



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:45 AM UTC

PDB ID : 3MBO / pdb_00003mbo
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

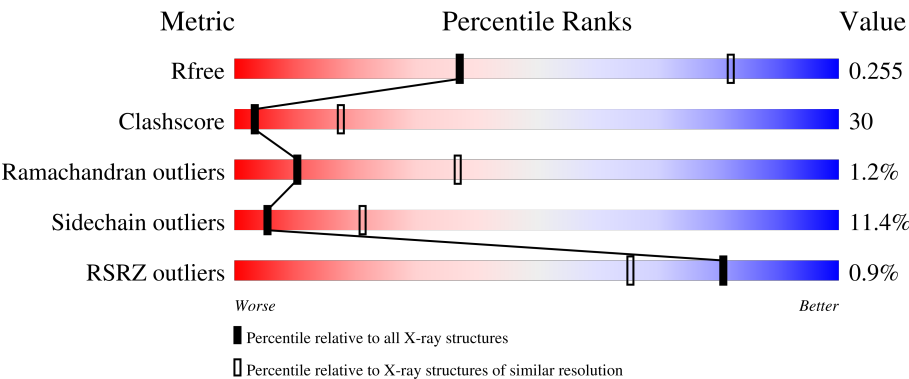
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	414	% 49%29%11%•10%
1	B	414	% 47%31%10%•11%
1	C	414	% 49%28%12%•10%
1	D	414	% 50%27%10%•11%
1	E	414	49%29%10%•9%

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Mol	Chain	Length	Quality of chain
1	F	414	
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	E	385	-	-	X	-
3	GOL	F	383	-	-	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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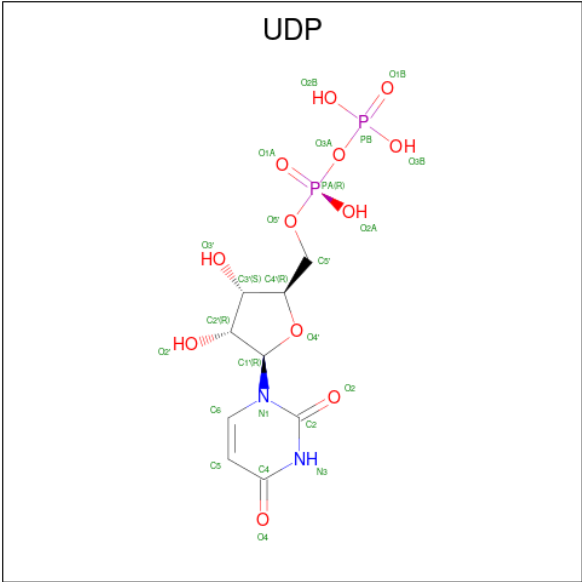
Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	GLY	-	expression tag	UNP Q81ST7
F	-15	SER	-	expression tag	UNP Q81ST7
F	-14	HIS	-	expression tag	UNP Q81ST7
F	-13	MET	-	expression tag	UNP Q81ST7
F	-12	ALA	-	expression tag	UNP Q81ST7
F	-11	SER	-	expression tag	UNP Q81ST7
F	-10	MET	-	expression tag	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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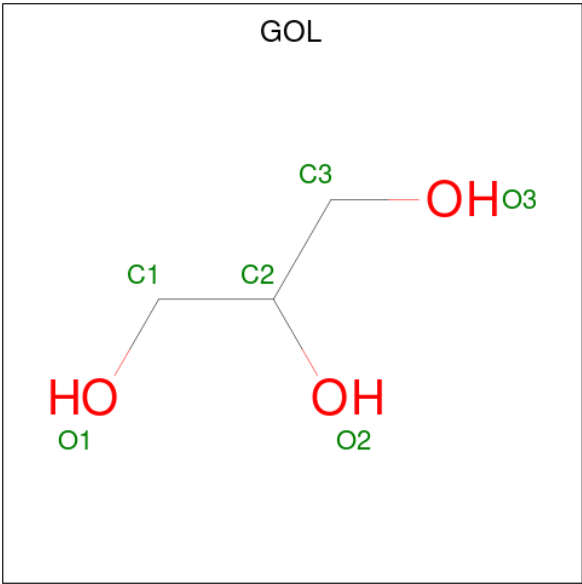
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLY	-	expression tag	UNP Q81ST7
G	-6	GLN	-	expression tag	UNP Q81ST7
G	-5	GLN	-	expression tag	UNP Q81ST7
G	-4	MET	-	expression tag	UNP Q81ST7
G	-3	GLY	-	expression tag	UNP Q81ST7
G	-2	ARG	-	expression tag	UNP Q81ST7
G	-1	GLY	-	expression tag	UNP Q81ST7
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 (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



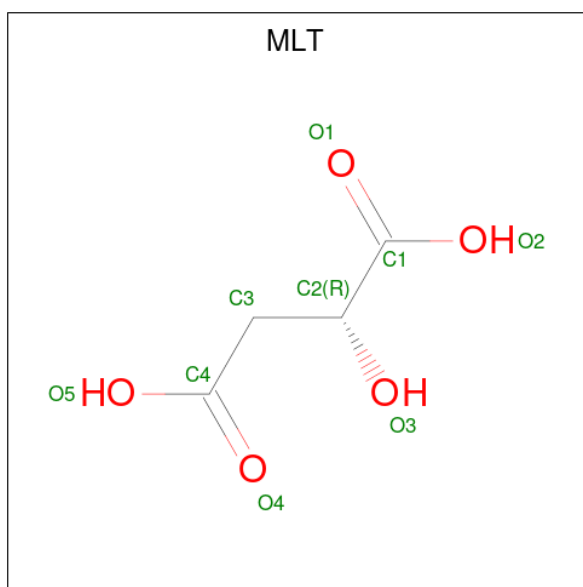
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	H	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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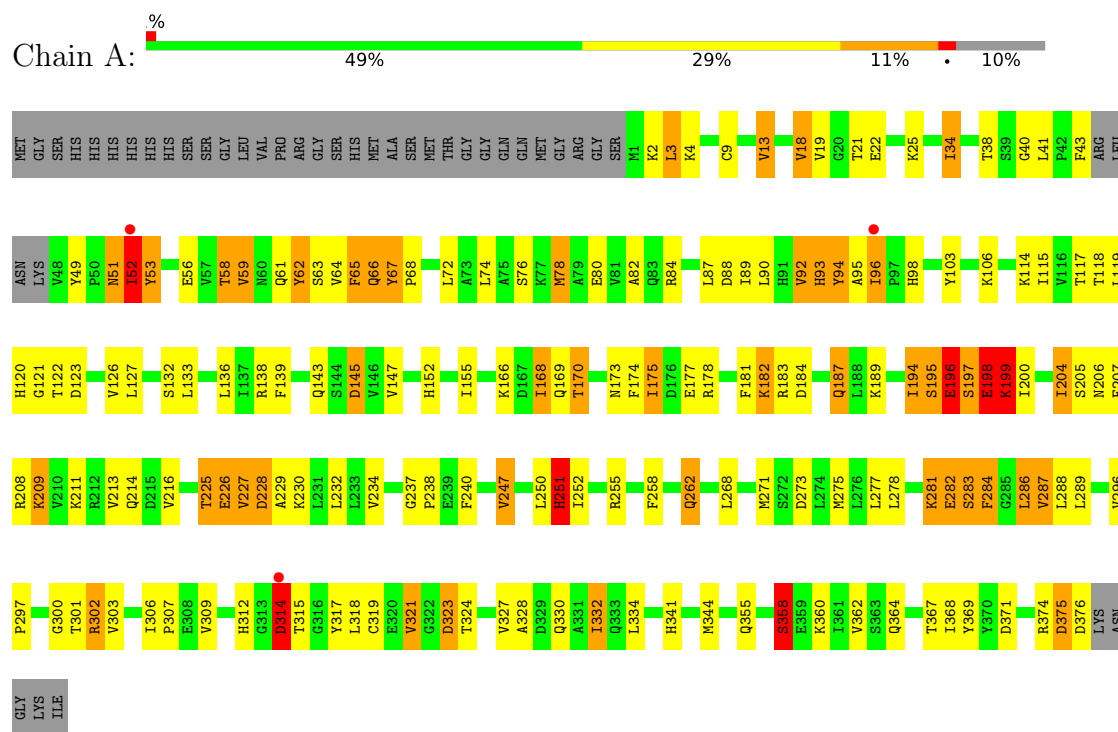
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	37	Total 37	O 37	0	0
6	E	41	Total 41	O 41	0	0
6	F	32	Total 32	O 32	0	0
6	G	33	Total 33	O 33	0	0
6	H	46	Total 46	O 46	0	0

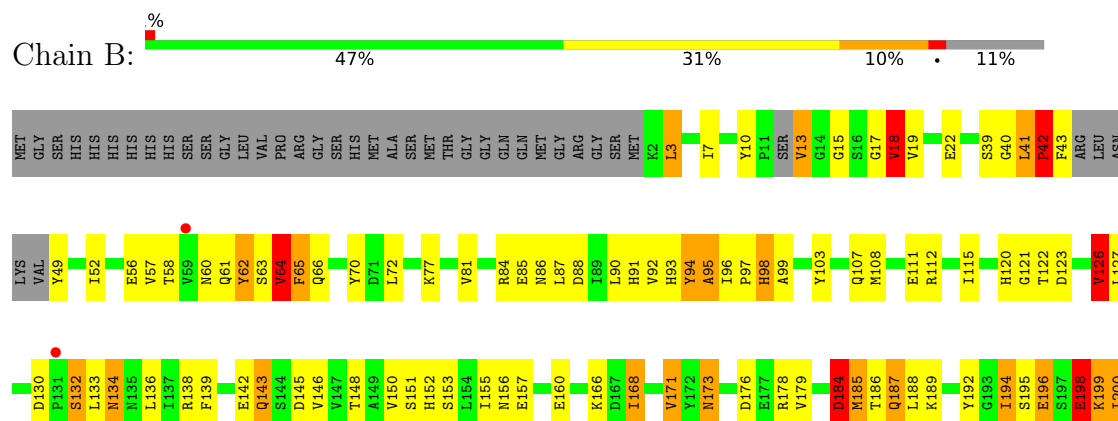
3 Residue-property plots

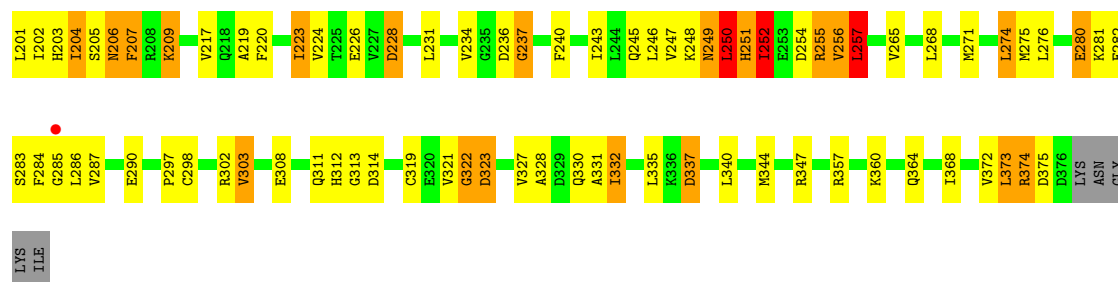
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glycosyltransferase, group 1 family

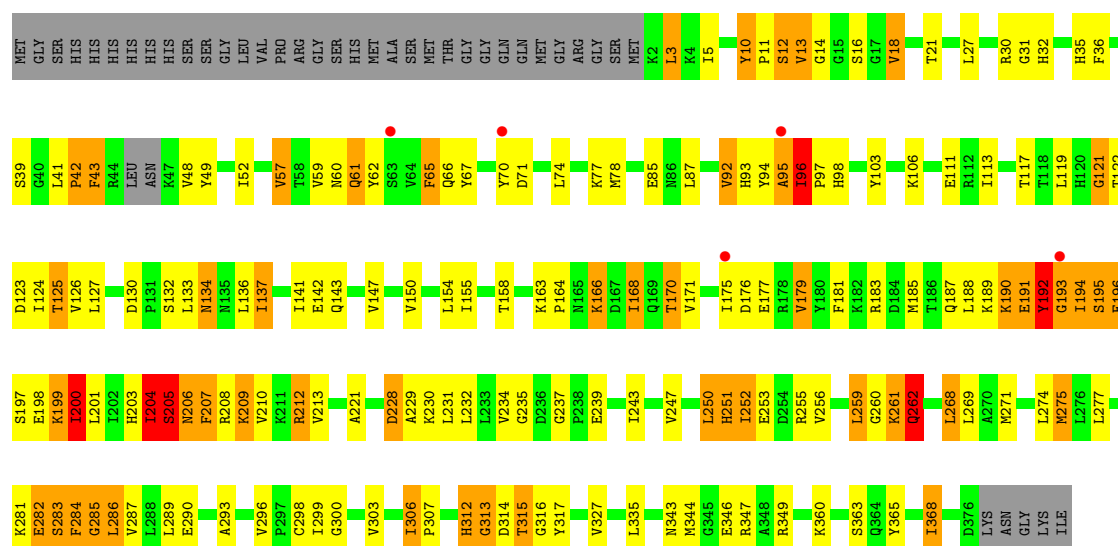


- Molecule 1: Glycosyltransferase, group 1 family

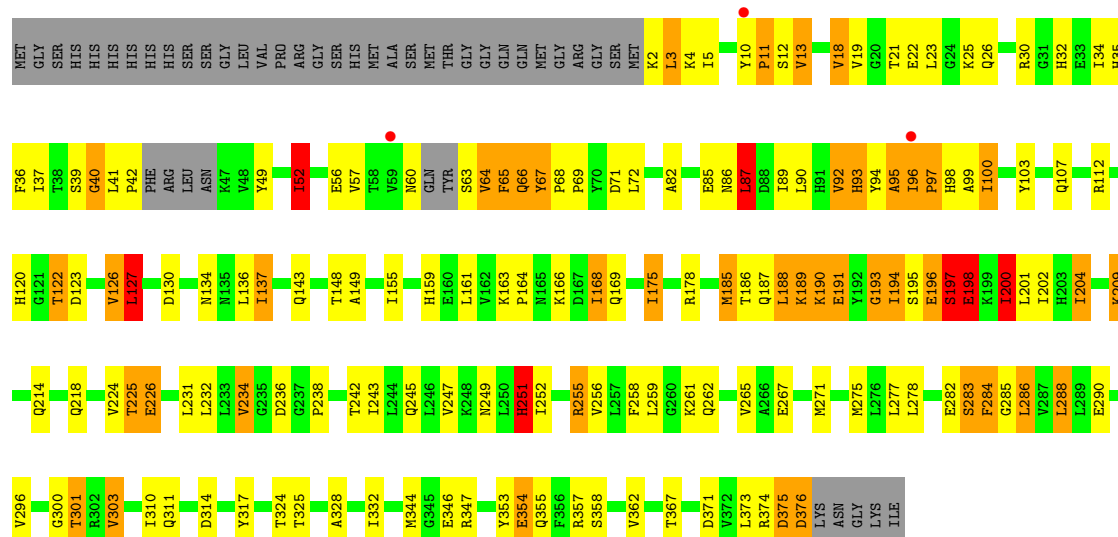




• Molecule 1: Glycosyltransferase, group 1 family

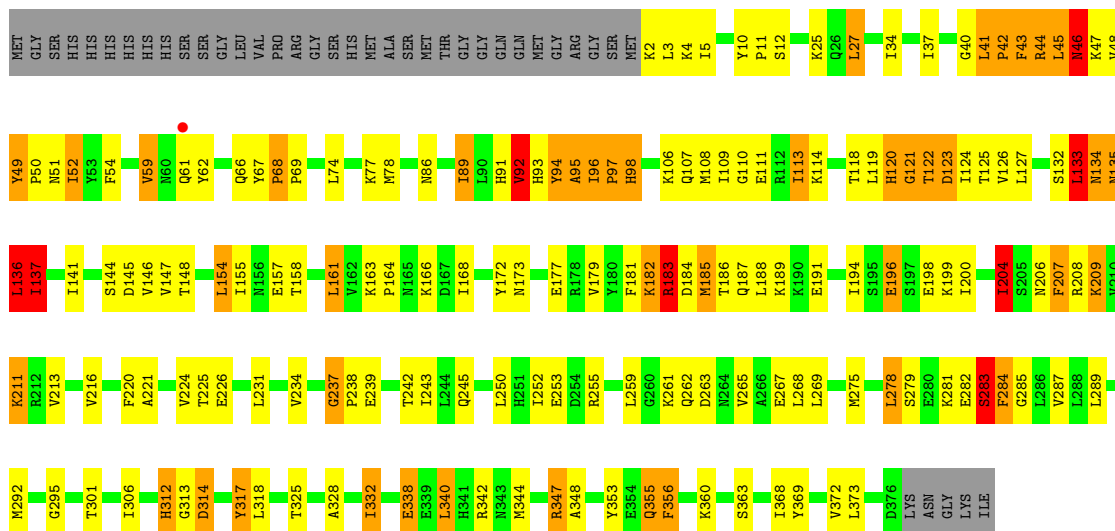


• Molecule 1: Glycosyltransferase, group 1 family



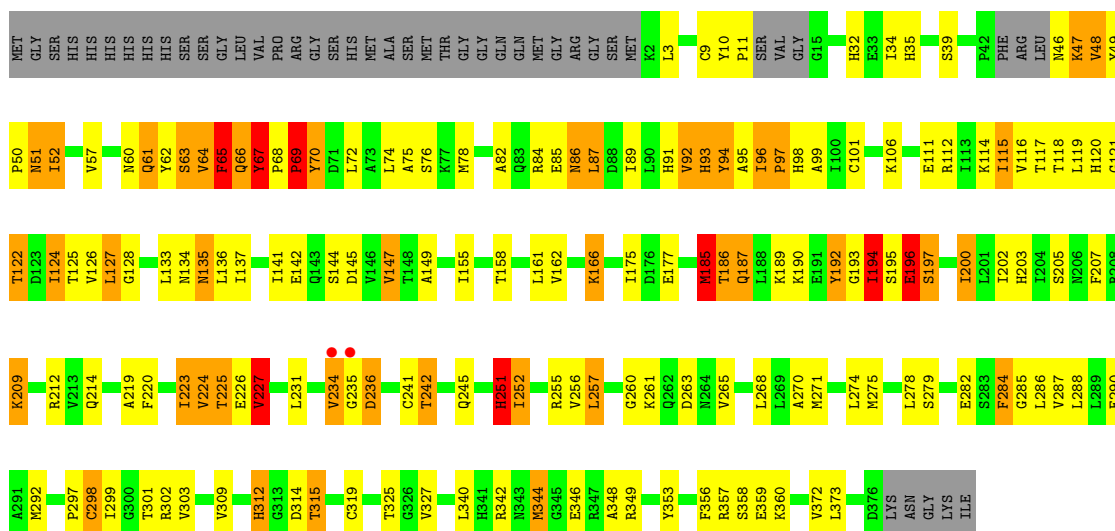
- Molecule 1: Glycosyltransferase, group 1 family

Chain E: 

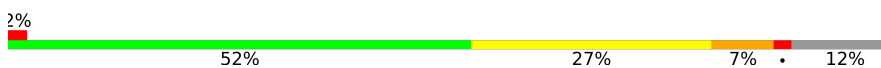


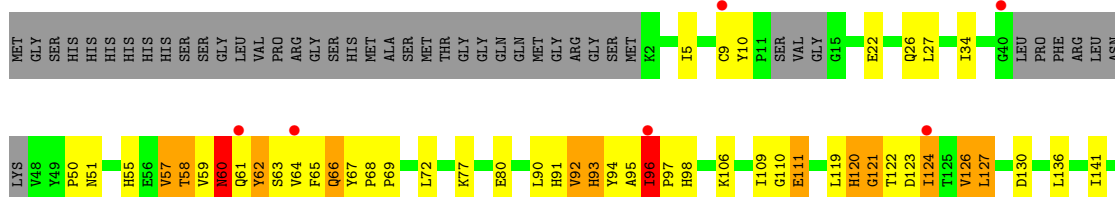
- Molecule 1: Glycosyltransferase, group 1 family

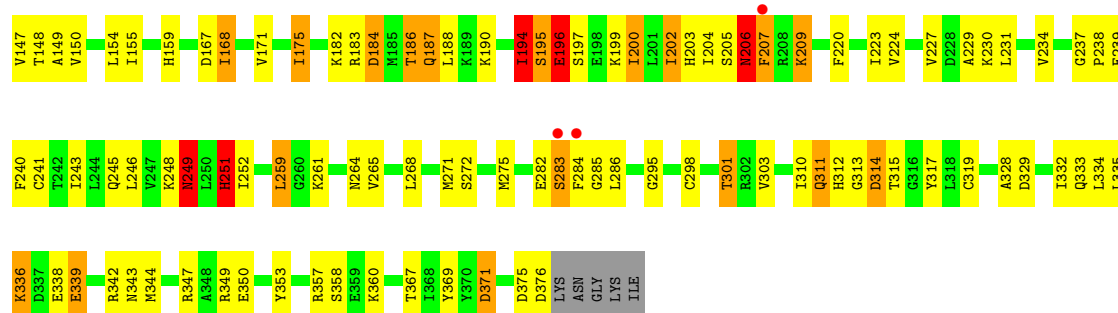
Chain F: 



- Molecule 1: Glycosyltransferase, group 1 family

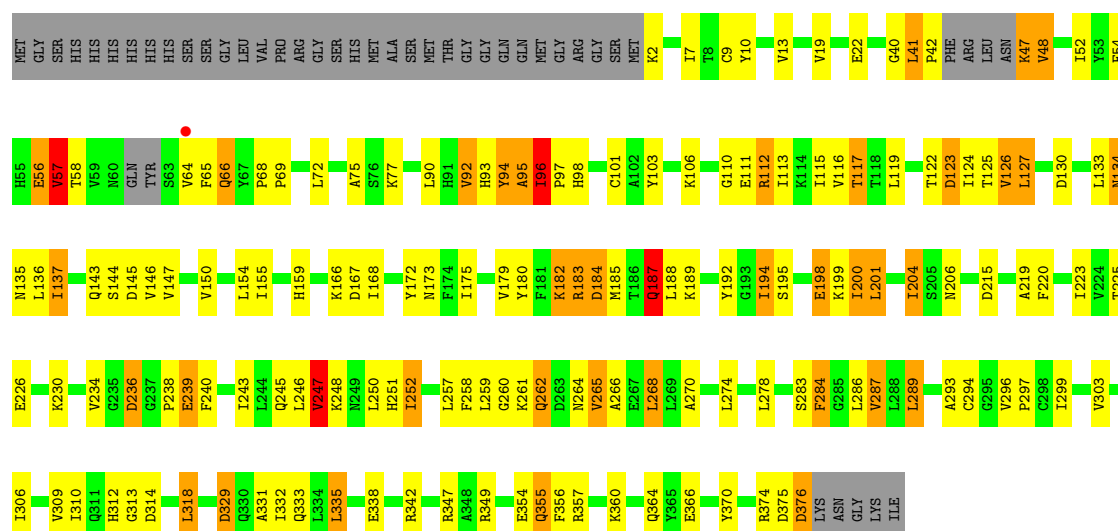
Chain G: 





● Molecule 1: Glycosyltransferase, group 1 family

Chain H: 50% 29% 9% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.257 0.226 , 0.255	Depositor DCC
R_{free} test set	2910 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.64	1/2974 (0.0%)	1.34	57/4027 (1.4%)
1	B	0.59	0/2956	1.42	68/4000 (1.7%)
1	C	0.67	3/2980 (0.1%)	1.35	59/4034 (1.5%)
1	D	0.62	3/2951 (0.1%)	1.36	40/3991 (1.0%)
1	E	0.66	2/3011 (0.1%)	1.38	60/4075 (1.5%)
1	F	0.59	1/2968 (0.0%)	1.53	66/4014 (1.6%)
1	G	0.57	0/2929	1.35	58/3961 (1.5%)
1	H	0.60	1/2955 (0.0%)	1.33	44/3996 (1.1%)
All	All	0.62	11/23724 (0.0%)	1.39	452/32098 (1.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	ILE	CA-CB	8.06	1.58	1.54
1	D	196	GLU	N-CA	7.18	1.55	1.45
1	E	92	VAL	CA-CB	-6.08	1.47	1.54
1	D	196	GLU	CA-C	5.79	1.61	1.53
1	A	68	PRO	N-CD	5.58	1.55	1.47
1	D	198	GLU	CA-C	-5.54	1.45	1.52
1	C	96	ILE	CA-CB	-5.36	1.47	1.54
1	H	306	ILE	CA-CB	5.33	1.57	1.54
1	C	204	ILE	CA-CB	-5.25	1.48	1.54
1	E	306	ILE	CA-CB	5.12	1.57	1.54
1	F	227	VAL	CA-CB	-5.03	1.48	1.54

All (452) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	234	VAL	N-CA-C	30.45	140.92	112.29
1	D	126	VAL	N-CA-C	27.63	135.57	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	284	PHE	N-CA-C	-21.73	81.07	108.45
1	E	284	PHE	N-CA-C	-18.76	79.53	108.42
1	H	194	ILE	N-CA-C	18.73	128.59	111.91
1	F	70	TYR	N-CA-C	-17.82	91.96	113.88
1	H	182	LYS	N-CA-C	-17.75	82.09	109.25
1	B	374	ARG	N-CA-C	17.39	130.23	111.28
1	B	206	ASN	N-CA-C	-16.56	84.69	110.36
1	D	93	HIS	N-CA-C	15.88	133.70	112.90
1	C	65	PHE	N-CA-C	-15.43	86.81	109.96
1	G	303	VAL	N-CA-CB	-15.40	94.51	112.07
1	B	256	VAL	CB-CA-C	-15.24	86.30	111.29
1	F	64	VAL	N-CA-C	15.15	124.96	110.42
1	C	261	LYS	N-CA-C	15.11	132.16	111.92
1	D	126	VAL	CB-CA-C	-14.91	94.40	111.55
1	F	63	SER	N-CA-C	-14.70	88.92	110.23
1	H	65	PHE	N-CA-C	14.66	127.34	111.36
1	A	93	HIS	N-CA-C	14.42	132.81	112.04
1	C	314	ASP	N-CA-C	14.32	132.36	112.45
1	E	95	ALA	N-CA-C	14.29	126.36	111.07
1	F	196	GLU	N-CA-C	14.17	126.23	111.07
1	G	194	ILE	N-CA-C	13.84	125.30	112.29
1	C	42	PRO	N-CA-C	-13.48	90.11	111.14
1	D	197	SER	N-CA-C	-13.43	89.96	109.96
1	C	207	PHE	N-CA-C	13.28	127.58	112.57
1	A	375	ASP	CB-CA-C	-13.27	93.58	111.63
1	D	12	SER	N-CA-C	13.22	128.60	110.35
1	F	93	HIS	N-CA-C	13.19	130.47	112.93
1	A	196	GLU	N-CA-C	-13.16	92.45	110.35
1	F	135	ASN	CB-CA-C	-13.07	91.14	111.66
1	D	12	SER	N-CA-CB	-12.95	92.52	110.38
1	G	199	LYS	N-CA-C	12.76	129.39	111.52
1	D	188	LEU	N-CA-C	-12.74	97.78	113.20
1	F	65	PHE	N-CA-C	12.70	125.12	111.28
1	F	263	ASP	N-CA-C	12.65	126.83	111.40
1	G	126	VAL	N-CA-C	12.63	122.67	111.81
1	A	52	ILE	N-CA-C	12.46	121.46	111.62
1	C	66	GLN	N-CA-CB	-12.41	90.31	110.42
1	F	285	GLY	N-CA-C	-12.40	83.78	113.18
1	B	250	LEU	N-CA-C	-12.33	94.25	110.53
1	G	121	GLY	N-CA-C	12.29	127.48	112.73
1	D	200	ILE	N-CA-C	12.25	125.87	107.99
1	C	60	ASN	N-CA-C	12.16	127.61	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	PHE	N-CA-CB	-12.15	92.51	110.49
1	F	127	LEU	N-CA-C	12.03	128.14	113.23
1	F	192	TYR	N-CA-C	-11.77	98.94	113.18
1	A	94	TYR	N-CA-C	-11.66	90.82	109.59
1	E	278	LEU	N-CA-C	-11.64	87.67	107.80
1	D	314	ASP	N-CA-C	11.44	125.35	111.40
1	G	10	TYR	N-CA-C	11.43	124.05	109.65
1	F	314	ASP	N-CA-C	11.42	127.82	113.43
1	C	251	HIS	CB-CA-C	-11.35	89.61	111.06
1	H	199	LYS	N-CA-C	11.25	126.84	111.54
1	H	126	VAL	N-CA-C	11.20	121.53	112.12
1	G	207	PHE	N-CA-CB	-11.17	89.79	110.56
1	E	313	GLY	N-CA-C	11.10	129.64	115.21
1	G	251	HIS	CB-CA-C	-11.04	93.93	111.48
1	B	254	ASP	N-CA-C	-10.87	98.67	112.90
1	H	303	VAL	N-CA-C	10.87	122.49	110.21
1	A	281	LYS	N-CA-C	-10.71	90.76	108.32
1	H	246	LEU	N-CA-CB	-10.65	94.12	110.42
1	C	262	GLN	N-CA-C	10.64	124.08	110.24
1	B	42	PRO	CB-CA-C	-10.63	94.02	111.56
1	A	197	SER	N-CA-C	10.56	122.79	111.28
1	G	195	SER	N-CA-C	10.55	122.78	111.28
1	B	375	ASP	N-CA-C	10.54	122.77	111.28
1	E	279	SER	N-CA-C	-10.51	92.90	109.50
1	H	200	ILE	N-CA-C	10.38	123.53	108.58
1	B	196	GLU	N-CA-C	-10.33	96.30	110.35
1	B	252	ILE	N-CA-C	10.25	122.88	108.12
1	E	46	ASN	N-CA-CB	-10.22	93.22	110.49
1	D	200	ILE	N-CA-CB	-10.20	99.27	111.21
1	B	251	HIS	N-CA-C	10.19	122.39	111.28
1	H	66	GLN	N-CA-CB	-10.13	93.37	110.49
1	B	200	ILE	N-CA-C	10.08	125.71	109.78
1	A	226	GLU	N-CA-C	9.96	126.72	113.97
1	H	134	ASN	N-CA-C	9.96	123.06	111.11
1	G	303	VAL	N-CA-C	9.95	123.19	109.46
1	F	197	SER	N-CA-C	-9.95	99.97	114.39
1	A	51	ASN	N-CA-C	9.93	127.81	113.02
1	G	206	ASN	N-CA-C	-9.89	97.47	110.53
1	G	249	ASN	N-CA-CB	-9.88	96.08	110.80
1	C	259	LEU	CB-CA-C	-9.77	95.37	111.68
1	G	329	ASP	N-CA-C	9.73	121.65	111.14
1	C	315	THR	N-CA-C	-9.72	96.68	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	186	THR	N-CA-C	-9.71	101.57	113.41
1	D	127	LEU	N-CA-C	-9.70	101.11	113.72
1	F	84	ARG	N-CA-C	9.67	123.58	111.69
1	E	121	GLY	N-CA-C	9.67	124.33	112.73
1	E	52	ILE	N-CA-C	9.55	122.33	108.58
1	G	283	SER	N-CA-C	-9.53	90.51	110.80
1	B	303	VAL	N-CA-CB	9.53	124.05	111.19
1	F	234	VAL	CB-CA-C	-9.52	98.84	111.88
1	D	11	PRO	N-CA-C	-9.46	92.98	112.47
1	D	40	GLY	N-CA-C	9.43	135.52	113.18
1	F	127	LEU	CB-CA-C	-9.32	90.62	109.55
1	A	227	VAL	N-CA-C	9.25	120.94	112.43
1	H	195	SER	CB-CA-C	-9.20	97.68	112.03
1	H	64	VAL	N-CA-C	-9.17	96.55	108.93
1	D	251	HIS	CB-CA-C	-9.14	96.46	111.36
1	E	285	GLY	N-CA-C	-9.10	91.61	113.18
1	E	284	PHE	CB-CA-C	-9.05	95.22	110.43
1	E	312	HIS	N-CA-C	-9.03	96.50	109.96
1	F	185	MET	N-CA-C	9.03	124.22	108.52
1	E	120	HIS	N-CA-C	-9.02	95.60	109.85
1	H	309	VAL	CB-CA-C	-8.91	102.18	110.91
1	C	200	ILE	N-CA-C	8.90	120.77	107.51
1	F	312	HIS	N-CA-C	8.87	129.70	110.80
1	C	42	PRO	CB-CA-C	8.84	122.86	111.46
1	H	195	SER	N-CA-CB	-8.82	98.66	110.57
1	D	67	TYR	N-CA-C	-8.81	94.43	109.15
1	A	358	SER	N-CA-C	8.79	121.97	111.33
1	A	13	VAL	N-CA-C	8.77	127.58	109.34
1	A	376	ASP	N-CA-CB	8.77	125.40	110.50
1	B	120	HIS	N-CA-C	-8.74	96.42	110.32
1	E	196	GLU	N-CA-C	8.74	124.00	113.16
1	E	267	GLU	N-CA-C	8.74	120.50	110.97
1	F	94	TYR	N-CA-C	-8.72	94.51	108.73
1	D	303	VAL	N-CA-C	8.68	119.51	110.05
1	C	252	ILE	N-CA-C	-8.67	91.31	109.34
1	A	133	LEU	N-CA-CB	-8.65	98.64	110.67
1	E	48	VAL	N-CA-C	-8.64	97.26	108.93
1	A	95	ALA	CA-C-N	8.64	127.24	120.33
1	A	95	ALA	C-N-CA	8.64	127.24	120.33
1	A	281	LYS	CB-CA-C	8.63	124.48	109.89
1	G	248	LYS	CB-CA-C	8.63	127.21	110.46
1	F	185	MET	CB-CA-C	-8.63	98.02	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	PHE	N-CA-C	8.61	124.02	113.17
1	H	126	VAL	CB-CA-C	-8.60	102.49	110.91
1	E	226	GLU	N-CA-CB	-8.57	99.19	110.59
1	B	185	MET	N-CA-CB	8.54	124.71	111.39
1	H	112	ARG	CB-CA-C	-8.54	95.27	109.27
1	B	184	ASP	CB-CA-C	-8.53	97.35	111.68
1	D	11	PRO	CB-CA-C	-8.51	97.53	111.56
1	G	51	ASN	N-CA-C	-8.50	94.46	108.49
1	B	194	ILE	N-CA-C	8.49	127.01	109.34
1	B	95	ALA	N-CA-C	8.47	120.52	111.28
1	G	60	ASN	N-CA-C	8.46	120.59	111.36
1	G	109	ILE	CB-CA-C	-8.45	97.43	111.29
1	H	312	HIS	CB-CA-C	8.41	123.02	109.90
1	F	251	HIS	CB-CA-C	-8.36	95.25	111.06
1	B	120	HIS	CB-CA-C	8.35	123.78	109.51
1	D	226	GLU	N-CA-CB	-8.34	99.37	110.88
1	G	58	THR	CB-CA-C	8.32	121.28	109.71
1	B	322	GLY	N-CA-C	8.32	126.42	115.36
1	A	49	TYR	C-N-CD	-8.31	90.94	125.00
1	E	312	HIS	CB-CA-C	8.25	122.05	110.16
1	G	50	PRO	N-CA-C	8.24	129.46	112.47
1	A	182	LYS	N-CA-C	-8.19	99.21	110.35
1	C	48	VAL	N-CA-C	8.19	126.38	109.34
1	F	85	GLU	N-CA-C	-8.16	102.89	113.17
1	B	133	LEU	N-CA-CB	-8.15	99.62	110.88
1	F	136	LEU	N-CA-C	-8.05	93.64	110.80
1	F	121	GLY	N-CA-C	8.04	132.23	113.18
1	E	61	GLN	N-CA-C	-8.03	91.94	107.44
1	G	200	ILE	N-CA-C	8.02	121.08	108.89
1	C	61	GLN	N-CA-C	8.01	122.62	113.01
1	C	133	LEU	N-CA-CB	-7.99	99.97	110.59
1	F	252	ILE	N-CA-CB	7.97	124.38	111.23
1	A	52	ILE	CB-CA-C	-7.97	103.96	111.05
1	D	190	LYS	N-CA-C	7.97	120.04	111.36
1	F	314	ASP	CB-CA-C	-7.96	96.28	109.65
1	B	257	LEU	N-CA-CB	-7.95	97.62	109.95
1	F	186	THR	N-CA-CB	-7.92	100.06	110.59
1	D	252	ILE	N-CA-C	-7.91	105.15	112.43
1	E	43	PHE	CB-CA-C	-7.91	99.27	112.00
1	E	182	LYS	N-CA-C	-7.90	98.33	110.10
1	B	199	LYS	N-CA-C	7.80	122.71	111.56
1	F	67	TYR	N-CA-C	-7.79	92.59	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	PHE	CB-CA-C	-7.78	97.45	109.89
1	G	314	ASP	N-CA-C	7.75	120.63	111.71
1	H	57	VAL	N-CA-C	7.75	125.45	109.34
1	D	194	ILE	N-CA-CB	-7.75	98.45	111.23
1	C	12	SER	N-CA-C	7.72	120.60	108.79
1	B	184	ASP	N-CA-C	-7.71	93.48	107.98
1	D	225	THR	CB-CA-C	7.71	124.88	110.63
1	H	313	GLY	N-CA-C	7.69	126.38	115.30
1	F	51	ASN	N-CA-C	7.69	122.71	111.87
1	A	183	ARG	N-CA-C	-7.68	97.39	108.60
1	G	126	VAL	CB-CA-C	-7.61	102.80	111.55
1	A	126	VAL	N-CA-C	7.58	118.49	112.12
1	A	314	ASP	CB-CA-C	-7.54	97.37	109.13
1	A	195	SER	CB-CA-C	-7.54	93.71	110.21
1	E	62	TYR	N-CA-C	-7.53	103.66	114.12
1	G	51	ASN	N-CA-CB	7.52	122.74	111.23
1	C	194	ILE	N-CA-C	-7.51	93.71	109.34
1	E	253	GLU	N-CA-C	-7.49	104.17	113.38
1	E	204	ILE	N-CA-C	7.47	118.66	107.75
1	E	208	ARG	N-CA-C	-7.45	97.69	109.23
1	A	61	GLN	N-CA-C	7.44	121.89	111.92
1	F	251	HIS	N-CA-C	7.43	123.89	113.56
1	E	185	MET	N-CA-C	-7.43	93.16	107.57
1	F	86	ASN	N-CA-C	7.41	121.62	111.39
1	A	315	THR	N-CA-C	-7.39	104.29	113.38
1	E	340	LEU	N-CA-C	-7.36	104.11	113.23
1	C	194	ILE	CB-CA-C	-7.33	99.26	111.29
1	G	187	GLN	N-CA-C	-7.32	104.33	113.55
1	B	126	VAL	N-CA-C	7.30	118.60	111.67
1	A	132	SER	CB-CA-C	7.28	124.03	110.70
1	E	136	LEU	N-CA-C	7.28	119.00	111.14
1	D	36	PHE	N-CA-C	-7.23	98.97	109.59
1	B	87	LEU	N-CA-C	7.21	119.61	110.24
1	B	64	VAL	CB-CA-C	-7.20	99.49	111.29
1	H	182	LYS	CB-CA-C	-7.19	98.50	110.29
1	H	238	PRO	N-CA-C	7.18	123.02	113.40
1	B	43	PHE	N-CA-CB	7.16	122.68	110.50
1	B	302	ARG	N-CA-C	-7.16	95.91	108.23
1	B	132	SER	CB-CA-C	7.09	124.21	110.46
1	A	303	VAL	N-CA-C	7.07	124.05	109.34
1	C	283	SER	N-CA-C	-7.07	103.64	112.90
1	D	67	TYR	CB-CA-C	7.05	118.25	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	263	ASP	N-CA-C	7.05	118.96	111.28
1	E	135	ASN	N-CA-C	-7.04	103.60	111.28
1	G	124	ILE	CB-CA-C	-7.02	102.83	112.24
1	B	198	GLU	N-CA-C	7.01	119.95	111.82
1	E	200	ILE	N-CA-C	6.99	119.50	108.87
1	G	375	ASP	CB-CA-C	-6.98	99.98	111.36
1	A	315	THR	N-CA-CB	6.97	120.92	110.53
1	G	186	THR	N-CA-C	6.96	122.32	113.55
1	H	259	LEU	N-CA-C	-6.93	103.33	111.03
1	A	58	THR	N-CA-C	-6.93	99.56	109.96
1	B	171	VAL	N-CA-C	-6.93	97.46	107.78
1	H	248	LYS	N-CA-C	6.91	119.45	111.02
1	F	136	LEU	N-CA-CB	6.91	122.16	110.49
1	B	281	LYS	N-CA-C	6.87	120.69	107.44
1	C	315	THR	CB-CA-C	6.86	123.85	111.03
1	G	339	GLU	N-CA-C	6.85	121.81	113.38
1	G	124	ILE	N-CA-C	6.84	118.46	111.00
1	B	280	GLU	CB-CA-C	6.84	124.34	110.38
1	F	315	THR	N-CA-CB	6.83	124.28	111.43
1	G	252	ILE	N-CA-CB	6.83	122.50	111.23
1	A	195	SER	N-CA-C	6.82	121.06	112.87
1	G	336	LYS	N-CA-C	6.81	121.64	113.12
1	D	191	GLU	N-CA-C	-6.81	103.88	111.71
1	G	150	VAL	N-CA-C	6.80	118.63	112.17
1	C	30	ARG	CB-CA-C	-6.79	99.06	110.81
1	G	194	ILE	CB-CA-C	-6.79	102.58	111.88
1	D	95	ALA	N-CA-C	6.78	118.46	111.14
1	E	96	ILE	CA-C-N	-6.78	111.37	119.84
1	E	96	ILE	C-N-CA	-6.78	111.37	119.84
1	G	301	THR	CB-CA-C	6.77	122.16	110.45
1	C	95	ALA	N-CA-C	6.76	125.20	110.80
1	B	121	GLY	N-CA-C	6.71	120.75	112.64
1	A	199	LYS	N-CA-C	6.68	125.04	110.80
1	A	51	ASN	CA-C-N	-6.66	116.10	123.16
1	A	51	ASN	C-N-CA	-6.66	116.10	123.16
1	A	355	GLN	N-CA-C	-6.65	105.70	113.88
1	B	65	PHE	N-CA-C	-6.63	95.42	107.75
1	H	135	ASN	N-CA-C	-6.62	105.20	113.28
1	C	121	GLY	N-CA-C	6.61	128.85	113.18
1	C	296	VAL	N-CA-C	6.60	115.25	107.73
1	E	110	GLY	N-CA-C	6.60	127.35	114.16
1	H	247	VAL	CB-CA-C	6.58	120.67	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	VAL	N-CA-C	6.56	117.55	111.45
1	H	58	THR	N-CA-C	6.56	119.74	109.96
1	F	315	THR	N-CA-C	-6.55	102.84	113.19
1	B	179	VAL	CB-CA-C	6.54	116.82	111.06
1	E	237	GLY	CA-C-N	6.54	126.12	119.19
1	E	237	GLY	C-N-CA	6.54	126.12	119.19
1	E	199	LYS	N-CA-C	6.51	120.64	111.52
1	F	200	ILE	N-CA-C	6.50	118.75	108.87
1	C	193	GLY	N-CA-C	-6.50	97.79	113.18
1	G	57	VAL	N-CA-C	6.49	122.84	109.34
1	H	238	PRO	CB-CA-C	-6.49	102.82	112.55
1	C	134	ASN	N-CA-C	6.46	119.15	111.33
1	B	321	VAL	CB-CA-C	6.46	120.96	111.33
1	F	52	ILE	N-CA-C	6.45	117.58	108.36
1	H	252	ILE	N-CA-C	-6.44	105.05	111.88
1	C	177	GLU	N-CA-C	-6.43	105.72	112.93
1	B	171	VAL	CB-CA-C	6.40	118.82	110.12
1	F	302	ARG	N-CA-C	-6.37	98.43	108.63
1	C	314	ASP	N-CA-CB	-6.37	100.77	110.26
1	D	36	PHE	CB-CA-C	6.37	119.81	110.26
1	E	48	VAL	CB-CA-C	6.37	121.62	111.69
1	A	324	THR	N-CA-C	-6.36	103.86	111.69
1	C	285	GLY	N-CA-C	6.36	128.26	113.18
1	B	86	ASN	N-CA-C	6.36	120.42	111.52
1	C	252	ILE	N-CA-CB	6.35	121.71	111.23
1	B	66	GLN	CA-C-N	6.35	130.57	122.64
1	B	66	GLN	C-N-CA	6.35	130.57	122.64
1	A	126	VAL	CB-CA-C	-6.34	104.69	110.91
1	C	192	TYR	N-CA-C	6.30	118.53	109.14
1	H	354	GLU	N-CA-C	6.30	121.20	111.56
1	A	198	GLU	N-CA-C	6.29	117.42	108.74
1	B	323	ASP	N-CA-C	6.28	119.49	108.56
1	C	207	PHE	N-CA-CB	-6.28	100.99	110.91
1	E	206	ASN	N-CA-C	-6.27	102.41	110.19
1	G	336	LYS	CB-CA-C	-6.27	99.22	109.56
1	D	196	GLU	N-CA-C	6.27	118.12	110.41
1	B	323	ASP	N-CA-CB	-6.26	102.12	110.57
1	B	281	LYS	N-CA-CB	-6.26	100.12	110.95
1	F	312	HIS	CB-CA-C	-6.21	98.06	110.42
1	D	296	VAL	N-CA-CB	6.19	119.63	111.40
1	H	56	GLU	N-CA-C	6.19	121.01	112.90
1	A	314	ASP	N-CA-C	6.18	122.41	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	TYR	N-CA-CB	-6.18	100.46	110.71
1	B	186	THR	N-CA-CB	-6.16	101.48	110.53
1	G	127	LEU	N-CA-C	-6.16	105.59	113.23
1	G	110	GLY	N-CA-C	6.15	124.38	114.90
1	A	229	ALA	N-CA-C	6.13	119.48	110.59
1	A	282	GLU	N-CA-C	-6.13	99.41	108.79
1	D	197	SER	CA-CB-OG	6.13	123.36	111.10
1	E	92	VAL	CB-CA-C	-6.12	103.18	111.63
1	C	312	HIS	N-CA-C	6.12	117.62	111.07
1	F	279	SER	N-CA-C	-6.12	100.93	110.42
1	G	186	THR	CB-CA-C	-6.10	99.88	109.34
1	B	255	ARG	N-CA-C	6.10	121.54	112.94
1	A	323	ASP	N-CA-C	-6.09	97.75	108.23
1	H	187	GLN	N-CA-CB	-6.09	102.20	110.67
1	D	252	ILE	N-CA-CB	6.08	120.06	112.16
1	C	313	GLY	N-CA-C	-6.07	105.15	112.49
1	E	211	LYS	CB-CA-C	6.06	120.98	110.68
1	E	356	PHE	N-CA-CB	-6.05	103.00	110.98
1	C	130	ASP	CA-C-N	6.04	125.93	119.28
1	C	130	ASP	C-N-CA	6.04	125.93	119.28
1	A	96	ILE	N-CA-C	6.04	119.60	112.35
1	B	186	THR	N-CA-C	6.03	120.92	113.50
1	H	179	VAL	N-CA-CB	-6.03	105.57	112.21
1	E	86	ASN	CB-CA-C	6.03	118.83	110.16
1	B	187	GLN	N-CA-C	6.00	118.72	111.40
1	F	194	ILE	CB-CA-C	-5.98	103.61	110.73
1	F	84	ARG	CB-CA-C	-5.97	99.77	110.70
1	A	251	HIS	CB-CA-C	-5.96	99.79	111.06
1	B	188	LEU	N-CA-C	-5.95	106.02	113.28
1	F	87	LEU	N-CA-C	5.94	118.62	110.24
1	G	63	SER	N-CA-C	-5.92	105.14	112.72
1	G	202	ILE	CB-CA-C	-5.92	100.47	110.71
1	H	312	HIS	N-CA-C	-5.90	101.31	110.10
1	C	132	SER	CB-CA-C	5.90	121.54	110.63
1	D	251	HIS	N-CA-C	5.88	120.04	112.86
1	H	247	VAL	N-CA-C	-5.88	103.92	110.62
1	G	315	THR	N-CA-C	5.87	117.68	111.28
1	B	18	VAL	CB-CA-C	5.87	120.91	111.29
1	E	43	PHE	N-CA-CB	-5.86	101.75	110.60
1	B	66	GLN	N-CA-C	-5.86	104.31	112.45
1	A	96	ILE	CA-C-N	-5.85	112.53	119.84
1	A	96	ILE	C-N-CA	-5.85	112.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	LEU	CB-CA-C	5.85	122.31	110.38
1	A	166	LYS	N-CA-CB	-5.84	101.10	110.63
1	A	358	SER	CB-CA-C	-5.84	100.76	110.68
1	E	267	GLU	CB-CA-C	-5.84	101.97	110.96
1	B	43	PHE	N-CA-C	-5.83	94.66	111.00
1	B	312	HIS	N-CA-C	-5.83	101.41	110.10
1	F	227	VAL	CB-CA-C	-5.83	101.82	110.33
1	H	200	ILE	N-CA-CB	-5.83	104.37	110.72
1	A	95	ALA	N-CA-C	5.82	118.84	111.69
1	C	49	TYR	N-CA-C	5.82	117.92	109.84
1	B	42	PRO	N-CA-C	5.81	124.43	112.47
1	C	204	ILE	CB-CA-C	-5.80	103.28	111.28
1	H	198	GLU	N-CA-C	5.79	117.11	108.31
1	C	212	ARG	N-CA-C	5.77	119.21	111.24
1	G	93	HIS	N-CA-C	5.74	119.97	111.87
1	A	34	ILE	N-CA-C	5.73	114.99	106.85
1	C	195	SER	CB-CA-C	-5.72	99.91	113.02
1	F	93	HIS	CB-CA-C	-5.72	101.10	110.08
1	H	187	GLN	N-CA-C	5.71	121.28	113.97
1	G	120	HIS	N-CA-C	-5.67	102.37	110.59
1	F	128	GLY	N-CA-C	5.66	119.49	112.64
1	H	134	ASN	CB-CA-C	-5.66	101.76	110.81
1	F	64	VAL	CB-CA-C	-5.65	104.74	111.97
1	F	236	ASP	N-CA-CB	-5.63	101.04	111.13
1	G	339	GLU	N-CA-CB	-5.61	102.17	110.53
1	D	193	GLY	N-CA-C	5.59	123.76	114.48
1	D	189	LYS	N-CA-C	5.57	119.24	112.23
1	H	239	GLU	N-CA-C	-5.55	106.39	112.72
1	C	282	GLU	CB-CA-C	5.53	118.31	110.24
1	G	202	ILE	N-CA-C	5.53	116.63	108.45
1	C	13	VAL	N-CA-C	5.52	120.82	109.34
1	G	66	GLN	N-CA-C	-5.51	104.50	111.11
1	A	302	ARG	N-CA-C	5.50	120.95	113.37
1	G	130	ASP	CA-C-N	5.50	125.02	119.19
1	G	130	ASP	C-N-CA	5.50	125.02	119.19
1	F	223	ILE	CB-CA-C	-5.48	104.75	112.14
1	C	284	PHE	CB-CA-C	-5.47	99.53	110.42
1	F	271	MET	N-CA-CB	-5.46	102.14	110.33
1	E	133	LEU	N-CA-C	5.42	122.35	110.80
1	G	96	ILE	N-CA-C	5.42	120.58	108.88
1	B	237	GLY	CA-C-N	5.41	125.05	119.05
1	B	237	GLY	C-N-CA	5.41	125.05	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	329	ASP	CB-CA-C	-5.40	102.37	110.90
1	B	130	ASP	CA-C-N	5.38	125.09	119.82
1	B	130	ASP	C-N-CA	5.38	125.09	119.82
1	C	113	ILE	N-CA-CB	-5.35	104.38	112.35
1	E	86	ASN	N-CA-C	-5.34	102.00	109.96
1	C	286	LEU	N-CA-C	5.34	122.17	110.80
1	F	224	VAL	N-CA-C	5.33	120.44	109.34
1	G	9	CYS	CB-CA-C	-5.33	99.80	110.42
1	F	122	THR	N-CA-C	-5.33	106.83	113.38
1	F	373	LEU	N-CA-C	5.31	120.41	113.30
1	H	96	ILE	CA-C-N	-5.29	113.22	119.84
1	H	96	ILE	C-N-CA	-5.29	113.22	119.84
1	F	186	THR	N-CA-C	5.29	120.39	113.88
1	D	37	ILE	N-CA-C	-5.29	98.31	106.72
1	B	254	ASP	N-CA-CB	5.29	118.26	110.33
1	H	113	ILE	N-CA-C	-5.28	100.88	108.48
1	D	52	ILE	N-CA-C	5.28	113.97	106.53
1	G	284	PHE	N-CA-C	5.27	118.50	111.75
1	D	196	GLU	CA-C-O	-5.26	116.00	121.99
1	G	59	VAL	CA-C-N	5.26	127.75	120.29
1	G	59	VAL	C-N-CA	5.26	127.75	120.29
1	F	69	PRO	N-CA-C	-5.25	101.64	112.47
1	F	96	ILE	CA-C-N	-5.25	113.27	119.84
1	F	96	ILE	C-N-CA	-5.25	113.27	119.84
1	E	68	PRO	CB-CA-C	5.25	117.33	110.92
1	C	41	LEU	CA-C-N	5.24	125.16	119.76
1	C	41	LEU	C-N-CA	5.24	125.16	119.76
1	F	373	LEU	N-CA-CB	-5.24	102.70	110.61
1	E	225	THR	CB-CA-C	5.24	121.68	110.21
1	H	355	GLN	N-CA-C	-5.23	107.55	114.04
1	E	98	HIS	N-CA-C	5.23	118.12	111.69
1	B	41	LEU	CB-CA-C	5.23	115.66	110.33
1	A	314	ASP	N-CA-CB	5.22	117.94	111.00
1	H	184	ASP	N-CA-C	5.20	119.61	113.16
1	G	111	GLU	N-CA-C	5.19	118.88	111.92
1	C	237	GLY	CA-C-N	5.19	124.81	119.05
1	C	237	GLY	C-N-CA	5.19	124.81	119.05
1	C	31	GLY	N-CA-C	5.19	123.09	114.48
1	E	183	ARG	CA-C-N	-5.18	115.31	122.30
1	E	183	ARG	C-N-CA	-5.18	115.31	122.30
1	C	96	ILE	CB-CA-C	-5.17	101.95	111.36
1	E	49	TYR	CA-C-N	5.17	126.30	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	49	TYR	C-N-CA	5.17	126.30	119.84
1	D	94	TYR	N-CA-C	-5.16	99.19	108.48
1	E	211	LYS	N-CA-C	-5.16	105.08	111.33
1	B	373	LEU	CA-C-N	5.15	127.18	120.28
1	B	373	LEU	C-N-CA	5.15	127.18	120.28
1	F	271	MET	N-CA-C	5.15	119.64	112.90
1	C	284	PHE	N-CA-C	5.14	121.74	110.80
1	F	303	VAL	N-CA-CB	5.13	120.67	111.63
1	F	166	LYS	N-CA-C	5.13	118.58	109.96
1	E	51	ASN	N-CA-C	5.12	120.66	113.02
1	E	137	ILE	CB-CA-C	-5.12	105.41	111.97
1	B	198	GLU	CA-C-N	-5.12	114.84	122.36
1	B	198	GLU	C-N-CA	-5.12	114.84	122.36
1	E	45	LEU	N-CA-C	-5.11	99.62	108.52
1	F	194	ILE	N-CA-C	5.11	115.83	107.24
1	E	283	SER	N-CA-C	5.11	116.93	111.36
1	B	19	VAL	N-CA-C	5.10	115.32	110.53
1	G	5	ILE	N-CA-C	5.10	115.19	107.75
1	F	122	THR	N-CA-CB	5.10	118.12	110.53
1	D	37	ILE	N-CA-CB	5.08	118.30	112.15
1	F	225	THR	N-CA-CB	-5.08	102.64	110.56
1	F	358	SER	N-CA-C	5.08	117.20	111.11
1	A	68	PRO	N-CA-C	-5.07	104.51	110.70
1	A	93	HIS	CB-CA-C	-5.07	101.29	110.56
1	A	225	THR	N-CA-C	-5.05	105.77	111.28
1	E	207	PHE	N-CA-C	-5.05	97.67	107.62
1	C	10	TYR	CA-C-N	5.03	124.64	119.05
1	C	10	TYR	C-N-CA	5.03	124.64	119.05
1	A	59	VAL	N-CA-C	-5.03	107.39	112.17
1	B	228	ASP	N-CA-C	-5.02	98.89	108.17

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	213	0
1	B	2907	0	2916	204	0
1	C	2929	0	2940	177	0
1	D	2903	0	2929	172	0
1	E	2959	0	2977	204	0
1	F	2919	0	2941	194	0
1	G	2881	0	2885	179	0
1	H	2907	0	2934	158	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
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	1431	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 30.

All (1431) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:D:251:HIS:CD2	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:194:ILE:HG13	6:G:395:HOH:O	1.07	1.24
1:G:203:HIS:O	1:G:204:ILE:HG22	1.30	1.24
1:B:62:TYR:HB2	1:B:65:PHE:CG	1.71	1.23
1:A:34:ILE:C	1:A:52:ILE:HG22	1.64	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
1:G:251:HIS:CG	1:G:251:HIS:O	1.82	1.21
1:G:62:TYR:CD2	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:CG	1:G:65:PHE:CE1	2.30	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:C:206:ASN:OD1	1:C:207:PHE:N	1.72	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:12:SER:OG	1:E:42:PRO:O	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:MET:HE3	1:F:135:ASN:O	1.47	1.14
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:B:196:GLU:CG	1:B:198:GLU:HG3	1.78	1.13
1:G:62:TYR:CE2	1:G:65:PHE:CE1	2.35	1.13
1:D:93:HIS:O	1:D:120:HIS:HD2	1.32	1.13
1:E:40:GLY:C	1:E:41:LEU:HD13	1.73	1.13
1:A:66:GLN:CB	1:A:67:TYR:CE2	2.30	1.13
1:E:41:LEU:HD22	1:E:41:LEU:H	0.97	1.13
1:G:62:TYR:CE1	1:G:65:PHE:CE1	2.35	1.13
1:F:193:GLY:C	1:F:194:ILE:HD12	1.74	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:63:SER:C	1:A:65:PHE:HD2	1.58	1.11
1:A:96:ILE:CB	6:A:393:HOH:O	1.88	1.11
1:F:194:ILE:HD12	1:F:194:ILE:N	1.60	1.11
1:D:60:ASN:OD1	1:D:64:VAL:HB	1.51	1.10
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: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
1:E:134:ASN:C	1:E:134:ASN:HD22	1.55	1.10
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:E:282:GLU:OE2	1:E:284:PHE:O	1.68	1.09
1:F:234:VAL:O	1:F:234:VAL:HG12	1.38	1.09
1:B:314:ASP:OD2	1:B:347:ARG:HG3	1.53	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:C:260:GLY:C	1:C:261:LYS:HG2	1.76	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:CD2	2.33	1.06
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:THR:O	1:G:126:VAL:HG22	1.56	1.05
1:B:252:ILE:HD12	1:B:252:ILE:H	1.22	1.04
1:B:63:SER:C	1:B:64:VAL:HG12	1.77	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: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:O	1:E:44:ARG:HG3	1.54	1.03
1:B:252:ILE:HD13	1:B:252:ILE:O	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:D:93:HIS:O	1:D:120:HIS:CD2	2.11	1.02
1:E:108:MET:CE	1:F:135:ASN:O	2.05	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:B:41:LEU:HB2	1:C:190:LYS:NZ	1.76	1.01
1:B:256:VAL:O	1:B:256:VAL:HG12	1.20	1.01
1:E:11:PRO:HA	1:E:42:PRO:CB	1.90	1.01
1:G:62:TYR:HD1	1:G:62:TYR:O	1.40	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:G:194:ILE:HD12	1:G:271:MET:HE2	1.43	0.99
1:A:251:HIS:O	1:A:251:HIS:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:G:249:ASN:H	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:O	1:G:251:HIS:CD2	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:66:GLN:HB3	1:A:67:TYR:CD2	1.99	0.97
1:A:286:LEU:O	1:A:288:LEU:N	1.98	0.97
1:F:78:MET:HE1	1:F:101:CYS:HB3	1.45	0.97
1:F:190:LYS:O	1:F:193:GLY:CA	2.12	0.96
1:G:194:ILE:HD12	1:G:271:MET:HE1	1.47	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:HD12	1:E:137:ILE:H	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
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:HE21	1:A:66:GLN:HA	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:262:GLN:NE2	1:C:262:GLN:N	2.17	0.93
1:C:262:GLN:N	1:C:262:GLN:HE21	1.67	0.93
1:E:11:PRO:HA	1:E:42:PRO:HB3	0.95	0.93
1:E:252:ILE:HD12	1:E:252:ILE:O	1.69	0.92
1:A:66:GLN:OE1	1:B:10:TYR:CE1	2.23	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:TYR:O	1:C:193:GLY:C	2.13	0.92
1:D:82:ALA:O	1:D:86:ASN:O	1.87	0.92
1:F:190:LYS:C	1:F:193:GLY:H	1.77	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:A:66:GLN:C	1:A:67:TYR:CG	2.48	0.91
1:C:260:GLY:C	1:C:261:LYS:CG	2.42	0.91
1:G:203:HIS:C	1:G:204:ILE:HG22	1.96	0.90
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:O	1:D:251:HIS:CG	2.19	0.89
1:B:196:GLU:O	1:B:198:GLU:HG3	1.72	0.89
1:A:65:PHE:CD2	1:A:65:PHE:N	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:G:209:LYS:H	1:G:209:LYS:HD2	1.38	0.88
1:B:196:GLU:CD	1:B:255:ARG:HH21	1.80	0.88
1:C:96:ILE:CG2	1:C:97:PRO:N	2.30	0.88
1:B:94:TYR:HH	1:B:122:THR:HB	1.37	0.88
1:H:57:VAL:HG23	1:H:57:VAL:O	1.71	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:D:198:GLU:CG	6:D:421:HOH:O	2.22	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:F:196:GLU:CD	1:F:196:GLU:H	1.80	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:E:43:PHE:O	1:E:43:PHE:CD1	2.29	0.85
1:D:251:HIS:O	1:D:251:HIS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	1:G:62:TYR:O	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:E:10:TYR:HE1	1:E:98:HIS:HE2	1.24	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: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:D:63:SER:O	1:D:64:VAL:HG13	1.79	0.83
1:F:190:LYS:C	1:F:193:GLY:HA2	2.04	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
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:A:184:ASP:HB3	1:D:261:LYS:HE3	1.60	0.81
1:B:62:TYR:HB2	1:B:65:PHE:CD2	2.14	0.81
1:C:96:ILE:HG22	1:C:97:PRO:N	1.89	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:62:TYR:CB	1:B:65:PHE:HB2	2.08	0.81
1:B:196:GLU:HG2	1:B:198:GLU:HG3	0.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:HIS:HD1	1:G:369:TYR:HE1	1.28	0.81
1:G:207:PHE:O	1:G:207:PHE:HD1	1.64	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:62:TYR:CD1	1:A:65:PHE:CE1	2.70	0.80
1:A:227:VAL:O	1:A:228:ASP:OD1	2.00	0.80
1:B:252:ILE:HD12	1:B:252:ILE:N	1.92	0.80
1:B:252:ILE:O	1:B:252:ILE:CD1	2.30	0.80
1:D:65:PHE:O	1:D:66:GLN:CG	2.30	0.80
1:D:283:SER:O	1:D:284:PHE:HB2	1.80	0.80
1:F:192:TYR:O	1:F:194:ILE:CD1	2.30	0.80
1:D:186:THR:HG22	1:D:186:THR:O	1.80	0.80
1:H:194:ILE:O	1:H:194:ILE:HG13	1.80	0.80
1:E:134:ASN:C	1:E:134:ASN:ND2	2.29	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
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:10:TYR:OH	1:C:97:PRO:HG3	1.82	0.79
1:C:13:VAL:O	1:C:13:VAL:CG1	2.29	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:O	1:C:198:GLU:HG2	1.81	0.79
1:E:11:PRO:C	1:E:42:PRO:HB3	2.08	0.79
1:F:66:GLN:H	1:F:66:GLN:CD	1.89	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:O	1:G:207:PHE:CD1	2.36	0.79
1:E:59:VAL:HG23	1:E:59:VAL:O	1.81	0.79
1:F:66:GLN:O	1:F:67:TYR:CB	2.30	0.79
1:D:375:ASP:C	1:D:376:ASP:CG	2.49	0.79
1:H:194:ILE:O	1:H:194:ILE:CD1	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:GLN:CD	1:G:67:TYR:CE1	2.61	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:H:338:GLU:O	1:H:342:ARG:HD3	1.83	0.78
1:D:64:VAL:CG2	1:D:64:VAL:O	2.30	0.78
1:D:65:PHE:C	1:D:66:GLN:HG3	2.07	0.78
1:E:66:GLN:HE22	1:H:187:GLN:HE22	1.32	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:A:66:GLN:C	1:A:67:TYR:CD2	2.62	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:CA	1:A:66:GLN:NE2	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:G:249:ASN:H	1:G:249:ASN:ND2	1.74	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:F:190:LYS:C	1:F:193:GLY:N	2.42	0.77
1:A:66:GLN:HE21	1:A:66:GLN:N	1.81	0.77
1:A:286:LEU:O	1:A:289:LEU:N	2.17	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
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:E:66:GLN:NE2	1:H:185:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:ARG:HE	1:G:342:ARG:HA	1.50	0.76
1:A:286:LEU:O	1:A:287:VAL:C	2.28	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:41:LEU:CA	1:E:43:PHE:HE2	1.99	0.75
1:E:185:MET:O	1:E:189:LYS:HG3	1.85	0.75
1:C:260:GLY:O	1:C:261:LYS:HG3	1.87	0.75
1:D:375:ASP:O	1:D:376:ASP:CG	2.29	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:D:375:ASP:C	1:D:376:ASP:OD2	2.30	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:B:196:GLU:O	1:B:198:GLU:CD	2.29	0.74
1:B:198:GLU:O	1:B:228:ASP:O	2.06	0.74
1:D:63:SER:C	1:D:64:VAL:HG13	2.13	0.74
1:C:206:ASN:OD1	1:C:206:ASN:C	2.29	0.74
1:B:196:GLU:CD	1:B:198:GLU:HG2	2.13	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:G:206:ASN:OD1	1:G:206:ASN:C	2.30	0.73
1:D:374:ARG:C	1:D:375:ASP:OD2	2.30	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:O	1:A:194:ILE:CG2	2.34	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:E:245:GLN:HG2	1:H:245:GLN:HE22	1.46	0.73
1:F:75:ALA:HA	1:F:78:MET:HE3	1.69	0.73
1:B:314:ASP:O	1:B:344:MET:HG3	1.89	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:ILE:O	1:G:194:ILE:CG2	2.30	0.72
1:G:60:ASN:C	1:G:60:ASN:OD1	2.33	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:A:204:ILE:C	1:A:205:SER:OG	2.33	0.72
1:A:62:TYR:C	1:A:65:PHE:CE2	2.68	0.72
1:H:94:TYR:O	1:H:95:ALA:HB2	1.88	0.72
1:D:175:ILE:HD11	1:D:290:GLU:HG3	1.72	0.72
1:D:185:MET:O	1:D:188:LEU:HD23	1.89	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:C:136:LEU:HD21	1:D:72:LEU:HB3	1.72	0.71
1:D:282:GLU:HG3	1:D:284:PHE:H	1.54	0.71
1:D:65:PHE:O	1:D:66:GLN:HG3	1.90	0.71
1:D:198:GLU:HG3	6:D:421:HOH:O	1.89	0.71
1:F:69:PRO:HG2	1:F:69:PRO:O	1.90	0.71
1:F:189:LYS:HB3	1:F:195:SER:OG	1.90	0.71
1:G:194:ILE:O	6:G:401:HOH:O	2.07	0.71
1:F:190:LYS:C	1:F:193:GLY:CA	2.64	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:O	1:D:64:VAL:HG22	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: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:D:63:SER:C	1:D:64:VAL:CG1	2.64	0.70
1:F:207:PHE:CE1	1:F:235:GLY:O	2.44	0.70
1:E:44:ARG:O	1:E:44:ARG:CG	2.36	0.70
1:G:207:PHE:CD1	1:G:237:GLY:HA3	2.27	0.70
1:A:227:VAL:O	1:A:227:VAL:HG12	1.91	0.70
1:E:173:ASN:HB2	1:E:284:PHE:CE1	2.26	0.70
1:E:119:LEU:HD23	1:E:124:ILE:CG1	2.21	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:TYR:CG	1:G:65:PHE:CD1	2.79	0.69
1:G:301:THR:HA	1:G:319:CYS:O	1.92	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:A:66:GLN:CB	1:A:67:TYR:CD2	2.68	0.69
1:B:92:VAL:HG11	1:B:98:HIS:O	1.92	0.69
1:B:157:GLU:HG3	3:B:382:GOL:H32	1.75	0.69
1:G:311:GLN:C	1:G:313:GLY:H	1.99	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:A:209:LYS:H	1:A:209:LYS:HD2	1.57	0.69
1:C:192:TYR:HD2	1:C:192:TYR:N	1.91	0.69
1:F:207:PHE:CD1	1:F:235:GLY:O	2.46	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:G:66:GLN:CD	1:G:67:TYR:CD1	2.71	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
1:A:251:HIS:O	1:A:251:HIS:CD2	2.47	0.68
1:E:137:ILE:HD12	1:E:137:ILE:N	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:O	1:C:94:TYR:CD2	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:O	1:G:251:HIS:ND1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASN:C	1:A:52:ILE:HD13	2.20	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: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: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:34:ILE:CG2	1:A:52:ILE:HG21	2.24	0.66
1:A:206:ASN:CB	1:A:211:LYS:HE3	2.26	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: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: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:O	1:F:67:TYR:CG	2.49	0.65
1:F:66:GLN:N	1:F:66:GLN:OE1	2.30	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:60:ASN:OD1	1:G:61:GLN:N	2.30	0.65
1:G:209:LYS:HD2	1:G:209:LYS:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:N	1:A:65:PHE:CD2	2.65	0.65
1:A:119:LEU:HD12	1:A:168:ILE:HD12	1.79	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:G:66:GLN:CD	1:G:67:TYR:HE1	2.04	0.65
1:A:34:ILE:HG22	1:A:52:ILE:HG21	1.79	0.65
1:F:49:TYR:CE2	3:F:383:GOL:O1	2.42	0.65
1:F:342:ARG:O	1:F:346:GLU:HB2	1.97	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: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:245:GLN:O	1:G:246:LEU:HB2	1.97	0.64
1:C:198:GLU:O	1:C:198:GLU:CG	2.45	0.64
1:A:52:ILE:C	1:A:53:TYR:CG	2.75	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:C:57:VAL:HG23	1:C:57:VAL:O	1.98	0.64
1:C:282:GLU:HG2	1:C:306:ILE:HD11	1.80	0.64
1:E:92:VAL:HG22	1:E:98:HIS:HB3	1.80	0.64
1:H:40:GLY:C	1:H:42:PRO:HD2	2.23	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:H:122:THR:O	1:H:123:ASP:C	2.40	0.63
1:C:96:ILE:O	1:C:96:ILE:CD1	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:H	1:A:209:LYS:CD	2.11	0.63
1:A:209:LYS:HD2	1:A:209:LYS:N	2.13	0.63
1:G:126:VAL:HG23	1:G:127:LEU:HD12	1.80	0.63
1:F:69:PRO:O	1:F:69:PRO:CG	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:GLU:OE2	1:F:196:GLU:N	2.30	0.62
1:A:67:TYR:CD2	1:A:67:TYR:N	2.67	0.62
1:A:237:GLY:H	1:A:240:PHE:HB2	1.64	0.62
1:D:204:ILE:HG22	1:D:234:VAL:HB	1.81	0.62
1:G:67:TYR:OH	1:H:10:TYR:CZ	2.52	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:O	1:E:43:PHE:HD1	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:93:HIS:O	1:F:120:HIS:HD2	1.83	0.62
1:F:192:TYR:O	1:F:194:ILE:HD11	1.99	0.62
1:D:163:LYS:N	1:D:164:PRO:HD3	2.14	0.62
1:G:61:GLN:OE1	1:H:130:ASP:CG	2.42	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:286:LEU:C	1:A:288:LEU:N	2.58	0.61
1:A:360:LYS:HE2	3:A:387:GOL:H12	1.81	0.61
1:D:196:GLU:O	1:D:197:SER:C	2.43	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:E:182:LYS:HB2	3:E:385:GOL:HO1	1.65	0.61
1:F:62:TYR:O	1:F:63:SER:C	2.41	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:C:74:LEU:HG	1:C:78:MET:HE3	1.82	0.61
1:D:358:SER:O	1:D:362:VAL:HG12	2.00	0.61
1:C:119:LEU:HD22	1:C:124:ILE:HD11	1.83	0.61
1:D:251:HIS:CD2	1:D:251:HIS:C	2.65	0.61
1:G:194:ILE:CD1	1:G:271:MET:HE1	2.26	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:HE2	1:B:209:LYS:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:VAL:HG13	1:C:98:HIS:HB2	1.83	0.60
1:G:61:GLN:CD	1:H:133:LEU:HD22	2.26	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:B:313:GLY:O	1:B:344:MET:HE2	2.00	0.60
1:B:196:GLU:CD	1:B:255:ARG:NH2	2.50	0.60
1:C:96:ILE:CD1	1:C:96:ILE:C	2.73	0.60
1:E:42:PRO:HD2	1:E:43:PHE:HD2	0.53	0.60
1:E:137:ILE:HG22	1:E:141:ILE:HG13	1.83	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: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:O	1:F:224:VAL:HG22	2.01	0.59
1:A:66:GLN:CD	1:B:10:TYR:CE1	2.80	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: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:G:65:PHE:O	1:G:66:GLN:C	2.43	0.59
1:B:62:TYR:C	1:B:65:PHE:HB3	2.27	0.59
1:B:323:ASP:O	1:B:327:VAL:HG23	2.02	0.59
1:C:96:ILE:HG23	1:C:97:PRO:N	2.10	0.59
1:E:66:GLN:NE2	1:H:185:MET:CE	2.66	0.59
1:G:342:ARG:HA	1:G:342:ARG:NE	2.17	0.59
1:A:96:ILE:HG12	1:A:123:ASP:HB3	1.84	0.59
1:B:62:TYR:CA	1:B:65:PHE:HB3	2.33	0.59
1:B:112:ARG:O	1:B:112:ARG:HD3	2.03	0.59
1:F:196:GLU:CD	1:F:196:GLU:N	2.57	0.59
1:G:282:GLU:HG3	1:G:283:SER:N	2.15	0.59
1:C:204:ILE:HA	1:C:234:VAL:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:VAL:O	1:D:22:GLU:HG2	2.02	0.59
1:F:65:PHE:N	1:F:65:PHE:CD1	2.30	0.59
1:H:251:HIS:CD2	1:H:251:HIS:O	2.55	0.59
1:B:63:SER:C	1:B:64:VAL:CG1	2.43	0.59
1:D:190:LYS:C	1:D:193:GLY:H	2.10	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: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:B:196:GLU:C	1:B:198:GLU:HG3	2.27	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:F:312:HIS:C	1:F:312:HIS:CD2	2.82	0.58
1:G:61:GLN:OE1	1:H:133:LEU:HD22	2.02	0.58
1:H:103:TYR:CE1	1:H:143:GLN:HG2	2.39	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:HD12	1:F:257:LEU:H	1.67	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: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:E:11:PRO:C	1:E:42:PRO:CB	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:245:GLN:HG2	1:H:357:ARG:HH12	1.69	0.57
1:H:57:VAL:O	1:H:57:VAL:CG2	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: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:64:VAL:HG12	1:A:64:VAL:O	2.04	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: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:A:65:PHE:HD2	1:A:65:PHE:N	2.01	0.56
1:A:96:ILE:HG12	1:A:123:ASP:HB2	1.87	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:B:150:VAL:O	1:B:284:PHE:CE2	2.58	0.56
1:C:198:GLU:O	1:C:199:LYS:CE	2.53	0.56
1:C:231:LEU:HB3	1:C:256:VAL:HG22	1.86	0.56
1:E:66:GLN:HE22	1:H:185:MET:HE3	1.68	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: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
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:95:ALA:HB3	1:G:123:ASP:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:314:ASP:O	1:G:344:MET:SD	2.63	0.56
1:B:94:TYR:OH	1:B:122:THR:C	2.48	0.56
1:B:205:SER:CB	1:B:206:ASN:O	2.54	0.56
1:H:251:HIS:HB3	6:H:411:HOH:O	2.05	0.56
1:A:80:GLU:O	1:A:84:ARG:HG2	2.06	0.56
1:A:273:ASP:O	1:A:297:PRO:HD2	2.05	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:O	1:D:112:ARG:HD3	2.05	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:194:ILE:HG12	1:D:194:ILE:O	2.04	0.55
1:D:373:LEU:O	1:D:376:ASP:O	2.23	0.55
1:E:42:PRO:CD	1:E:43:PHE:N	2.66	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: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:H:194:ILE:HD12	1:H:194:ILE:C	2.32	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:77:LYS:O	1:B:81:VAL:HG23	2.07	0.55
1:B:223:ILE:HG22	1:B:328:ALA:HA	1.89	0.55
1:E:245:GLN:HG2	1:H:245:GLN:NE2	2.10	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:A:319:CYS:SG	1:A:327:VAL:HG22	2.46	0.55
1:G:314:ASP:HA	1:G:344:MET:HE2	1.87	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
1:A:262:GLN:HG2	1:A:268:LEU:HD11	1.87	0.55
1:D:96:ILE:HD12	1:D:127:LEU:HD11	1.89	0.55
1:D:214:GLN:HG3	1:D:243:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD2	1:D:375:ASP:N	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:HD22	1:G:249:ASN:N	1.81	0.55
1:F:86:ASN:O	1:F:86:ASN:ND2	2.38	0.54
1:A:230:LYS:HD3	1:A:255:ARG:HA	1.89	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:204:ILE:CG2	1:G:275:MET:HE3	2.37	0.54
1:D:65:PHE:CG	1:D:66:GLN:N	2.76	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: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:G:240:PHE:C	1:G:240:PHE:CD2	2.85	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:26:GLN:O	1:D:30:ARG:HG2	2.06	0.54
1:D:204:ILE:HG21	1:D:265:VAL:HG11	1.90	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:G:240:PHE:C	1:G:240:PHE:HD2	2.15	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
1:E:74:LEU:HG	1:E:78:MET:HE3	1.90	0.54
1:B:364:GLN:O	1:B:368:ILE:HG12	2.07	0.54
1:H:201:LEU:HD21	1:H:223:ILE:HG21	1.88	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:LEU:HB3	1:D:256:VAL:HG22	1.90	0.53
1:B:18:VAL:O	1:B:22:GLU:HG2	2.08	0.53
1:B:153:SER:O	1:B:157:GLU:HG2	2.08	0.53
1:D:185:MET:HG3	1:D:188:LEU:HB2	1.90	0.53
1:B:198:GLU:O	1:B:199:LYS:HB2	2.06	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:H:92:VAL:HG13	1:H:98:HIS:HB2	1.89	0.53
1:E:43:PHE:CD2	1:E:43:PHE:N	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:G:311:GLN:C	1:G:313:GLY:N	2.61	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:187:GLN:C	1:D:189:LYS:H	2.14	0.53
1:D:209:LYS:HB3	6:D:409:HOH:O	2.09	0.53
1:F:47:LYS:HD3	1:F:47:LYS:C	2.09	0.53
1:F:66:GLN:CD	1:F:66:GLN:N	2.60	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:O	1:C:96:ILE:HD13	2.09	0.52
1:D:187:GLN:C	1:D:189:LYS:N	2.67	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:H:374:ARG:O	1:H:375:ASP:CB	2.54	0.52
1:A:63:SER:C	1:A:65:PHE:CE2	2.71	0.52
1:E:45:LEU:C	1:E:47:LYS:N	2.67	0.52
1:E:137:ILE:CG2	1:E:141:ILE:HD11	2.39	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:225:THR:C	1:F:227:VAL:H	2.17	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:F:74:LEU:HG	1:F:78:MET:HE2	1.92	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:A:232:LEU:HD21	1:A:271:MET:HE3	1.92	0.51
1:G:204:ILE:O	1:G:204:ILE:HG12	2.11	0.51
1:B:151:SER:O	1:B:155:ILE:HG13	2.10	0.51
1:F:312:HIS:CD2	1:F:312:HIS:O	2.63	0.51
1:G:61:GLN:HE22	1:H:127:LEU:HA	1.76	0.51
1:G:195:SER:O	1:G:197:SER:N	2.43	0.51
1:B:223:ILE:HG13	1:B:224:VAL:N	2.25	0.51
1:C:11:PRO:O	1:C:12:SER:OG	2.26	0.51
1:C:94:TYR:O	1:C:95:ALA:HB3	2.11	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

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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: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:H	1:H:268:LEU:HD23	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:A:275:MET:HE1	1:A:287:VAL:HB	1.93	0.51
1:C:196:GLU:HA	1:C:197:SER:C	2.36	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:65:PHE:CD2	1:D:65:PHE:C	2.88	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:B:103:TYR:O	1:B:107:GLN:HG2	2.11	0.51
1:C:67:TYR:HB2	6:D:405:HOH:O	2.11	0.51
1:C:176:ASP:HB3	1:C:179:VAL:HG12	1.92	0.51
1:C:191:GLU:C	1:C:191:GLU:OE1	2.53	0.51
1:C:198:GLU:O	1:C:199:LYS:HE2	2.09	0.51
1:C:204:ILE:CG1	1:C:205:SER:N	2.68	0.51
1:D:65:PHE:O	1:D:66:GLN:NE2	2.42	0.51
1:D:367:THR:O	1:D:371:ASP:HB2	2.11	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:H:122:THR:C	1:H:124:ILE:N	2.68	0.51
1:A:207:PHE:CD1	1:A:237:GLY:HA3	2.46	0.51
1:B:205:SER:C	1:B:206:ASN:O	2.41	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: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:H:251:HIS:CD2	1:H:251:HIS:C	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:VAL:O	1:D:64:VAL:HG23	2.11	0.50
1:D:214:GLN:O	1:D:218:GLN:HG2	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:82:ALA:O	1:F:86:ASN:HA	2.11	0.50
1:F:286:LEU:O	1:F:290:GLU:HG3	2.11	0.50
1:C:313:GLY:O	1:C:344:MET:HE3	2.12	0.50
1:D:317:TYR:CE2	1:D:344:MET:HE1	2.47	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:40:GLY:CA	1:H:54:PHE:HZ	2.10	0.50
1:H:112:ARG:O	1:H:112:ARG:CD	2.60	0.50
1:H:251:HIS:O	1:H:251:HIS:HD2	1.93	0.50
1:A:62:TYR:HD1	1:A:65:PHE:CZ	2.30	0.50
1:C:92:VAL:CG1	1:C:98:HIS:HB2	2.41	0.50
1:C:200:ILE:HD13	1:C:200:ILE:H	1.76	0.50
1:E:46:ASN:HD22	1:E:46:ASN:H	1.59	0.50
1:H:173:ASN:HB2	1:H:284:PHE:HE1	1.76	0.50
1:F:96:ILE:HG21	1:F:127:LEU:CD2	2.42	0.50
1:F:278:LEU:HD11	1:F:327:VAL:HG11	1.93	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:OE1	1:C:191:GLU:O	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:C:199:LYS:HA	1:C:199:LYS:CE	2.39	0.49
1:C:252:ILE:C	6:C:396:HOH:O	2.56	0.49
1:E:97:PRO:HB2	1:E:98:HIS:CD2	2.46	0.49
1:F:75:ALA:HA	1:F:78:MET:CE	2.40	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:B:93:HIS:O	1:B:94:TYR:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:TYR:CE2	1:C:94:TYR:CD2	3.01	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:D:185:MET:O	1:D:186:THR:C	2.52	0.49
1:F:127:LEU:HD23	1:F:133:LEU:CD2	2.42	0.49
1:A:282:GLU:HG3	1:A:284:PHE:H	1.76	0.49
1:C:27:LEU:O	1:C:32:HIS:HB2	2.13	0.49
1:C:141:ILE:HG23	1:C:147:VAL:HG21	1.95	0.49
1:E:207:PHE:O	1:E:237:GLY:HA3	2.13	0.49
1:F:91:HIS:CD2	1:F:116:VAL:HG12	2.48	0.49
1:F:114:LYS:HA	1:F:145:ASP:OD2	2.12	0.49
1:B:199:LYS:HD2	1:B:335:LEU:HD12	1.94	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:C:11:PRO:C	1:C:12:SER:OG	2.56	0.48
1:C:204:ILE:HG12	1:C:205:SER:N	2.15	0.48
1:E:108:MET:HE1	1:F:135:ASN:O	2.05	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: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:A:66:GLN:CD	1:C:187:GLN:HE22	2.21	0.48
1:B:57:VAL:HG22	1:B:77:LYS:HG2	1.94	0.48
1:G:123:ASP:OD1	1:G:123:ASP:N	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:48:VAL:HG23	1.90	0.48
1:H:226:GLU:HG3	1:H:332:ILE:HD12	1.96	0.48
1:C:3:LEU:HB3	1:C:5:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LYS:O	1:C:229:ALA:CB	2.57	0.48
1:F:202:ILE:HG23	1:F:275:MET:HG3	1.94	0.48
1:F:209:LYS:HD2	1:F:209:LYS:N	2.28	0.48
1:C:192:TYR:HD2	1:C:192:TYR:H	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:F:225:THR:C	1:F:227:VAL:N	2.70	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:F:227:VAL:O	1:F:227:VAL:HG12	2.01	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:49:TYR:H	1:D:52:ILE:HD11	1.79	0.47
1:D:189:LYS:HE3	1:D:271:MET:HG3	1.95	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:49:TYR:CG	1:F:52:ILE:HD11	2.49	0.47
1:F:186:THR:HG23	1:F:187:GLN:NE2	2.29	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:49:TYR:CD1	1:E:50:PRO:HD2	2.50	0.47
1:E:268:LEU:H	1:E:268:LEU:HD23	1.79	0.47
1:F:278:LEU:HA	1:F:301:THR:HG23	1.96	0.47
1:G:62:TYR:CD1	1:G:62:TYR:C	2.90	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:E:177:GLU:C	1:E:179:VAL:H	2.22	0.47
1:G:357:ARG:HG2	1:G:360:LYS:H	1.80	0.47
1:B:49:TYR:HB2	1:B:52:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:HG11	1:B:98:HIS:HB2	1.97	0.47
1:B:195:SER:O	1:B:196:GLU:C	2.57	0.47
1:C:12:SER:HA	1:C:43:PHE:HE2	1.78	0.47
1:C:221:ALA:HB2	1:C:250:LEU:HD13	1.97	0.47
1:C:228:ASP:HB2	1:C:255:ARG:NH1	2.29	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:G:61:GLN:HE21	1:H:127:LEU:CD1	2.10	0.47
1:G:205:SER:C	1:G:206:ASN:O	2.52	0.47
1:H:223:ILE:CD1	1:H:331:ALA:HB3	2.45	0.47
1:H:264:ASN:C	1:H:266:ALA:H	2.23	0.47
1:A:63:SER:O	1:A:64:VAL:C	2.58	0.47
1:C:21:THR:HA	1:C:36:PHE:HZ	1.79	0.47
1:C:253:GLU:O	1:C:253:GLU:HG2	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:D:10:TYR:C	1:D:11:PRO:O	2.51	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:CZ	1:D:374:ARG:HB3	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:OD1	1:E:123:ASP:N	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:5:ILE:HD12	1:D:89:ILE:HB	1.96	0.46
1:D:204:ILE:CG2	1:D:234:VAL:HB	2.44	0.46
1:F:241:CYS:SG	1:F:242:THR:N	2.88	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:E:45:LEU:C	1:E:47:LYS:H	2.23	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:HG22	1:H:265:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:149:ALA:CB	1:D:168:ILE:HD11	2.45	0.46
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: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:A:204:ILE:C	1:A:204:ILE:HD13	2.40	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:E:45:LEU:O	1:E:46:ASN:C	2.59	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:88:ASP:HB3	1:B:373:LEU:HD21	1.98	0.46
1:B:94:TYR:HH	1:B:122:THR:CB	2.09	0.46
1:B:286:LEU:HD12	1:B:286:LEU:HA	1.61	0.46
1:D:39:SER:HA	1:D:57:VAL:HG22	1.97	0.46
1:E:317:TYR:N	1:E:317:TYR:CD1	2.83	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:207:PHE:HD1	1:F:235:GLY:C	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:ILE:HG23	1:F:97:PRO:HD3	1.97	0.45
1:B:91:HIS:CD2	1:B:93:HIS:HE2	2.34	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
1:E:59:VAL:O	1:E:59:VAL:CG2	2.53	0.45
1:F:91:HIS:HD2	1:F:116:VAL:O	2.00	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: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:95:ALA:O	1:B:99:ALA:HB3	2.17	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:C:155:ILE:HD11	1:C:170:THR:OG1	2.16	0.45
1:D:72:LEU:HD12	1:D:72:LEU:H	1.81	0.45
1:D:259:LEU:HB3	1:D:262:GLN:NE2	2.31	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:114:LYS:HD2	1:E:372:VAL:HG22	1.99	0.45
1:E:122:THR:HA	1:E:125:THR:HB	1.99	0.45
1:A:92:VAL:CG2	1:A:98:HIS:HB3	2.47	0.45
1:B:176:ASP:C	1:B:178:ARG:H	2.25	0.45
1:B:196:GLU:C	1:B:198:GLU:N	2.74	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:A:228:ASP:CG	1:A:228:ASP:O	2.60	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:85:GLU:O	1:D:86:ASN:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:GLY:O	1:D:288:LEU:CB	2.65	0.45
1:E:252:ILE:H	1:E:252:ILE:HG13	1.64	0.45
1:A:302:ARG:O	1:A:302:ARG:HG2	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:E:164:PRO:C	1:E:166:LYS:H	2.25	0.44
1:E:281:LYS:O	1:E:282:GLU:C	2.56	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:201:LEU:N	1:D:201:LEU:HD12	2.31	0.44
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:NH1	1:E:44:ARG:CA	2.80	0.44
1:E:353:TYR:HH	1:G:241:CYS:HG	1.63	0.44
1:F:57:VAL:HG11	1:F:74:LEU:HD12	1.98	0.44
1:F:106:LYS:CE	1:F:111:GLU:HG3	2.44	0.44
1:H:96:ILE:HG22	1:H:97:PRO:HD3	1.99	0.44
1:B:374:ARG:HG2	1:B:374:ARG:HH11	1.82	0.44
1:H:106:LYS:HB2	1:H:115:ILE:CD1	2.47	0.44
1:A:72:LEU:HG	1:B:136:LEU:HD21	1.98	0.44
1:A:281:LYS:HB3	1:A:281:LYS:HE2	1.80	0.44
1:G:175:ILE:HD12	1:G:175:ILE:HA	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:66:GLN:CG	1:B:10:TYR:CE1	3.00	0.44
1:A:302:ARG:HA	1:A:318:LEU:HD23	2.00	0.44
1:A:306:ILE:N	1:A:307:PRO:CD	2.80	0.44
1:A:371:ASP:OD1	1:A:374:ARG:NH1	2.51	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:D:13:VAL:HG12	1:D:13:VAL:O	2.17	0.44
1:D:68:PRO:HA	1:D:69:PRO:HD3	1.81	0.44
1:D:247:VAL:HG11	1:D:258:PHE:CE2	2.52	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:126:VAL:HG23	1:D:127:LEU:N	2.32	0.44
1:D:189:LYS:HZ3	1:D:198:GLU:CD	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:SER:HG	1:E:42:PRO:C	2.13	0.44
1:D:204:ILE:H	1:D:204:ILE:HG12	1.53	0.44
1:G:57:VAL:O	1:G:58:THR:C	2.60	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:35:HIS:CE1	1:C:85:GLU:HG3	2.53	0.43
1:C:200:ILE:HD13	1:C:200:ILE:N	2.32	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:F:135:ASN:O	1:F:135:ASN:CG	2.57	0.43
1:H:41:LEU:N	1:H:42:PRO:CD	2.81	0.43
1:H:173:ASN:HB3	1:H:286:LEU:HD13	2.00	0.43
1:H:184:ASP:OD1	1:H:184:ASP:N	2.47	0.43
1:H:189:LYS:HZ1	1:H:198:GLU:HG3	1.83	0.43
1:A:136:LEU:HD12	1:B:108:MET:SD	2.58	0.43
1:A:227:VAL:O	1:A:227:VAL:CG1	2.62	0.43
1:F:94:TYR:CE2	1:F:96:ILE:HG22	2.53	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:F:66:GLN:C	1:F:67:TYR:CG	2.97	0.43
1:C:122:THR:O	1:C:126:VAL:HG12	2.18	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:D:190:LYS:O	1:D:191:GLU:C	2.60	0.43
1:E:27:LEU:HD11	1:E:369:TYR:HE2	1.83	0.43
1:E:67:TYR:O	1:E:68:PRO:C	2.62	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:H	1:D:191:GLU:HG3	1.60	0.43
1:F:190:LYS:HA	1:F:193:GLY:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:CB	1:B:132:SER:O	2.64	0.43
1:A:247:VAL:HG11	1:A:258:PHE:HE2	1.84	0.43
1:B:40:GLY:O	1:B:42:PRO:HD3	2.19	0.43
1:B:249:ASN:C	1:B:250:LEU:O	2.55	0.43
1:C:59:VAL:HG22	1:C:59:VAL:O	2.18	0.43
1:C:134:ASN:ND2	1:C:134:ASN:C	2.77	0.43
1:D:63:SER:OG	1:D:64:VAL:HG12	2.18	0.43
1:H:180:TYR:HB3	1:H:294:CYS:HB3	2.00	0.43
1:H:200:ILE:HG13	1:H:200:ILE:O	2.19	0.43
1:B:10:TYR:O	1:B:17:GLY:HA3	2.19	0.43
1:B:195:SER:C	1:B:196:GLU:O	2.57	0.43
1:C:213:VAL:HB	1:C:243:ILE:HG13	1.99	0.43
1:E:317:TYR:HE1	1:E:344:MET:HE1	1.83	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:C:192:TYR:O	1:C:194:ILE:N	2.50	0.43
1:H:92:VAL:CG2	1:H:98:HIS:HB3	2.48	0.43
1:H:116:VAL:HG23	1:H:146:VAL:HB	2.00	0.43
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:O	1:F:372:VAL:HG22	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:39:SER:O	1:D:56:GLU:HG3	2.18	0.42
1:D:375:ASP:HB2	1:D:376:ASP:OD2	2.19	0.42
1:E:12:SER:HA	6:E:413:HOH:O	2.18	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:G:314:ASP:O	1:G:344:MET:HE2	2.19	0.42
1:H:94:TYR:O	1:H:95:ALA:HB3	2.16	0.42
1:H:236:ASP:OD2	1:H:260:GLY:HA2	2.19	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:HA	1:E:77:LYS:HD3	1.93	0.42
1:E:134:ASN:O	1:E:135:ASN:C	2.58	0.42
1:F:149:ALA:HB3	1:F:155:ILE:HG13	2.02	0.42
1:H:133:LEU:C	1:H:137:ILE:HD12	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:VAL:HG22	2:H:382:UDP:H5'2	2.01	0.42
1:A:286:LEU:C	1:A:288:LEU:H	2.26	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:41:LEU:N	1:D:42:PRO:CD	2.56	0.42
1:D:163:LYS:HB3	6:D:411:HOH:O	2.18	0.42
1:E:220:PHE:CE2	1:E:231:LEU:HB2	2.55	0.42
1:E:317:TYR:N	1:E:317:TYR:HD1	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:65:PHE:CG	1:B:65:PHE:O	2.72	0.42
1:B:103:TYR:CE1	1:B:143:GLN:HG2	2.54	0.42
1:B:274:LEU:HA	1:B:297:PRO:O	2.20	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:F:67:TYR:O	1:F:68:PRO:C	2.61	0.42
1:G:149:ALA:O	1:G:171:VAL:O	2.37	0.42
1:C:125:THR:HB	1:C:281:LYS:CE	2.47	0.42
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: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:22:GLU:HG3	1:A:174:PHE:HE1	1.85	0.42
1:A:62:TYR:CD1	1:A:62:TYR:C	2.90	0.42
1:A:106:LYS:HB2	1:A:115:ILE:HD11	2.01	0.42
1:A:195:SER:C	1:A:196:GLU:O	2.56	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:C:96:ILE:C	1:C:96:ILE:HD12	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:SER:O	1:G:196:GLU:C	2.63	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:A:66:GLN:HG3	1:C:187:GLN:OE1	2.20	0.41
1:B:146:VAL:HG21	1:B:372:VAL:HB	2.02	0.41
1:B:331:ALA:O	1:B:335:LEU:HD23	2.20	0.41
1:C:43:PHE:CD2	1:C:43:PHE:N	2.74	0.41
1:C:57:VAL:O	1:C:57:VAL:CG2	2.68	0.41
1:C:121:GLY:HA2	1:C:283:SER:HB2	2.02	0.41
1:C:209:LYS:O	1:C:212:ARG:HG2	2.20	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:43:PHE:O	1:E:45:LEU:N	2.53	0.41
1:E:109:ILE:O	1:E:109:ILE:HG13	2.20	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
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:F:260:GLY:O	1:F:261:LYS:C	2.63	0.41
1:G:92:VAL:HG13	1:G:98:HIS:HB2	2.03	0.41
1:G:349:ARG:H	1:G:349:ARG:HG2	1.65	0.41
1:H:68:PRO:HA	1:H:69:PRO:HD3	1.93	0.41
1:A:334:LEU:HD11	1:A:341:HIS:HA	2.01	0.41
1:D:255:ARG:HE	1:D:255:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:D:107:GLN:OE1	2.21	0.41
1:D:166:LYS:HD2	1:D:166:LYS:HA	1.88	0.41
1:D:374:ARG:CZ	1:D:374:ARG:CB	2.98	0.41
1:E:155:ILE:O	1:E:158:THR:HB	2.21	0.41
1:E:196:GLU:C	1:E:198:GLU:H	2.27	0.41
1:F:214:GLN:H	1:F:214:GLN:CD	2.28	0.41
1:G:202:ILE:O	1:G:202:ILE:CG2	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:60:ASN:OD1	1:G:61:GLN:CA	2.68	0.41
1:G:106:LYS:HG3	1:G:111:GLU:HA	2.02	0.41
1:G:251:HIS:O	1:G:251:HIS:CE1	2.74	0.41
1:H:264:ASN:C	1:H:266:ALA:N	2.78	0.41
1:A:136:LEU:CD2	1:B:72:LEU:HB3	2.51	0.41
1:A:181:PHE:O	1:A:182:LYS:C	2.63	0.41
1:B:94:TYR:OH	1:B:123:ASP:N	2.54	0.41
1:B:187:GLN:H	1:B:187:GLN:HG2	1.70	0.41
1:B:337:ASP:CG	1:B:340:LEU:HB3	2.46	0.41
1:B:374:ARG:HG2	1:B:374:ARG:NH1	2.35	0.41
1:C:239:GLU:O	1:C:243:ILE:HG12	2.21	0.41
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:E:132:SER:C	1:E:133:LEU:CD1	2.94	0.41
1:F:312:HIS:O	1:F:312:HIS:CG	2.71	0.41
1:G:126:VAL:CG2	1:G:127:LEU:HD12	2.48	0.41
1:G:203:HIS:O	1:G:204:ILE:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:TYR:CE2	1:G:123:ASP:HB3	2.56	0.41
1:G:234:VAL:HG22	1:G:259:LEU:HD13	2.03	0.41
1:G:240:PHE:HD2	1:G:240:PHE:O	2.04	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:H:19:VAL:HG21	1:H:173:ASN:CG	2.46	0.40
1:A:90:LEU:HD12	1:A:90:LEU:HA	1.82	0.40
1:C:122:THR:HB	1:C:126:VAL:HG12	2.03	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:E:181:PHE:CG	1:G:237:GLY:HA2	2.56	0.40
1:F:142:GLU:HA	1:F:166:LYS:HB2	2.03	0.40
1:G:27:LEU:HB3	1:G:34:ILE:HD11	2.02	0.40
1:G:264:ASN:O	1:G:268:LEU:HD23	2.21	0.40
1:G:332:ILE:HG13	1:G:333:GLN:N	2.35	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:91:HIS:CD2	1:G:93:HIS:NE2	2.88	0.40
1:G:246:LEU:CA	1:G:249:ASN:HD21	2.34	0.40
1:G:282:GLU:C	1:G:283:SER:O	2.58	0.40
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.69	0.40
1:C:35:HIS:CD2	1:C:87:LEU:HD21	2.55	0.40
1:C:317:TYR:CZ	1:C:344:MET:HE1	2.56	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:C:269:LEU:C	1:C:271:MET:H	2.30	0.40
1:D:286:LEU:C	1:D:288:LEU:N	2.77	0.40
1:F:39:SER:HA	1:F:57:VAL:HG22	2.04	0.40
1:F:231:LEU:HB3	1:F:256:VAL:HG22	2.03	0.40
1:H:122:THR:HG21	4:H:384:MLT:O1	2.22	0.40
1:H:130:ASP:O	1:H:134:ASN:HB2	2.21	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%)	11	39
1	B	363/414 (88%)	335 (92%)	24 (7%)	4 (1%)	11	39
1	C	369/414 (89%)	331 (90%)	36 (10%)	2 (0%)	24	55
1	D	363/414 (88%)	332 (92%)	25 (7%)	6 (2%)	7	30
1	E	373/414 (90%)	331 (89%)	36 (10%)	6 (2%)	7	31
1	F	363/414 (88%)	326 (90%)	34 (9%)	3 (1%)	16	45
1	G	359/414 (87%)	335 (93%)	22 (6%)	2 (1%)	21	52
1	H	363/414 (88%)	329 (91%)	26 (7%)	8 (2%)	5	26
All	All	2921/3312 (88%)	2651 (91%)	235 (8%)	35 (1%)	10	37

All (35) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	285 (88%)	37 (12%)	5	21
1	B	321/359 (89%)	286 (89%)	35 (11%)	6	23
1	C	322/359 (90%)	286 (89%)	36 (11%)	6	22
1	D	322/359 (90%)	276 (86%)	46 (14%)	3	14
1	E	327/359 (91%)	282 (86%)	45 (14%)	3	15
1	F	324/359 (90%)	286 (88%)	38 (12%)	5	20
1	G	317/359 (88%)	294 (93%)	23 (7%)	13	39
1	H	323/359 (90%)	289 (90%)	34 (10%)	6	25
All	All	2578/2872 (90%)	2284 (89%)	294 (11%)	5	21

All (294) 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	58	THR
1	A	62	TYR
1	A	65	PHE
1	A	66	GLN
1	A	67	TYR
1	A	78	MET
1	A	88	ASP
1	A	92	VAL
1	A	122	THR
1	A	143	GLN
1	A	145	ASP
1	A	168	ILE
1	A	170	THR
1	A	175	ILE
1	A	187	GLN
1	A	194	ILE
1	A	196	GLU
1	A	198	GLU
1	A	204	ILE
1	A	209	LYS
1	A	214	GLN
1	A	228	ASP
1	A	247	VAL
1	A	251	HIS
1	A	262	GLN
1	A	283	SER
1	A	286	LEU
1	A	314	ASP
1	A	321	VAL
1	A	332	ILE
1	A	358	SER
1	B	3	LEU
1	B	7	ILE
1	B	13	VAL
1	B	18	VAL
1	B	56	GLU
1	B	58	THR

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Mol	Chain	Res	Type
1	B	61	GLN
1	B	62	TYR
1	B	64	VAL
1	B	90	LEU
1	B	96	ILE
1	B	98	HIS
1	B	111	GLU
1	B	126	VAL
1	B	134	ASN
1	B	143	GLN
1	B	148	THR
1	B	168	ILE
1	B	173	ASN
1	B	184	ASP
1	B	198	GLU
1	B	204	ILE
1	B	209	LYS
1	B	223	ILE
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	283	SER
1	B	311	GLN
1	B	330	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	57	VAL
1	C	71	ASP
1	C	92	VAL
1	C	96	ILE
1	C	125	THR
1	C	137	ILE
1	C	166	LYS
1	C	168	ILE
1	C	170	THR

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Mol	Chain	Res	Type
1	C	179	VAL
1	C	183	ARG
1	C	185	MET
1	C	188	LEU
1	C	190	LYS
1	C	191	GLU
1	C	192	TYR
1	C	196	GLU
1	C	199	LYS
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	347	ARG
1	C	368	ILE
1	D	3	LEU
1	D	18	VAL
1	D	19	VAL
1	D	34	ILE
1	D	52	ILE
1	D	64	VAL
1	D	65	PHE
1	D	71	ASP
1	D	87	LEU
1	D	90	LEU
1	D	92	VAL
1	D	96	ILE
1	D	100	ILE
1	D	122	THR
1	D	127	LEU
1	D	134	ASN
1	D	137	ILE
1	D	161	LEU
1	D	168	ILE

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Mol	Chain	Res	Type
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
1	D	204	ILE
1	D	209	LYS
1	D	225	THR
1	D	226	GLU
1	D	234	VAL
1	D	236	ASP
1	D	242	THR
1	D	251	HIS
1	D	255	ARG
1	D	283	SER
1	D	286	LEU
1	D	288	LEU
1	D	301	THR
1	D	303	VAL
1	D	325	THR
1	D	346	GLU
1	D	347	ARG
1	D	354	GLU
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	41	LEU
1	E	44	ARG
1	E	52	ILE
1	E	54	PHE
1	E	59	VAL
1	E	89	ILE
1	E	92	VAL
1	E	122	THR
1	E	123	ASP
1	E	133	LEU

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Mol	Chain	Res	Type
1	E	134	ASN
1	E	136	LEU
1	E	137	ILE
1	E	154	LEU
1	E	161	LEU
1	E	183	ARG
1	E	187	GLN
1	E	188	LEU
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	265	VAL
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	338	GLU
1	E	340	LEU
1	E	347	ARG
1	E	355	GLN
1	E	363	SER
1	E	368	ILE
1	F	3	LEU
1	F	9	CYS
1	F	46	ASN
1	F	47	LYS
1	F	48	VAL
1	F	50	PRO
1	F	61	GLN
1	F	64	VAL
1	F	65	PHE
1	F	66	GLN
1	F	70	TYR
1	F	72	LEU

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Mol	Chain	Res	Type
1	F	92	VAL
1	F	115	ILE
1	F	124	ILE
1	F	147	VAL
1	F	161	LEU
1	F	175	ILE
1	F	177	GLU
1	F	185	MET
1	F	187	GLN
1	F	194	ILE
1	F	196	GLU
1	F	200	ILE
1	F	209	LYS
1	F	227	VAL
1	F	242	THR
1	F	251	HIS
1	F	252	ILE
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	344	MET
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	92	VAL
1	G	96	ILE
1	G	148	THR
1	G	167	ASP
1	G	168	ILE
1	G	175	ILE
1	G	184	ASP
1	G	194	ILE
1	G	196	GLU
1	G	206	ASN
1	G	209	LYS
1	G	249	ASN

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Mol	Chain	Res	Type
1	G	251	HIS
1	G	259	LEU
1	G	265	VAL
1	G	286	LEU
1	G	311	GLN
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
1	H	90	LEU
1	H	92	VAL
1	H	96	ILE
1	H	117	THR
1	H	127	LEU
1	H	137	ILE
1	H	183	ARG
1	H	187	GLN
1	H	188	LEU
1	H	201	LEU
1	H	204	ILE
1	H	206	ASN
1	H	225	THR
1	H	236	ASP
1	H	247	VAL
1	H	252	ILE
1	H	261	LYS
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	349	ARG
1	H	366	GLU
1	H	376	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	98	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	311	GLN
1	A	330	GLN
1	A	355	GLN
1	B	35	HIS
1	B	86	ASN
1	B	91	HIS
1	B	134	ASN
1	B	165	ASN
1	B	173	ASN
1	B	249	ASN
1	B	251	HIS
1	B	311	GLN
1	B	333	GLN
1	B	364	GLN
1	C	35	HIS
1	C	66	GLN
1	C	83	GLN
1	C	98	HIS
1	C	134	ASN
1	C	165	ASN
1	C	169	GLN
1	C	173	ASN
1	C	187	GLN
1	C	251	HIS
1	C	262	GLN
1	D	35	HIS
1	D	66	GLN
1	D	120	HIS
1	D	159	HIS
1	D	173	ASN
1	D	251	HIS
1	D	262	GLN
1	D	311	GLN
1	E	46	ASN

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Mol	Chain	Res	Type
1	E	55	HIS
1	E	66	GLN
1	E	91	HIS
1	E	134	ASN
1	E	135	ASN
1	E	152	HIS
1	E	165	ASN
1	E	169	GLN
1	E	173	ASN
1	E	245	GLN
1	E	262	GLN
1	E	264	ASN
1	E	330	GLN
1	E	333	GLN
1	E	355	GLN
1	F	51	ASN
1	F	55	HIS
1	F	86	ASN
1	F	98	HIS
1	F	107	GLN
1	F	120	HIS
1	F	134	ASN
1	F	159	HIS
1	F	169	GLN
1	F	173	ASN
1	F	187	GLN
1	F	249	ASN
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	165	ASN
1	G	173	ASN
1	G	187	GLN
1	G	249	ASN
1	G	262	GLN
1	G	311	GLN

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Mol	Chain	Res	Type
1	H	60	ASN
1	H	83	GLN
1	H	134	ASN
1	H	152	HIS
1	H	165	ASN
1	H	169	GLN
1	H	173	ASN
1	H	187	GLN
1	H	206	ASN
1	H	245	GLN
1	H	249	ASN
1	H	251	HIS
1	H	262	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
4	MLT	H	384	-	8,8,8	1.11	0	10,10,10	1.57	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLT	C	385	-	8,8,8	1.02	0	10,10,10	1.82	2 (20%)
3	GOL	C	384	-	5,5,5	0.40	0	5,5,5	0.19	0
3	GOL	F	384	-	5,5,5	0.41	0	5,5,5	0.25	0
2	UDP	E	382	5	25,26,26	1.03	0	38,40,40	1.95	7 (18%)
3	GOL	A	386	-	5,5,5	0.36	0	5,5,5	0.19	0
3	GOL	D	384	-	5,5,5	0.40	0	5,5,5	0.41	0
3	GOL	E	386	-	5,5,5	0.33	0	5,5,5	0.40	0
4	MLT	E	387	-	8,8,8	1.08	0	10,10,10	1.74	4 (40%)
2	UDP	A	382	-	25,26,26	1.02	1 (4%)	38,40,40	1.61	5 (13%)
3	GOL	H	383	-	5,5,5	0.32	0	5,5,5	0.42	0
3	GOL	B	382	-	5,5,5	0.40	0	5,5,5	0.34	0
3	GOL	D	383	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	E	385	-	5,5,5	0.39	0	5,5,5	0.49	0
2	UDP	C	382	5	25,26,26	1.03	2 (8%)	38,40,40	1.56	4 (10%)
3	GOL	A	387	-	5,5,5	0.37	0	5,5,5	0.46	0
2	UDP	H	382	-	25,26,26	1.08	1 (4%)	38,40,40	1.71	7 (18%)
3	GOL	B	383	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	E	384	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	D	382	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	A	384	-	5,5,5	0.40	0	5,5,5	0.17	0
3	GOL	F	383	-	5,5,5	0.41	0	5,5,5	0.28	0
4	MLT	A	388	-	8,8,8	1.10	0	10,10,10	1.68	2 (20%)
3	GOL	A	385	-	5,5,5	0.40	0	5,5,5	0.29	0
3	GOL	F	382	-	5,5,5	0.39	0	5,5,5	0.23	0
3	GOL	A	383	-	5,5,5	0.36	0	5,5,5	0.22	0
3	GOL	E	383	-	5,5,5	0.40	0	5,5,5	0.30	0
3	GOL	F	385	-	5,5,5	0.41	0	5,5,5	0.31	0
3	GOL	C	383	-	5,5,5	0.37	0	5,5,5	0.28	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
4	MLT	H	384	-	-	6/8/8/8	-
4	MLT	C	385	-	-	2/8/8/8	-
3	GOL	C	384	-	-	0/4/4/4	-
3	GOL	F	384	-	-	4/4/4/4	-
2	UDP	E	382	5	-	6/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	386	-	-	4/4/4/4	-
3	GOL	D	384	-	-	4/4/4/4	-
3	GOL	E	386	-	-	3/4/4/4	-
4	MLT	E	387	-	-	3/8/8/8	-
2	UDP	A	382	-	-	5/16/32/32	0/2/2/2
3	GOL	H	383	-	-	4/4/4/4	-
3	GOL	B	382	-	-	4/4/4/4	-
3	GOL	D	383	-	-	2/4/4/4	-
3	GOL	E	385	-	-	0/4/4/4	-
2	UDP	C	382	5	-	7/16/32/32	0/2/2/2
3	GOL	A	387	-	-	2/4/4/4	-
2	UDP	H	382	-	-	3/16/32/32	0/2/2/2
3	GOL	B	383	-	-	4/4/4/4	-
3	GOL	E	384	-	-	1/4/4/4	-
3	GOL	D	382	-	-	4/4/4/4	-
3	GOL	A	384	-	-	2/4/4/4	-
3	GOL	F	383	-	-	2/4/4/4	-
4	MLT	A	388	-	-	0/8/8/8	-
3	GOL	A	385	-	-	1/4/4/4	-
3	GOL	F	382	-	-	2/4/4/4	-
3	GOL	A	383	-	-	0/4/4/4	-
3	GOL	E	383	-	-	2/4/4/4	-
3	GOL	F	385	-	-	2/4/4/4	-
3	GOL	C	383	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	382	UDP	PA-O3A	2.42	1.62	1.59
2	A	382	UDP	PA-O3A	2.16	1.61	1.59
2	C	382	UDP	PA-O3A	2.01	1.61	1.59
2	C	382	UDP	C5-C4	-2.00	1.39	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	382	UDP	C4-N3-C2	-5.66	119.59	126.61
2	C	382	UDP	C4-N3-C2	-5.29	120.05	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	382	UDP	C4-N3-C2	-5.16	120.21	126.61
2	A	382	UDP	C4-N3-C2	-5.01	120.39	126.61
2	E	382	UDP	C1'-N1-C2	4.39	125.47	117.59
2	E	382	UDP	C5-C4-N3	4.28	120.79	114.80
2	E	382	UDP	O4'-C1'-N1	4.24	117.97	108.36
2	H	382	UDP	N3-C2-N1	4.18	120.34	114.89
4	C	385	MLT	O2-C1-C2	3.95	121.09	112.74
2	A	382	UDP	N3-C2-N1	3.86	119.92	114.89
2	A	382	UDP	C5-C4-N3	3.78	120.10	114.80
2	C	382	UDP	N3-C2-N1	3.78	119.81	114.89
4	E	387	MLT	O2-C1-C2	3.72	120.60	112.74
2	E	382	UDP	O4-C4-C5	-3.60	118.95	125.16
4	A	388	MLT	O2-C1-C2	3.55	120.26	112.74
2	H	382	UDP	C5-C4-N3	3.52	119.74	114.80
2	C	382	UDP	C5-C4-N3	3.44	119.62	114.80
2	E	382	UDP	N3-C2-N1	3.42	119.34	114.89
2	H	382	UDP	O4-C4-C5	-3.26	119.54	125.16
4	H	384	MLT	O2-C1-C2	3.18	119.47	112.74
2	H	382	UDP	C1'-N1-C2	3.01	123.00	117.59
2	A	382	UDP	O4-C4-C5	-2.96	120.05	125.16
2	E	382	UDP	C1'-N1-C6	-2.80	114.79	120.78
2	C	382	UDP	O4-C4-C5	-2.44	120.95	125.16
2	H	382	UDP	C3'-C2'-C1'	2.40	106.01	101.46
4	A	388	MLT	O5-C4-C3	2.39	121.42	114.00
4	E	387	MLT	O5-C4-C3	2.35	121.32	114.00
4	C	385	MLT	O5-C4-C3	2.17	120.75	114.00
4	H	384	MLT	O2-C1-O1	-2.16	119.17	124.08
2	A	382	UDP	C1'-N1-C2	2.14	121.44	117.59
4	E	387	MLT	O5-C4-O4	-2.02	118.13	123.33
2	H	382	UDP	O2-C2-N3	-2.02	117.77	121.49
4	E	387	MLT	O2-C1-O1	-2.00	119.54	124.08

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	E	382	UDP	O4'-C1'-N1-C2
2	E	382	UDP	O4'-C1'-N1-C6
2	E	382	UDP	C5'-O5'-PA-O1A

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

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

There are no ring outliers.

21 monomers are involved in 35 short contacts:

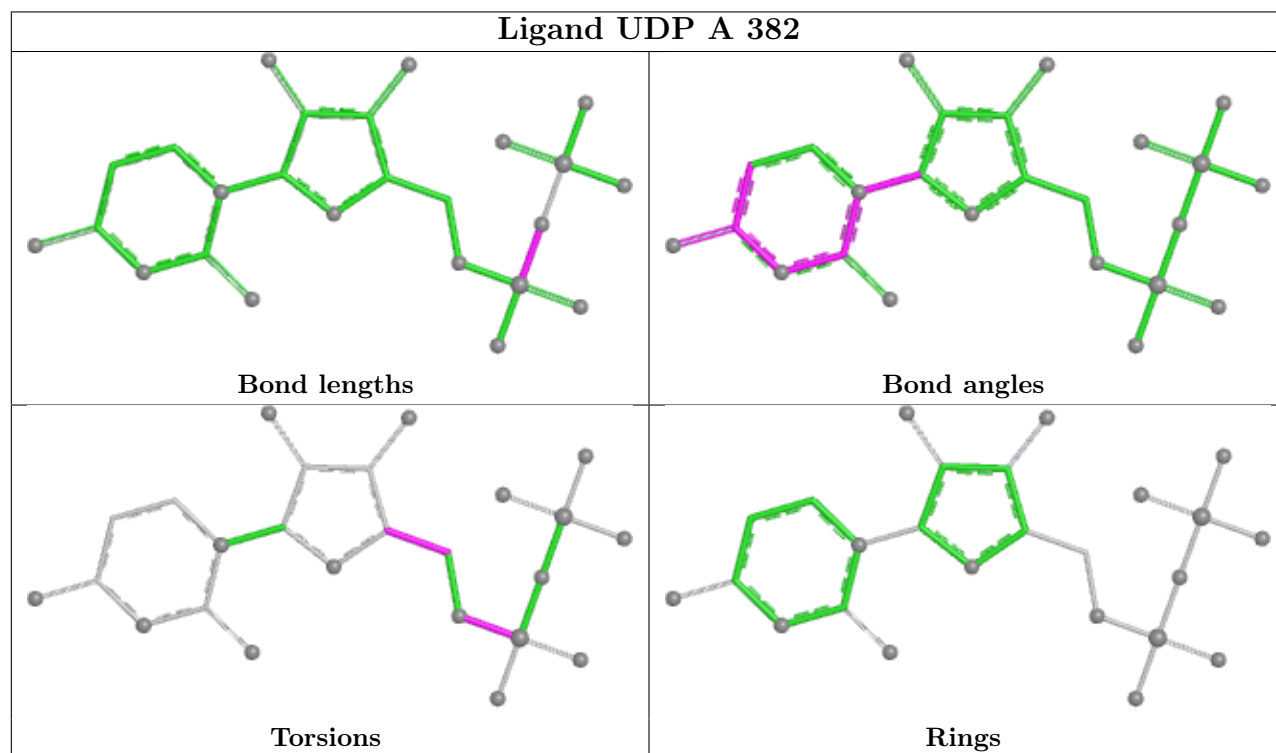
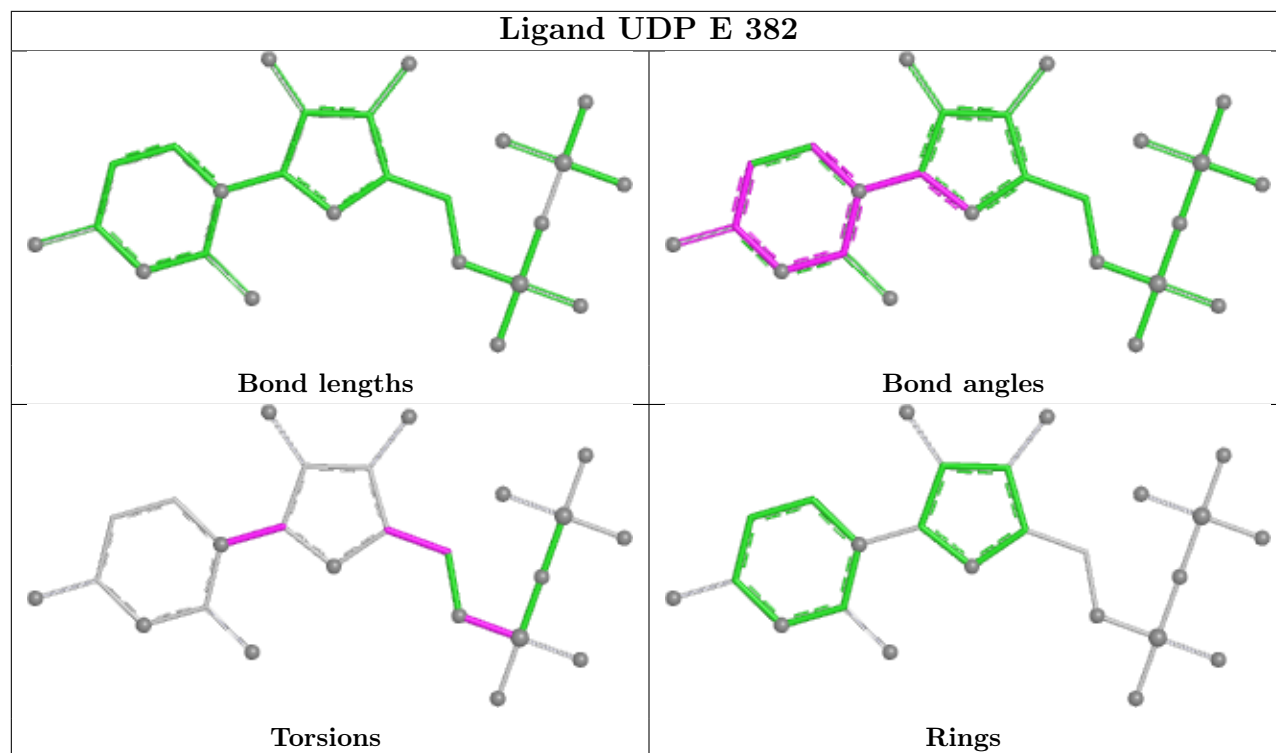
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	384	MLT	1	0
4	C	385	MLT	1	0

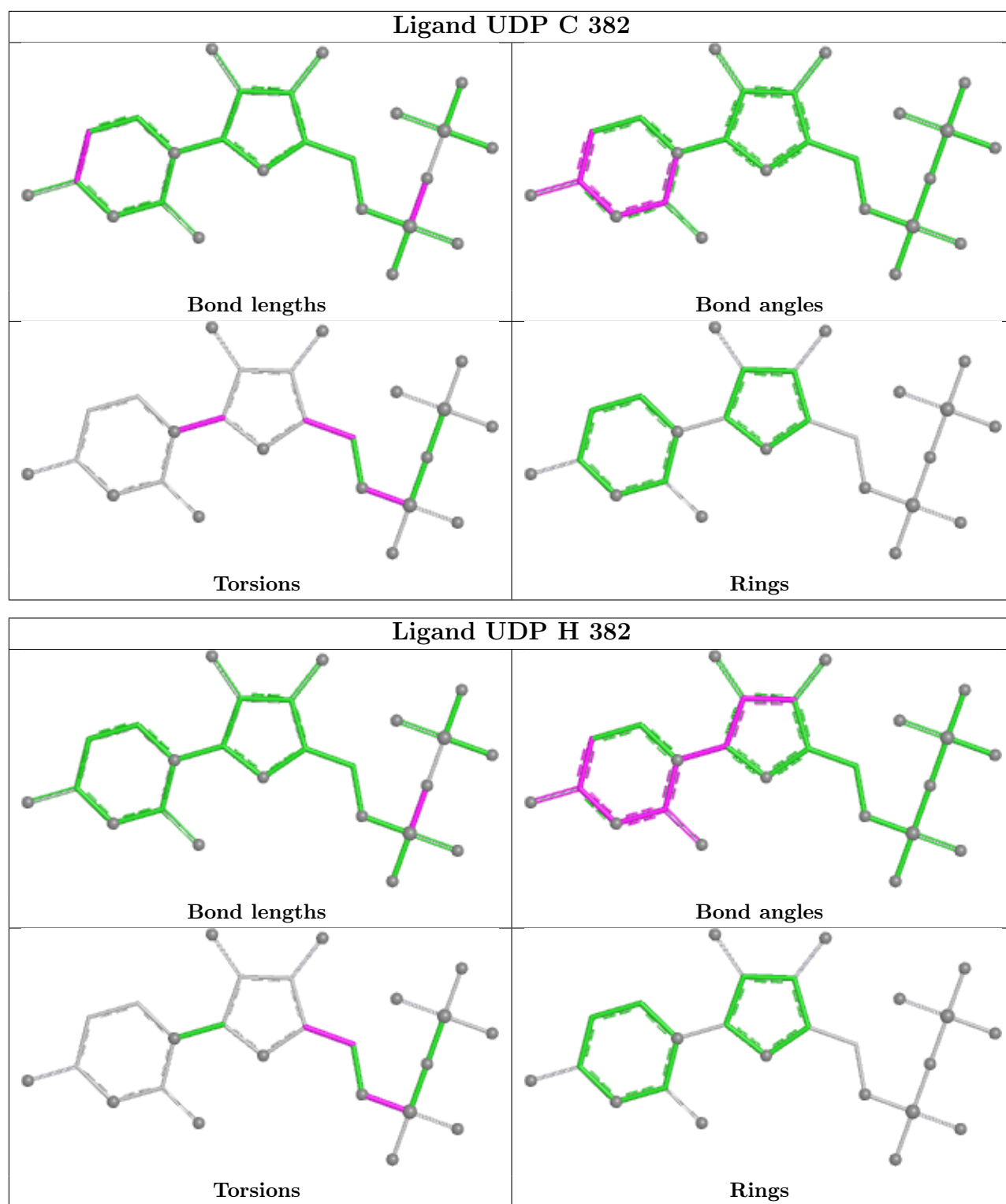
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	384	GOL	1	0
3	F	384	GOL	2	0
2	E	382	UDP	2	0
3	A	386	GOL	1	0
3	E	386	GOL	1	0
3	H	383	GOL	1	0
3	B	382	GOL	1	0
3	D	383	GOL	1	0
3	E	385	GOL	6	0
2	C	382	UDP	2	0
3	A	387	GOL	1	0
2	H	382	UDP	2	0
3	D	382	GOL	2	0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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	372/414 (89%)	-0.12	3 (0%) 82 68	34, 57, 107, 153	0
1	B	369/414 (89%)	0.12	3 (0%) 82 68	41, 85, 124, 147	0
1	C	373/414 (90%)	-0.06	5 (1%) 75 56	35, 60, 104, 133	0
1	D	369/414 (89%)	-0.11	3 (0%) 82 68	35, 56, 109, 139	0
1	E	375/414 (90%)	-0.01	1 (0%) 90 82	37, 66, 116, 149	0
1	F	369/414 (89%)	0.00	2 (0%) 87 76	42, 69, 115, 146	0
1	G	365/414 (88%)	0.23	9 (2%) 58 39	55, 96, 135, 152	0
1	H	369/414 (89%)	-0.10	1 (0%) 90 82	48, 69, 110, 140	0
All	All	2961/3312 (89%)	-0.01	27 (0%) 81 65	34, 68, 120, 153	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	SER	2.9
1	C	95	ALA	2.9
1	D	96	ILE	2.7
1	A	96	ILE	2.7
1	B	285	GLY	2.7
1	H	64	VAL	2.7
1	C	193	GLY	2.6
1	D	10	TYR	2.6
1	G	96	ILE	2.5
1	G	64	VAL	2.5
1	E	61	GLN	2.3
1	G	124	ILE	2.2
1	A	52	ILE	2.2
1	G	40	GLY	2.2
1	F	235	GLY	2.1
1	G	207	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	314	ASP	2.1
1	B	131	PRO	2.1
1	G	284	PHE	2.1
1	D	59	VAL	2.1
1	G	61	GLN	2.1
1	G	283	SER	2.1
1	C	175	ILE	2.1
1	C	70	TYR	2.1
1	G	9	CYS	2.1
1	F	234	VAL	2.0
1	B	59	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	H	383	6/6	0.55	0.13	89,91,91,92	0
3	GOL	E	385	6/6	0.61	0.18	80,81,81,81	6
3	GOL	B	382	6/6	0.65	0.24	107,108,108,108	0
3	GOL	F	383	6/6	0.72	0.12	144,145,145,146	0
3	GOL	E	383	6/6	0.74	0.12	103,104,105,105	0
3	GOL	A	387	6/6	0.74	0.16	84,86,86,90	0
4	MLT	H	384	9/9	0.74	0.19	80,82,86,86	9
3	GOL	F	385	6/6	0.76	0.20	77,82,82,85	6
4	MLT	C	385	9/9	0.77	0.17	61,62,62,62	9
3	GOL	A	385	6/6	0.77	0.13	75,78,78,79	0
3	GOL	D	383	6/6	0.78	0.14	102,107,107,110	0
3	GOL	C	384	6/6	0.78	0.14	72,73,73,74	6

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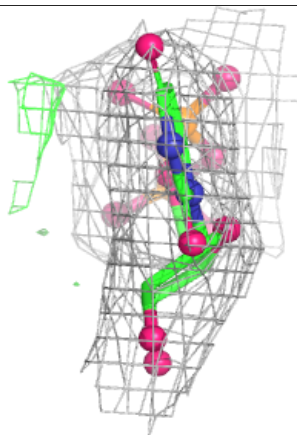
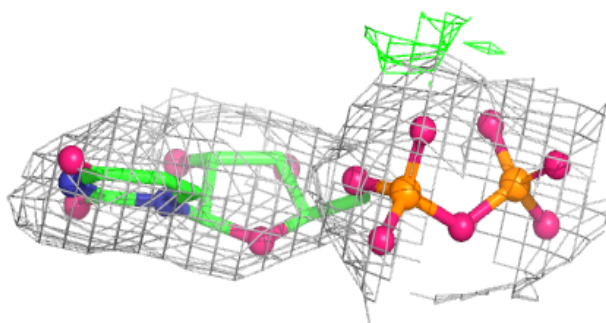
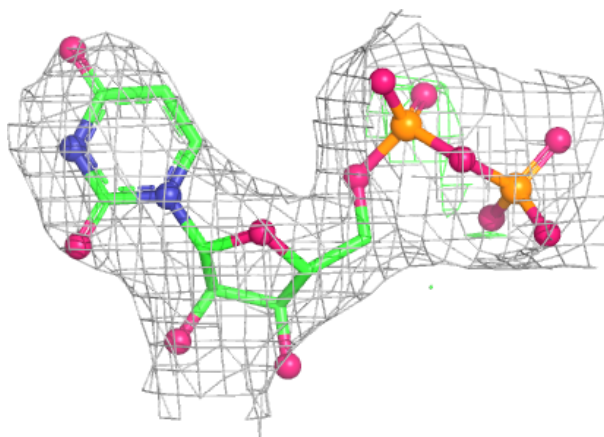
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	F	382	6/6	0.79	0.18	83,84,85,85	0
4	MLT	A	388	9/9	0.79	0.18	76,80,86,86	9
3	GOL	F	384	6/6	0.82	0.17	110,111,111,112	0
3	GOL	E	384	6/6	0.82	0.13	92,92,92,93	0
3	GOL	A	384	6/6	0.82	0.12	100,101,101,102	0
4	MLT	E	387	9/9	0.83	0.12	90,91,91,91	0
5	MG	E	388	1/1	0.84	0.15	72,72,72,72	0
3	GOL	A	386	6/6	0.85	0.14	71,73,73,73	0
2	UDP	A	382	25/25	0.85	0.12	70,78,98,99	0
2	UDP	H	382	25/25	0.85	0.11	91,94,121,121	0
3	GOL	D	384	6/6	0.86	0.09	77,79,79,80	0
3	GOL	E	386	6/6	0.86	0.13	52,53,54,56	6
3	GOL	D	382	6/6	0.86	0.15	100,100,100,100	0
2	UDP	E	382	25/25	0.86	0.12	82,85,96,97	2
3	GOL	B	383	6/6	0.88	0.10	81,82,82,82	0
3	GOL	C	383	6/6	0.88	0.11	78,84,85,85	0
3	GOL	A	383	6/6	0.89	0.09	57,58,59,60	0
2	UDP	C	382	25/25	0.91	0.10	65,67,76,76	0
5	MG	C	386	1/1	0.93	0.13	43,43,43,43	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.

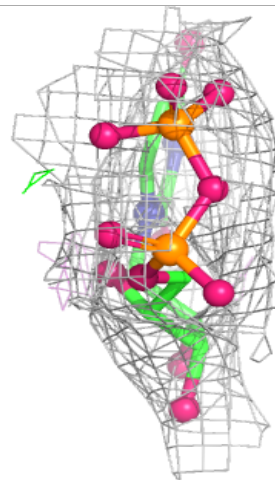
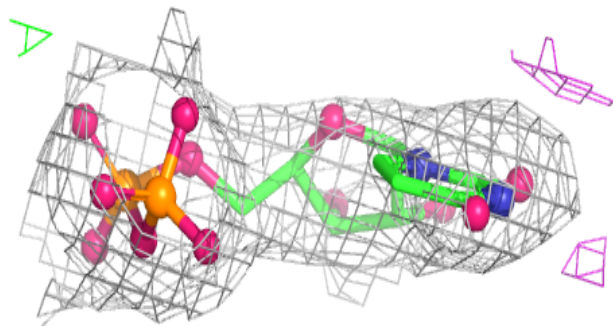
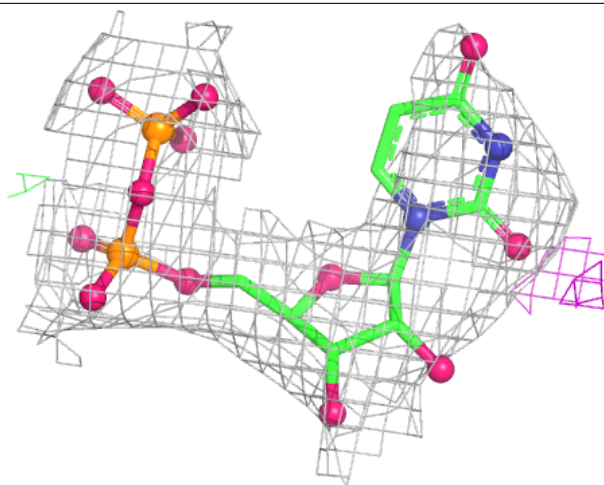
Electron density around UDP A 382:

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



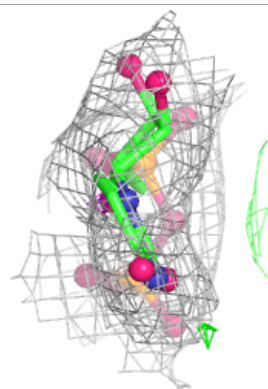
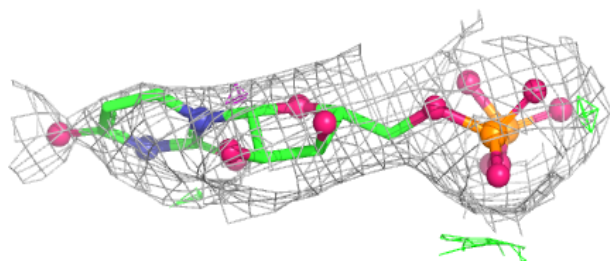
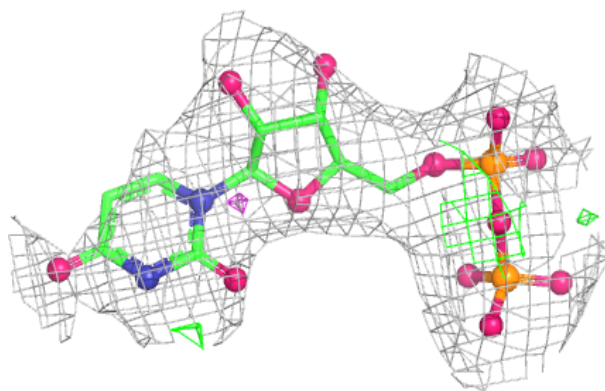
Electron density around UDP H 382:

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

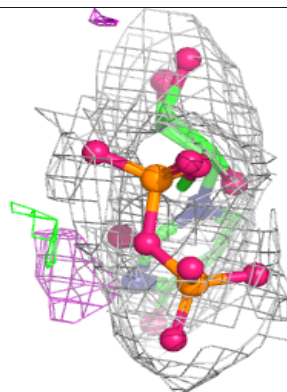
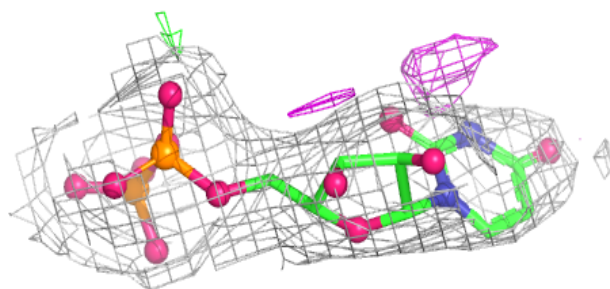


Electron density around UDP E 382:

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

**Electron density around UDP C 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.