E:119:LEU:HD23	1:E:124:ILE:CG1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:PHE:HE1	1:E:183:ARG:CZ	2.04	0.70
1:G:200:ILE:HG22	1:G:230:LYS:HB2	1.71	0.70
1:A:59:VAL:O	1:A:62:TYR:CD2	2.43	0.70
1:E:41:LEU:CA	1:E:43:PHE:CE2	2.74	0.70
1:H:192:TYR:HB3	1:H:257:LEU:HD21	1.74	0.70
1:C:39:SER:HB2	1:C:70:TYR:CE1	2.27	0.70
1:G:62:TYR:CZ	1:G:65:PHE:CZ	2.75	0.70
1:F:126:VAL:HG23	1:F:127:LEU:HD12	1.73	0.69
1:G:301:THR:HA	1:G:319:CYS:O	1.92	0.69
1:G:62:TYR:CG	1:G:65:PHE:CD1	2.79	0.69
1:B:196:GLU:O	1:B:198:GLU:CD	2.29	0.69
1:B:226:GLU:HB3	1:B:332:ILE:HD13	1.74	0.69
1:H:159:HIS:HD2	6:H:415:HOH:O	1.74	0.69
1:C:196:GLU:CG	1:C:197:SER:HA	2.22	0.69
1:F:194:ILE:HG22	1:F:196:GLU:OE2	1.93	0.69
1:F:319:CYS:SG	1:F:327:VAL:HG22	2.32	0.69
1:A:64:VAL:CG1	1:B:13:VAL:HG22	2.22	0.69
1:B:319:CYS:SG	1:B:327:VAL:HG22	2.31	0.69
1:D:63:SER:C	1:D:64:VAL:HG13	2.13	0.69
1:A:66:GLN:CB	1:A:67:TYR:CD2	2.68	0.69
1:B:157:GLU:HG3	3:B:382:GOL:H32	1.75	0.69
1:B:92:VAL:HG11	1:B:98:HIS:O	1.92	0.69
1:C:206:ASN:C	1:C:206:ASN:OD1	2.29	0.69
1:B:196:GLU:CD	1:B:198:GLU:HG2	2.13	0.69
1:A:247:VAL:HG23	1:A:252:ILE:HG13	1.73	0.69
1:G:61:GLN:NE2	1:H:127:LEU:HD12	2.05	0.69
1:G:206:ASN:C	1:G:206:ASN:OD1	2.30	0.69
1:A:209:LYS:HD2	1:A:209:LYS:H	1.57	0.69
1:C:192:TYR:N	1:C:192:TYR:HD2	1.91	0.69
1:F:207:PHE:CD1	1:F:235:GLY:O	2.46	0.69
1:D:374:ARG:C	1:D:375:ASP:OD2	2.30	0.69
1:E:355:GLN:HA	1:E:360:LYS:HE2	1.75	0.69
1:F:47:LYS:O	1:F:49:TYR:CE2	2.46	0.69
1:H:375:ASP:O	6:H:410:HOH:O	2.11	0.69
1:A:96:ILE:CG1	1:A:127:LEU:HD12	2.17	0.68
1:G:121:GLY:HA3	1:G:283:SER:HB3	1.75	0.68
1:B:143:GLN:HG3	6:B:401:HOH:O	1.92	0.68
1:A:78:MET:HG2	1:A:90:LEU:HD21	1.75	0.68
1:B:205:SER:OG	1:B:206:ASN:O	2.09	0.68
1:E:182:LYS:HB2	3:E:385:GOL:C1	2.23	0.68
1:A:206:ASN:HB2	1:A:211:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:HIS:O	1:A:251:HIS:CD2	2.47	0.68
1:E:137:ILE:N	1:E:137:ILE:HD12	2.07	0.68
1:E:183:ARG:HD2	1:E:185:MET:SD	2.34	0.68
1:D:209:LYS:HD2	1:D:209:LYS:H	1.59	0.68
1:A:207:PHE:HD1	1:A:238:PRO:HD2	1.59	0.68
1:C:94:TYR:CD2	1:C:94:TYR:O	2.46	0.68
1:D:155:ILE:HG12	1:D:168:ILE:HD11	1.75	0.68
1:F:219:ALA:O	1:F:223:ILE:HG13	1.93	0.68
1:G:251:HIS:ND1	1:G:251:HIS:O	2.26	0.68
1:G:60:ASN:OD1	1:G:60:ASN:C	2.33	0.67
1:A:204:ILE:C	1:A:205:SER:OG	2.33	0.67
1:C:96:ILE:HG23	1:C:97:PRO:N	2.10	0.67
1:A:96:ILE:HG12	1:A:123:ASP:CB	2.25	0.67
1:D:103:TYR:CE1	1:D:143:GLN:HG2	2.29	0.67
1:G:282:GLU:O	6:G:386:HOH:O	2.12	0.67
1:C:281:LYS:HD3	6:C:412:HOH:O	1.95	0.67
1:C:125:THR:HB	1:C:281:LYS:HE3	1.76	0.67
1:A:59:VAL:O	1:A:62:TYR:HE2	1.74	0.67
1:F:96:ILE:HD13	1:F:137:ILE:CG1	2.24	0.67
1:B:150:VAL:O	1:B:284:PHE:CD2	2.48	0.67
1:D:23:LEU:HD12	1:D:362:VAL:HG23	1.77	0.67
1:F:49:TYR:CD2	1:F:52:ILE:HD11	2.30	0.67
1:H:112:ARG:HD2	1:H:112:ARG:O	1.94	0.67
1:A:314:ASP:O	1:A:344:MET:HG3	1.94	0.66
1:A:62:TYR:C	1:A:65:PHE:CE2	2.68	0.66
1:E:119:LEU:CD2	1:E:124:ILE:HD11	2.25	0.66
1:G:66:GLN:NE2	1:G:67:TYR:HE1	1.91	0.66
1:C:189:LYS:HB3	1:C:194:ILE:HG12	1.78	0.66
1:F:190:LYS:C	1:F:193:GLY:CA	2.64	0.66
1:H:201:LEU:HD12	1:H:201:LEU:H	1.61	0.66
1:A:34:ILE:CA	1:A:52:ILE:HG22	2.26	0.66
1:F:122:THR:HB	1:F:126:VAL:HG22	1.78	0.66
1:A:206:ASN:CB	1:A:211:LYS:HE3	2.26	0.66
1:A:34:ILE:CG2	1:A:52:ILE:HG21	2.24	0.66
1:B:185:MET:O	1:B:189:LYS:HB2	1.96	0.66
1:C:198:GLU:HB2	1:C:200:ILE:HD11	1.77	0.66
1:D:63:SER:C	1:D:64:VAL:CG1	2.64	0.66
1:F:49:TYR:HB2	1:F:52:ILE:CD1	2.25	0.66
1:G:66:GLN:HE21	1:G:67:TYR:HD1	1.43	0.66
1:D:285:GLY:O	1:D:288:LEU:HB2	1.96	0.66
1:E:66:GLN:HE22	1:H:185:MET:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:VAL:CG2	1:F:224:VAL:O	2.42	0.65
1:C:62:TYR:HB2	1:C:65:PHE:HB2	1.77	0.65
1:F:35:HIS:HD2	1:F:87:LEU:HD21	1.60	0.65
1:F:66:GLN:OE1	1:F:66:GLN:N	2.30	0.65
1:F:66:GLN:O	1:F:67:TYR:CG	2.49	0.65
1:B:247:VAL:HG11	1:B:256:VAL:HG11	1.78	0.65
1:D:198:GLU:HG2	6:D:421:HOH:O	1.87	0.65
1:E:41:LEU:N	1:E:41:LEU:CD1	2.46	0.65
1:F:96:ILE:CG2	1:F:97:PRO:HD3	2.27	0.65
1:C:199:LYS:HE2	1:C:199:LYS:HA	1.79	0.65
1:D:122:THR:HG22	1:D:126:VAL:HG22	1.78	0.65
1:A:93:HIS:O	1:A:120:HIS:HD2	1.80	0.65
1:F:106:LYS:HE2	1:F:111:GLU:HG3	1.79	0.65
1:G:209:LYS:N	1:G:209:LYS:HD2	2.10	0.65
1:G:60:ASN:OD1	1:G:61:GLN:N	2.30	0.65
1:A:119:LEU:HD12	1:A:168:ILE:HD12	1.79	0.65
1:A:64:VAL:N	1:A:65:PHE:CD2	2.65	0.65
1:G:64:VAL:O	6:G:410:HOH:O	2.14	0.65
1:B:236:ASP:OD1	1:B:240:PHE:HD1	1.80	0.65
1:E:181:PHE:CE1	1:E:183:ARG:CZ	2.79	0.65
1:A:34:ILE:HG22	1:A:52:ILE:HG21	1.79	0.65
1:F:342:ARG:O	1:F:346:GLU:HB2	1.97	0.65
1:F:49:TYR:CE2	3:F:383:GOL:O1	2.42	0.65
1:G:367:THR:O	1:G:371:ASP:HB2	1.96	0.65
1:B:196:GLU:OE1	1:B:255:ARG:NE	2.30	0.64
1:G:311:GLN:C	1:G:313:GLY:H	1.99	0.64
1:D:65:PHE:O	1:D:66:GLN:HB2	1.96	0.64
1:E:92:VAL:CG1	1:E:93:HIS:N	2.58	0.64
1:F:190:LYS:O	1:F:193:GLY:N	2.31	0.64
1:H:201:LEU:HD11	1:H:220:PHE:HE2	1.61	0.64
1:B:257:LEU:H	1:B:257:LEU:CD1	2.02	0.64
1:A:62:TYR:CD1	1:A:65:PHE:CZ	2.86	0.64
1:E:10:TYR:HE1	1:E:98:HIS:NE2	1.96	0.64
1:G:66:GLN:CD	1:G:67:TYR:CD1	2.71	0.64
1:G:245:GLN:O	1:G:246:LEU:HB2	1.97	0.64
1:C:198:GLU:CG	1:C:198:GLU:O	2.45	0.64
1:A:277:LEU:O	1:A:300:GLY:HA2	1.98	0.64
1:F:224:VAL:CG2	1:F:255:ARG:CZ	2.75	0.64
1:F:75:ALA:HA	1:F:78:MET:HE2	1.78	0.64
1:C:282:GLU:HG2	1:C:306:ILE:HD11	1.80	0.64
1:C:57:VAL:HG23	1:C:57:VAL:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:VAL:HG22	1:E:98:HIS:HB3	1.80	0.64
1:H:173:ASN:HB2	1:H:284:PHE:CE1	2.33	0.64
1:C:192:TYR:N	1:C:192:TYR:CD2	2.65	0.63
1:F:274:LEU:HD11	1:F:299:ILE:HG13	1.79	0.63
1:A:18:VAL:HG12	1:A:43:PHE:CZ	2.27	0.63
1:C:96:ILE:CD1	1:C:96:ILE:O	2.46	0.63
1:G:55:HIS:HB3	1:G:77:LYS:HE2	1.80	0.63
1:C:11:PRO:O	1:C:42:PRO:HA	1.97	0.63
1:E:91:HIS:HE1	1:E:118:THR:HG23	1.63	0.63
1:H:47:LYS:HD2	1:H:48:VAL:H	1.63	0.63
1:A:209:LYS:CD	1:A:209:LYS:H	2.11	0.63
1:A:209:LYS:N	1:A:209:LYS:HD2	2.13	0.63
1:G:126:VAL:HG23	1:G:127:LEU:HD12	1.80	0.63
1:F:196:GLU:N	1:F:196:GLU:OE2	2.30	0.62
1:F:69:PRO:CG	1:F:69:PRO:O	2.43	0.62
1:A:237:GLY:H	1:A:240:PHE:HB2	1.64	0.62
1:A:51:ASN:C	1:A:52:ILE:HD13	2.20	0.62
1:A:67:TYR:CD2	1:A:67:TYR:N	2.67	0.62
1:D:204:ILE:HG22	1:D:234:VAL:HB	1.81	0.62
1:H:106:LYS:HB2	1:H:115:ILE:HD11	1.81	0.62
1:H:122:THR:OG1	1:H:123:ASP:N	2.31	0.62
1:E:43:PHE:HD1	1:E:43:PHE:O	1.83	0.62
1:B:91:HIS:CD2	1:B:93:HIS:NE2	2.67	0.62
1:F:106:LYS:HD2	1:F:115:ILE:HD11	1.81	0.62
1:A:34:ILE:CB	1:A:52:ILE:HG21	2.29	0.62
1:F:192:TYR:O	1:F:194:ILE:HD11	1.99	0.62
1:F:93:HIS:O	1:F:120:HIS:HD2	1.83	0.62
1:D:163:LYS:N	1:D:164:PRO:HD3	2.14	0.62
1:E:168:ILE:HD12	1:E:168:ILE:H	1.65	0.62
1:A:63:SER:N	1:A:65:PHE:CE2	2.68	0.61
1:B:94:TYR:OH	1:B:122:THR:CA	2.49	0.61
1:C:235:GLY:H	1:C:261:LYS:H	1.46	0.61
1:E:41:LEU:CB	1:E:43:PHE:HE2	2.13	0.61
1:A:360:LYS:HE2	3:A:387:GOL:H12	1.81	0.61
1:E:45:LEU:O	1:E:47:LYS:O	2.19	0.61
1:F:225:THR:O	1:F:226:GLU:CB	2.36	0.61
1:F:236:ASP:HB3	1:H:182:LYS:O	2.00	0.61
1:B:39:SER:HB3	1:B:70:TYR:HE1	1.66	0.61
1:D:96:ILE:HG12	1:D:137:ILE:HG23	1.82	0.61
1:B:282:GLU:OE2	1:B:285:GLY:HA2	2.00	0.61
1:D:358:SER:O	1:D:362:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD22	1:C:124:ILE:HD11	1.83	0.61
1:C:234:VAL:HA	1:C:259:LEU:O	2.00	0.61
6:C:416:HOH:O	1:D:67:TYR:HD2	1.83	0.61
1:A:93:HIS:O	1:A:118:THR:O	2.19	0.61
1:H:347:ARG:HE	1:H:347:ARG:HA	1.65	0.61
1:B:209:LYS:H	1:B:209:LYS:HE2	1.65	0.60
1:C:92:VAL:HG13	1:C:98:HIS:HB2	1.83	0.60
1:B:328:ALA:O	1:B:332:ILE:HG22	2.01	0.60
1:A:66:GLN:HA	1:A:66:GLN:NE2	2.12	0.60
1:E:137:ILE:HG22	1:E:141:ILE:HG13	1.83	0.60
1:E:42:PRO:HD2	1:E:43:PHE:HD2	0.53	0.60
1:F:78:MET:CE	1:F:101:CYS:HB3	2.27	0.60
1:F:96:ILE:HG22	1:F:97:PRO:HD3	1.84	0.60
1:E:134:ASN:ND2	1:E:134:ASN:O	2.30	0.60
1:F:122:THR:HA	1:F:125:THR:HB	1.83	0.60
1:G:282:GLU:HG3	1:G:283:SER:N	2.15	0.60
1:A:358:SER:O	1:A:362:VAL:HG23	2.01	0.60
1:A:374:ARG:O	1:A:375:ASP:HB2	2.01	0.59
1:C:121:GLY:O	1:C:125:THR:OG1	2.20	0.59
1:E:182:LYS:HD2	3:E:385:GOL:H2	1.83	0.59
1:F:224:VAL:HG22	1:F:224:VAL:O	2.01	0.59
1:A:198:GLU:O	1:A:199:LYS:HB2	2.00	0.59
1:H:93:HIS:O	1:H:94:TYR:CB	2.49	0.59
1:H:215:ASP:HB3	1:H:278:LEU:HD12	1.83	0.59
1:C:93:HIS:O	1:C:98:HIS:CD2	2.55	0.59
1:D:324:THR:HG21	6:D:385:HOH:O	2.02	0.59
1:E:41:LEU:CD2	1:E:41:LEU:O	2.50	0.59
1:F:49:TYR:HB2	1:F:52:ILE:HG12	1.85	0.59
1:G:94:TYR:OH	1:G:122:THR:OG1	1.58	0.59
1:E:66:GLN:NE2	1:H:185:MET:CE	2.66	0.59
1:B:155:ILE:HG12	1:B:168:ILE:HD11	1.84	0.59
1:B:257:LEU:HD13	1:B:257:LEU:N	2.14	0.59
1:A:52:ILE:C	1:A:53:TYR:CG	2.75	0.59
1:B:323:ASP:O	1:B:327:VAL:HG23	2.02	0.59
1:G:342:ARG:NE	1:G:342:ARG:HA	2.17	0.59
1:A:96:ILE:HG12	1:A:123:ASP:HB3	1.84	0.59
1:B:112:ARG:O	1:B:112:ARG:HD3	2.03	0.59
1:B:62:TYR:CA	1:B:65:PHE:HB3	2.33	0.59
1:C:204:ILE:HA	1:C:234:VAL:HB	1.85	0.59
1:D:18:VAL:O	1:D:22:GLU:HG2	2.02	0.59
1:F:65:PHE:CD1	1:F:65:PHE:N	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:251:HIS:CD2	1:H:251:HIS:O	2.55	0.59
1:E:5:ILE:HG23	1:E:89:ILE:HG22	1.85	0.59
1:E:41:LEU:O	1:E:41:LEU:HD23	2.03	0.58
1:F:225:THR:O	1:F:227:VAL:N	2.34	0.58
1:F:227:VAL:HG12	1:F:227:VAL:O	2.01	0.58
1:D:224:VAL:HG21	1:D:255:ARG:HD3	1.84	0.58
1:E:92:VAL:HG13	1:E:93:HIS:N	2.18	0.58
1:G:122:THR:HG21	6:G:408:HOH:O	2.02	0.58
1:H:122:THR:O	1:H:123:ASP:C	2.40	0.58
1:H:40:GLY:C	1:H:42:PRO:HD2	2.23	0.58
1:F:62:TYR:O	1:F:62:TYR:CG	2.54	0.58
1:H:122:THR:HB	1:H:126:VAL:HG22	1.85	0.58
1:A:34:ILE:HB	1:A:52:ILE:HG21	1.75	0.58
1:A:34:ILE:CA	1:A:52:ILE:CG2	2.81	0.58
1:E:106:LYS:HE3	1:E:145:ASP:OD1	2.02	0.58
1:H:103:TYR:CE1	1:H:143:GLN:HG2	2.39	0.58
1:G:61:GLN:OE1	1:H:133:LEU:HD22	2.02	0.58
1:H:167:ASP:HA	6:H:394:HOH:O	2.03	0.58
1:C:14:GLY:O	1:C:18:VAL:HG13	2.01	0.58
1:C:43:PHE:H	1:C:43:PHE:HD2	1.50	0.58
1:D:122:THR:HG22	1:D:126:VAL:CG2	2.34	0.58
1:E:119:LEU:CD2	1:E:124:ILE:CG1	2.82	0.58
1:E:137:ILE:HG22	1:E:141:ILE:CD1	2.33	0.58
1:F:257:LEU:H	1:F:257:LEU:HD12	1.67	0.58
1:B:196:GLU:CD	1:B:255:ARG:NH2	2.50	0.58
1:B:275:MET:HG2	1:B:298:CYS:HB3	1.84	0.58
1:D:66:GLN:HE22	3:D:382:GOL:H32	1.68	0.58
1:A:64:VAL:HG12	1:A:64:VAL:O	2.04	0.58
1:E:137:ILE:HG22	1:E:141:ILE:HD11	1.85	0.58
1:F:209:LYS:H	1:F:209:LYS:HD2	1.69	0.58
1:G:227:VAL:HG11	1:G:335:LEU:HB3	1.85	0.58
1:B:91:HIS:CD2	1:B:93:HIS:CD2	2.92	0.57
1:A:52:ILE:O	1:A:53:TYR:CB	2.51	0.57
1:G:182:LYS:HE3	1:G:295:GLY:HA3	1.86	0.57
1:H:92:VAL:HG22	1:H:98:HIS:HB3	1.86	0.57
1:B:122:THR:O	1:B:126:VAL:HG22	2.03	0.57
1:H:119:LEU:HD12	1:H:168:ILE:HD12	1.86	0.57
1:H:250:LEU:O	1:H:251:HIS:CG	2.57	0.57
1:A:96:ILE:HG21	6:A:393:HOH:O	1.83	0.57
1:G:93:HIS:O	1:G:120:HIS:HD2	1.86	0.57
1:H:201:LEU:HD11	1:H:220:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ILE:O	1:C:205:SER:CB	2.32	0.57
1:C:275:MET:HG2	1:C:298:CYS:SG	2.44	0.57
1:E:239:GLU:O	1:E:243:ILE:HG12	2.04	0.57
1:G:61:GLN:OE1	1:H:130:ASP:CG	2.42	0.57
1:F:245:GLN:HG2	1:H:357:ARG:HH12	1.69	0.57
1:H:57:VAL:CG2	1:H:57:VAL:O	2.43	0.57
1:C:277:LEU:O	1:C:300:GLY:HA2	2.04	0.57
1:F:245:GLN:HG2	1:H:357:ARG:NH1	2.20	0.57
1:C:155:ILE:HG12	1:C:168:ILE:HD11	1.85	0.57
1:C:96:ILE:C	1:C:96:ILE:CD1	2.73	0.57
1:G:66:GLN:CD	1:G:67:TYR:HE1	2.04	0.57
1:A:286:LEU:C	1:A:288:LEU:N	2.58	0.57
1:A:40:GLY:HA2	1:A:56:GLU:HG3	1.86	0.57
1:A:66:GLN:HG2	1:B:10:TYR:HE1	1.70	0.57
1:E:204:ILE:O	1:E:204:ILE:HG13	2.02	0.57
1:F:92:VAL:HG13	1:F:98:HIS:HB2	1.87	0.57
1:A:207:PHE:CD1	1:A:238:PRO:HD2	2.40	0.57
1:C:228:ASP:HB2	1:C:255:ARG:HH12	1.70	0.57
1:D:196:GLU:O	1:D:197:SER:C	2.43	0.57
1:D:97:PRO:CD	6:D:407:HOH:O	2.53	0.57
1:E:119:LEU:HD23	1:E:124:ILE:HD11	1.87	0.57
1:E:132:SER:O	1:E:133:LEU:HD12	2.03	0.57
1:H:262:GLN:HE21	1:H:262:GLN:HA	1.70	0.57
1:E:119:LEU:HD23	1:E:124:ILE:HG12	1.87	0.56
1:F:62:TYR:O	1:F:63:SER:C	2.41	0.56
1:A:96:ILE:HG12	1:A:123:ASP:HB2	1.87	0.56
1:A:65:PHE:N	1:A:65:PHE:HD2	2.01	0.56
1:D:194:ILE:HG12	1:D:194:ILE:O	2.04	0.56
1:G:61:GLN:NE2	1:H:127:LEU:HA	2.20	0.56
1:A:66:GLN:HG2	1:B:10:TYR:CE1	2.40	0.56
1:C:198:GLU:O	1:C:199:LYS:CE	2.53	0.56
1:E:182:LYS:HD2	3:E:385:GOL:C2	2.35	0.56
1:F:282:GLU:HG3	1:F:284:PHE:O	2.05	0.56
1:G:202:ILE:HG23	1:G:202:ILE:O	2.03	0.56
1:H:57:VAL:HG12	1:H:77:LYS:HG2	1.87	0.56
1:B:150:VAL:O	1:B:284:PHE:CE2	2.58	0.56
1:C:231:LEU:HB3	1:C:256:VAL:HG22	1.86	0.56
1:D:251:HIS:CD2	1:D:251:HIS:C	2.65	0.56
1:A:82:ALA:HA	1:A:87:LEU:HG	1.88	0.56
1:E:141:ILE:HG23	1:E:147:VAL:HG11	1.87	0.56
1:A:63:SER:N	1:A:65:PHE:CD2	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:HG12	1:B:15:GLY:H	1.67	0.56
1:E:66:GLN:NE2	1:H:187:GLN:HE22	2.00	0.56
1:E:181:PHE:CD2	1:G:237:GLY:HA2	2.41	0.56
1:G:314:ASP:O	1:G:344:MET:SD	2.63	0.56
1:G:95:ALA:HB3	1:G:123:ASP:CB	2.35	0.56
1:B:205:SER:CB	1:B:206:ASN:O	2.54	0.56
1:E:182:LYS:HB2	3:E:385:GOL:HO1	1.70	0.56
1:H:251:HIS:HB3	6:H:411:HOH:O	2.05	0.56
1:A:273:ASP:O	1:A:297:PRO:HD2	2.05	0.56
1:A:80:GLU:O	1:A:84:ARG:HG2	2.06	0.56
1:B:198:GLU:O	1:B:199:LYS:HB2	2.06	0.56
1:F:10:TYR:HB3	6:F:394:HOH:O	2.06	0.56
1:B:64:VAL:O	1:B:64:VAL:HG13	2.06	0.56
1:D:112:ARG:HD3	1:D:112:ARG:O	2.05	0.56
1:G:61:GLN:CD	1:H:133:LEU:HD22	2.26	0.56
1:F:274:LEU:HD12	1:F:297:PRO:O	2.06	0.56
1:C:206:ASN:OD1	1:C:207:PHE:CA	2.51	0.55
1:E:91:HIS:CE1	1:E:118:THR:CG2	2.87	0.55
1:E:136:LEU:HD22	1:F:76:SER:HB2	1.88	0.55
1:B:219:ALA:O	1:B:223:ILE:HG23	2.06	0.55
1:D:373:LEU:O	1:D:376:ASP:O	2.23	0.55
1:E:183:ARG:CD	1:E:185:MET:SD	2.93	0.55
1:E:209:LYS:H	1:E:209:LYS:CD	2.19	0.55
1:E:42:PRO:CD	1:E:43:PHE:N	2.66	0.55
1:A:92:VAL:HG22	1:A:98:HIS:HB3	1.87	0.55
1:E:12:SER:N	1:E:42:PRO:CB	2.70	0.55
1:E:252:ILE:O	1:E:252:ILE:CD1	2.48	0.55
1:C:230:LYS:HD3	1:C:255:ARG:HA	1.88	0.55
1:F:196:GLU:HG2	1:F:197:SER:H	1.71	0.55
1:G:72:LEU:HD23	1:H:136:LEU:HD21	1.88	0.55
1:H:155:ILE:HA	1:H:168:ILE:HD11	1.87	0.55
1:H:201:LEU:HB3	1:H:274:LEU:HB3	1.87	0.55
1:B:223:ILE:HG22	1:B:328:ALA:HA	1.89	0.55
1:B:77:LYS:O	1:B:81:VAL:HG23	2.07	0.55
1:E:245:GLN:HG2	1:H:245:GLN:NE2	2.10	0.55
1:A:319:CYS:SG	1:A:327:VAL:HG22	2.46	0.55
1:A:3:LEU:HD21	1:A:89:ILE:HD12	1.88	0.55
1:A:63:SER:O	1:A:65:PHE:HD2	1.88	0.55
1:D:185:MET:HG2	1:D:271:MET:HB2	1.88	0.55
1:E:118:THR:HG22	1:E:148:THR:OG1	2.06	0.55
1:A:177:GLU:OE2	1:A:358:SER:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLN:HG2	1:A:268:LEU:HD11	1.87	0.55
1:A:66:GLN:CD	1:B:10:TYR:CE1	2.80	0.55
1:D:214:GLN:HG3	1:D:243:ILE:HD11	1.89	0.55
1:D:96:ILE:HD12	1:D:127:LEU:HD11	1.89	0.55
1:G:220:PHE:CE2	1:G:231:LEU:HB2	2.42	0.55
1:B:196:GLU:O	1:B:198:GLU:N	2.36	0.55
1:D:375:ASP:N	1:D:375:ASP:OD2	2.38	0.55
1:F:127:LEU:HD23	1:F:133:LEU:HD23	1.89	0.55
1:D:204:ILE:HD13	1:D:265:VAL:HG11	1.89	0.55
1:G:249:ASN:N	1:G:249:ASN:HD22	1.81	0.55
1:F:86:ASN:ND2	1:F:86:ASN:O	2.38	0.54
1:A:230:LYS:HD3	1:A:255:ARG:HA	1.89	0.54
1:B:62:TYR:C	1:B:65:PHE:HB3	2.27	0.54
1:C:315:THR:O	1:C:344:MET:HG2	2.07	0.54
1:E:154:LEU:HD23	1:E:283:SER:HB3	1.89	0.54
1:F:194:ILE:HG23	1:F:196:GLU:OE1	2.07	0.54
1:G:65:PHE:O	1:G:66:GLN:C	2.43	0.54
1:D:148:THR:HA	1:D:169:GLN:O	2.07	0.54
1:D:196:GLU:O	1:D:198:GLU:N	2.39	0.54
1:D:65:PHE:CG	1:D:66:GLN:N	2.76	0.54
1:F:63:SER:HG	1:F:65:PHE:HE1	1.55	0.54
1:G:183:ARG:HG2	1:G:184:ASP:H	1.73	0.54
1:H:236:ASP:HB3	1:H:240:PHE:CD1	2.42	0.54
1:E:137:ILE:HG22	1:E:141:ILE:CG1	2.37	0.54
1:G:67:TYR:OH	1:H:10:TYR:CE1	2.60	0.54
1:G:96:ILE:HG12	1:G:97:PRO:HD3	1.88	0.54
1:E:184:ASP:HB3	1:G:261:LYS:HD2	1.90	0.54
1:E:259:LEU:HD23	1:E:268:LEU:CD1	2.36	0.54
1:F:11:PRO:HG2	1:H:187:GLN:HG3	1.90	0.54
1:B:63:SER:C	1:B:64:VAL:CG1	2.43	0.54
1:B:39:SER:HB3	1:B:70:TYR:CE1	2.42	0.54
1:C:61:GLN:CB	1:D:130:ASP:OD1	2.55	0.54
1:D:204:ILE:HG21	1:D:265:VAL:HG11	1.90	0.54
1:D:26:GLN:O	1:D:30:ARG:HG2	2.06	0.54
1:A:323:ASP:O	1:A:327:VAL:HG23	2.07	0.54
1:B:207:PHE:CB	1:B:237:GLY:HA3	2.34	0.54
1:C:62:TYR:HD1	1:C:65:PHE:H	1.55	0.54
1:D:278:LEU:HA	1:D:301:THR:HG23	1.89	0.54
1:G:187:GLN:HG3	1:G:188:LEU:HD12	1.90	0.54
1:H:355:GLN:HG3	1:H:356:PHE:CD2	2.43	0.54
1:A:21:THR:O	1:A:25:LYS:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLN:O	1:B:368:ILE:HG12	2.07	0.54
1:G:311:GLN:C	1:G:313:GLY:N	2.61	0.54
1:H:201:LEU:HD21	1:H:223:ILE:HG21	1.88	0.54
1:B:196:GLU:C	1:B:198:GLU:HG3	2.27	0.53
1:B:84:ARG:HG3	1:B:85:GLU:HG2	1.90	0.53
1:C:175:ILE:HG12	1:C:290:GLU:HG2	1.91	0.53
1:D:231:LEU:HB3	1:D:256:VAL:HG22	1.90	0.53
1:F:312:HIS:C	1:F:312:HIS:CD2	2.82	0.53
1:B:153:SER:O	1:B:157:GLU:HG2	2.08	0.53
1:B:18:VAL:O	1:B:22:GLU:HG2	2.08	0.53
1:B:205:SER:C	1:B:206:ASN:O	2.41	0.53
1:D:185:MET:HG3	1:D:188:LEU:HB2	1.90	0.53
1:C:204:ILE:CG1	1:C:205:SER:N	2.68	0.53
1:E:12:SER:H	1:E:42:PRO:HA	1.73	0.53
1:F:224:VAL:CG2	1:F:255:ARG:NH1	2.72	0.53
1:E:66:GLN:NE2	1:H:185:MET:HE2	2.24	0.53
1:H:92:VAL:HG13	1:H:98:HIS:HB2	1.89	0.53
1:E:43:PHE:N	1:E:43:PHE:CD2	2.69	0.53
1:E:66:GLN:HE22	1:H:185:MET:CE	2.22	0.53
1:F:193:GLY:CA	1:F:194:ILE:HD12	2.38	0.53
1:G:298:CYS:HB2	1:G:310:ILE:HD11	1.90	0.53
1:D:85:GLU:O	1:D:86:ASN:HB3	2.09	0.53
1:F:288:LEU:HB3	1:F:309:VAL:HG11	1.90	0.53
1:A:52:ILE:N	1:A:52:ILE:CD1	2.54	0.53
1:C:96:ILE:O	1:C:96:ILE:HD12	2.07	0.53
1:D:209:LYS:HB3	6:D:409:HOH:O	2.09	0.53
1:F:190:LYS:CA	1:F:193:GLY:HA2	2.39	0.53
1:E:209:LYS:HD2	1:E:209:LYS:N	2.22	0.53
1:F:224:VAL:HG21	1:F:255:ARG:CZ	2.39	0.53
1:G:239:GLU:O	1:G:243:ILE:HG12	2.09	0.53
1:H:126:VAL:HG23	1:H:127:LEU:HD13	1.91	0.53
1:B:17:GLY:O	1:B:18:VAL:HG22	2.09	0.52
1:E:125:THR:CG2	1:E:281:LYS:HD2	2.39	0.52
1:F:117:THR:HB	1:F:147:VAL:HG12	1.92	0.52
1:G:26:GLN:HE22	1:G:358:SER:HB2	1.73	0.52
1:C:96:ILE:HD13	1:C:96:ILE:O	2.09	0.52
1:E:44:ARG:NH1	1:E:44:ARG:HA	2.24	0.52
1:F:134:ASN:ND2	1:F:162:VAL:HA	2.18	0.52
1:F:196:GLU:CD	1:F:196:GLU:N	2.57	0.52
1:H:374:ARG:O	1:H:375:ASP:CB	2.54	0.52
1:E:137:ILE:CG2	1:E:141:ILE:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:424:HOH:O	1:F:61:GLN:HB3	2.09	0.52
1:G:317:TYR:HE2	1:G:334:LEU:HD11	1.74	0.52
1:A:9:CYS:H	1:A:38:THR:HG22	1.74	0.52
1:C:285:GLY:O	1:C:287:VAL:N	2.42	0.52
1:F:35:HIS:CD2	1:F:87:LEU:HD21	2.43	0.52
1:B:314:ASP:OD2	1:B:347:ARG:HB3	1.99	0.52
1:D:97:PRO:HD3	6:D:407:HOH:O	2.08	0.52
1:F:68:PRO:HB2	3:F:384:GOL:O3	2.09	0.52
1:G:209:LYS:HA	1:G:239:GLU:HG3	1.91	0.52
1:G:224:VAL:HG23	1:G:229:ALA:HB3	1.91	0.52
1:B:84:ARG:HG3	1:B:85:GLU:N	2.25	0.52
1:B:91:HIS:HD2	1:B:93:HIS:CD2	2.28	0.52
1:D:200:ILE:HD11	1:D:232:LEU:HD22	1.92	0.52
1:B:94:TYR:CE2	1:B:123:ASP:HB3	2.45	0.52
1:D:100:ILE:HD13	1:D:136:LEU:HG	1.91	0.52
1:D:317:TYR:CE2	1:D:344:MET:HE1	2.45	0.52
1:E:44:ARG:HA	1:E:44:ARG:CZ	2.40	0.52
1:G:338:GLU:O	1:G:342:ARG:HB2	2.10	0.52
1:A:34:ILE:O	1:A:52:ILE:HG21	1.92	0.52
1:E:41:LEU:HB3	1:E:43:PHE:CZ	2.44	0.52
1:E:97:PRO:HB2	1:E:98:HIS:HD2	1.75	0.52
1:G:27:LEU:HD11	1:G:369:TYR:HE2	1.75	0.52
1:A:181:PHE:HD1	1:A:182:LYS:O	1.92	0.52
1:B:203:HIS:NE2	1:B:205:SER:HB3	2.25	0.52
1:D:4:LYS:O	1:D:87:LEU:HD22	2.10	0.52
1:B:237:GLY:HA2	1:C:181:PHE:CD1	2.45	0.52
1:A:206:ASN:HB3	1:A:211:LYS:CG	2.38	0.51
1:C:123:ASP:HA	1:C:127:LEU:HD12	1.93	0.51
1:D:35:HIS:CD2	1:D:87:LEU:HD21	2.45	0.51
1:F:49:TYR:CB	1:F:52:ILE:HD11	2.39	0.51
1:H:155:ILE:HG12	1:H:168:ILE:HG13	1.91	0.51
1:A:169:GLN:HE21	3:A:385:GOL:H11	1.76	0.51
1:G:204:ILE:HG12	1:G:204:ILE:O	2.11	0.51
1:B:151:SER:O	1:B:155:ILE:HG13	2.10	0.51
1:E:11:PRO:C	1:E:42:PRO:CB	2.77	0.51
1:F:312:HIS:O	1:F:312:HIS:CD2	2.63	0.51
1:G:195:SER:O	1:G:197:SER:N	2.43	0.51
1:G:61:GLN:HE22	1:H:127:LEU:HA	1.76	0.51
1:B:223:ILE:HG13	1:B:224:VAL:N	2.25	0.51
1:B:94:TYR:OH	1:B:122:THR:C	2.48	0.51
1:C:94:TYR:O	1:C:95:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:LEU:HD23	1:E:124:ILE:CD1	2.40	0.51
1:E:91:HIS:HE1	1:E:118:THR:CG2	2.23	0.51
1:E:95:ALA:HB3	1:E:123:ASP:HB2	1.91	0.51
1:F:60:ASN:HB2	6:F:410:HOH:O	2.11	0.51
1:G:332:ILE:O	1:G:336:LYS:HG2	2.11	0.51
1:H:268:LEU:HD23	1:H:268:LEU:H	1.76	0.51
1:H:314:ASP:OD1	1:H:347:ARG:HD3	2.11	0.51
1:A:225:THR:OG1	1:A:226:GLU:HG3	2.10	0.51
1:E:204:ILE:O	1:E:287:VAL:HG11	2.10	0.51
1:H:123:ASP:N	1:H:123:ASP:OD1	2.43	0.51
1:A:19:VAL:HG21	1:A:173:ASN:OD1	2.10	0.51
1:B:134:ASN:HD21	1:B:138:ARG:NH2	2.08	0.51
1:C:250:LEU:O	1:C:251:HIS:HB2	2.11	0.51
1:D:196:GLU:O	1:D:198:GLU:CB	2.59	0.51
1:D:247:VAL:HG11	1:D:258:PHE:CZ	2.45	0.51
1:F:75:ALA:HA	1:F:78:MET:CE	2.40	0.51
1:B:103:TYR:O	1:B:107:GLN:HG2	2.11	0.51
1:C:176:ASP:HB3	1:C:179:VAL:HG12	1.92	0.51
1:C:198:GLU:O	1:C:199:LYS:HE2	2.09	0.51
1:C:67:TYR:HB2	6:D:405:HOH:O	2.11	0.51
1:D:367:THR:O	1:D:371:ASP:HB2	2.11	0.51
1:D:65:PHE:O	1:D:66:GLN:NE2	2.42	0.51
1:E:259:LEU:HD23	1:E:268:LEU:HD13	1.92	0.51
1:F:190:LYS:HA	1:F:193:GLY:CA	2.40	0.51
1:C:343:ASN:HA	1:C:346:GLU:HB2	1.93	0.51
1:G:200:ILE:HG13	1:G:272:SER:HA	1.93	0.51
1:A:207:PHE:CD1	1:A:237:GLY:HA3	2.46	0.51
1:D:92:VAL:HG13	1:D:98:HIS:HB2	1.92	0.51
1:E:44:ARG:HD3	1:E:46:ASN:HA	1.93	0.51
1:C:92:VAL:HG22	1:C:98:HIS:HB3	1.93	0.51
1:F:292:MET:HG2	1:F:348:ALA:HB1	1.92	0.51
1:G:67:TYR:OH	1:H:10:TYR:CZ	2.52	0.51
1:H:194:ILE:C	1:H:194:ILE:HD12	2.32	0.51
1:A:207:PHE:CG	1:A:237:GLY:HA3	2.47	0.50
1:D:196:GLU:O	1:D:198:GLU:HG2	2.10	0.50
1:A:74:LEU:O	1:A:78:MET:HB2	2.11	0.50
1:D:354:GLU:OE2	1:D:355:GLN:HB3	2.12	0.50
1:G:207:PHE:CG	1:G:237:GLY:HA3	2.46	0.50
1:A:74:LEU:HD21	1:A:98:HIS:HD2	1.76	0.50
1:C:235:GLY:N	1:C:261:LYS:H	2.10	0.50
1:D:214:GLN:O	1:D:218:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:VAL:O	1:D:64:VAL:HG23	2.11	0.50
1:E:295:GLY:HA3	3:E:385:GOL:H11	1.94	0.50
1:A:197:SER:O	1:A:198:GLU:OE1	2.30	0.50
1:F:11:PRO:HD3	6:F:390:HOH:O	2.09	0.50
1:F:286:LEU:O	1:F:290:GLU:HG3	2.11	0.50
1:F:82:ALA:O	1:F:86:ASN:HA	2.11	0.50
1:F:32:HIS:O	1:F:51:ASN:ND2	2.44	0.50
1:G:120:HIS:O	1:G:123:ASP:OD1	2.30	0.50
1:H:112:ARG:CD	1:H:112:ARG:O	2.60	0.50
1:H:251:HIS:O	1:H:251:HIS:HD2	1.93	0.50
1:H:40:GLY:CA	1:H:54:PHE:HZ	2.10	0.50
1:A:62:TYR:HD1	1:A:65:PHE:CZ	2.30	0.50
1:C:200:ILE:H	1:C:200:ILE:HD13	1.76	0.50
1:C:92:VAL:CG1	1:C:98:HIS:HB2	2.41	0.50
1:E:46:ASN:H	1:E:46:ASN:HD22	1.59	0.50
1:H:173:ASN:HB2	1:H:284:PHE:HE1	1.76	0.50
1:F:278:LEU:HD11	1:F:327:VAL:HG11	1.93	0.50
1:F:96:ILE:HG21	1:F:127:LEU:CD2	2.42	0.50
1:A:187:GLN:HB2	1:D:11:PRO:HG2	1.93	0.49
1:A:204:ILE:HA	1:A:234:VAL:HB	1.94	0.49
1:C:191:GLU:O	1:C:191:GLU:OE1	2.30	0.49
1:D:189:LYS:O	1:D:194:ILE:CG2	2.56	0.49
1:H:117:THR:HG22	1:H:147:VAL:HG22	1.92	0.49
1:A:155:ILE:HG12	1:A:168:ILE:HD11	1.93	0.49
1:C:198:GLU:O	1:C:199:LYS:HE3	2.12	0.49
1:E:328:ALA:O	1:E:332:ILE:HG22	2.12	0.49
1:G:240:PHE:C	1:G:240:PHE:CD2	2.85	0.49
1:C:199:LYS:CE	1:C:199:LYS:HA	2.39	0.49
1:E:97:PRO:HB2	1:E:98:HIS:CD2	2.46	0.49
1:F:96:ILE:HG21	1:F:127:LEU:HD22	1.94	0.49
1:H:310:ILE:HB	1:H:318:LEU:HD23	1.94	0.49
1:A:213:VAL:HG23	6:A:390:HOH:O	2.11	0.49
1:E:121:GLY:HA2	1:E:154:LEU:CD2	2.30	0.49
1:F:124:ILE:HG21	1:F:158:THR:HA	1.94	0.49
1:G:240:PHE:HD2	1:G:240:PHE:C	2.15	0.49
1:B:93:HIS:O	1:B:94:TYR:O	2.30	0.49
1:C:10:TYR:CE2	1:C:94:TYR:CD2	3.01	0.49
1:G:194:ILE:CD1	1:G:271:MET:HE1	2.38	0.49
1:G:311:GLN:O	1:G:313:GLY:N	2.45	0.49
1:A:199:LYS:HD2	1:A:199:LYS:N	2.27	0.49
1:F:127:LEU:HD23	1:F:133:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:HG3	1:A:284:PHE:H	1.76	0.49
1:C:141:ILE:HG23	1:C:147:VAL:HG21	1.95	0.49
1:C:27:LEU:O	1:C:32:HIS:HB2	2.13	0.49
1:E:207:PHE:O	1:E:237:GLY:HA3	2.13	0.49
1:F:114:LYS:HA	1:F:145:ASP:OD2	2.12	0.49
1:F:91:HIS:CD2	1:F:116:VAL:HG12	2.48	0.49
1:B:199:LYS:HD2	1:B:335:LEU:HD12	1.94	0.49
1:C:11:PRO:O	1:C:12:SER:OG	2.26	0.49
1:D:374:ARG:HG3	1:D:375:ASP:OD2	2.13	0.49
1:F:68:PRO:HG2	3:F:384:GOL:O2	2.13	0.49
1:A:63:SER:C	1:A:65:PHE:CE2	2.71	0.48
1:C:204:ILE:HG12	1:C:205:SER:N	2.15	0.48
1:E:133:LEU:O	1:E:137:ILE:HD12	2.13	0.48
1:G:141:ILE:HG23	1:G:147:VAL:HG21	1.95	0.48
1:A:94:TYR:CE2	1:A:123:ASP:HB3	2.48	0.48
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.41	0.48
1:A:367:THR:HB	3:A:384:GOL:H31	1.95	0.48
1:C:293:ALA:O	1:C:349:ARG:CD	2.61	0.48
1:E:119:LEU:CD2	1:E:124:ILE:CD1	2.91	0.48
1:F:353:TYR:O	1:F:357:ARG:HB3	2.12	0.48
1:H:98:HIS:HA	1:H:101:CYS:HB2	1.95	0.48
1:H:332:ILE:HG13	1:H:333:GLN:N	2.27	0.48
1:D:187:GLN:C	1:D:189:LYS:H	2.14	0.48
1:D:97:PRO:HD2	6:D:407:HOH:O	2.13	0.48
1:E:107:GLN:OE1	1:E:111:GLU:HG3	2.12	0.48
1:G:121:GLY:HA2	1:G:154:LEU:CD1	2.44	0.48
1:A:123:ASP:HA	1:A:127:LEU:HD12	1.95	0.48
1:B:57:VAL:HG22	1:B:77:LYS:HG2	1.94	0.48
1:G:123:ASP:N	1:G:123:ASP:OD1	2.46	0.48
1:H:106:LYS:O	1:H:110:GLY:O	2.31	0.48
1:B:217:VAL:HG21	1:B:243:ILE:HG23	1.95	0.48
1:C:201:LEU:HG	1:C:274:LEU:HB3	1.95	0.48
1:D:95:ALA:O	1:D:99:ALA:HB3	2.14	0.48
1:F:47:LYS:HD3	1:F:47:LYS:C	2.09	0.48
1:F:47:LYS:HD3	1:F:48:VAL:HG23	1.90	0.48
1:H:226:GLU:HG3	1:H:332:ILE:HD12	1.96	0.48
1:C:199:LYS:O	1:C:229:ALA:CB	2.57	0.48
1:C:3:LEU:HB3	1:C:5:ILE:HD11	1.96	0.48
1:D:10:TYR:C	1:D:11:PRO:O	2.51	0.48
1:F:209:LYS:N	1:F:209:LYS:HD2	2.28	0.48
1:F:202:ILE:HG23	1:F:275:MET:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:TYR:H	1:C:192:TYR:HD2	1.59	0.48
1:D:196:GLU:O	1:D:198:GLU:HG3	2.10	0.48
1:F:119:LEU:HD13	1:F:124:ILE:HD11	1.96	0.48
1:B:94:TYR:CD2	1:B:123:ASP:HB3	2.49	0.48
1:B:155:ILE:HA	1:B:168:ILE:HD11	1.96	0.48
1:D:310:ILE:HG22	1:D:311:GLN:N	2.29	0.48
1:H:117:THR:CG2	1:H:147:VAL:HG13	2.43	0.48
1:H:375:ASP:O	1:H:376:ASP:CB	2.38	0.48
1:A:328:ALA:O	1:A:332:ILE:HG12	2.13	0.47
1:E:45:LEU:C	1:E:47:LYS:N	2.67	0.47
1:F:270:ALA:O	3:F:382:GOL:H31	2.14	0.47
1:B:204:ILE:HD13	1:B:265:VAL:HG21	1.96	0.47
1:C:154:LEU:O	1:C:158:THR:N	2.44	0.47
1:D:189:LYS:HE3	1:D:271:MET:HG3	1.95	0.47
1:D:49:TYR:H	1:D:52:ILE:HD11	1.79	0.47
1:A:34:ILE:CG2	1:A:52:ILE:CG2	2.88	0.47
1:B:194:ILE:HA	1:B:196:GLU:OE2	2.13	0.47
1:B:287:VAL:HA	1:B:290:GLU:HB2	1.95	0.47
1:D:2:LYS:HD3	6:D:414:HOH:O	2.14	0.47
1:G:77:LYS:HA	1:G:80:GLU:HG2	1.96	0.47
1:A:170:THR:H	3:A:385:GOL:H32	1.79	0.47
1:B:223:ILE:CG2	1:B:328:ALA:HA	2.44	0.47
1:F:186:THR:HG23	1:F:187:GLN:NE2	2.29	0.47
1:F:49:TYR:CG	1:F:52:ILE:HD11	2.49	0.47
1:H:95:ALA:O	1:H:98:HIS:N	2.48	0.47
1:C:96:ILE:HD11	1:C:137:ILE:HD13	1.96	0.47
1:E:268:LEU:H	1:E:268:LEU:HD23	1.79	0.47
1:E:49:TYR:CD1	1:E:50:PRO:HD2	2.50	0.47
1:F:278:LEU:HA	1:F:301:THR:HG23	1.96	0.47
1:G:282:GLU:CG	1:G:283:SER:N	2.78	0.47
1:H:7:ILE:HG23	1:H:93:HIS:HD2	1.79	0.47
1:D:122:THR:O	1:D:126:VAL:HG22	2.15	0.47
1:E:94:TYR:HD1	6:E:396:HOH:O	1.96	0.47
1:F:225:THR:C	1:F:227:VAL:H	2.17	0.47
1:G:357:ARG:HG2	1:G:360:LYS:H	1.80	0.47
1:C:221:ALA:HB2	1:C:250:LEU:HD13	1.97	0.47
1:G:61:GLN:HE21	1:H:127:LEU:CD1	2.10	0.47
1:H:223:ILE:CD1	1:H:331:ALA:HB3	2.45	0.47
1:B:49:TYR:HB2	1:B:52:ILE:HG12	1.97	0.47
1:B:92:VAL:HG11	1:B:98:HIS:HB2	1.97	0.47
1:C:228:ASP:HB2	1:C:255:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:SER:HA	1:C:43:PHE:HE2	1.78	0.47
1:D:96:ILE:HG12	1:D:137:ILE:HG12	1.96	0.47
1:F:141:ILE:HD12	1:F:162:VAL:HG11	1.97	0.47
1:F:241:CYS:SG	1:F:242:THR:N	2.88	0.47
1:C:191:GLU:C	1:C:191:GLU:OE1	2.53	0.47
1:C:21:THR:HA	1:C:36:PHE:HZ	1.79	0.47
1:C:253:GLU:HG2	1:C:253:GLU:O	2.10	0.47
1:C:312:HIS:O	1:C:316:GLY:O	2.33	0.47
1:C:360:LYS:HG2	6:C:398:HOH:O	2.14	0.47
1:E:119:LEU:HD21	1:E:124:ILE:HD11	1.97	0.47
1:C:365:TYR:O	1:C:368:ILE:HB	2.15	0.47
1:D:10:TYR:HB3	1:D:11:PRO:HD2	1.97	0.47
1:D:204:ILE:CD1	1:D:265:VAL:HG11	2.44	0.47
1:D:374:ARG:HB3	1:D:374:ARG:CZ	2.44	0.47
1:F:209:LYS:H	1:F:209:LYS:CD	2.28	0.47
1:F:212:ARG:HB2	1:F:278:LEU:O	2.14	0.47
1:D:149:ALA:HB2	1:D:168:ILE:CD1	2.45	0.47
1:E:123:ASP:N	1:E:123:ASP:OD1	2.45	0.47
1:H:54:PHE:CE2	1:H:56:GLU:HG2	2.49	0.47
1:A:34:ILE:O	1:A:52:ILE:CB	2.57	0.46
1:D:204:ILE:CG2	1:D:234:VAL:HB	2.44	0.46
1:D:5:ILE:HD12	1:D:89:ILE:HB	1.96	0.46
1:H:75:ALA:HB2	1:H:101:CYS:SG	2.55	0.46
1:B:155:ILE:HG23	1:B:168:ILE:HG12	1.96	0.46
1:C:194:ILE:HG13	1:C:195:SER:N	2.30	0.46
1:C:196:GLU:HA	1:C:197:SER:C	2.36	0.46
1:G:282:GLU:OE2	1:G:285:GLY:N	2.48	0.46
1:H:94:TYR:OH	1:H:122:THR:OG1	2.28	0.46
1:H:189:LYS:NZ	1:H:198:GLU:HG3	2.30	0.46
1:H:265:VAL:O	1:H:265:VAL:HG22	2.16	0.46
1:C:287:VAL:HG12	2:C:382:UDP:H3'	1.98	0.46
1:D:267:GLU:OE1	1:D:267:GLU:HA	2.15	0.46
1:D:65:PHE:C	1:D:65:PHE:CD2	2.88	0.46
1:E:204:ILE:HB	1:E:234:VAL:HB	1.96	0.46
1:H:370:TYR:CE1	3:H:383:GOL:H2	2.51	0.46
1:B:91:HIS:NE2	1:B:93:HIS:NE2	2.62	0.46
1:D:283:SER:O	1:D:284:PHE:CB	2.55	0.46
1:E:119:LEU:CD2	1:E:124:ILE:HG13	2.44	0.46
1:A:200:ILE:HG23	1:A:232:LEU:HD13	1.97	0.46
1:B:94:TYR:HH	1:B:122:THR:CB	2.10	0.46
1:D:149:ALA:CB	1:D:168:ILE:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ASP:OD2	1:D:376:ASP:N	2.48	0.46
1:E:189:LYS:HD3	1:E:194:ILE:HD11	1.97	0.46
1:E:369:TYR:O	1:E:373:LEU:HG	2.16	0.46
1:H:122:THR:C	1:H:124:ILE:N	2.68	0.46
1:A:138:ARG:HD3	3:A:383:GOL:H32	1.98	0.46
1:E:37:ILE:HG23	1:E:77:LYS:HG3	1.97	0.46
1:G:126:VAL:HG23	1:G:127:LEU:N	2.30	0.46
1:G:347:ARG:HA	1:G:350:GLU:HB2	1.98	0.46
1:H:144:SER:O	1:H:166:LYS:NZ	2.48	0.46
1:A:216:VAL:HA	1:A:278:LEU:HD12	1.98	0.46
1:B:139:PHE:O	1:B:143:GLN:HB2	2.16	0.46
1:B:192:TYR:O	1:B:194:ILE:HG12	2.15	0.46
1:G:68:PRO:HA	1:G:69:PRO:HD3	1.83	0.46
1:H:103:TYR:CD1	1:H:143:GLN:HG2	2.51	0.46
1:A:103:TYR:CE2	1:A:139:PHE:HE2	2.34	0.46
1:A:189:LYS:HB3	1:A:194:ILE:HG22	1.97	0.46
1:B:286:LEU:HD12	1:B:286:LEU:HA	1.61	0.46
1:B:88:ASP:HB3	1:B:373:LEU:HD21	1.98	0.46
1:D:39:SER:HA	1:D:57:VAL:HG22	1.97	0.46
1:E:317:TYR:CD1	1:E:317:TYR:N	2.83	0.46
1:F:66:GLN:N	1:F:66:GLN:CD	2.60	0.46
1:H:251:HIS:CD2	1:H:251:HIS:C	2.90	0.46
1:C:284:PHE:CZ	1:C:289:LEU:HD11	2.51	0.46
1:F:190:LYS:CA	1:F:193:GLY:CA	2.94	0.46
1:G:155:ILE:O	1:G:159:HIS:HD2	1.98	0.46
1:G:223:ILE:CG1	1:G:328:ALA:HA	2.45	0.46
1:B:65:PHE:HA	6:B:389:HOH:O	2.16	0.45
1:B:94:TYR:CZ	1:B:123:ASP:N	2.83	0.45
1:F:186:THR:O	1:F:189:LYS:HB2	2.15	0.45
1:F:315:THR:HB	1:F:348:ALA:HA	1.97	0.45
1:G:136:LEU:HD21	1:H:72:LEU:HG	1.98	0.45
1:H:274:LEU:HD22	1:H:335:LEU:HD21	1.98	0.45
1:A:368:ILE:HG13	6:A:419:HOH:O	2.15	0.45
1:E:338:GLU:O	1:E:342:ARG:HB2	2.16	0.45
1:H:111:GLU:CB	6:H:413:HOH:O	2.63	0.45
1:C:62:TYR:CB	1:C:65:PHE:HB2	2.43	0.45
1:E:221:ALA:HB2	1:E:250:LEU:HD23	1.98	0.45
1:F:225:THR:C	1:F:227:VAL:N	2.70	0.45
1:F:96:ILE:HG23	1:F:97:PRO:HD3	1.97	0.45
1:B:200:ILE:HD11	1:B:271:MET:HG2	1.98	0.45
1:D:155:ILE:O	1:D:159:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:VAL:O	1:E:59:VAL:CG2	2.53	0.45
1:F:144:SER:O	1:F:166:LYS:NZ	2.49	0.45
1:F:357:ARG:HG2	1:F:360:LYS:HB2	1.98	0.45
1:F:91:HIS:HD2	1:F:116:VAL:O	2.00	0.45
1:H:360:LYS:O	1:H:364:GLN:HG3	2.17	0.45
1:A:136:LEU:HD21	1:B:72:LEU:HD12	1.98	0.45
1:B:150:VAL:O	1:B:284:PHE:HD2	1.96	0.45
1:B:196:GLU:O	1:B:198:GLU:OE2	2.34	0.45
1:B:204:ILE:HG21	1:B:265:VAL:HG21	1.99	0.45
1:B:95:ALA:O	1:B:99:ALA:HB3	2.17	0.45
1:C:155:ILE:HD11	1:C:170:THR:OG1	2.16	0.45
1:D:259:LEU:HB3	1:D:262:GLN:NE2	2.31	0.45
1:D:72:LEU:H	1:D:72:LEU:HD12	1.81	0.45
1:F:86:ASN:HD21	1:F:112:ARG:NH2	2.14	0.45
1:A:178:ARG:HG2	1:D:238:PRO:HB3	1.98	0.45
1:C:150:VAL:HA	1:C:171:VAL:O	2.17	0.45
1:D:21:THR:HG22	1:D:25:LYS:HE2	1.99	0.45
1:E:122:THR:HA	1:E:125:THR:HB	1.99	0.45
1:E:114:LYS:HD2	1:E:372:VAL:HG22	1.99	0.45
1:A:92:VAL:CG2	1:A:98:HIS:HB3	2.47	0.45
1:C:103:TYR:CE1	1:C:143:GLN:HG2	2.51	0.45
1:D:23:LEU:CD1	1:D:362:VAL:HG23	2.45	0.45
1:E:146:VAL:HA	3:E:386:GOL:H11	1.97	0.45
1:F:35:HIS:HD2	1:F:87:LEU:CD2	2.26	0.45
1:B:60:ASN:HA	1:B:62:TYR:CZ	2.52	0.45
1:C:96:ILE:HG12	1:C:137:ILE:HD12	1.99	0.45
1:A:206:ASN:OD1	1:A:208:ARG:HG3	2.16	0.45
1:A:301:THR:HB	1:A:321:VAL:HG12	1.99	0.45
1:B:220:PHE:CE2	1:B:231:LEU:HB2	2.51	0.45
1:D:285:GLY:O	1:D:288:LEU:CB	2.65	0.45
1:D:85:GLU:O	1:D:86:ASN:CB	2.65	0.45
1:E:252:ILE:H	1:E:252:ILE:HG13	1.64	0.45
1:A:302:ARG:HG2	1:A:302:ARG:O	2.16	0.45
1:F:359:GLU:HG3	1:F:360:LYS:N	2.32	0.45
1:C:122:THR:OG1	4:C:385:MLT:H32	2.17	0.44
1:D:209:LYS:HE3	6:D:409:HOH:O	2.17	0.44
1:F:95:ALA:O	1:F:99:ALA:HB3	2.16	0.44
1:G:119:LEU:HD13	1:G:124:ILE:HD11	1.99	0.44
1:B:204:ILE:HB	1:B:234:VAL:HB	1.98	0.44
1:D:126:VAL:HG23	1:D:127:LEU:N	2.32	0.44
1:D:201:LEU:HD12	1:D:201:LEU:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:LEU:O	1:D:300:GLY:HA2	2.17	0.44
1:E:5:ILE:HB	1:E:34:ILE:HD13	1.99	0.44
1:E:44:ARG:CA	1:E:44:ARG:NH1	2.80	0.44
1:F:106:LYS:CE	1:F:111:GLU:HG3	2.44	0.44
1:F:57:VAL:HG11	1:F:74:LEU:HD12	1.98	0.44
1:H:96:ILE:HG22	1:H:97:PRO:HD3	1.99	0.44
1:B:374:ARG:HH11	1:B:374:ARG:HG2	1.82	0.44
1:D:190:LYS:C	1:D:193:GLY:H	2.10	0.44
1:H:106:LYS:HB2	1:H:115:ILE:CD1	2.47	0.44
1:A:281:LYS:HE2	1:A:281:LYS:HB3	1.80	0.44
1:A:72:LEU:HG	1:B:136:LEU:HD21	1.98	0.44
1:D:185:MET:O	1:D:186:THR:C	2.52	0.44
1:G:175:ILE:HA	1:G:175:ILE:HD12	1.88	0.44
1:H:111:GLU:HB3	6:H:413:HOH:O	2.16	0.44
1:H:124:ILE:HB	1:H:154:LEU:HD11	2.00	0.44
1:A:306:ILE:N	1:A:307:PRO:CD	2.80	0.44
1:A:302:ARG:HA	1:A:318:LEU:HD23	2.00	0.44
1:A:371:ASP:OD1	1:A:374:ARG:NH1	2.51	0.44
1:A:66:GLN:CG	1:B:10:TYR:CE1	3.00	0.44
1:B:3:LEU:HD11	1:B:373:LEU:HD13	2.00	0.44
1:C:209:LYS:H	1:C:209:LYS:HD2	1.82	0.44
1:C:11:PRO:C	1:C:12:SER:OG	2.56	0.44
1:A:66:GLN:CD	1:C:187:GLN:HE22	2.21	0.44
1:D:13:VAL:O	1:D:13:VAL:HG12	2.17	0.44
1:D:247:VAL:HG11	1:D:258:PHE:CE2	2.52	0.44
1:D:68:PRO:HA	1:D:69:PRO:HD3	1.81	0.44
1:E:42:PRO:N	1:E:43:PHE:CD2	2.85	0.44
1:A:312:HIS:HB2	1:A:318:LEU:HD12	1.99	0.44
1:C:142:GLU:HA	1:C:166:LYS:HB2	1.99	0.44
1:D:69:PRO:HD2	3:D:382:GOL:H12	2.00	0.44
1:D:204:ILE:H	1:D:204:ILE:HG12	1.53	0.44
1:H:219:ALA:O	1:H:223:ILE:HG12	2.17	0.44
1:B:142:GLU:HA	1:B:166:LYS:HB2	2.00	0.43
1:C:200:ILE:N	1:C:200:ILE:HD13	2.32	0.43
1:C:35:HIS:CE1	1:C:85:GLU:HG3	2.53	0.43
1:D:137:ILE:H	1:D:137:ILE:HG13	1.65	0.43
1:E:289:LEU:HD11	1:E:356:PHE:CG	2.52	0.43
1:H:184:ASP:N	1:H:184:ASP:OD1	2.47	0.43
1:H:189:LYS:HZ1	1:H:198:GLU:HG3	1.83	0.43
1:H:173:ASN:HB3	1:H:286:LEU:HD13	2.00	0.43
1:H:41:LEU:N	1:H:42:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:CG1	1:A:227:VAL:O	2.62	0.43
1:A:136:LEU:HD12	1:B:108:MET:SD	2.58	0.43
1:F:94:TYR:CE2	1:F:96:ILE:HG22	2.53	0.43
1:C:252:ILE:C	6:C:396:HOH:O	2.56	0.43
1:D:123:ASP:OD1	1:D:123:ASP:N	2.51	0.43
1:E:119:LEU:HD22	1:E:124:ILE:HG13	2.00	0.43
1:F:66:GLN:HG2	1:F:67:TYR:N	2.33	0.43
1:F:94:TYR:HD2	1:F:97:PRO:HD3	1.84	0.43
1:G:207:PHE:HB2	1:G:237:GLY:HA3	1.99	0.43
1:H:194:ILE:HD13	1:H:230:LYS:HG3	2.00	0.43
1:D:245:GLN:O	1:D:249:ASN:OD1	2.36	0.43
1:D:328:ALA:O	1:D:332:ILE:HG23	2.17	0.43
1:E:10:TYR:OH	1:E:97:PRO:HG2	2.17	0.43
1:C:122:THR:O	1:C:126:VAL:HG12	2.18	0.43
1:C:192:TYR:O	1:C:194:ILE:N	2.50	0.43
1:H:150:VAL:O	1:H:172:TYR:HD1	2.00	0.43
1:C:306:ILE:HB	1:C:307:PRO:HD3	2.00	0.43
1:E:27:LEU:HD11	1:E:369:TYR:HE2	1.83	0.43
1:H:274:LEU:HD21	1:H:299:ILE:HD12	2.00	0.43
1:A:89:ILE:CD1	1:A:369:TYR:HB3	2.49	0.43
1:B:63:SER:N	1:B:65:PHE:HB3	2.34	0.43
1:D:191:GLU:HG3	1:D:191:GLU:H	1.60	0.43
1:G:349:ARG:HB2	1:G:353:TYR:CE2	2.54	0.43
1:H:175:ILE:HD12	6:H:393:HOH:O	2.17	0.43
1:H:247:VAL:HG11	1:H:258:PHE:CE2	2.53	0.43
1:A:247:VAL:HG11	1:A:258:PHE:HE2	1.84	0.43
1:A:76:SER:CB	1:B:132:SER:O	2.64	0.43
1:B:40:GLY:O	1:B:42:PRO:HD3	2.19	0.43
1:C:59:VAL:O	1:C:59:VAL:HG22	2.18	0.43
1:D:63:SER:OG	1:D:64:VAL:HG12	2.18	0.43
1:H:200:ILE:HG13	1:H:200:ILE:O	2.19	0.43
1:H:180:TYR:HB3	1:H:294:CYS:HB3	2.00	0.43
1:B:10:TYR:O	1:B:17:GLY:HA3	2.19	0.43
1:C:213:VAL:HB	1:C:243:ILE:HG13	1.99	0.43
1:E:281:LYS:O	1:E:282:GLU:C	2.56	0.43
1:F:47:LYS:NZ	1:F:48:VAL:HG23	2.30	0.43
1:H:239:GLU:O	1:H:243:ILE:HG12	2.19	0.43
1:A:64:VAL:HG11	1:B:13:VAL:HG22	1.98	0.43
1:B:173:ASN:HD22	1:B:173:ASN:HA	1.61	0.43
1:H:116:VAL:HG23	1:H:146:VAL:HB	2.00	0.43
1:H:92:VAL:CG2	1:H:98:HIS:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:VAL:HG12	1:E:213:VAL:O	2.19	0.42
1:F:134:ASN:O	1:F:135:ASN:CB	2.67	0.42
1:F:203:HIS:CE1	1:F:205:SER:HB2	2.54	0.42
1:F:372:VAL:HG22	1:F:372:VAL:O	2.19	0.42
1:A:367:THR:HG23	6:A:419:HOH:O	2.20	0.42
1:B:357:ARG:CB	1:B:360:LYS:HB2	2.44	0.42
1:C:259:LEU:HD23	1:C:268:LEU:CD1	2.49	0.42
1:D:375:ASP:HB2	1:D:376:ASP:OD2	2.19	0.42
1:D:39:SER:O	1:D:56:GLU:HG3	2.18	0.42
1:E:12:SER:HA	6:E:413:HOH:O	2.18	0.42
1:E:177:GLU:C	1:E:179:VAL:H	2.22	0.42
1:E:292:MET:HG2	1:E:348:ALA:HB1	2.01	0.42
1:F:141:ILE:HG23	1:F:147:VAL:HG11	2.00	0.42
1:H:236:ASP:OD2	1:H:260:GLY:HA2	2.19	0.42
1:H:94:TYR:O	1:H:95:ALA:HB3	2.16	0.42
1:A:282:GLU:HG3	1:A:283:SER:N	2.34	0.42
1:C:203:HIS:O	1:C:203:HIS:CG	2.71	0.42
1:E:77:LYS:HD3	1:E:77:LYS:HA	1.93	0.42
1:F:149:ALA:HB3	1:F:155:ILE:HG13	2.02	0.42
1:H:287:VAL:HG22	2:H:382:UDP:H5'2	2.01	0.42
1:B:184:ASP:OD1	1:B:184:ASP:N	2.52	0.42
1:B:282:GLU:OE2	1:B:284:PHE:O	2.37	0.42
1:C:92:VAL:HG12	1:C:117:THR:HG23	2.02	0.42
1:D:163:LYS:HB3	6:D:411:HOH:O	2.18	0.42
1:D:41:LEU:N	1:D:42:PRO:CD	2.56	0.42
1:E:220:PHE:CE2	1:E:231:LEU:HB2	2.55	0.42
1:E:317:TYR:HD1	1:E:317:TYR:N	2.18	0.42
1:F:187:GLN:N	1:F:187:GLN:HE21	2.18	0.42
1:G:121:GLY:HA2	1:G:154:LEU:HD11	2.01	0.42
1:H:93:HIS:O	1:H:94:TYR:HB3	2.18	0.42
1:B:103:TYR:CE1	1:B:143:GLN:HG2	2.54	0.42
1:B:195:SER:O	1:B:196:GLU:C	2.57	0.42
1:B:274:LEU:HA	1:B:297:PRO:O	2.20	0.42
1:B:65:PHE:O	1:B:65:PHE:CG	2.72	0.42
1:C:299:ILE:HG21	1:C:327:VAL:HG13	2.00	0.42
1:E:172:TYR:HD2	6:E:394:HOH:O	2.01	0.42
1:G:149:ALA:O	1:G:171:VAL:O	2.37	0.42
1:G:205:SER:C	1:G:206:ASN:O	2.52	0.42
1:H:264:ASN:C	1:H:266:ALA:H	2.23	0.42
1:A:63:SER:O	1:A:64:VAL:C	2.58	0.42
1:C:125:THR:HB	1:C:281:LYS:CE	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LEU:HB2	1:D:32:HIS:ND1	2.34	0.42
1:F:93:HIS:O	1:F:120:HIS:CD2	2.68	0.42
1:A:114:LYS:HD3	1:A:145:ASP:OD2	2.20	0.42
1:E:74:LEU:HD13	6:E:390:HOH:O	2.19	0.42
1:F:227:VAL:CG1	1:F:228:ASP:N	2.76	0.42
1:G:206:ASN:OD1	1:G:207:PHE:CA	2.63	0.42
1:H:192:TYR:HB2	1:H:194:ILE:HG22	2.01	0.42
1:A:106:LYS:HB2	1:A:115:ILE:HD11	2.01	0.42
1:A:22:GLU:HG3	1:A:174:PHE:HE1	1.85	0.42
1:B:249:ASN:C	1:B:250:LEU:O	2.55	0.42
1:D:251:HIS:HE1	3:D:383:GOL:O2	2.03	0.42
1:E:181:PHE:HE1	1:E:183:ARG:NE	2.18	0.42
1:A:117:THR:HB	1:A:147:VAL:HG13	2.02	0.42
1:A:206:ASN:HB3	1:A:211:LYS:HE3	2.00	0.42
1:A:317:TYR:CG	1:A:330:GLN:HG2	2.55	0.42
1:B:156:ASN:O	1:B:160:GLU:HG2	2.19	0.42
1:B:202:ILE:HG12	1:B:203:HIS:N	2.35	0.42
1:B:226:GLU:CB	1:B:332:ILE:HD13	2.47	0.42
1:E:98:HIS:CD2	1:E:98:HIS:N	2.88	0.42
1:F:223:ILE:O	1:F:225:THR:O	2.38	0.42
1:G:332:ILE:HG13	1:G:333:GLN:N	2.35	0.42
1:H:289:LEU:O	1:H:293:ALA:HB2	2.19	0.42
1:B:152:HIS:HB2	1:B:308:GLU:OE1	2.19	0.42
1:C:10:TYR:HA	1:C:11:PRO:HD3	1.83	0.42
1:F:149:ALA:CB	1:F:155:ILE:HG13	2.50	0.42
1:F:207:PHE:HE1	1:F:235:GLY:O	1.98	0.42
1:G:96:ILE:HG13	1:G:127:LEU:HD22	2.01	0.42
1:B:331:ALA:O	1:B:335:LEU:HD23	2.20	0.41
1:B:146:VAL:HG21	1:B:372:VAL:HB	2.02	0.41
1:A:66:GLN:HG3	1:C:187:GLN:OE1	2.20	0.41
1:C:209:LYS:O	1:C:212:ARG:HG2	2.20	0.41
1:C:121:GLY:HA2	1:C:283:SER:HB2	2.02	0.41
1:C:43:PHE:N	1:C:43:PHE:CD2	2.74	0.41
1:C:57:VAL:CG2	1:C:57:VAL:O	2.68	0.41
1:F:89:ILE:HG12	1:F:114:LYS:HB2	2.01	0.41
1:H:96:ILE:HG13	1:H:127:LEU:HD23	2.02	0.41
1:D:149:ALA:HB2	1:D:168:ILE:HD11	2.02	0.41
1:E:109:ILE:HG13	1:E:109:ILE:O	2.20	0.41
1:E:43:PHE:O	1:E:45:LEU:N	2.53	0.41
1:H:94:TYR:HB2	6:H:390:HOH:O	2.20	0.41
1:A:364:GLN:HA	1:A:367:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:HB2	1:B:237:GLY:CA	2.43	0.41
1:C:201:LEU:HD11	1:C:335:LEU:HD11	2.02	0.41
1:F:134:ASN:O	1:F:135:ASN:HB3	2.19	0.41
1:G:61:GLN:O	1:G:61:GLN:HG2	2.20	0.41
1:A:247:VAL:HG11	1:A:258:PHE:CE2	2.55	0.41
1:A:296:VAL:HA	1:A:297:PRO:HD3	1.86	0.41
1:B:115:ILE:H	1:B:145:ASP:HB2	1.85	0.41
1:D:353:TYR:O	1:D:357:ARG:HB3	2.19	0.41
1:E:118:THR:HA	1:E:148:THR:O	2.19	0.41
1:F:141:ILE:O	1:F:166:LYS:HG2	2.20	0.41
1:G:349:ARG:H	1:G:349:ARG:HG2	1.65	0.41
1:G:92:VAL:HG13	1:G:98:HIS:HB2	2.03	0.41
1:H:68:PRO:HA	1:H:69:PRO:HD3	1.93	0.41
1:A:204:ILE:C	1:A:204:ILE:HD13	2.40	0.41
1:A:334:LEU:HD11	1:A:341:HIS:HA	2.01	0.41
1:D:255:ARG:HB3	1:D:255:ARG:HE	1.64	0.41
1:E:144:SER:O	1:E:166:LYS:HE2	2.21	0.41
1:A:250:LEU:O	1:A:251:HIS:HB3	2.20	0.41
1:B:245:GLN:HA	1:B:248:LYS:HB3	2.02	0.41
1:C:12:SER:HA	1:C:43:PHE:CE2	2.54	0.41
1:D:357:ARG:NH1	6:D:412:HOH:O	2.53	0.41
1:E:113:ILE:HG12	1:E:114:LYS:H	1.85	0.41
1:E:163:LYS:O	6:E:401:HOH:O	2.22	0.41
1:H:122:THR:HA	1:H:125:THR:OG1	2.21	0.41
1:H:183:ARG:HB3	1:H:270:ALA:CB	2.50	0.41
1:C:124:ILE:HG21	1:C:158:THR:HA	2.02	0.41
1:C:194:ILE:HG13	1:C:195:SER:H	1.85	0.41
1:C:199:LYS:HB3	1:C:229:ALA:HB2	2.01	0.41
1:D:107:GLN:OE1	1:D:107:GLN:HA	2.21	0.41
1:D:166:LYS:HA	1:D:166:LYS:HD2	1.88	0.41
1:D:374:ARG:CB	1:D:374:ARG:CZ	2.98	0.41
1:E:155:ILE:O	1:E:158:THR:HB	2.21	0.41
1:G:202:ILE:CG2	1:G:202:ILE:O	2.69	0.41
1:G:227:VAL:HG22	1:G:336:LYS:HE2	2.02	0.41
1:C:96:ILE:HG13	1:C:127:LEU:HD13	2.02	0.41
1:C:163:LYS:N	1:C:164:PRO:HD3	2.36	0.41
1:C:243:ILE:O	1:C:247:VAL:HG23	2.21	0.41
1:G:106:LYS:HG3	1:G:111:GLU:HA	2.02	0.41
1:G:251:HIS:CE1	1:G:251:HIS:O	2.74	0.41
1:G:60:ASN:OD1	1:G:61:GLN:CA	2.68	0.41
1:A:136:LEU:CD2	1:B:72:LEU:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:GLU:HG3	1:D:355:GLN:N	2.35	0.41
1:D:374:ARG:O	1:D:375:ASP:CB	2.68	0.41
1:E:96:ILE:HB	1:E:127:LEU:HD23	2.03	0.41
1:F:207:PHE:HD1	1:F:235:GLY:C	2.25	0.41
1:B:187:GLN:H	1:B:187:GLN:HG2	1.70	0.41
1:B:374:ARG:NH1	1:B:374:ARG:HG2	2.35	0.41
1:B:94:TYR:OH	1:B:123:ASP:N	2.54	0.41
1:C:239:GLU:O	1:C:243:ILE:HG12	2.21	0.41
1:F:312:HIS:CG	1:F:312:HIS:O	2.71	0.41
1:G:126:VAL:CG2	1:G:127:LEU:HD12	2.48	0.41
1:H:95:ALA:HB1	6:H:422:HOH:O	2.21	0.41
1:B:126:VAL:CG2	1:B:127:LEU:HD12	2.51	0.41
1:C:21:THR:HA	1:C:36:PHE:CZ	2.56	0.41
1:C:262:GLN:O	2:C:382:UDP:H5	2.03	0.41
1:D:200:ILE:H	1:D:200:ILE:HG22	1.55	0.41
1:E:314:ASP:HB3	1:E:347:ARG:NH1	2.36	0.41
1:G:234:VAL:HG22	1:G:259:LEU:HD13	2.03	0.41
1:G:240:PHE:O	1:G:240:PHE:HD2	2.04	0.41
1:G:94:TYR:CE2	1:G:123:ASP:HB3	2.56	0.41
1:H:296:VAL:HA	1:H:297:PRO:HD3	1.86	0.41
1:D:190:LYS:O	1:D:193:GLY:CA	2.69	0.40
1:E:157:GLU:O	1:E:161:LEU:HB2	2.21	0.40
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.82	0.40
1:C:122:THR:HB	1:C:126:VAL:HG12	2.03	0.40
1:D:187:GLN:C	1:D:189:LYS:N	2.67	0.40
1:E:10:TYR:CE1	1:E:98:HIS:NE2	2.80	0.40
1:E:126:VAL:HG23	1:E:127:LEU:HD13	2.03	0.40
1:F:142:GLU:HA	1:F:166:LYS:HB2	2.03	0.40
1:E:181:PHE:CG	1:G:237:GLY:HA2	2.56	0.40
1:G:264:ASN:O	1:G:268:LEU:HD23	2.21	0.40
1:G:27:LEU:HB3	1:G:34:ILE:HD11	2.02	0.40
1:A:228:ASP:CG	1:A:228:ASP:O	2.60	0.40
1:C:10:TYR:CE2	1:C:94:TYR:CE2	3.09	0.40
1:E:134:ASN:HA	1:E:137:ILE:CD1	2.52	0.40
1:F:340:LEU:O	1:F:344:MET:HB3	2.21	0.40
1:G:246:LEU:CA	1:G:249:ASN:HD21	2.34	0.40
1:G:91:HIS:CD2	1:G:93:HIS:NE2	2.88	0.40
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.69	0.40
1:B:176:ASP:C	1:B:178:ARG:H	2.25	0.40
1:B:196:GLU:C	1:B:198:GLU:N	2.74	0.40
1:C:35:HIS:CD2	1:C:87:LEU:HD21	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:PHE:CG	1:E:43:PHE:O	2.54	0.40
1:H:115:ILE:O	1:H:145:ASP:HB2	2.22	0.40
1:A:64:VAL:N	1:A:65:PHE:CE2	2.89	0.40
1:B:209:LYS:H	1:B:209:LYS:CE	2.33	0.40
1:F:231:LEU:HB3	1:F:256:VAL:HG22	2.03	0.40
1:F:39:SER:HA	1:F:57:VAL:HG22	2.04	0.40
1:H:130:ASP:O	1:H:134:ASN:HB2	2.21	0.40
1:H:122:THR:HG21	4:H:384:MLT:O1	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/414 (89%)	332 (90%)	32 (9%)	4 (1%)	14	45
1	B	363/414 (88%)	335 (92%)	24 (7%)	4 (1%)	14	45
1	C	369/414 (89%)	331 (90%)	36 (10%)	2 (0%)	29	61
1	D	363/414 (88%)	332 (92%)	25 (7%)	6 (2%)	9	35
1	E	373/414 (90%)	331 (89%)	36 (10%)	6 (2%)	9	36
1	F	363/414 (88%)	326 (90%)	34 (9%)	3 (1%)	19	51
1	G	359/414 (87%)	335 (93%)	22 (6%)	2 (1%)	25	57
1	H	363/414 (88%)	329 (91%)	26 (7%)	8 (2%)	6	30
All	All	2921/3312 (88%)	2651 (91%)	235 (8%)	35 (1%)	13	42

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	PHE
1	A	287	VAL

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Mol	Chain	Res	Type
1	B	42	PRO
1	C	205	SER
1	C	286	LEU
1	D	66	GLN
1	D	284	PHE
1	E	42	PRO
1	E	46	ASN
1	G	196	GLU
1	H	66	GLN
1	H	94	TYR
1	H	95	ALA
1	H	123	ASP
1	A	199	LYS
1	D	87	LEU
1	B	94	TYR
1	B	274	LEU
1	E	94	TYR
1	F	67	TYR
1	G	312	HIS
1	H	284	PHE
1	E	97	PRO
1	A	53	TYR
1	D	13	VAL
1	D	97	PRO
1	H	41	LEU
1	E	69	PRO
1	H	265	VAL
1	D	40	GLY
1	H	13	VAL
1	F	69	PRO
1	E	113	ILE
1	B	97	PRO
1	F	97	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/359 (90%)	293 (91%)	29 (9%)	9	32
1	B	321/359 (89%)	292 (91%)	29 (9%)	9	32
1	C	322/359 (90%)	289 (90%)	33 (10%)	7	27
1	D	322/359 (90%)	282 (88%)	40 (12%)	4	19
1	E	327/359 (91%)	284 (87%)	43 (13%)	4	17
1	F	324/359 (90%)	292 (90%)	32 (10%)	8	28
1	G	317/359 (88%)	292 (92%)	25 (8%)	12	37
1	H	323/359 (90%)	290 (90%)	33 (10%)	7	27
All	All	2578/2872 (90%)	2314 (90%)	264 (10%)	7	27

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	LEU
1	A	4	LYS
1	A	18	VAL
1	A	41	LEU
1	A	52	ILE
1	A	62	TYR
1	A	65	PHE
1	A	66	GLN
1	A	67	TYR
1	A	122	THR
1	A	143	GLN
1	A	168	ILE
1	A	173	ASN
1	A	175	ILE
1	A	187	GLN
1	A	194	ILE
1	A	196	GLU
1	A	204	ILE
1	A	207	PHE
1	A	209	LYS
1	A	228	ASP
1	A	236	ASP
1	A	251	HIS
1	A	283	SER
1	A	286	LEU
1	A	314	ASP

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Mol	Chain	Res	Type
1	A	332	ILE
1	A	358	SER
1	B	3	LEU
1	B	61	GLN
1	B	62	TYR
1	B	90	LEU
1	B	94	TYR
1	B	96	ILE
1	B	98	HIS
1	B	111	GLU
1	B	112	ARG
1	B	126	VAL
1	B	148	THR
1	B	168	ILE
1	B	173	ASN
1	B	184	ASP
1	B	198	GLU
1	B	207	PHE
1	B	209	LYS
1	B	240	PHE
1	B	249	ASN
1	B	250	LEU
1	B	251	HIS
1	B	252	ILE
1	B	257	LEU
1	B	268	LEU
1	B	273	ASP
1	B	283	SER
1	B	311	GLN
1	B	332	ILE
1	B	337	ASP
1	C	3	LEU
1	C	18	VAL
1	C	43	PHE
1	C	52	ILE
1	C	65	PHE
1	C	71	ASP
1	C	92	VAL
1	C	96	ILE
1	C	125	THR
1	C	137	ILE
1	C	166	LYS

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Mol	Chain	Res	Type
1	C	168	ILE
1	C	170	THR
1	C	179	VAL
1	C	183	ARG
1	C	185	MET
1	C	190	LYS
1	C	191	GLU
1	C	192	TYR
1	C	200	ILE
1	C	204	ILE
1	C	205	SER
1	C	206	ASN
1	C	209	LYS
1	C	210	VAL
1	C	228	ASP
1	C	232	LEU
1	C	262	GLN
1	C	268	LEU
1	C	275	MET
1	C	303	VAL
1	C	344	MET
1	C	347	ARG
1	D	3	LEU
1	D	18	VAL
1	D	64	VAL
1	D	65	PHE
1	D	71	ASP
1	D	87	LEU
1	D	90	LEU
1	D	122	THR
1	D	127	LEU
1	D	134	ASN
1	D	137	ILE
1	D	161	LEU
1	D	168	ILE
1	D	175	ILE
1	D	178	ARG
1	D	185	MET
1	D	195	SER
1	D	197	SER
1	D	198	GLU
1	D	200	ILE

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Mol	Chain	Res	Type
1	D	204	ILE
1	D	209	LYS
1	D	225	THR
1	D	226	GLU
1	D	236	ASP
1	D	242	THR
1	D	249	ASN
1	D	251	HIS
1	D	255	ARG
1	D	283	SER
1	D	286	LEU
1	D	288	LEU
1	D	303	VAL
1	D	325	THR
1	D	346	GLU
1	D	347	ARG
1	D	354	GLU
1	D	363	SER
1	D	375	ASP
1	D	376	ASP
1	E	2	LYS
1	E	3	LEU
1	E	4	LYS
1	E	25	LYS
1	E	27	LEU
1	E	30	ARG
1	E	41	LEU
1	E	44	ARG
1	E	52	ILE
1	E	54	PHE
1	E	65	PHE
1	E	70	TYR
1	E	89	ILE
1	E	92	VAL
1	E	122	THR
1	E	123	ASP
1	E	134	ASN
1	E	136	LEU
1	E	154	LEU
1	E	161	LEU
1	E	181	PHE
1	E	183	ARG

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Mol	Chain	Res	Type
1	E	187	GLN
1	E	191	GLU
1	E	204	ILE
1	E	209	LYS
1	E	216	VAL
1	E	242	THR
1	E	261	LYS
1	E	262	GLN
1	E	269	LEU
1	E	275	MET
1	E	283	SER
1	E	301	THR
1	E	314	ASP
1	E	317	TYR
1	E	318	LEU
1	E	325	THR
1	E	332	ILE
1	E	340	LEU
1	E	347	ARG
1	E	355	GLN
1	E	363	SER
1	F	3	LEU
1	F	9	CYS
1	F	46	ASN
1	F	47	LYS
1	F	48	VAL
1	F	61	GLN
1	F	64	VAL
1	F	65	PHE
1	F	66	GLN
1	F	70	TYR
1	F	72	LEU
1	F	115	ILE
1	F	123	ASP
1	F	147	VAL
1	F	161	LEU
1	F	177	GLU
1	F	185	MET
1	F	187	GLN
1	F	190	LYS
1	F	194	ILE
1	F	196	GLU

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Mol	Chain	Res	Type
1	F	200	ILE
1	F	209	LYS
1	F	242	THR
1	F	257	LEU
1	F	265	VAL
1	F	268	LEU
1	F	287	VAL
1	F	298	CYS
1	F	325	THR
1	F	349	ARG
1	F	356	PHE
1	G	22	GLU
1	G	60	ASN
1	G	62	TYR
1	G	90	LEU
1	G	96	ILE
1	G	112	ARG
1	G	148	THR
1	G	167	ASP
1	G	168	ILE
1	G	184	ASP
1	G	206	ASN
1	G	209	LYS
1	G	240	PHE
1	G	249	ASN
1	G	251	HIS
1	G	254	ASP
1	G	259	LEU
1	G	265	VAL
1	G	273	ASP
1	G	286	LEU
1	G	311	GLN
1	G	329	ASP
1	G	349	ARG
1	G	371	ASP
1	G	376	ASP
1	H	2	LYS
1	H	9	CYS
1	H	47	LYS
1	H	48	VAL
1	H	52	ILE
1	H	57	VAL

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Mol	Chain	Res	Type
1	H	88	ASP
1	H	90	LEU
1	H	92	VAL
1	H	96	ILE
1	H	112	ARG
1	H	117	THR
1	H	127	LEU
1	H	187	GLN
1	H	188	LEU
1	H	190	LYS
1	H	201	LEU
1	H	204	ILE
1	H	206	ASN
1	H	236	ASP
1	H	247	VAL
1	H	252	ILE
1	H	262	GLN
1	H	268	LEU
1	H	283	SER
1	H	287	VAL
1	H	289	LEU
1	H	318	LEU
1	H	329	ASP
1	H	335	LEU
1	H	347	ARG
1	H	349	ARG
1	H	376	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	83	GLN
1	A	120	HIS
1	A	165	ASN
1	A	169	GLN
1	A	173	ASN
1	A	187	GLN
1	A	214	GLN
1	A	262	GLN
1	A	355	GLN
1	B	35	HIS

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Mol	Chain	Res	Type
1	B	61	GLN
1	B	134	ASN
1	B	165	ASN
1	B	173	ASN
1	B	251	HIS
1	B	311	GLN
1	B	333	GLN
1	B	364	GLN
1	C	98	HIS
1	C	134	ASN
1	C	165	ASN
1	C	173	ASN
1	C	187	GLN
1	C	262	GLN
1	D	35	HIS
1	D	66	GLN
1	D	120	HIS
1	D	134	ASN
1	D	159	HIS
1	D	173	ASN
1	D	251	HIS
1	D	262	GLN
1	D	311	GLN
1	E	46	ASN
1	E	66	GLN
1	E	91	HIS
1	E	134	ASN
1	E	152	HIS
1	E	165	ASN
1	E	173	ASN
1	E	245	GLN
1	E	262	GLN
1	E	330	GLN
1	E	355	GLN
1	F	51	ASN
1	F	60	ASN
1	F	86	ASN
1	F	98	HIS
1	F	107	GLN
1	F	120	HIS
1	F	134	ASN
1	F	173	ASN

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Mol	Chain	Res	Type
1	F	187	GLN
1	F	251	HIS
1	F	262	GLN
1	F	311	GLN
1	F	312	HIS
1	G	26	GLN
1	G	61	GLN
1	G	66	GLN
1	G	120	HIS
1	G	134	ASN
1	G	159	HIS
1	G	165	ASN
1	G	173	ASN
1	G	187	GLN
1	G	249	ASN
1	G	262	GLN
1	G	311	GLN
1	H	60	ASN
1	H	83	GLN
1	H	107	GLN
1	H	152	HIS
1	H	165	ASN
1	H	173	ASN
1	H	187	GLN
1	H	206	ASN
1	H	245	GLN
1	H	251	HIS
1	H	262	GLN
1	H	343	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	GOL	B	382	-	5,5,5	0.39	0	5,5,5	0.34	0
3	GOL	E	383	-	5,5,5	0.39	0	5,5,5	0.28	0
3	GOL	F	385	-	5,5,5	0.41	0	5,5,5	0.29	0
3	GOL	C	384	-	5,5,5	0.40	0	5,5,5	0.18	0
2	UDP	E	382	5	20,26,26	1.23	1 (5%)	25,40,40	1.09	1 (4%)
3	GOL	A	385	-	5,5,5	0.39	0	5,5,5	0.28	0
3	GOL	B	383	-	5,5,5	0.36	0	5,5,5	0.24	0
2	UDP	A	382	-	20,26,26	1.15	1 (5%)	25,40,40	1.18	2 (8%)
2	UDP	C	382	5	20,26,26	1.12	1 (5%)	25,40,40	1.14	1 (4%)
3	GOL	A	387	-	5,5,5	0.36	0	5,5,5	0.44	0
3	GOL	A	384	-	5,5,5	0.39	0	5,5,5	0.18	0
3	GOL	A	383	-	5,5,5	0.35	0	5,5,5	0.23	0
4	MLT	C	385	-	2,8,8	0.38	0	3,10,10	0.86	0
3	GOL	E	384	-	5,5,5	0.36	0	5,5,5	0.27	0
3	GOL	H	383	-	5,5,5	0.32	0	5,5,5	0.38	0
3	GOL	A	386	-	5,5,5	0.35	0	5,5,5	0.18	0
3	GOL	F	382	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	D	382	-	5,5,5	0.36	0	5,5,5	0.27	0
4	MLT	E	387	-	2,8,8	0.44	0	3,10,10	0.62	0
3	GOL	D	384	-	5,5,5	0.39	0	5,5,5	0.39	0
3	GOL	F	384	-	5,5,5	0.40	0	5,5,5	0.24	0
4	MLT	A	388	-	2,8,8	0.44	0	3,10,10	0.89	0
4	MLT	H	384	-	2,8,8	0.47	0	3,10,10	1.13	0
3	GOL	E	386	-	5,5,5	0.33	0	5,5,5	0.38	0
2	UDP	H	382	-	20,26,26	1.25	1 (5%)	25,40,40	1.18	2 (8%)
3	GOL	C	383	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	F	383	-	5,5,5	0.40	0	5,5,5	0.27	0
3	GOL	D	383	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	E	385	-	5,5,5	0.38	0	5,5,5	0.46	0

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	GOL	B	382	-	-	4/4/4/4	-
3	GOL	E	383	-	-	2/4/4/4	-
3	GOL	F	385	-	-	2/4/4/4	-
3	GOL	C	384	-	-	0/4/4/4	-
2	UDP	E	382	5	-	4/14/32/32	0/2/2/2
3	GOL	A	385	-	-	2/4/4/4	-
3	GOL	B	383	-	-	4/4/4/4	-
2	UDP	A	382	-	-	5/14/32/32	0/2/2/2
2	UDP	C	382	5	-	5/14/32/32	0/2/2/2
3	GOL	A	387	-	-	2/4/4/4	-
3	GOL	A	384	-	-	2/4/4/4	-
3	GOL	A	383	-	-	0/4/4/4	-
4	MLT	C	385	-	-	0/2/8/8	-
3	GOL	E	384	-	-	1/4/4/4	-
3	GOL	H	383	-	-	4/4/4/4	-
3	GOL	A	386	-	-	4/4/4/4	-
3	GOL	F	382	-	-	2/4/4/4	-
3	GOL	D	382	-	-	4/4/4/4	-
4	MLT	E	387	-	-	1/2/8/8	-
3	GOL	D	384	-	-	4/4/4/4	-
3	GOL	F	384	-	-	4/4/4/4	-
4	MLT	A	388	-	-	0/2/8/8	-
4	MLT	H	384	-	-	2/2/8/8	-
3	GOL	E	386	-	-	3/4/4/4	-
2	UDP	H	382	-	-	4/14/32/32	0/2/2/2
3	GOL	C	383	-	-	3/4/4/4	-
3	GOL	F	383	-	-	2/4/4/4	-
3	GOL	D	383	-	-	2/4/4/4	-
3	GOL	E	385	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	382	UDP	C4-N3	3.54	1.39	1.33
2	H	382	UDP	C4-N3	3.47	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	382	UDP	C4-N3	3.13	1.38	1.33
2	C	382	UDP	C4-N3	2.88	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	382	UDP	PA-O3A-PB	-3.64	120.34	132.83
2	C	382	UDP	PA-O3A-PB	-3.61	120.44	132.83
2	H	382	UDP	C3'-C2'-C1'	3.34	106.01	100.98
2	A	382	UDP	PA-O3A-PB	-3.04	122.38	132.83
2	H	382	UDP	PA-O3A-PB	-2.74	123.42	132.83
2	A	382	UDP	C3'-C2'-C1'	2.71	105.06	100.98

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	382	GOL	O1-C1-C2-C3
3	E	383	GOL	O1-C1-C2-O2
3	E	383	GOL	O1-C1-C2-C3
3	F	385	GOL	C1-C2-C3-O3
2	E	382	UDP	C5'-O5'-PA-O1A
3	B	383	GOL	O1-C1-C2-O2
3	B	383	GOL	O1-C1-C2-C3
2	A	382	UDP	C5'-O5'-PA-O1A
2	A	382	UDP	C5'-O5'-PA-O2A
2	A	382	UDP	C5'-O5'-PA-O3A
2	C	382	UDP	C2'-C1'-N1-C6
2	C	382	UDP	O4'-C1'-N1-C6
3	A	387	GOL	O1-C1-C2-C3
3	A	384	GOL	O1-C1-C2-O2
3	A	384	GOL	O1-C1-C2-C3
3	H	383	GOL	O1-C1-C2-C3
3	A	386	GOL	O1-C1-C2-O2
3	A	386	GOL	O1-C1-C2-C3
3	A	386	GOL	C1-C2-C3-O3
3	D	382	GOL	O1-C1-C2-O2
3	D	382	GOL	O1-C1-C2-C3
4	E	387	MLT	C1-C2-C3-C4
3	D	384	GOL	O1-C1-C2-C3
3	F	384	GOL	O1-C1-C2-O2
3	F	384	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	H	384	MLT	C1-C2-C3-C4
4	H	384	MLT	O3-C2-C3-C4
2	H	382	UDP	C3'-C4'-C5'-O5'
2	H	382	UDP	C5'-O5'-PA-O1A
3	C	383	GOL	O1-C1-C2-C3
3	F	383	GOL	O1-C1-C2-C3
2	E	382	UDP	C3'-C4'-C5'-O5'
2	E	382	UDP	O4'-C4'-C5'-O5'
2	A	382	UDP	C3'-C4'-C5'-O5'
2	A	382	UDP	O4'-C4'-C5'-O5'
2	C	382	UDP	C3'-C4'-C5'-O5'
2	C	382	UDP	O4'-C4'-C5'-O5'
3	H	383	GOL	O2-C2-C3-O3
3	D	384	GOL	O1-C1-C2-O2
3	C	383	GOL	O1-C1-C2-O2
3	B	382	GOL	C1-C2-C3-O3
3	B	383	GOL	C1-C2-C3-O3
3	E	384	GOL	C1-C2-C3-O3
3	H	383	GOL	C1-C2-C3-O3
3	F	382	GOL	C1-C2-C3-O3
3	D	384	GOL	C1-C2-C3-O3
3	F	384	GOL	C1-C2-C3-O3
3	C	383	GOL	C1-C2-C3-O3
3	D	383	GOL	O1-C1-C2-C3
3	B	382	GOL	O1-C1-C2-O2
3	F	385	GOL	O2-C2-C3-O3
3	H	383	GOL	O1-C1-C2-O2
3	A	386	GOL	O2-C2-C3-O3
3	F	384	GOL	O2-C2-C3-O3
3	F	383	GOL	O1-C1-C2-O2
2	H	382	UDP	O4'-C4'-C5'-O5'
3	A	387	GOL	O1-C1-C2-O2
3	D	384	GOL	O2-C2-C3-O3
3	F	382	GOL	O2-C2-C3-O3
3	E	386	GOL	O1-C1-C2-O2
2	E	382	UDP	C5'-O5'-PA-O3A
3	D	382	GOL	O2-C2-C3-O3
2	H	382	UDP	C5'-O5'-PA-O3A
3	D	383	GOL	O1-C1-C2-O2
3	D	382	GOL	C1-C2-C3-O3
3	B	383	GOL	O2-C2-C3-O3
3	A	385	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	E	386	GOL	C1-C2-C3-O3
3	A	385	GOL	O1-C1-C2-O2
3	B	382	GOL	O2-C2-C3-O3
3	E	386	GOL	O2-C2-C3-O3
2	C	382	UDP	C5'-O5'-PA-O1A

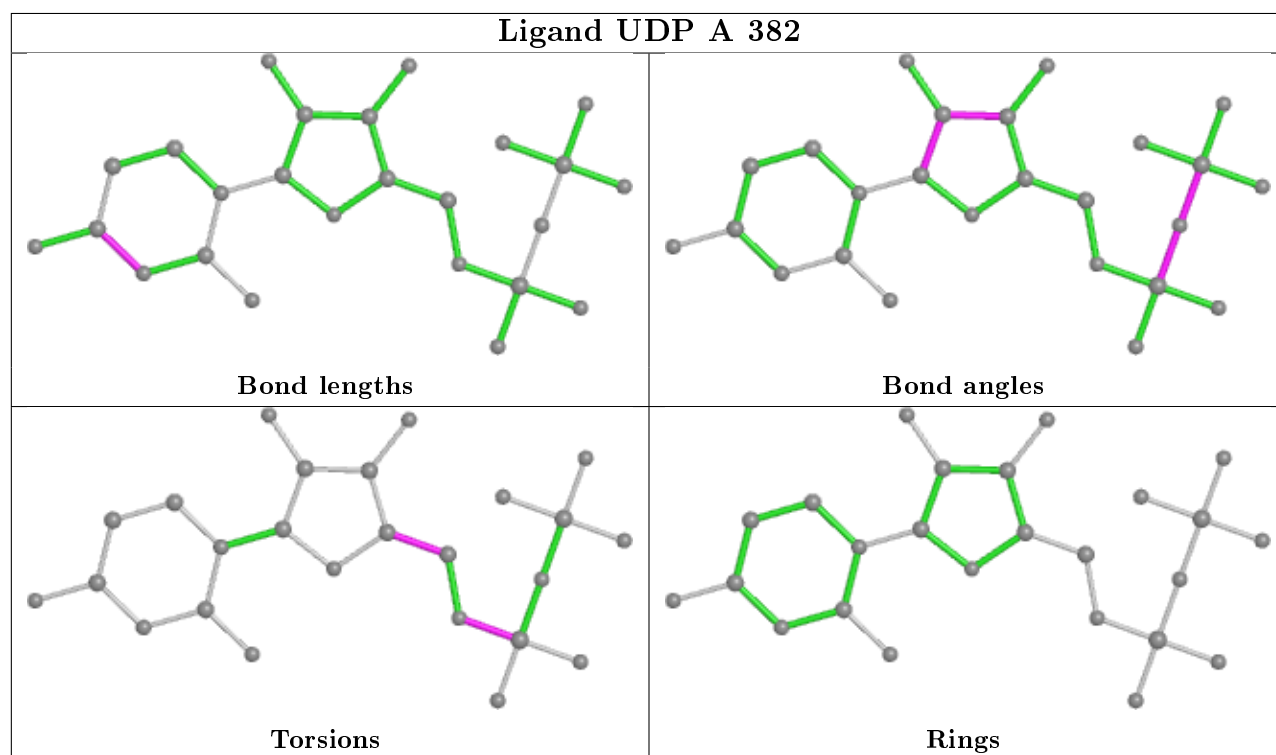
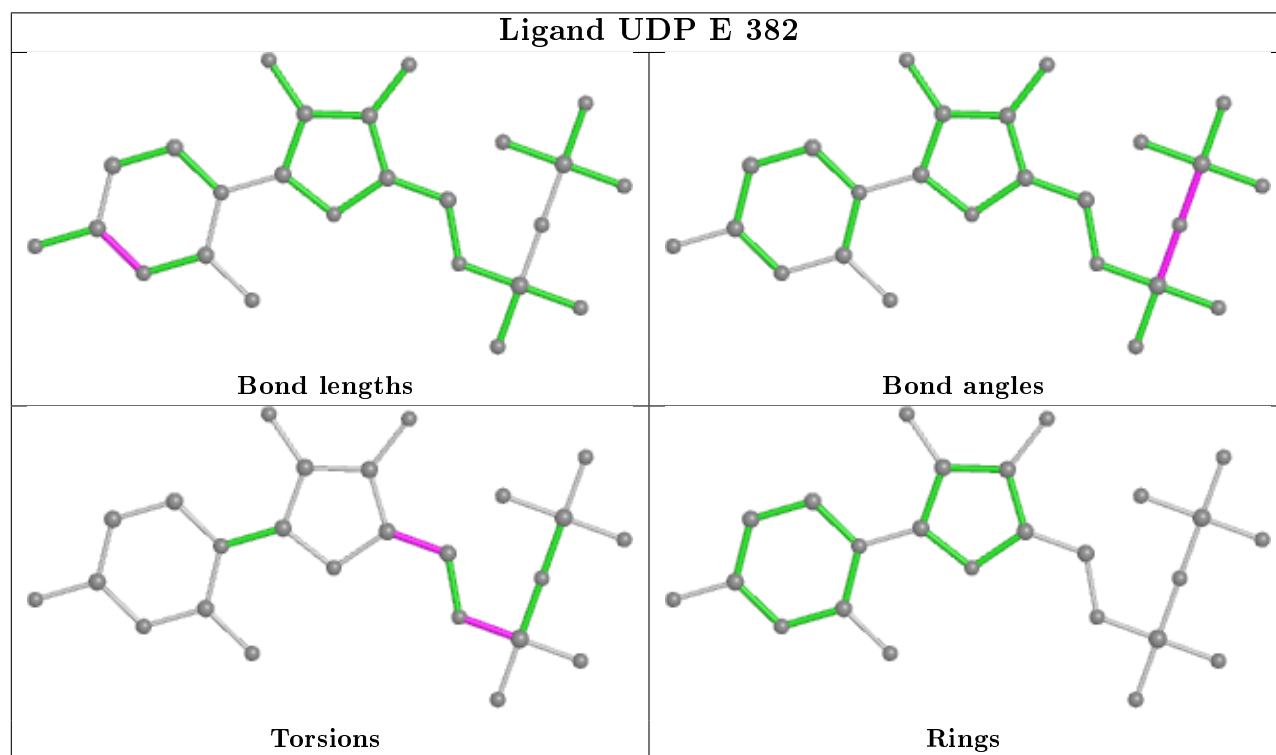
There are no ring outliers.

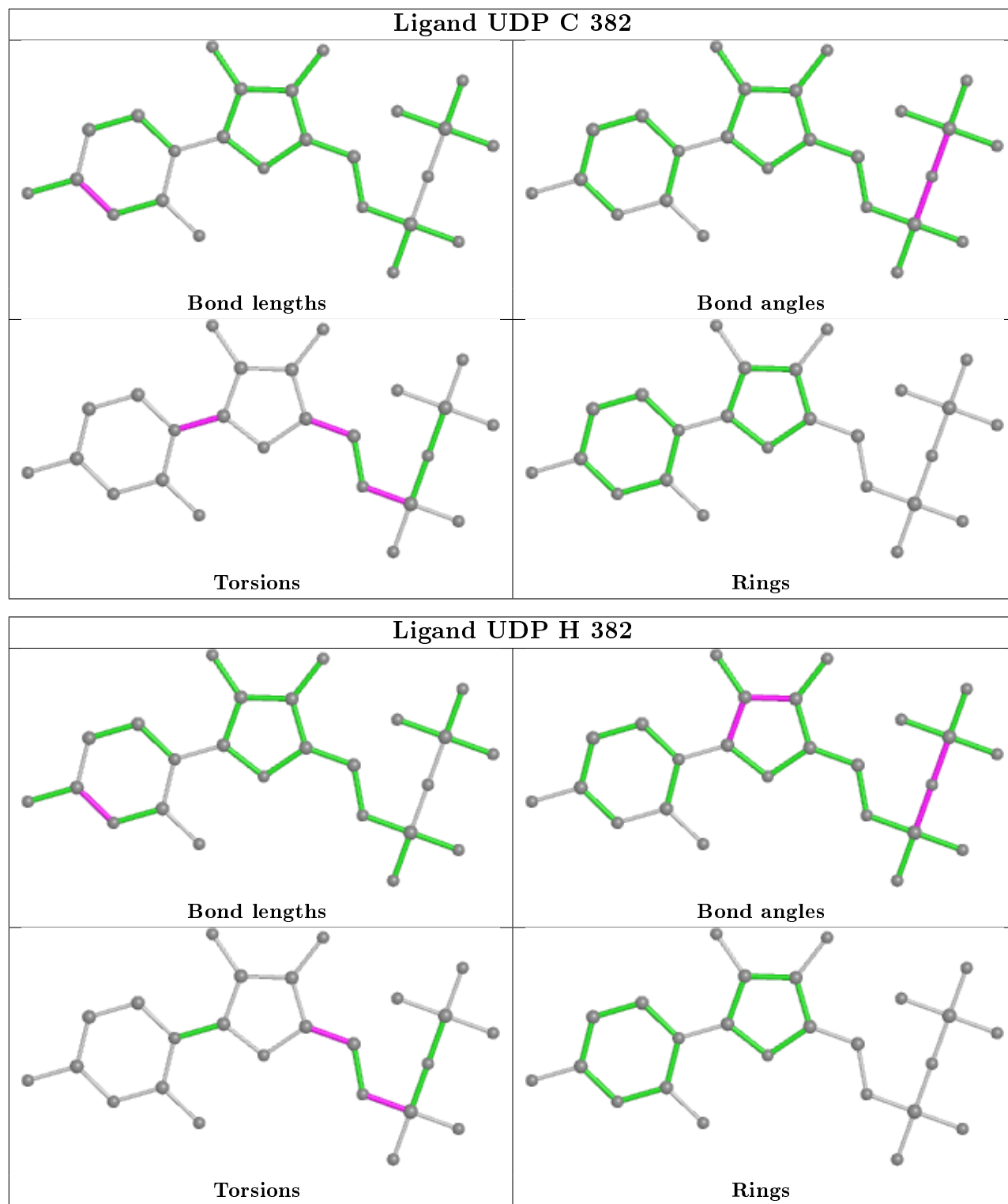
21 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	382	GOL	1	0
3	F	385	GOL	1	0
3	C	384	GOL	1	0
2	E	382	UDP	2	0
3	A	385	GOL	2	0
2	C	382	UDP	2	0
3	A	387	GOL	1	0
3	A	384	GOL	1	0
3	A	383	GOL	1	0
4	C	385	MLT	1	0
3	H	383	GOL	1	0
3	A	386	GOL	1	0
3	F	382	GOL	1	0
3	D	382	GOL	2	0
3	F	384	GOL	2	0
4	H	384	MLT	1	0
3	E	386	GOL	1	0
2	H	382	UDP	2	0
3	F	383	GOL	4	0
3	D	383	GOL	1	0
3	E	385	GOL	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	372/414 (89%)	-0.22	0 100 100	34, 57, 107, 153	0
1	B	369/414 (89%)	0.16	6 (1%) 72 70	41, 85, 124, 147	0
1	C	373/414 (90%)	-0.16	4 (1%) 80 81	35, 60, 104, 133	0
1	D	369/414 (89%)	-0.14	3 (0%) 86 86	35, 56, 109, 139	0
1	E	375/414 (90%)	-0.06	3 (0%) 86 86	37, 66, 116, 149	0
1	F	369/414 (89%)	-0.02	5 (1%) 75 75	42, 69, 115, 147	0
1	G	365/414 (88%)	0.26	15 (4%) 37 35	55, 96, 135, 152	0
1	H	369/414 (89%)	-0.09	3 (0%) 86 86	48, 69, 110, 140	0
All	All	2961/3312 (89%)	-0.03	39 (1%) 77 77	34, 68, 120, 153	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	ASN	3.8
1	G	15	GLY	3.5
1	F	376	ASP	3.5
1	E	61	GLN	3.3
1	G	376	ASP	3.3
1	G	229	ALA	3.2
1	G	50	PRO	3.1
1	G	218	GLN	2.9
1	B	324	THR	2.9
1	D	197	SER	2.8
1	H	194	ILE	2.8
1	C	193	GLY	2.7
1	B	49	TYR	2.7
1	D	5	ILE	2.6
1	G	48	VAL	2.5
1	G	32	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	49	TYR	2.4
1	B	35	HIS	2.4
1	F	15	GLY	2.3
1	F	48	VAL	2.3
1	C	63	SER	2.3
1	G	113	ILE	2.3
1	E	228	ASP	2.3
1	F	195	SER	2.3
1	G	3	LEU	2.2
1	C	60	ASN	2.2
1	B	15	GLY	2.2
1	B	50	PRO	2.2
1	C	61	GLN	2.2
1	D	263	ASP	2.2
1	G	40	GLY	2.2
1	G	199	LYS	2.2
1	B	87	LEU	2.1
1	G	186	THR	2.1
1	G	219	ALA	2.1
1	H	224	VAL	2.1
1	F	49	TYR	2.1
1	G	88	ASP	2.1
1	H	229	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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.

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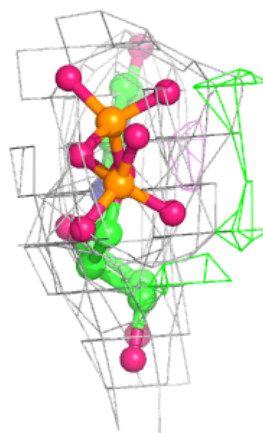
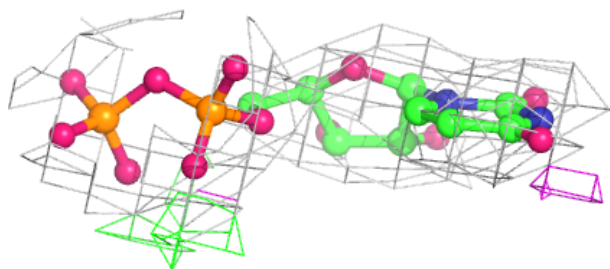
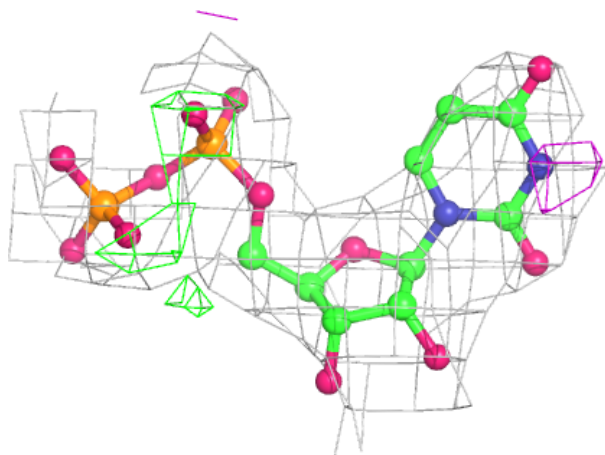
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	382	6/6	0.40	0.69	107,108,108,108	0
3	GOL	E	386	6/6	0.61	0.49	52,53,54,56	6
3	GOL	A	384	6/6	0.65	0.46	100,101,101,102	0
3	GOL	A	385	6/6	0.67	0.34	75,78,78,79	0
3	GOL	E	385	6/6	0.68	0.41	80,81,81,81	6
3	GOL	E	384	6/6	0.70	0.38	92,92,92,93	0
3	GOL	F	383	6/6	0.72	0.74	144,145,145,146	0
5	MG	E	388	1/1	0.72	0.59	72,72,72,72	0
3	GOL	E	383	6/6	0.73	0.40	103,104,105,105	0
3	GOL	F	385	6/6	0.74	0.39	77,82,82,85	6
3	GOL	D	383	6/6	0.75	0.70	102,107,107,110	0
3	GOL	D	384	6/6	0.75	0.31	77,79,79,80	0
3	GOL	A	387	6/6	0.78	0.42	84,86,86,90	0
4	MLT	H	384	9/9	0.79	0.38	80,82,86,86	9
3	GOL	D	382	6/6	0.79	0.44	100,100,100,100	0
3	GOL	A	386	6/6	0.79	0.29	71,73,73,73	0
3	GOL	F	382	6/6	0.80	0.32	83,84,85,85	0
4	MLT	C	385	9/9	0.81	0.34	61,62,62,62	9
4	MLT	A	388	9/9	0.81	0.40	76,80,86,86	9
3	GOL	H	383	6/6	0.85	0.30	89,91,91,92	0
3	GOL	F	384	6/6	0.85	0.47	110,111,111,112	0
3	GOL	B	383	6/6	0.85	0.33	81,82,82,82	0
4	MLT	E	387	9/9	0.86	0.25	90,91,91,91	0
3	GOL	C	384	6/6	0.87	0.53	72,73,73,74	6
3	GOL	A	383	6/6	0.87	0.22	57,58,59,60	0
2	UDP	A	382	25/25	0.89	0.22	70,78,98,99	0
2	UDP	E	382	25/25	0.89	0.22	82,85,96,97	2
2	UDP	H	382	25/25	0.90	0.17	91,94,121,121	0
5	MG	C	386	1/1	0.91	0.33	43,43,43,43	0
3	GOL	C	383	6/6	0.93	0.24	78,84,85,85	0
2	UDP	C	382	25/25	0.94	0.18	65,67,76,76	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.

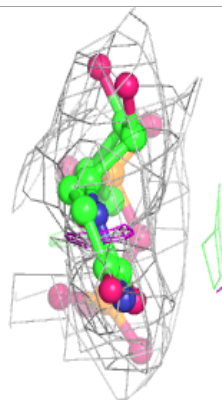
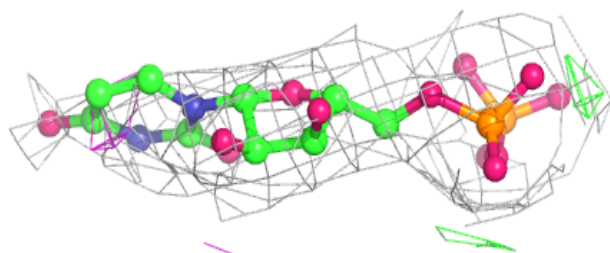
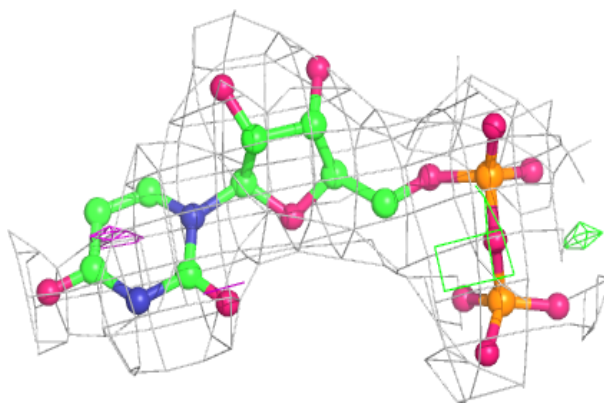
**Electron density around UDP A 382:**

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



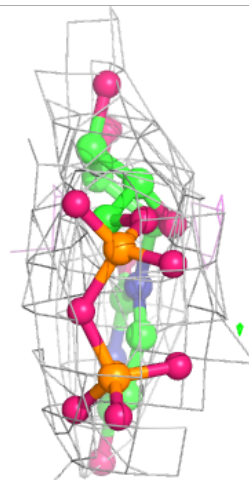
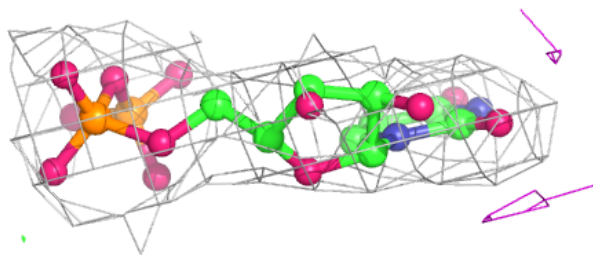
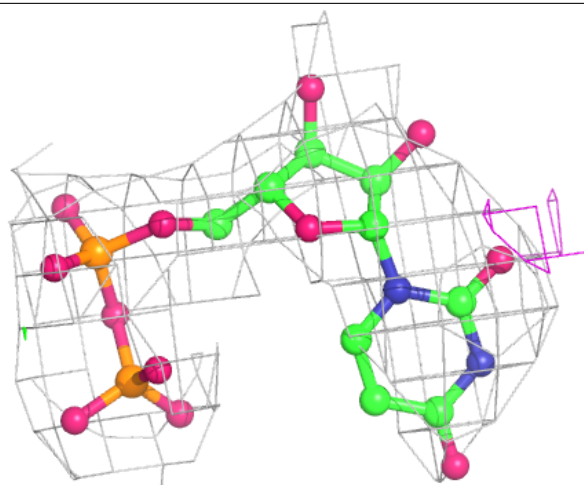
**Electron density around UDP E 382:**

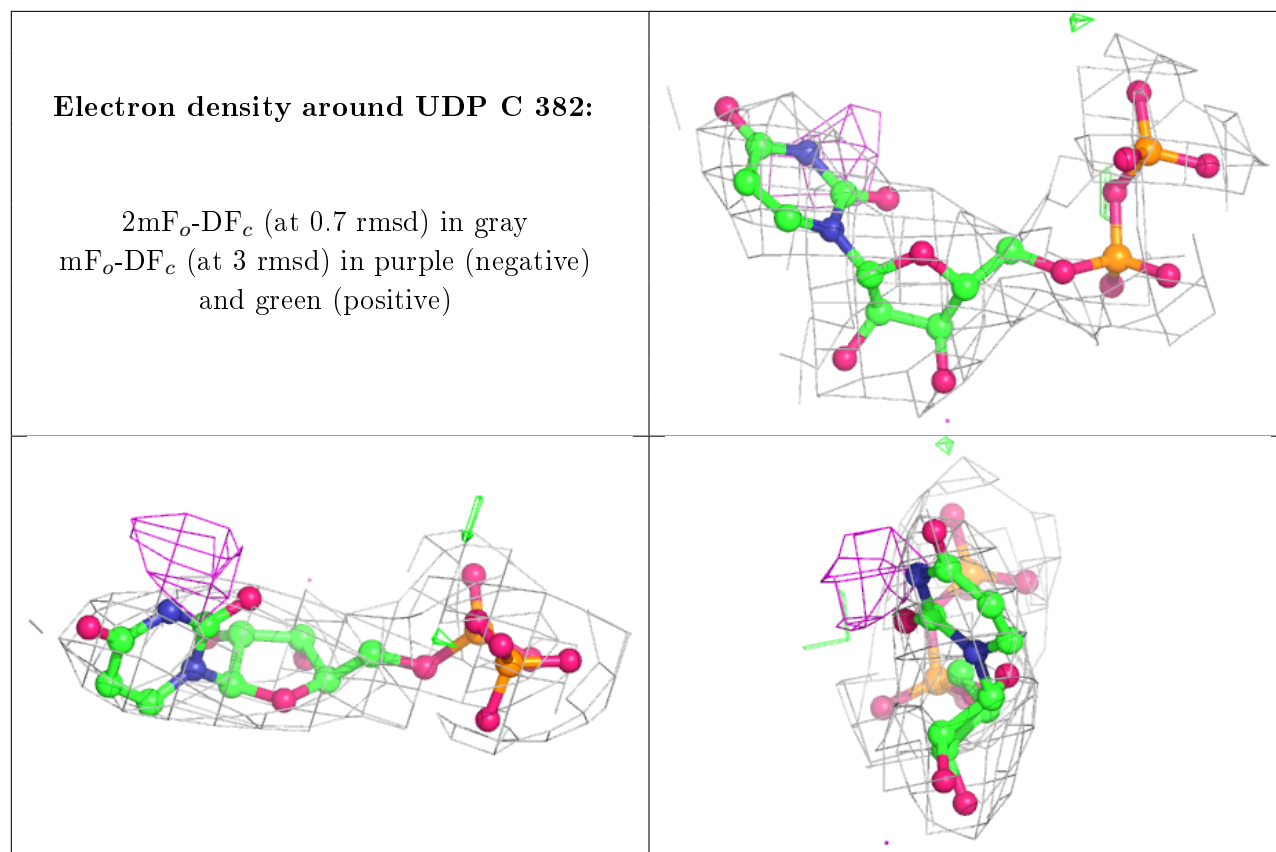
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UDP H 382:**

$2mF_o-DF_c$  (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.