



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:35 PM BST

PDB ID : 3S29
Title : The crystal structure of sucrose synthase-1 from Arabidopsis thaliana and its functional implications.
Authors : Zheng, Y.I.; Garavito, R.M.
Deposited on : 2011-05-16
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

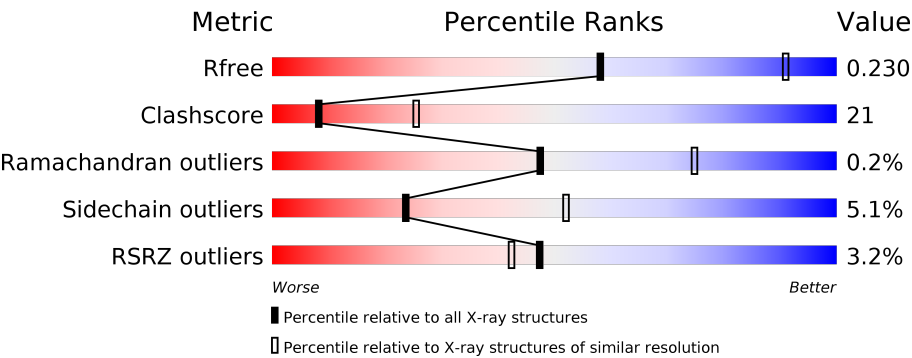
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	816	<div><div>3%</div><div><div></div><div>65%</div><div>28%</div><div>.</div><div>.</div></div></div>
1	B	816	<div><div>4%</div><div><div></div><div>62%</div><div>33%</div><div>.</div><div>.</div></div></div>
1	C	816	<div><div>3%</div><div><div></div><div>63%</div><div>31%</div><div>.</div><div>.</div></div></div>
1	D	816	<div><div>2%</div><div><div></div><div>67%</div><div>26%</div><div>.</div><div>.</div></div></div>
1	E	816	<div><div>4%</div><div><div></div><div>66%</div><div>28%</div><div>.</div><div>.</div></div></div>
1	F	816	<div><div>3%</div><div><div></div><div>63%</div><div>29%</div><div>.</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	816	
1	H	816	

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	FRU	A	902	-	-	X	-
3	FRU	B	902	-	-	X	-
3	FRU	E	902	-	-	X	-
4	SO4	B	913	-	-	X	-
4	SO4	E	913	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 51504 atoms, of which 24 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 Sucrose synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6280	4033	1066	1159	22			
1	B	791	Total	C	N	O	S	0	0	0
			6321	4056	1073	1170	22			
1	C	781	Total	C	N	O	S	0	0	0
			6294	4047	1065	1160	22			
1	D	781	Total	C	N	O	S	0	0	0
			6275	4032	1062	1159	22			
1	E	781	Total	C	N	O	S	0	0	0
			6275	4031	1063	1159	22			
1	F	781	Total	C	N	O	S	0	0	0
			6299	4047	1070	1160	22			
1	G	781	Total	C	N	O	S	0	0	0
			6301	4047	1070	1162	22			
1	H	797	Total	C	N	O	S	0	0	0
			6398	4101	1091	1184	22			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	809	VAL	-	expression tag	UNP P49040
A	810	GLU	-	expression tag	UNP P49040
A	811	HIS	-	expression tag	UNP P49040
A	812	HIS	-	expression tag	UNP P49040
A	813	HIS	-	expression tag	UNP P49040
A	814	HIS	-	expression tag	UNP P49040
A	815	HIS	-	expression tag	UNP P49040
A	816	HIS	-	expression tag	UNP P49040
B	809	VAL	-	expression tag	UNP P49040
B	810	GLU	-	expression tag	UNP P49040
B	811	HIS	-	expression tag	UNP P49040
B	812	HIS	-	expression tag	UNP P49040
B	813	HIS	-	expression tag	UNP P49040

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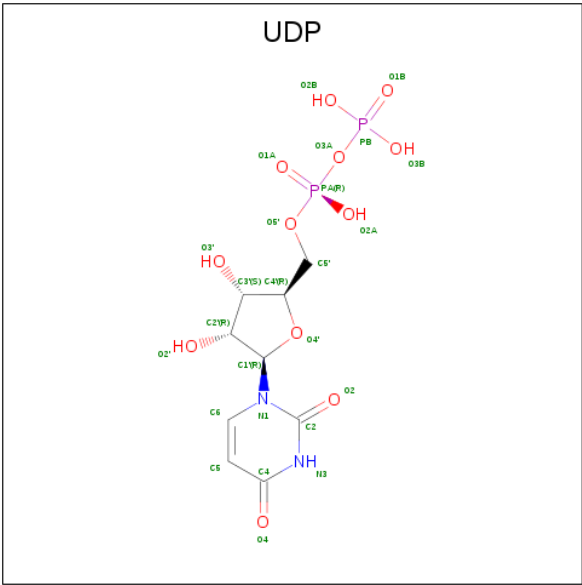
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	expression tag	UNP P49040
B	815	HIS	-	expression tag	UNP P49040
B	816	HIS	-	expression tag	UNP P49040
C	809	VAL	-	expression tag	UNP P49040
C	810	GLU	-	expression tag	UNP P49040
C	811	HIS	-	expression tag	UNP P49040
C	812	HIS	-	expression tag	UNP P49040
C	813	HIS	-	expression tag	UNP P49040
C	814	HIS	-	expression tag	UNP P49040
C	815	HIS	-	expression tag	UNP P49040
C	816	HIS	-	expression tag	UNP P49040
D	809	VAL	-	expression tag	UNP P49040
D	810	GLU	-	expression tag	UNP P49040
D	811	HIS	-	expression tag	UNP P49040
D	812	HIS	-	expression tag	UNP P49040
D	813	HIS	-	expression tag	UNP P49040
D	814	HIS	-	expression tag	UNP P49040
D	815	HIS	-	expression tag	UNP P49040
D	816	HIS	-	expression tag	UNP P49040
E	809	VAL	-	expression tag	UNP P49040
E	810	GLU	-	expression tag	UNP P49040
E	811	HIS	-	expression tag	UNP P49040
E	812	HIS	-	expression tag	UNP P49040
E	813	HIS	-	expression tag	UNP P49040
E	814	HIS	-	expression tag	UNP P49040
E	815	HIS	-	expression tag	UNP P49040
E	816	HIS	-	expression tag	UNP P49040
F	809	VAL	-	expression tag	UNP P49040
F	810	GLU	-	expression tag	UNP P49040
F	811	HIS	-	expression tag	UNP P49040
F	812	HIS	-	expression tag	UNP P49040
F	813	HIS	-	expression tag	UNP P49040
F	814	HIS	-	expression tag	UNP P49040
F	815	HIS	-	expression tag	UNP P49040
F	816	HIS	-	expression tag	UNP P49040
G	809	VAL	-	expression tag	UNP P49040
G	810	GLU	-	expression tag	UNP P49040
G	811	HIS	-	expression tag	UNP P49040
G	812	HIS	-	expression tag	UNP P49040
G	813	HIS	-	expression tag	UNP P49040
G	814	HIS	-	expression tag	UNP P49040
G	815	HIS	-	expression tag	UNP P49040

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Chain	Residue	Modelled	Actual	Comment	Reference
G	816	HIS	-	expression tag	UNP P49040
H	809	VAL	-	expression tag	UNP P49040
H	810	GLU	-	expression tag	UNP P49040
H	811	HIS	-	expression tag	UNP P49040
H	812	HIS	-	expression tag	UNP P49040
H	813	HIS	-	expression tag	UNP P49040
H	814	HIS	-	expression tag	UNP P49040
H	815	HIS	-	expression tag	UNP P49040
H	816	HIS	-	expression tag	UNP P49040

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



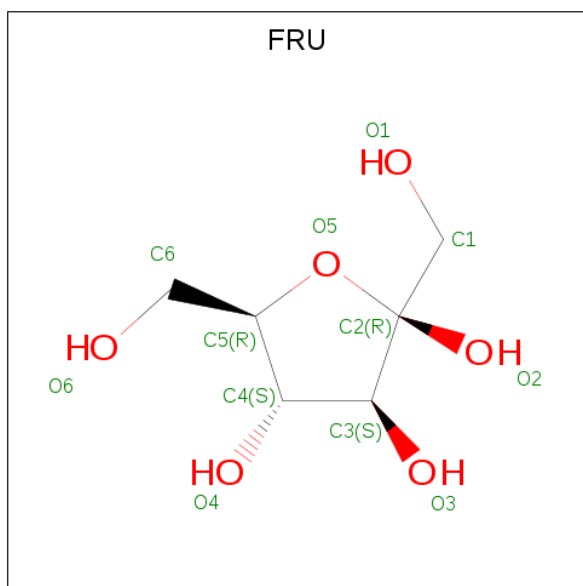
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	G	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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

- Molecule 3 is beta-D-fructofuranose (three-letter code: FRU) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		
3	G	1	Total	C	O	0	0
			12	6	6		
3	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



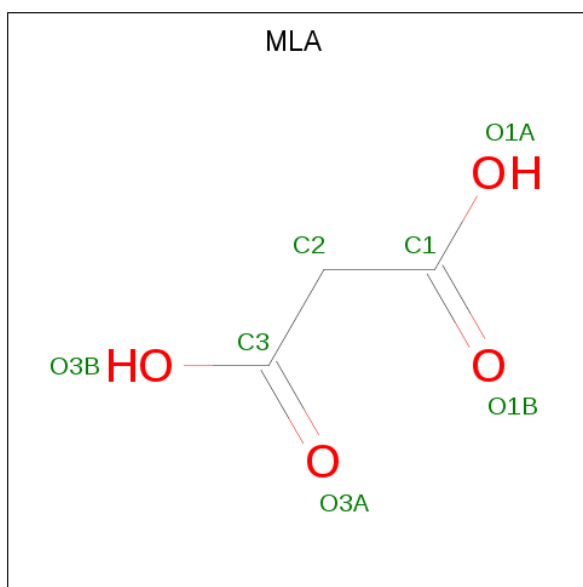
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			9	3	2	4		
5	B	1	Total	C	H	O	0	0
			9	3	2	4		
5	C	1	Total	C	H	O	0	0
			9	3	2	4		
5	D	1	Total	C	H	O	0	0
			9	3	2	4		
5	D	1	Total	C	H	O	0	0
			9	3	2	4		
5	E	1	Total	C	H	O	0	0
			9	3	2	4		
5	F	1	Total	C	H	O	0	0
			9	3	2	4		
5	F	1	Total	C	H	O	0	0
			9	3	2	4		
5	G	1	Total	C	H	O	0	0
			9	3	2	4		
5	G	1	Total	C	H	O	0	0
			9	3	2	4		
5	H	1	Total	C	H	O	0	0
			9	3	2	4		
5	H	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

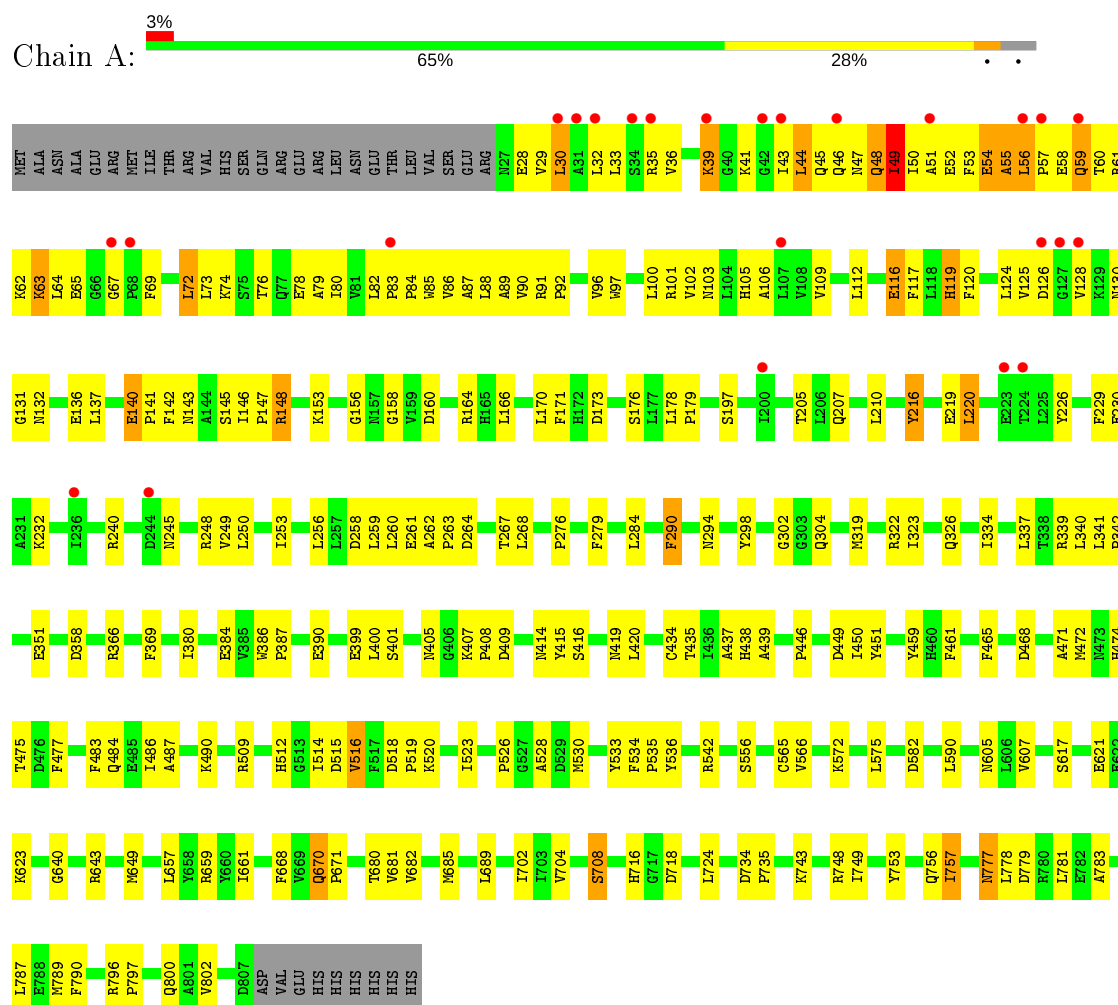
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	76	Total O 76 76	0	0
7	B	62	Total O 62 62	0	0
7	C	38	Total O 38 38	0	0
7	D	64	Total O 64 64	0	0
7	E	58	Total O 58 58	0	0
7	F	80	Total O 80 80	0	0
7	G	71	Total O 71 71	0	0
7	H	50	Total O 50 50	0	0

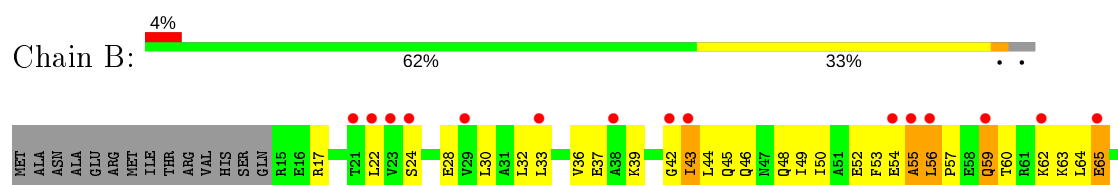
3 Residue-property plots

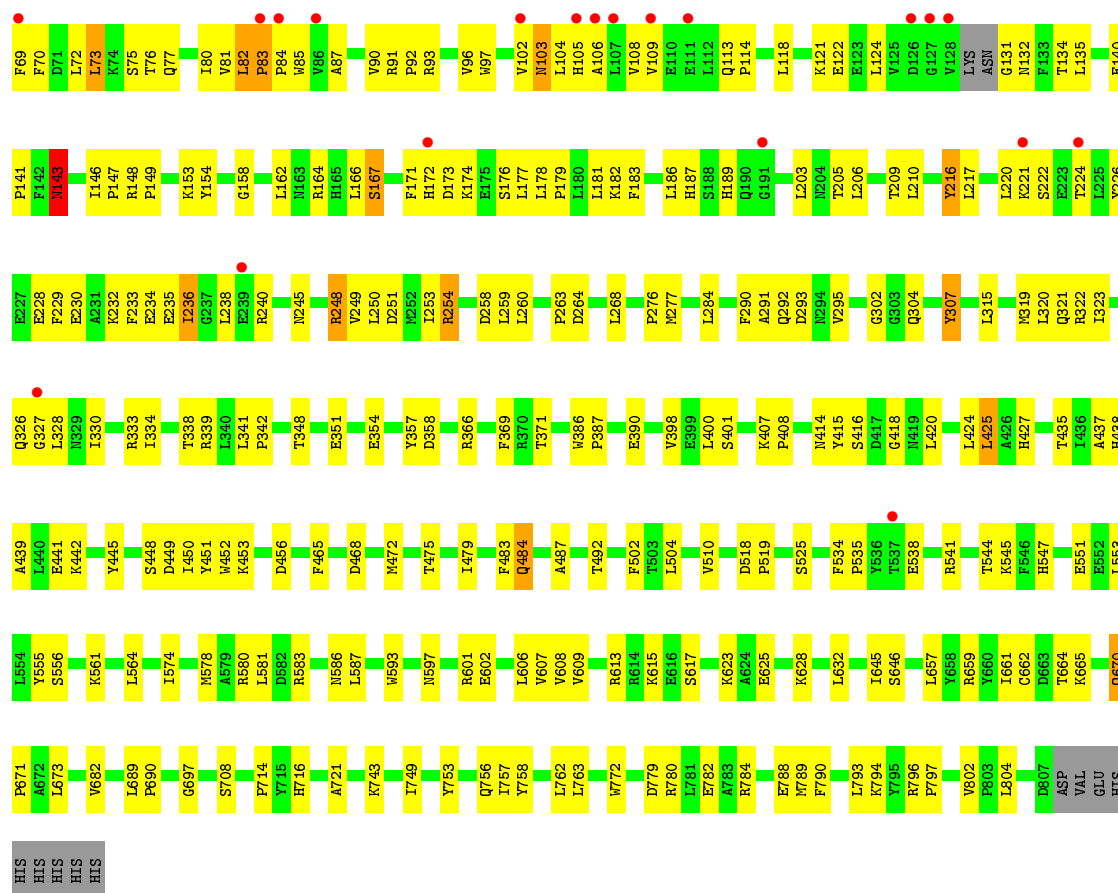
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sucrose synthase 1

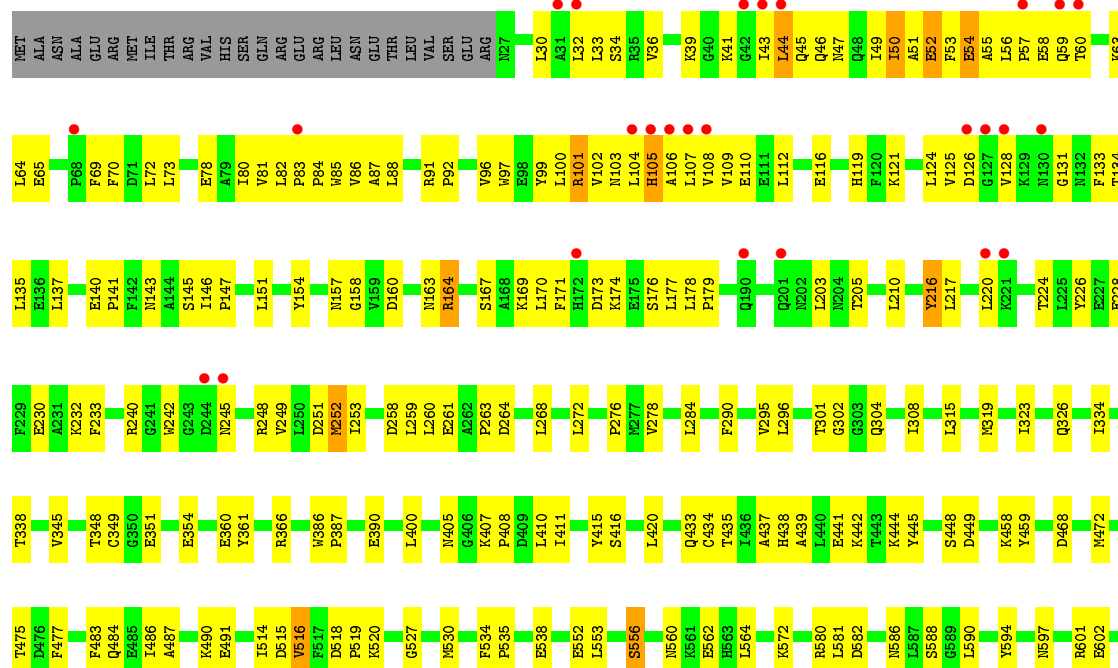


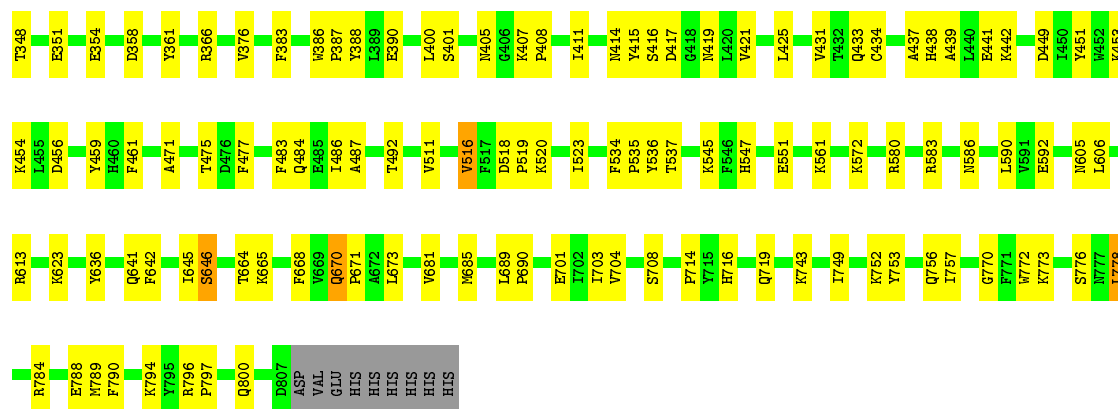
• Molecule 1: Sucrose synthase 1



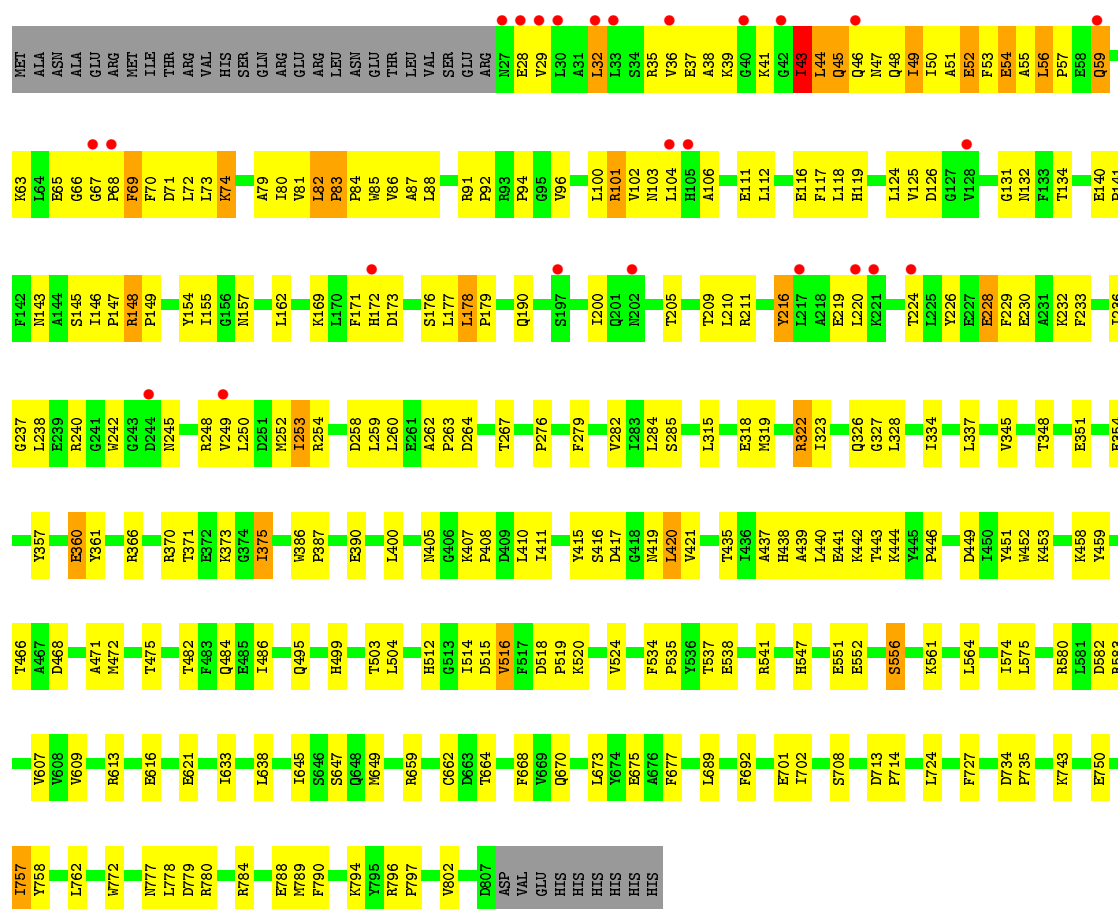


• Molecule 1: Sucrose synthase 1



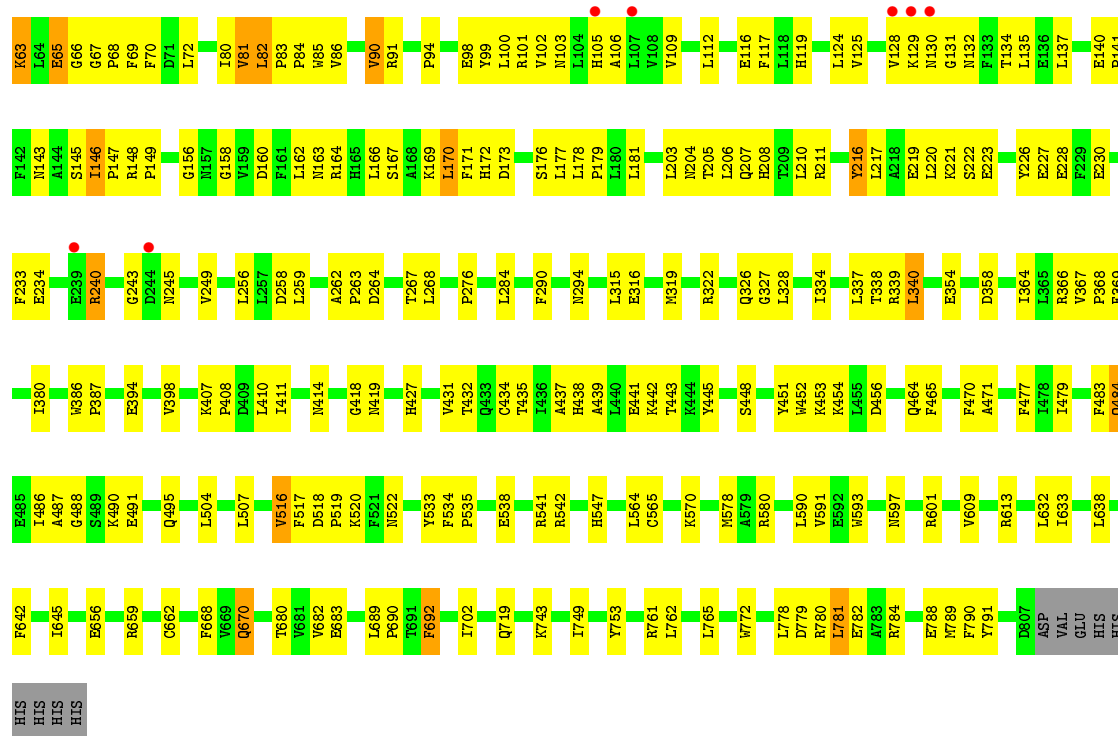


• Molecule 1: Sucrose synthase 1

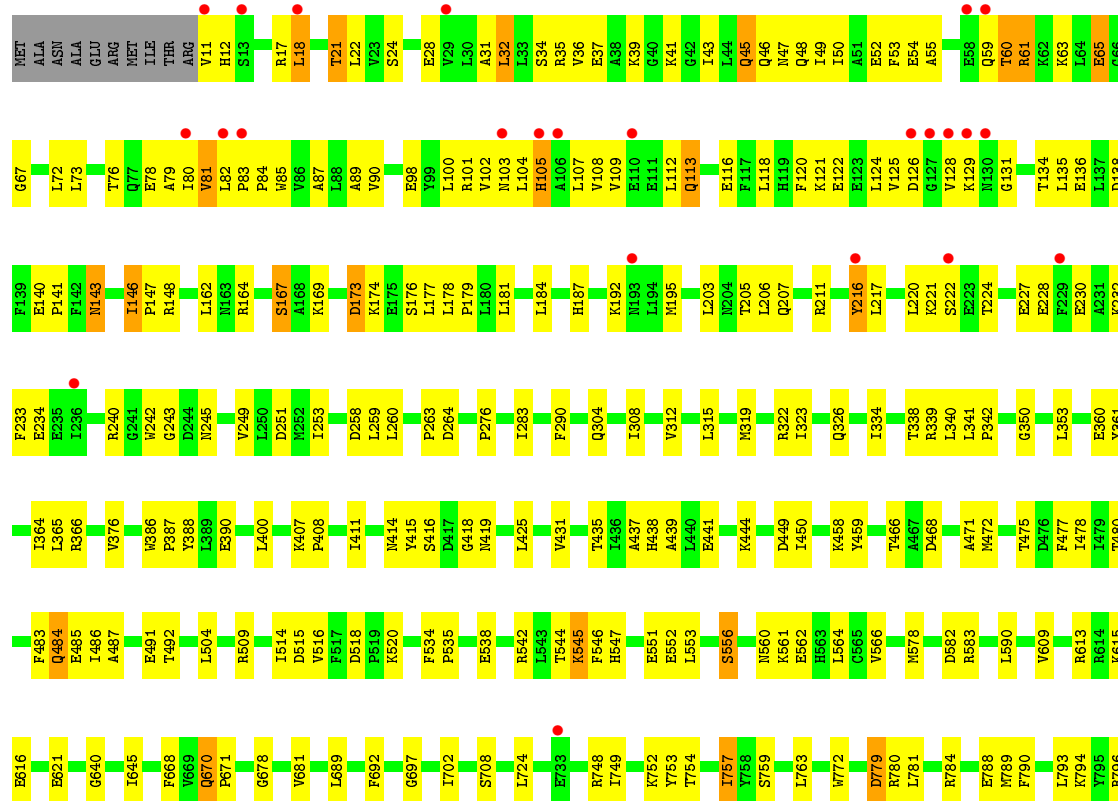


• Molecule 1: Sucrose synthase 1





• Molecule 1: Sucrose synthase 1



P797			
V802			
P803			
L804			
D807			
ASP			
VAL			
GLU			
HIS			
HIS			
HIS			
HIS			
HIS			
HIS			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	277.16 Å 261.50 Å 161.10 Å 90.00° 109.27° 90.00°	Depositor
Resolution (Å)	24.96 – 2.85 48.88 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.96-2.85) 99.3 (48.88-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.86 Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.185 , 0.234 0.181 , 0.230	Depositor DCC
R_{free} test set	11907 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51504	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8124e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UDP, MLA, K, FRU, SO4

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	0.36	0/6427	0.54	0/8703
1	B	0.35	0/6467	0.54	0/8761
1	C	0.33	0/6441	0.52	0/8723
1	D	0.35	0/6422	0.55	0/8700
1	E	0.34	0/6421	0.54	0/8697
1	F	0.35	0/6446	0.54	0/8728
1	G	0.35	0/6448	0.53	0/8731
1	H	0.34	0/6546	0.54	0/8867
All	All	0.35	0/51618	0.54	0/69910

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	ASN	Peptide
1	F	83	PRO	Peptide

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	6280	0	6200	278	0
1	B	6321	0	6203	312	0
1	C	6294	0	6244	272	0
1	D	6275	0	6197	257	0
1	E	6275	0	6205	272	0
1	F	6299	0	6247	283	0
1	G	6301	0	6247	280	0
1	H	6398	0	6301	285	0
2	A	25	0	11	1	0
2	B	25	0	11	2	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
2	E	25	0	11	1	0
2	F	25	0	11	1	0
2	G	25	0	11	1	0
2	H	25	0	11	0	0
3	A	12	0	12	7	0
3	B	12	0	12	6	0
3	C	12	0	12	4	0
3	D	12	0	12	0	0
3	E	12	0	12	11	0
3	F	12	0	12	0	0
3	G	12	0	12	0	0
3	H	12	0	12	1	0
4	A	25	0	0	2	0
4	B	15	0	0	3	0
4	C	15	0	0	0	0
4	D	20	0	0	1	0
4	E	20	0	0	4	0
4	F	20	0	0	0	0
4	G	20	0	0	1	0
4	H	15	0	0	0	0
5	A	7	2	2	0	0
5	B	7	2	2	0	0
5	C	7	2	2	0	0
5	D	14	4	4	2	0
5	E	7	2	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	14	4	4	2	0
5	G	14	4	4	0	0
5	H	14	4	4	1	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	76	0	0	3	0
7	B	62	0	0	4	0
7	C	38	0	0	1	0
7	D	64	0	0	2	0
7	E	58	0	0	4	0
7	F	80	0	0	0	0
7	G	71	0	0	3	0
7	H	50	0	0	2	0
All	All	51480	24	50052	2131	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 21.

All (2131) 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:D:145:SER:HB3	1:D:779:ASP:OD2	1.16	1.31
1:G:66:GLY:C	1:G:68:PRO:HD3	1.57	1.23
1:G:119:HIS:CE1	1:G:129:LYS:HD2	1.73	1.21
1:H:46:GLN:HB2	1:H:79:ALA:HB3	1.20	1.18
1:B:83:PRO:HB2	1:B:84:PRO:HD2	1.26	1.15
1:G:82:LEU:CD1	1:G:83:PRO:HD3	1.77	1.14
1:D:145:SER:CB	1:D:779:ASP:OD2	1.96	1.13
1:E:789:MET:HE2	1:H:789:MET:HE2	1.14	1.11
1:F:789:MET:HE2	1:G:789:MET:HE2	1.14	1.09
1:F:789:MET:HB3	1:G:789:MET:CE	1.82	1.09
1:G:82:LEU:HD12	1:G:83:PRO:HD3	1.09	1.09
1:E:789:MET:HB3	1:H:789:MET:CE	1.81	1.09
1:H:76:THR:HG22	1:H:90:VAL:HG22	1.30	1.07
1:B:113:GLN:CG	1:B:114:PRO:HD2	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:PRO:HG2	1:G:85:TRP:HB2	1.30	1.06
1:G:143:ASN:HA	1:G:780:ARG:HH12	1.20	1.05
1:F:789:MET:HE2	1:G:789:MET:CE	1.86	1.05
1:F:82:LEU:HD12	1:F:83:PRO:HD3	1.08	1.05
1:A:83:PRO:HG2	1:A:84:PRO:HD3	1.37	1.04
1:G:83:PRO:CG	1:G:85:TRP:HB2	1.87	1.04
1:E:53:PHE:O	1:E:57:PRO:HG2	1.59	1.03
1:C:39:LYS:HB2	1:C:104:LEU:HD13	1.40	1.02
1:A:262:ALA:HB1	1:B:164:ARG:HD3	1.42	1.02
1:A:146:ILE:HG13	1:A:147:PRO:HD2	1.37	1.02
1:A:319:MET:CE	1:A:334:ILE:HD11	1.90	1.01
1:G:45:GLN:HE21	1:G:45:GLN:HA	1.21	1.01
1:F:53:PHE:C	1:F:57:PRO:HG2	1.80	1.01
1:G:119:HIS:HE1	1:G:129:LYS:HD2	1.07	1.01
1:B:113:GLN:HG3	1:B:114:PRO:HD2	1.04	1.00
1:G:83:PRO:HB2	1:G:84:PRO:HD2	1.43	1.00
1:B:789:MET:CE	1:C:789:MET:HB3	1.91	1.00
1:G:81:VAL:HB	1:G:86:VAL:HG23	1.42	1.00
1:H:32:LEU:HD22	1:H:35:ARG:NH1	1.76	1.00
1:H:216:TYR:HE1	1:H:220:LEU:HD11	1.26	0.99
1:B:82:LEU:CB	1:B:83:PRO:HD2	1.91	0.99
1:C:83:PRO:HG2	1:C:84:PRO:HD3	1.44	0.99
1:G:49:ILE:HD12	1:G:49:ILE:H	1.25	0.99
1:F:82:LEU:HD12	1:F:83:PRO:CD	1.92	0.99
1:B:39:LYS:CB	1:B:104:LEU:HD22	1.92	0.99
1:G:82:LEU:HD12	1:G:83:PRO:CD	1.92	0.99
1:D:217:LEU:HD11	1:D:233:PHE:HZ	1.24	0.98
1:B:56:LEU:HB3	1:B:57:PRO:HD3	1.46	0.98
1:E:789:MET:HE2	1:H:789:MET:CE	1.92	0.98
1:F:82:LEU:CD1	1:F:83:PRO:HD3	1.95	0.97
1:E:30:LEU:HD22	1:E:62:LYS:HD3	1.46	0.97
1:G:56:LEU:HB3	1:G:57:PRO:HD3	1.46	0.97
1:A:54:GLU:HG3	1:A:55:ALA:N	1.80	0.97
1:F:143:ASN:HA	1:F:780:ARG:HH12	1.24	0.97
1:B:54:GLU:HG3	1:B:55:ALA:H	1.27	0.97
1:B:113:GLN:HG3	1:B:114:PRO:CD	1.94	0.96
1:B:121:LYS:HD3	1:B:450:ILE:HD11	1.45	0.96
1:B:793:LEU:HD11	1:C:135:LEU:HD22	1.47	0.96
1:E:83:PRO:HG2	1:E:84:PRO:HD3	1.46	0.96
1:E:789:MET:HB3	1:H:789:MET:HE2	1.46	0.95
1:D:319:MET:CE	1:D:334:ILE:HD11	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:MET:HE3	1:C:789:MET:HB3	1.47	0.95
1:B:319:MET:HE3	1:B:334:ILE:HD11	1.47	0.95
1:E:46:GLN:HB3	1:E:50:ILE:HD12	1.49	0.95
1:G:143:ASN:HA	1:G:780:ARG:NH1	1.80	0.95
1:F:81:VAL:HG13	1:F:86:VAL:HG23	1.49	0.95
1:E:55:ALA:O	1:E:59:GLN:HB2	1.66	0.94
1:D:113:GLN:HG3	1:D:114:PRO:HD2	1.50	0.94
1:B:319:MET:CE	1:B:334:ILE:HD11	1.98	0.93
1:D:171:PHE:HD1	1:D:263:PRO:HD2	1.30	0.93
1:F:146:ILE:HG13	1:F:147:PRO:HD2	1.48	0.93
1:B:55:ALA:O	1:B:59:GLN:HB2	1.67	0.93
1:H:82:LEU:HD21	1:H:85:TRP:HB2	1.51	0.92
1:F:66:GLY:C	1:F:68:PRO:HD2	1.89	0.92
1:G:83:PRO:HG2	1:G:85:TRP:CB	1.99	0.92
1:A:789:MET:CE	1:D:789:MET:HB3	1.98	0.92
1:D:52:GLU:O	1:D:57:PRO:HD2	1.70	0.92
1:E:319:MET:CE	1:E:334:ILE:HD11	2.00	0.92
1:B:53:PHE:HA	1:B:57:PRO:HG2	1.52	0.91
1:D:173:ASP:HB3	1:D:176:SER:HB3	1.53	0.91
1:E:216:TYR:CE1	1:E:220:LEU:HD11	2.06	0.91
1:G:32:LEU:O	1:G:36:VAL:HG23	1.67	0.91
1:H:146:ILE:HG13	1:H:147:PRO:HD2	1.53	0.91
1:E:304:GLN:CB	3:E:902:FRU:H12	1.99	0.91
1:G:486:ILE:HG22	1:G:516:VAL:HG22	1.51	0.91
1:F:319:MET:CE	1:F:334:ILE:HD11	2.01	0.91
1:H:39:LYS:HG3	1:H:104:LEU:CB	2.00	0.91
1:B:17:ARG:O	1:B:72:LEU:HD21	1.72	0.90
1:H:46:GLN:CB	1:H:79:ALA:HB3	1.99	0.90
1:G:45:GLN:NE2	1:G:45:GLN:HA	1.86	0.90
1:A:302:GLY:CA	3:A:902:FRU:O1	2.20	0.90
1:F:46:GLN:HB3	1:F:50:ILE:HG22	1.51	0.90
1:G:66:GLY:C	1:G:68:PRO:CD	2.39	0.89
1:A:789:MET:HE3	1:D:789:MET:HG2	1.54	0.89
1:H:216:TYR:CE1	1:H:220:LEU:HD11	2.06	0.89
1:G:63:LYS:O	1:G:65:GLU:HG2	1.72	0.89
1:E:304:GLN:H	3:E:902:FRU:H12	1.37	0.88
1:A:56:LEU:HB3	1:A:57:PRO:HD3	1.54	0.88
1:C:143:ASN:HA	1:C:780:ARG:HH12	1.37	0.88
1:A:32:LEU:O	1:A:36:VAL:HG23	1.73	0.88
1:H:319:MET:HE3	1:H:334:ILE:HD11	1.55	0.88
1:A:777:ASN:HD22	1:A:778:LEU:N	1.69	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:789:MET:HB3	1:G:789:MET:HE1	1.53	0.88
1:H:31:ALA:HB1	1:H:35:ARG:NH2	1.88	0.88
1:A:789:MET:HB3	1:D:789:MET:CE	2.03	0.87
1:G:216:TYR:CE1	1:G:220:LEU:HD11	2.09	0.87
1:A:45:GLN:HA	1:A:45:GLN:HE21	1.40	0.87
1:F:789:MET:CE	1:G:789:MET:HB3	2.04	0.87
1:D:45:GLN:HE22	1:D:80:ILE:HG13	1.39	0.87
1:D:82:LEU:HD13	1:D:84:PRO:HD2	1.57	0.87
1:F:789:MET:CE	1:G:789:MET:HE2	2.03	0.87
1:E:60:THR:HG23	1:E:62:LYS:HG3	1.53	0.86
1:H:319:MET:CE	1:H:334:ILE:HD11	2.05	0.86
1:A:103:ASN:CB	1:A:106:ALA:HB3	2.06	0.86
1:C:319:MET:HE3	1:C:334:ILE:HD11	1.55	0.86
1:D:319:MET:HE3	1:D:334:ILE:HD11	1.57	0.86
1:F:315:LEU:HD11	1:F:762:LEU:HD23	1.57	0.85
1:C:224:THR:CG2	1:C:228:GLU:HG3	2.06	0.85
1:D:83:PRO:HB2	1:D:84:PRO:HD3	1.58	0.85
1:A:319:MET:HE3	1:A:334:ILE:HD11	1.57	0.85
1:A:777:ASN:C	1:A:777:ASN:ND2	2.30	0.85
1:C:50:ILE:CD1	1:C:54:GLU:HG2	2.06	0.85
1:E:778:LEU:HD12	1:E:778:LEU:H	1.42	0.85
1:B:304:GLN:HB3	3:B:902:FRU:H12	1.58	0.85
1:A:789:MET:HE3	1:D:789:MET:CG	2.07	0.84
1:A:302:GLY:HA3	3:A:902:FRU:O1	1.77	0.84
1:A:83:PRO:CG	1:A:84:PRO:HD3	2.07	0.84
1:B:46:GLN:HB2	1:B:50:ILE:HB	1.55	0.84
1:D:39:LYS:HB2	1:D:104:LEU:HD13	1.59	0.84
1:B:83:PRO:HB2	1:B:84:PRO:CD	2.06	0.84
1:D:552:GLU:O	1:D:556:SER:HB3	1.77	0.84
1:E:124:LEU:HD12	1:E:124:LEU:O	1.77	0.84
1:D:173:ASP:HB3	1:D:176:SER:CB	2.08	0.84
1:H:82:LEU:HG	1:H:84:PRO:HD2	1.57	0.84
1:F:59:GLN:HA	1:F:59:GLN:HE21	1.42	0.84
1:H:668:PHE:HB2	1:H:689:LEU:HD23	1.59	0.84
1:H:143:ASN:HB3	1:H:780:ARG:HH12	1.43	0.84
1:A:216:TYR:CE1	1:A:220:LEU:HD11	2.13	0.83
1:E:45:GLN:HB3	1:E:80:ILE:HA	1.60	0.83
1:F:143:ASN:HA	1:F:780:ARG:NH1	1.93	0.83
1:F:43:ILE:HG23	1:F:44:LEU:N	1.92	0.83
1:D:54:GLU:HG3	1:D:55:ALA:N	1.93	0.83
1:G:32:LEU:HD22	1:G:35:ARG:NH1	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:789:MET:HG3	1:H:135:LEU:HD21	1.59	0.83
1:H:84:PRO:HG2	1:H:85:TRP:HD1	1.41	0.83
1:E:143:ASN:HB3	1:E:148:ARG:HH22	1.41	0.83
1:H:216:TYR:CE2	1:H:232:LYS:HG2	2.13	0.83
1:H:24:SER:O	1:H:28:GLU:HB2	1.79	0.83
1:A:45:GLN:HA	1:A:45:GLN:NE2	1.92	0.82
1:C:32:LEU:O	1:C:36:VAL:HG23	1.77	0.82
1:F:81:VAL:CG1	1:F:86:VAL:HG23	2.09	0.82
1:H:55:ALA:O	1:H:59:GLN:HB2	1.79	0.82
1:H:82:LEU:CD2	1:H:85:TRP:HB2	2.09	0.82
1:B:217:LEU:HD11	1:B:233:PHE:HZ	1.43	0.82
1:E:486:ILE:HG22	1:E:516:VAL:HG22	1.61	0.82
1:B:143:ASN:HB3	1:B:780:ARG:HH12	1.44	0.82
1:G:84:PRO:HB2	1:G:103:ASN:HD21	1.44	0.82
1:H:143:ASN:HB3	1:H:780:ARG:NH1	1.94	0.82
1:B:54:GLU:O	1:B:57:PRO:HD2	1.79	0.81
1:E:217:LEU:HD11	1:E:233:PHE:HZ	1.44	0.81
1:E:85:TRP:HB3	1:E:103:ASN:HA	1.60	0.81
1:A:46:GLN:HB3	1:A:79:ALA:HB3	1.60	0.81
1:G:366:ARG:HD3	7:G:827:HOH:O	1.81	0.81
1:G:83:PRO:HB2	1:G:84:PRO:CD	2.11	0.81
1:D:217:LEU:HD11	1:D:233:PHE:CZ	2.13	0.81
1:H:17:ARG:HE	1:H:72:LEU:HD23	1.45	0.81
1:E:319:MET:HE3	1:E:334:ILE:HD11	1.61	0.81
1:C:83:PRO:CG	1:C:84:PRO:HD3	2.11	0.81
1:B:315:LEU:HG	1:B:319:MET:CE	2.10	0.81
1:H:72:LEU:O	1:H:76:THR:HG23	1.81	0.81
1:F:264:ASP:OD1	1:F:267:THR:HB	1.81	0.80
1:G:83:PRO:CB	1:G:84:PRO:HD2	2.12	0.80
1:B:37:GLU:HB3	1:B:55:ALA:HB2	1.63	0.80
1:F:146:ILE:CG1	1:F:147:PRO:HD2	2.10	0.80
1:C:32:LEU:HD13	1:C:32:LEU:O	1.81	0.80
1:D:45:GLN:HA	1:D:45:GLN:HE21	1.46	0.80
1:A:789:MET:HG2	1:D:789:MET:HE3	1.62	0.80
1:H:164:ARG:HH11	1:H:164:ARG:HG3	1.47	0.80
1:A:146:ILE:CG1	1:A:147:PRO:HD2	2.11	0.80
1:E:304:GLN:HB3	3:E:902:FRU:H12	1.62	0.80
1:H:509:ARG:HH12	5:H:922:MLA:HC22	1.45	0.80
1:G:338:THR:HG23	1:G:366:ARG:HG2	1.62	0.80
1:H:249:VAL:O	1:H:253:ILE:HG12	1.82	0.80
1:C:131:GLY:HA3	1:C:134:THR:HG23	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:MET:CE	1:C:334:ILE:HD11	2.12	0.79
1:B:174:LYS:HD2	1:B:203:LEU:HD12	1.63	0.79
1:A:49:ILE:HG22	1:A:50:ILE:N	1.95	0.79
1:B:39:LYS:CB	1:B:104:LEU:HD13	2.13	0.79
1:F:143:ASN:HB3	1:F:148:ARG:NH2	1.97	0.79
1:D:60:THR:O	1:D:63:LYS:HD3	1.83	0.79
1:B:24:SER:O	1:B:28:GLU:CB	2.31	0.79
1:F:319:MET:HE1	1:F:334:ILE:HD11	1.63	0.79
1:A:789:MET:HE1	1:D:789:MET:HB3	1.65	0.78
1:D:171:PHE:CD1	1:D:263:PRO:HD2	2.16	0.78
1:G:45:GLN:CA	1:G:45:GLN:HE21	1.88	0.78
1:A:60:THR:HG23	1:A:62:LYS:H	1.47	0.78
1:E:72:LEU:HD22	1:E:90:VAL:HG11	1.65	0.78
1:H:34:SER:OG	1:H:55:ALA:HB1	1.83	0.78
1:B:124:LEU:O	1:B:124:LEU:HD23	1.84	0.78
1:H:37:GLU:HG2	1:H:54:GLU:OE2	1.84	0.78
1:H:46:GLN:HB2	1:H:79:ALA:CB	2.08	0.78
1:H:315:LEU:HG	1:H:319:MET:CE	2.14	0.78
1:C:304:GLN:HB3	3:C:902:FRU:H12	1.65	0.78
1:A:789:MET:HE3	1:D:789:MET:CE	2.14	0.77
1:D:113:GLN:HA	1:D:113:GLN:HE21	1.47	0.77
1:D:292:GLN:OE1	1:D:356:VAL:HA	1.83	0.77
1:H:32:LEU:O	1:H:36:VAL:HG23	1.84	0.77
1:H:80:ILE:HG22	1:H:120:PHE:HE2	1.47	0.77
1:C:796:ARG:HB2	1:C:797:PRO:HD3	1.66	0.77
1:A:54:GLU:HG3	1:A:55:ALA:H	1.45	0.77
1:B:187:HIS:O	6:B:931:K:K	1.94	0.77
1:D:45:GLN:NE2	1:D:80:ILE:HG13	1.98	0.77
1:B:315:LEU:HG	1:B:319:MET:HE1	1.66	0.77
1:E:83:PRO:CG	1:E:84:PRO:HD3	2.14	0.77
1:A:43:ILE:O	1:A:44:LEU:HG	1.84	0.77
1:D:319:MET:HE1	1:D:334:ILE:HD11	1.65	0.77
1:G:48:GLN:HE21	1:G:48:GLN:HA	1.49	0.77
1:B:216:TYR:CE1	1:B:220:LEU:HD11	2.20	0.77
1:F:51:ALA:O	1:F:52:GLU:HB3	1.82	0.77
1:G:49:ILE:CD1	1:G:49:ILE:H	1.98	0.77
1:G:216:TYR:CD1	1:G:220:LEU:HD11	2.20	0.77
1:F:210:LEU:HD22	1:F:253:ILE:HG23	1.66	0.76
1:A:789:MET:HE3	1:D:789:MET:HE3	1.67	0.76
1:F:145:SER:HB3	1:F:779:ASP:CG	2.06	0.76
1:C:72:LEU:C	1:C:72:LEU:HD13	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ALA:O	1:D:59:GLN:HB2	1.84	0.76
1:A:351:GLU:O	1:A:366:ARG:HD2	1.86	0.76
1:B:230:GLU:O	1:B:234:GLU:HG3	1.86	0.76
1:F:85:TRP:CE3	1:F:101:ARG:HG2	2.20	0.76
1:G:83:PRO:HG2	1:G:85:TRP:CA	2.16	0.76
1:A:45:GLN:HE21	1:A:45:GLN:CA	1.98	0.76
1:B:789:MET:HE2	1:C:789:MET:HE2	1.67	0.76
1:A:302:GLY:HA3	3:A:902:FRU:HO1	1.50	0.76
1:D:103:ASN:CB	1:D:106:ALA:HB3	2.16	0.76
1:E:30:LEU:CD2	1:E:62:LYS:HD3	2.15	0.76
1:F:82:LEU:N	1:F:83:PRO:HD3	2.01	0.76
1:A:124:LEU:O	1:A:124:LEU:HD23	1.86	0.75
1:D:216:TYR:HE1	1:D:220:LEU:HD21	1.51	0.75
1:E:30:LEU:CD1	1:E:62:LYS:HB3	2.16	0.75
1:E:72:LEU:O	1:E:72:LEU:HD13	1.86	0.75
1:G:504:LEU:HD13	1:G:507:LEU:HD23	1.68	0.75
1:A:43:ILE:HD11	1:A:83:PRO:HD3	1.67	0.75
1:D:216:TYR:CE2	1:D:232:LYS:HG2	2.21	0.75
1:A:69:PHE:CE1	1:A:73:LEU:HD11	2.21	0.75
1:A:777:ASN:HD22	1:A:777:ASN:C	1.87	0.75
1:G:339:ARG:HH12	1:G:380:ILE:HG13	1.49	0.75
1:H:472:MET:HG2	1:H:514:ILE:HD13	1.65	0.75
1:G:319:MET:CE	1:G:334:ILE:HD11	2.16	0.75
1:C:107:LEU:O	1:C:108:VAL:HG12	1.85	0.75
1:F:81:VAL:HG12	1:F:86:VAL:HA	1.68	0.75
1:H:181:LEU:HD13	1:H:206:LEU:HD22	1.68	0.75
1:E:304:GLN:N	3:E:902:FRU:H12	2.02	0.74
1:F:66:GLY:C	1:F:68:PRO:CD	2.55	0.74
1:B:217:LEU:HD11	1:B:233:PHE:CZ	2.23	0.74
1:E:414:ASN:ND2	1:E:438:HIS:NE2	2.34	0.74
1:E:433:GLN:HG2	1:E:475:THR:OG1	1.88	0.74
1:F:327:GLY:O	1:F:328:LEU:HD23	1.88	0.74
1:H:173:ASP:HB3	1:H:176:SER:CB	2.17	0.74
1:A:789:MET:CG	1:D:789:MET:HE3	2.18	0.74
1:E:43:ILE:HG23	1:E:44:LEU:N	2.02	0.74
1:H:668:PHE:HB2	1:H:689:LEU:CD2	2.17	0.74
1:A:216:TYR:HE1	1:A:220:LEU:HD11	1.50	0.74
1:F:82:LEU:N	1:F:83:PRO:CD	2.50	0.74
1:C:146:ILE:HG13	1:C:147:PRO:HD2	1.69	0.73
1:H:177:LEU:HD22	1:H:260:LEU:HD23	1.70	0.73
1:H:315:LEU:HG	1:H:319:MET:HE2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PHE:HE1	1:A:73:LEU:HD11	1.54	0.73
1:A:789:MET:CE	1:D:789:MET:CE	2.66	0.73
1:E:30:LEU:HD13	1:E:62:LYS:HB3	1.71	0.73
1:G:784:ARG:O	1:G:788:GLU:HG3	1.89	0.73
1:C:46:GLN:HB3	1:C:50:ILE:HG13	1.69	0.73
1:F:43:ILE:HG23	1:F:44:LEU:H	1.54	0.72
1:G:160:ASP:O	1:G:164:ARG:HG3	1.89	0.72
1:G:48:GLN:HE21	1:G:48:GLN:CA	2.02	0.72
1:G:67:GLY:N	1:G:68:PRO:CD	2.52	0.72
1:A:210:LEU:HD22	1:A:253:ILE:HG23	1.71	0.72
1:E:173:ASP:OD2	1:E:176:SER:HB2	1.88	0.72
1:F:54:GLU:C	1:F:57:PRO:HD2	2.10	0.72
1:H:17:ARG:HH21	1:H:72:LEU:CB	2.02	0.72
1:G:32:LEU:HD22	1:G:35:ARG:HH12	1.53	0.72
1:G:31:ALA:HB1	1:G:35:ARG:HH21	1.53	0.72
1:A:46:GLN:HB2	1:A:79:ALA:O	1.89	0.72
1:F:69:PHE:C	1:F:69:PHE:CD1	2.62	0.72
1:G:146:ILE:HG13	1:G:147:PRO:HD2	1.70	0.72
1:G:53:PHE:O	1:G:57:PRO:HD2	1.90	0.72
1:H:72:LEU:HD13	1:H:72:LEU:O	1.88	0.72
1:G:48:GLN:NE2	1:G:48:GLN:HA	2.03	0.72
1:H:18:LEU:HD12	1:H:109:VAL:HG12	1.72	0.72
1:B:121:LYS:HD3	1:B:450:ILE:CD1	2.18	0.72
1:E:789:MET:HE1	1:H:789:MET:HB3	1.70	0.72
1:G:49:ILE:HD12	1:G:49:ILE:N	2.03	0.72
1:G:66:GLY:O	1:G:68:PRO:HD3	1.88	0.72
1:H:217:LEU:HD11	1:H:233:PHE:HZ	1.54	0.71
1:B:544:THR:HA	1:B:547:HIS:CD2	2.25	0.71
1:B:793:LEU:HD11	1:C:135:LEU:CD2	2.20	0.71
1:C:315:LEU:HG	1:C:319:MET:HE2	1.71	0.71
1:H:17:ARG:HH21	1:H:72:LEU:HD23	1.54	0.71
1:E:583:ARG:HH11	1:E:583:ARG:HG2	1.54	0.71
1:B:39:LYS:CB	1:B:104:LEU:CD2	2.67	0.71
1:A:390:GLU:OE1	1:A:796:ARG:HD2	1.90	0.71
1:F:83:PRO:HG2	1:F:85:TRP:H	1.56	0.71
1:F:131:GLY:O	1:F:134:THR:HG23	1.91	0.71
1:B:245:ASN:O	1:B:249:VAL:HG23	1.89	0.71
1:C:60:THR:O	1:C:63:LYS:HD3	1.91	0.71
1:H:80:ILE:HG22	1:H:120:PHE:CE2	2.24	0.71
1:D:56:LEU:HG	1:D:70:PHE:HE1	1.55	0.71
1:A:35:ARG:NH2	1:A:102:VAL:CB	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:MET:CE	1:C:789:MET:HE2	2.21	0.71
1:G:90:VAL:HG23	1:G:98:GLU:O	1.91	0.71
1:C:102:VAL:HG12	1:C:109:VAL:HG22	1.72	0.70
1:F:789:MET:CE	1:G:789:MET:CE	2.63	0.70
1:B:182:LYS:HE2	1:B:186:LEU:HD11	1.71	0.70
1:E:158:GLY:HA3	1:E:519:PRO:O	1.91	0.70
1:F:319:MET:HE3	1:F:334:ILE:HD11	1.70	0.70
1:G:131:GLY:O	1:G:134:THR:HG23	1.90	0.70
1:H:52:GLU:OE1	1:H:53:PHE:HA	1.89	0.70
1:H:31:ALA:HB1	1:H:35:ARG:HH22	1.53	0.70
1:F:52:GLU:O	1:F:57:PRO:HG3	1.90	0.70
1:G:778:LEU:H	1:G:778:LEU:HD12	1.56	0.70
1:C:615:LYS:NZ	1:C:618:LYS:HE2	2.07	0.70
1:D:83:PRO:CB	1:D:84:PRO:HD3	2.21	0.70
1:E:319:MET:HE1	1:E:334:ILE:HD11	1.72	0.70
1:E:46:GLN:HB3	1:E:50:ILE:HB	1.72	0.70
1:F:580:ARG:HD3	2:F:901:UDP:O3B	1.90	0.70
1:E:789:MET:CE	1:H:789:MET:HE2	2.07	0.70
1:B:789:MET:HB3	1:C:789:MET:CE	2.20	0.70
1:G:217:LEU:HD11	1:G:233:PHE:HZ	1.56	0.70
1:A:486:ILE:HG22	1:A:516:VAL:HG22	1.73	0.70
1:A:53:PHE:O	1:A:57:PRO:HD2	1.91	0.70
1:C:86:VAL:HG12	1:C:102:VAL:CG2	2.22	0.70
1:C:82:LEU:HB3	1:C:83:PRO:HD2	1.74	0.70
1:F:38:ALA:O	1:F:41:LYS:HB2	1.91	0.70
1:G:68:PRO:HG2	1:G:70:PHE:HB3	1.73	0.70
1:G:83:PRO:HG3	1:G:85:TRP:HB2	1.74	0.70
1:B:82:LEU:CB	1:B:83:PRO:CD	2.68	0.70
1:E:216:TYR:CD1	1:E:220:LEU:HD11	2.27	0.70
1:A:49:ILE:HG22	1:A:50:ILE:H	1.56	0.69
1:C:249:VAL:O	1:C:253:ILE:HG13	1.92	0.69
1:A:590:LEU:HB2	1:A:671:PRO:HG3	1.73	0.69
1:C:319:MET:O	1:C:323:ILE:HG13	1.92	0.69
1:C:34:SER:HA	1:C:59:GLN:HE22	1.56	0.69
1:C:63:LYS:O	1:C:65:GLU:HG2	1.93	0.69
1:C:778:LEU:HD12	1:C:778:LEU:H	1.57	0.69
1:G:83:PRO:HD2	1:G:85:TRP:O	1.92	0.69
1:H:17:ARG:HH21	1:H:72:LEU:CD2	2.04	0.69
1:A:79:ALA:HB2	1:A:88:LEU:HD23	1.72	0.69
1:B:216:TYR:CD1	1:B:220:LEU:HD11	2.28	0.69
1:F:233:PHE:CD1	1:F:238:LEU:HD12	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:GLN:CB	1:E:50:ILE:HB	2.22	0.69
1:E:789:MET:HB3	1:H:789:MET:HE1	1.73	0.69
1:A:681:VAL:O	1:A:685:MET:HG3	1.92	0.69
1:F:49:ILE:O	1:F:53:PHE:CB	2.41	0.69
1:G:216:TYR:HD1	1:G:216:TYR:C	1.96	0.69
1:H:84:PRO:HG2	1:H:85:TRP:CD1	2.26	0.69
1:D:56:LEU:HB3	1:D:57:PRO:HD3	1.75	0.69
1:E:143:ASN:CB	1:E:148:ARG:HH12	2.05	0.69
1:F:276:PRO:HG3	1:F:326:GLN:HG3	1.74	0.69
1:A:46:GLN:CB	1:A:79:ALA:HB3	2.22	0.69
1:F:39:LYS:HG2	1:F:104:LEU:HD13	1.74	0.69
1:F:789:MET:HE1	1:G:789:MET:HB3	1.75	0.69
1:F:86:VAL:HG12	1:F:102:VAL:O	1.93	0.69
1:F:83:PRO:CB	1:F:84:PRO:HD2	2.22	0.69
1:B:366:ARG:HD3	7:B:836:HOH:O	1.92	0.68
1:B:59:GLN:HG2	1:B:63:LYS:HB3	1.73	0.68
1:F:177:LEU:HD22	1:F:260:LEU:HD23	1.75	0.68
1:G:84:PRO:HB2	1:G:103:ASN:ND2	2.07	0.68
1:B:553:LEU:HG	1:B:645:ILE:HD13	1.74	0.68
1:E:216:TYR:HE1	1:E:220:LEU:HD11	1.57	0.68
1:H:17:ARG:NH2	1:H:72:LEU:HB2	2.08	0.68
1:F:53:PHE:CA	1:F:57:PRO:HG2	2.23	0.68
1:A:264:ASP:OD1	1:A:267:THR:HB	1.93	0.68
1:G:217:LEU:HA	1:G:220:LEU:HD13	1.74	0.68
1:E:60:THR:CG2	1:E:62:LYS:HG3	2.24	0.68
1:F:673:LEU:HD23	1:F:714:PRO:HB2	1.75	0.68
1:G:262:ALA:HB1	1:H:164:ARG:HD3	1.76	0.68
1:G:72:LEU:HD22	1:G:90:VAL:HG11	1.74	0.68
1:A:319:MET:HE1	1:A:334:ILE:HD11	1.76	0.68
1:D:220:LEU:N	1:D:220:LEU:HD12	2.09	0.68
1:F:83:PRO:HB2	1:F:84:PRO:HD2	1.76	0.68
1:G:137:LEU:HD11	1:G:790:PHE:CZ	2.29	0.68
1:A:171:PHE:HD1	1:A:263:PRO:HD2	1.59	0.68
1:B:538:GLU:OE1	1:B:541:ARG:HD3	1.94	0.68
1:F:82:LEU:H	1:F:83:PRO:HD3	1.57	0.68
1:G:220:LEU:H	1:G:220:LEU:HD12	1.59	0.68
1:A:262:ALA:HB1	1:B:164:ARG:CD	2.19	0.67
1:E:210:LEU:HD22	1:E:253:ILE:HG23	1.76	0.67
1:H:217:LEU:HD11	1:H:233:PHE:CZ	2.28	0.67
1:A:49:ILE:CG2	1:A:50:ILE:N	2.58	0.67
1:B:547:HIS:O	1:B:551:GLU:HG2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:794:LYS:HE2	1:C:794:LYS:HA	1.75	0.67
1:D:143:ASN:HB3	1:D:148:ARG:NH2	2.09	0.67
1:E:105:HIS:O	1:E:106:ALA:HB3	1.93	0.67
1:E:125:VAL:HG13	1:E:126:ASP:OD2	1.94	0.67
1:F:552:GLU:O	1:F:556:SER:HB3	1.94	0.67
1:B:43:ILE:HG23	1:B:43:ILE:O	1.93	0.67
1:B:56:LEU:CB	1:B:57:PRO:HD3	2.24	0.67
1:E:46:GLN:HB3	1:E:50:ILE:CD1	2.23	0.67
1:F:83:PRO:HG2	1:F:85:TRP:HB2	1.76	0.67
1:C:43:ILE:C	1:C:44:LEU:HD12	2.14	0.67
1:E:411:ILE:HG13	1:E:431:VAL:HG11	1.76	0.67
1:H:441:GLU:HA	1:H:441:GLU:OE1	1.94	0.67
1:D:210:LEU:HD22	1:D:253:ILE:HG23	1.76	0.67
1:G:66:GLY:CA	1:G:68:PRO:HD3	2.23	0.67
1:B:140:GLU:N	1:B:141:PRO:HD2	2.10	0.67
1:C:65:GLU:HA	1:C:65:GLU:OE2	1.93	0.67
1:D:33:LEU:O	1:D:37:GLU:HG2	1.93	0.67
1:G:219:GLU:OE1	1:G:219:GLU:HA	1.94	0.67
1:G:83:PRO:HG2	1:G:85:TRP:N	2.10	0.67
1:A:72:LEU:O	1:A:72:LEU:HD13	1.95	0.67
1:B:103:ASN:OD1	1:B:106:ALA:HB3	1.94	0.67
1:B:302:GLY:CA	3:B:902:FRU:O1	2.43	0.67
1:D:249:VAL:O	1:D:253:ILE:HG13	1.94	0.67
1:D:327:GLY:O	1:D:328:LEU:HD23	1.95	0.67
1:E:789:MET:CE	1:H:789:MET:HB3	2.23	0.67
1:F:71:ASP:O	1:F:74:LYS:HB3	1.94	0.67
1:G:262:ALA:HB1	1:H:164:ARG:CD	2.25	0.67
1:C:43:ILE:O	1:C:44:LEU:HG	1.94	0.67
1:F:83:PRO:CG	1:F:85:TRP:HB2	2.24	0.67
1:H:162:LEU:HD11	1:H:772:TRP:CD2	2.30	0.67
1:F:633:ILE:HA	1:F:638:LEU:HD12	1.77	0.67
1:F:83:PRO:HG2	1:F:85:TRP:CA	2.25	0.67
1:B:400:LEU:C	1:B:400:LEU:HD12	2.16	0.67
1:B:92:PRO:HG2	1:B:96:VAL:HG23	1.77	0.67
1:E:27:ASN:OD1	1:E:30:LEU:HB2	1.95	0.67
1:D:407:LYS:HB2	1:D:408:PRO:CD	2.25	0.66
1:E:304:GLN:HB3	3:E:902:FRU:C1	2.24	0.66
1:E:174:LYS:HD2	1:E:203:LEU:HD12	1.76	0.66
1:E:210:LEU:CD2	1:E:253:ILE:HG23	2.25	0.66
1:G:72:LEU:CD2	1:G:90:VAL:HG11	2.26	0.66
1:B:217:LEU:HA	1:B:220:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:HIS:O	1:C:106:ALA:HB3	1.94	0.66
1:C:224:THR:HG23	1:C:228:GLU:HG3	1.76	0.66
1:A:789:MET:CE	1:D:789:MET:CB	2.72	0.66
1:B:36:VAL:HG12	1:B:37:GLU:N	2.10	0.66
1:D:216:TYR:CD2	1:D:232:LYS:HG2	2.31	0.66
1:D:719:GLN:HG3	4:D:913:SO4:O4	1.96	0.66
1:F:407:LYS:HB2	1:F:408:PRO:CD	2.25	0.66
1:H:83:PRO:HG2	1:H:84:PRO:HD3	1.78	0.66
1:B:544:THR:HA	1:B:547:HIS:HD2	1.60	0.66
1:B:56:LEU:HD21	1:B:65:GLU:OE2	1.94	0.66
1:C:534:PHE:HB2	1:C:535:PRO:CD	2.26	0.66
1:E:790:PHE:N	1:H:789:MET:HE1	2.11	0.66
1:F:315:LEU:CD1	1:F:762:LEU:HD23	2.24	0.66
1:G:54:GLU:OE2	1:G:55:ALA:HA	1.94	0.66
1:C:30:LEU:O	1:C:33:LEU:HG	1.95	0.66
1:C:137:LEU:HD11	1:C:790:PHE:CE1	2.30	0.66
1:F:140:GLU:N	1:F:141:PRO:HD2	2.10	0.66
1:B:784:ARG:O	1:B:788:GLU:HG3	1.96	0.66
1:D:146:ILE:HG13	1:D:147:PRO:HD2	1.77	0.66
1:C:51:ALA:O	1:C:52:GLU:HB3	1.96	0.66
1:C:49:ILE:O	1:C:53:PHE:CB	2.44	0.66
1:F:233:PHE:CE1	1:F:238:LEU:HD12	2.31	0.66
1:H:17:ARG:HG2	1:H:98:GLU:OE1	1.96	0.65
1:H:17:ARG:NE	1:H:72:LEU:HD23	2.10	0.65
1:A:59:GLN:CG	1:A:60:THR:H	2.09	0.65
1:B:56:LEU:HD11	1:B:65:GLU:OE2	1.95	0.65
1:B:30:LEU:HD11	1:E:405:ASN:HD21	1.61	0.65
1:F:118:LEU:HD22	1:F:503:THR:HG22	1.77	0.65
1:G:319:MET:HE3	1:G:334:ILE:HD11	1.78	0.65
1:H:82:LEU:HD22	1:H:120:PHE:CZ	2.32	0.65
1:B:217:LEU:CD1	1:B:233:PHE:HZ	2.10	0.65
1:C:46:GLN:HB3	1:C:50:ILE:CG1	2.25	0.65
1:F:52:GLU:O	1:F:57:PRO:HD3	1.96	0.65
1:G:538:GLU:OE1	1:G:541:ARG:HD3	1.96	0.65
1:A:47:ASN:O	1:A:48:GLN:HB3	1.95	0.65
1:B:75:SER:O	1:B:90:VAL:HG13	1.95	0.65
1:C:108:VAL:HG13	1:C:108:VAL:O	1.96	0.65
1:F:518:ASP:OD1	1:F:520:LYS:HG2	1.97	0.65
1:B:319:MET:HE1	1:B:334:ILE:HD11	1.77	0.65
1:C:259:LEU:O	1:C:263:PRO:HG3	1.97	0.65
1:G:483:PHE:CE1	1:G:487:ALA:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD13	1:B:206:LEU:HD22	1.79	0.65
1:B:54:GLU:HG3	1:B:55:ALA:N	2.07	0.65
1:C:39:LYS:HB2	1:C:104:LEU:CD1	2.20	0.65
1:F:37:GLU:HG2	1:F:54:GLU:OE2	1.96	0.65
1:G:441:GLU:HA	1:G:441:GLU:OE1	1.97	0.65
1:G:156:GLY:O	1:G:522:ASN:HA	1.96	0.65
1:H:121:LYS:HE2	1:H:450:ILE:CD1	2.27	0.65
1:E:143:ASN:HB3	1:E:148:ARG:NH2	2.11	0.65
1:E:778:LEU:N	1:E:778:LEU:HD12	2.09	0.65
1:B:37:GLU:CB	1:B:55:ALA:HB2	2.27	0.65
1:C:739:ASP:O	1:C:743:LYS:HD3	1.96	0.65
1:E:156:GLY:HA3	1:E:523:ILE:HG13	1.79	0.65
1:F:83:PRO:HG2	1:F:85:TRP:N	2.12	0.65
1:C:170:LEU:HD22	1:C:177:LEU:HD23	1.77	0.64
1:D:82:LEU:C	1:D:82:LEU:HD12	2.17	0.64
1:E:60:THR:O	1:E:63:LYS:HG3	1.98	0.64
1:F:54:GLU:HG3	1:F:55:ALA:H	1.62	0.64
1:C:668:PHE:HB2	1:C:689:LEU:CD2	2.28	0.64
1:G:207:GLN:HG2	1:H:12:HIS:CE1	2.32	0.64
1:E:173:ASP:HB3	1:E:176:SER:HB3	1.80	0.64
1:E:226:TYR:CE2	1:E:240:ARG:HG2	2.32	0.64
1:G:216:TYR:HE1	1:G:220:LEU:HD11	1.63	0.64
1:B:250:LEU:O	1:B:254:ARG:HG3	1.98	0.64
1:B:73:LEU:O	1:B:76:THR:HG22	1.98	0.64
1:D:216:TYR:CE1	1:D:220:LEU:HD11	2.32	0.64
1:F:83:PRO:HB2	1:F:84:PRO:CD	2.28	0.64
1:H:31:ALA:CB	1:H:35:ARG:HH22	2.10	0.64
1:A:79:ALA:CB	1:A:88:LEU:HD23	2.28	0.64
1:D:137:LEU:HD11	1:D:790:PHE:CZ	2.33	0.64
1:D:41:LYS:HE3	1:D:54:GLU:HG2	1.78	0.64
1:G:216:TYR:CD1	1:G:216:TYR:C	2.70	0.64
1:A:158:GLY:HA3	1:A:519:PRO:O	1.97	0.64
1:G:483:PHE:CZ	1:G:487:ALA:HB3	2.33	0.64
1:G:778:LEU:HD12	1:G:778:LEU:N	2.13	0.64
1:B:146:ILE:HG13	1:B:147:PRO:HD2	1.80	0.64
1:C:224:THR:HG22	1:C:228:GLU:HG3	1.78	0.64
1:E:45:GLN:HG2	1:E:80:ILE:CD1	2.28	0.64
1:G:319:MET:HE1	1:G:334:ILE:HD11	1.80	0.64
1:G:34:SER:N	1:G:59:GLN:HE22	1.95	0.64
1:G:407:LYS:HB2	1:G:408:PRO:CD	2.27	0.64
1:G:597:ASN:O	1:G:601:ARG:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:GLU:O	1:H:234:GLU:HG3	1.97	0.64
1:H:34:SER:OG	1:H:55:ALA:CB	2.45	0.64
1:A:82:LEU:O	1:A:85:TRP:O	2.15	0.64
1:C:80:ILE:CD1	1:C:121:LYS:CG	2.76	0.64
1:F:52:GLU:O	1:F:57:PRO:CG	2.46	0.64
1:G:204:ASN:OD1	1:H:11:VAL:HG12	1.98	0.63
1:C:615:LYS:HZ1	1:C:618:LYS:HE2	1.62	0.63
1:C:92:PRO:HD2	1:C:96:VAL:O	1.99	0.63
1:F:67:GLY:N	1:F:68:PRO:CD	2.60	0.63
1:H:259:LEU:O	1:H:263:PRO:HG3	1.98	0.63
1:E:135:LEU:HD22	1:H:793:LEU:HD11	1.80	0.63
1:A:28:GLU:O	1:A:32:LEU:HG	1.98	0.63
1:C:34:SER:CA	1:C:59:GLN:HE22	2.11	0.63
1:E:778:LEU:CD1	1:E:778:LEU:H	2.09	0.63
1:G:533:TYR:CZ	1:G:683:GLU:HG2	2.33	0.63
1:G:778:LEU:H	1:G:778:LEU:CD1	2.11	0.63
1:C:41:LYS:O	1:C:44:LEU:HD11	1.98	0.63
1:F:125:VAL:HG12	1:F:126:ASP:OD1	1.98	0.63
1:G:56:LEU:HB3	1:G:57:PRO:CD	2.26	0.63
1:F:778:LEU:HD12	1:F:778:LEU:N	2.14	0.63
1:E:72:LEU:C	1:E:72:LEU:HD13	2.19	0.63
1:H:103:ASN:HB3	1:H:105:HIS:O	1.99	0.63
1:D:125:VAL:HG13	1:D:126:ASP:N	2.14	0.63
1:D:131:GLY:O	1:D:134:THR:HG23	1.99	0.63
1:A:400:LEU:C	1:A:400:LEU:HD12	2.19	0.63
1:C:407:LYS:HB2	1:C:408:PRO:CD	2.29	0.63
1:E:304:GLN:H	3:E:902:FRU:C1	2.11	0.63
1:H:17:ARG:HH21	1:H:72:LEU:HB2	1.61	0.63
1:B:441:GLU:OE1	1:B:441:GLU:HA	1.98	0.63
1:H:486:ILE:HG22	1:H:516:VAL:HG22	1.81	0.63
1:F:43:ILE:CG2	1:F:44:LEU:N	2.62	0.62
1:G:54:GLU:HG3	1:G:55:ALA:N	2.14	0.62
1:C:86:VAL:HG12	1:C:102:VAL:HG22	1.80	0.62
1:D:220:LEU:HD12	1:D:220:LEU:H	1.63	0.62
1:H:466:THR:HG23	1:H:790:PHE:CZ	2.34	0.62
1:A:101:ARG:HB2	1:A:112:LEU:HD11	1.81	0.62
1:A:789:MET:HE2	1:D:789:MET:HE2	1.80	0.62
1:B:56:LEU:HB3	1:B:57:PRO:CD	2.26	0.62
1:C:216:TYR:HD2	1:C:232:LYS:HE2	1.64	0.62
1:F:282:VAL:HG13	1:F:337:LEU:HD23	1.80	0.62
1:G:443:THR:HG21	1:G:495:GLN:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:ASN:CB	1:H:780:ARG:HH12	2.13	0.62
1:B:315:LEU:HG	1:B:319:MET:HE2	1.81	0.62
1:B:54:GLU:O	1:B:56:LEU:N	2.33	0.62
1:H:164:ARG:HH11	1:H:164:ARG:CG	2.13	0.62
1:D:216:TYR:HD2	1:D:232:LYS:HE2	1.63	0.62
1:E:354:GLU:OE1	1:E:366:ARG:NH2	2.32	0.62
1:E:583:ARG:NH1	1:E:583:ARG:HG2	2.15	0.62
1:F:209:THR:CG2	1:F:236:ILE:HG13	2.30	0.62
1:G:689:LEU:HD12	1:G:690:PRO:HD2	1.81	0.62
1:H:140:GLU:N	1:H:141:PRO:HD2	2.14	0.62
1:H:31:ALA:CB	1:H:35:ARG:NH2	2.61	0.62
1:H:32:LEU:HD22	1:H:35:ARG:HH11	1.62	0.62
1:H:796:ARG:HB2	1:H:797:PRO:HD3	1.82	0.62
1:C:39:LYS:HG3	1:C:104:LEU:HD12	1.80	0.62
1:D:56:LEU:HG	1:D:70:PHE:CE1	2.34	0.62
1:C:80:ILE:CD1	1:C:121:LYS:HG2	2.30	0.62
1:A:72:LEU:HD13	1:A:72:LEU:C	2.20	0.62
1:C:137:LEU:HD11	1:C:790:PHE:CZ	2.35	0.62
1:F:216:TYR:HE1	1:F:220:LEU:HD11	1.65	0.62
1:F:357:TYR:CD2	5:F:922:MLA:HC22	2.34	0.62
1:G:31:ALA:CB	1:G:35:ARG:NH2	2.63	0.62
1:H:17:ARG:NH2	1:H:72:LEU:HD23	2.15	0.62
1:C:171:PHE:CD1	1:C:263:PRO:HD2	2.35	0.61
1:D:34:SER:O	1:D:37:GLU:HB2	1.99	0.61
1:A:789:MET:CB	1:D:789:MET:CE	2.78	0.61
1:G:43:ILE:HA	1:G:81:VAL:O	2.00	0.61
1:B:609:VAL:HG22	1:B:645:ILE:HB	1.83	0.61
1:E:249:VAL:O	1:E:253:ILE:HG13	2.00	0.61
1:G:207:GLN:HG2	1:H:12:HIS:HE1	1.63	0.61
1:B:302:GLY:N	3:B:902:FRU:O1	2.33	0.61
1:E:217:LEU:HD11	1:E:233:PHE:CZ	2.31	0.61
1:F:200:ILE:HD11	1:F:237:GLY:HA3	1.82	0.61
1:A:142:PHE:HB3	1:A:783:ALA:HB2	1.82	0.61
1:C:102:VAL:CG1	1:C:109:VAL:HG22	2.28	0.61
1:E:30:LEU:HD12	1:E:65:GLU:OE2	2.00	0.61
1:A:29:VAL:O	1:A:33:LEU:HG	2.00	0.61
1:B:659:ARG:O	1:B:662:CYS:HB2	2.00	0.61
1:C:278:VAL:HG21	1:C:763:LEU:CD2	2.31	0.61
1:C:143:ASN:HA	1:C:780:ARG:NH1	2.11	0.61
1:D:248:ARG:HH11	1:D:248:ARG:HB3	1.65	0.61
1:D:407:LYS:HB2	1:D:408:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:CB	1:G:57:PRO:HD3	2.25	0.61
1:H:174:LYS:HD3	1:H:203:LEU:HD12	1.82	0.61
1:A:302:GLY:N	3:A:902:FRU:O1	2.34	0.61
1:B:103:ASN:N	1:B:103:ASN:HD22	1.99	0.61
1:E:45:GLN:HG2	1:E:80:ILE:HD12	1.82	0.61
1:G:419:ASN:HB3	1:G:471:ALA:CB	2.30	0.61
1:A:220:LEU:N	1:A:220:LEU:HD12	2.16	0.61
1:C:86:VAL:CG1	1:C:102:VAL:HG22	2.30	0.61
1:D:86:VAL:HG12	1:D:102:VAL:HG12	1.83	0.61
1:H:407:LYS:HB2	1:H:408:PRO:CD	2.30	0.61
1:H:17:ARG:HE	1:H:72:LEU:CD2	2.14	0.61
1:D:102:VAL:HG23	1:D:109:VAL:HG23	1.82	0.61
1:E:140:GLU:N	1:E:141:PRO:HD2	2.16	0.61
1:G:221:LYS:HD2	1:G:222:SER:H	1.65	0.61
1:G:35:ARG:HD3	1:G:102:VAL:HG11	1.83	0.61
1:H:103:ASN:ND2	1:H:108:VAL:HB	2.15	0.61
1:G:220:LEU:N	1:G:220:LEU:HD12	2.16	0.61
1:F:789:MET:CB	1:G:789:MET:CE	2.68	0.61
1:F:789:MET:HE2	1:G:789:MET:HB3	1.82	0.61
1:H:552:GLU:O	1:H:556:SER:HB3	2.01	0.61
1:B:30:LEU:HD23	1:B:63:LYS:O	2.01	0.61
1:B:37:GLU:HG2	1:B:54:GLU:OE2	2.01	0.61
1:D:102:VAL:HG23	1:D:109:VAL:CG2	2.30	0.61
1:E:414:ASN:HD22	1:E:438:HIS:CD2	2.18	0.61
1:H:173:ASP:HB3	1:H:176:SER:HB3	1.81	0.61
1:B:63:LYS:HG3	1:B:64:LEU:H	1.65	0.60
1:B:790:PHE:N	1:C:789:MET:HE1	2.16	0.60
1:D:48:GLN:HA	1:D:51:ALA:HB3	1.82	0.60
1:G:91:ARG:NH2	1:G:94:PRO:HA	2.16	0.60
1:H:82:LEU:HD23	1:H:85:TRP:O	2.00	0.60
1:B:93:ARG:HB2	1:B:96:VAL:CG2	2.31	0.60
1:D:116:GLU:O	1:D:119:HIS:HB2	2.00	0.60
1:A:91:ARG:HD2	1:A:97:TRP:CZ2	2.37	0.60
1:E:534:PHE:HB2	1:E:535:PRO:CD	2.31	0.60
1:E:796:ARG:HB2	1:E:797:PRO:HD3	1.83	0.60
1:G:533:TYR:CE1	1:G:683:GLU:HG2	2.36	0.60
1:H:338:THR:HG23	1:H:366:ARG:HG2	1.84	0.60
1:F:79:ALA:CB	1:F:88:LEU:HD23	2.30	0.60
1:H:146:ILE:HG12	1:H:147:PRO:O	2.00	0.60
1:B:54:GLU:CG	1:B:55:ALA:H	2.02	0.60
1:C:83:PRO:CB	1:C:84:PRO:HD3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:PHE:N	1:D:789:MET:HE1	2.16	0.60
1:E:116:GLU:O	1:E:119:HIS:HB2	2.01	0.60
1:A:178:LEU:HB2	1:A:179:PRO:HD3	1.82	0.60
1:A:518:ASP:OD1	1:A:520:LYS:HG2	2.01	0.60
1:B:42:GLY:HA2	1:B:81:VAL:HG11	1.83	0.60
1:G:31:ALA:CB	1:G:35:ARG:HH21	2.14	0.60
1:H:245:ASN:O	1:H:249:VAL:HG23	2.02	0.60
1:A:407:LYS:HB2	1:A:408:PRO:CD	2.32	0.60
1:D:130:ASN:HB3	1:D:134:THR:OG1	2.02	0.60
1:A:216:TYR:C	1:A:216:TYR:CD1	2.75	0.60
1:A:216:TYR:C	1:A:216:TYR:HD1	2.05	0.60
1:B:143:ASN:HB3	1:B:780:ARG:NH1	2.13	0.60
1:E:81:VAL:HG13	1:E:86:VAL:HG23	1.82	0.60
1:F:224:THR:CG2	1:F:228:GLU:HG3	2.32	0.60
1:A:302:GLY:CA	3:A:902:FRU:HO1	2.11	0.60
1:A:298:TYR:HE1	1:A:649:MET:HE1	1.67	0.60
1:D:784:ARG:O	1:D:788:GLU:HG3	2.02	0.60
1:B:420:LEU:C	1:B:420:LEU:HD13	2.22	0.59
1:G:451:TYR:HB3	1:G:454:LYS:HE2	1.84	0.59
1:C:633:ILE:HA	1:C:638:LEU:HD12	1.84	0.59
1:H:315:LEU:HG	1:H:319:MET:HE1	1.84	0.59
1:A:35:ARG:CZ	1:A:86:VAL:HG12	2.32	0.59
1:A:35:ARG:NH2	1:A:86:VAL:HG12	2.17	0.59
1:F:486:ILE:HG22	1:F:516:VAL:HG22	1.82	0.59
1:F:209:THR:HG21	1:F:236:ILE:O	2.02	0.59
1:H:45:GLN:NE2	1:H:80:ILE:HG13	2.18	0.59
1:E:752:LYS:HB3	1:E:753:TYR:CE2	2.37	0.59
1:G:143:ASN:CA	1:G:780:ARG:HH12	2.04	0.59
1:D:217:LEU:CD1	1:D:233:PHE:HZ	2.07	0.59
1:E:160:ASP:O	1:E:164:ARG:HG3	2.02	0.59
1:F:173:ASP:HB3	1:F:176:SER:HB3	1.85	0.59
1:F:72:LEU:C	1:F:72:LEU:HD13	2.23	0.59
1:H:754:THR:HA	7:H:864:HOH:O	2.01	0.59
1:A:796:ARG:O	1:A:800:GLN:HG3	2.03	0.59
1:D:315:LEU:HG	1:D:319:MET:CE	2.33	0.59
1:G:56:LEU:HD13	1:G:63:LYS:HG2	1.84	0.59
1:B:30:LEU:HD11	1:E:405:ASN:ND2	2.17	0.59
1:D:534:PHE:HB2	1:D:535:PRO:CD	2.33	0.59
1:D:86:VAL:CG1	1:D:102:VAL:HG12	2.32	0.59
1:G:169:LYS:HG2	1:G:176:SER:OG	2.02	0.59
1:G:410:LEU:HD12	1:G:411:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ARG:HD2	1:A:659:ARG:HD2	1.85	0.59
1:B:55:ALA:HB1	1:B:59:GLN:HE22	1.68	0.59
1:C:125:VAL:HG12	1:C:126:ASP:OD1	2.03	0.59
1:E:72:LEU:CD2	1:E:90:VAL:HG11	2.33	0.59
1:F:534:PHE:HB2	1:F:535:PRO:CD	2.32	0.59
1:A:220:LEU:N	1:A:220:LEU:CD1	2.66	0.58
1:B:55:ALA:HB1	1:B:59:GLN:NE2	2.17	0.58
1:C:147:PRO:HB2	1:D:172:HIS:ND1	2.18	0.58
1:E:112:LEU:N	1:E:112:LEU:HD23	2.16	0.58
1:B:561:LYS:HD3	1:B:613:ARG:O	2.02	0.58
1:C:83:PRO:HG2	1:C:84:PRO:CD	2.26	0.58
1:D:113:GLN:HG3	1:D:114:PRO:CD	2.30	0.58
1:F:65:GLU:OE2	1:F:68:PRO:HG2	2.03	0.58
1:G:259:LEU:O	1:G:263:PRO:HG3	2.02	0.58
1:G:534:PHE:HB2	1:G:535:PRO:CD	2.33	0.58
1:D:486:ILE:HG22	1:D:516:VAL:HG22	1.85	0.58
1:D:730:LYS:HE3	5:D:921:MLA:O3A	2.03	0.58
1:E:111:GLU:C	1:E:112:LEU:HD23	2.24	0.58
1:F:54:GLU:HG3	1:F:55:ALA:N	2.17	0.58
1:F:79:ALA:HB2	1:F:88:LEU:HD23	1.85	0.58
1:C:216:TYR:CE2	1:C:232:LYS:HG2	2.38	0.58
1:C:210:LEU:HD22	1:C:253:ILE:HG23	1.86	0.58
1:C:702:ILE:HA	1:C:753:TYR:OH	2.03	0.58
1:C:80:ILE:HD11	1:C:121:LYS:CG	2.33	0.58
1:E:304:GLN:CB	3:E:902:FRU:C1	2.78	0.58
1:E:315:LEU:HG	1:E:319:MET:HE2	1.85	0.58
1:E:37:GLU:HG2	1:E:54:GLU:OE2	2.02	0.58
1:B:484:GLN:OE1	1:B:697:GLY:HA2	2.03	0.58
1:F:56:LEU:N	1:F:57:PRO:CD	2.66	0.58
1:G:82:LEU:N	1:G:83:PRO:CD	2.67	0.58
1:B:248:ARG:HH11	1:B:248:ARG:HB3	1.69	0.58
1:C:140:GLU:N	1:C:141:PRO:HD2	2.17	0.58
1:C:534:PHE:HB2	1:C:535:PRO:HD2	1.86	0.58
1:F:145:SER:HB3	1:F:779:ASP:OD2	2.03	0.58
1:C:437:ALA:O	1:C:438:HIS:HB2	2.04	0.58
1:C:50:ILE:HD11	1:C:54:GLU:HG2	1.86	0.58
1:D:37:GLU:HB3	1:D:54:GLU:OE2	2.04	0.58
1:H:340:LEU:HD11	1:H:350:GLY:O	2.04	0.58
1:A:143:ASN:HB3	1:A:148:ARG:NH2	2.19	0.58
1:A:171:PHE:CD1	1:A:263:PRO:HD2	2.38	0.58
1:C:216:TYR:O	1:C:220:LEU:HD13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ILE:O	1:D:44:LEU:HB2	2.03	0.58
1:E:233:PHE:HB3	1:E:238:LEU:HB2	1.85	0.58
1:E:45:GLN:CB	1:E:80:ILE:HD13	2.34	0.58
1:A:176:SER:O	1:A:179:PRO:HD2	2.04	0.58
1:A:48:GLN:O	1:A:49:ILE:C	2.41	0.58
1:A:514:ILE:HG13	1:A:515:ASP:N	2.19	0.58
1:E:164:ARG:HD2	1:F:262:ALA:HB1	1.85	0.58
1:F:219:GLU:HA	1:F:219:GLU:OE1	2.03	0.58
1:G:564:LEU:HD22	1:G:613:ARG:CZ	2.34	0.58
1:A:216:TYR:CD1	1:A:220:LEU:HD11	2.39	0.58
1:B:146:ILE:HG12	1:B:147:PRO:O	2.04	0.58
1:C:107:LEU:O	1:C:108:VAL:CG1	2.52	0.58
1:D:82:LEU:CD1	1:D:84:PRO:HD2	2.30	0.58
1:A:63:LYS:C	1:A:65:GLU:H	2.05	0.57
1:A:85:TRP:CG	1:A:101:ARG:HD2	2.39	0.57
1:F:387:PRO:HD3	1:F:802:VAL:HB	1.85	0.57
1:F:582:ASP:HB2	1:F:621:GLU:OE1	2.03	0.57
1:F:789:MET:CE	1:G:789:MET:CB	2.80	0.57
1:H:85:TRP:CE3	1:H:101:ARG:NE	2.71	0.57
1:D:83:PRO:O	1:D:104:LEU:HD12	2.04	0.57
1:E:561:LYS:HD3	1:E:613:ARG:O	2.02	0.57
1:F:116:GLU:O	1:F:119:HIS:HB2	2.04	0.57
1:B:333:ARG:HG2	1:B:333:ARG:HH11	1.69	0.57
1:B:54:GLU:HA	1:B:54:GLU:OE1	2.04	0.57
1:C:65:GLU:O	1:C:70:PHE:HB2	2.04	0.57
1:F:45:GLN:HB3	1:F:80:ILE:HA	1.86	0.57
1:G:542:ARG:HD2	1:G:659:ARG:HD2	1.85	0.57
1:G:83:PRO:HG2	1:G:85:TRP:H	1.68	0.57
1:B:789:MET:HG2	1:C:789:MET:HE3	1.85	0.57
1:G:217:LEU:HD11	1:G:233:PHE:CZ	2.38	0.57
1:H:407:LYS:HB2	1:H:408:PRO:HD2	1.84	0.57
1:A:789:MET:CE	1:D:789:MET:HE3	2.31	0.57
1:B:210:LEU:HD22	1:B:253:ILE:HG23	1.85	0.57
1:D:220:LEU:CD1	1:D:220:LEU:H	2.18	0.57
1:D:56:LEU:HB3	1:D:57:PRO:CD	2.33	0.57
1:A:789:MET:CE	1:D:789:MET:HE2	2.33	0.57
1:H:748:ARG:HH12	1:H:752:LYS:HE3	1.70	0.57
1:C:80:ILE:CD1	1:C:121:LYS:HG3	2.34	0.57
1:E:216:TYR:CD2	1:E:232:LYS:HG2	2.39	0.57
1:F:32:LEU:O	1:F:36:VAL:HG23	2.04	0.57
1:A:407:LYS:HB2	1:A:408:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:LYS:O	1:B:632:LEU:HG	2.04	0.57
1:C:790:PHE:O	1:C:794:LYS:HB3	2.04	0.57
1:G:172:HIS:ND1	1:H:147:PRO:HB2	2.19	0.57
1:G:504:LEU:CD1	1:G:507:LEU:HD23	2.34	0.57
1:H:173:ASP:CB	1:H:176:SER:HB3	2.34	0.57
1:D:173:ASP:HB3	1:D:176:SER:HB2	1.86	0.57
1:E:52:GLU:OE1	1:E:57:PRO:HD3	2.04	0.57
1:F:101:ARG:HB2	1:F:112:LEU:HD21	1.87	0.57
1:G:386:TRP:N	1:G:387:PRO:HD2	2.19	0.57
1:A:49:ILE:O	1:A:53:PHE:CB	2.53	0.57
1:B:103:ASN:HD22	1:B:103:ASN:H	1.51	0.57
1:F:789:MET:HE1	1:G:790:PHE:N	2.18	0.57
1:B:284:LEU:HD22	1:B:284:LEU:N	2.19	0.57
1:C:54:GLU:HG3	1:C:55:ALA:N	2.20	0.57
1:D:216:TYR:CD1	1:D:220:LEU:HD11	2.40	0.57
1:E:171:PHE:CD1	1:E:263:PRO:HD2	2.40	0.57
1:H:319:MET:HE1	1:H:334:ILE:HD11	1.85	0.57
1:A:46:GLN:OE1	1:A:46:GLN:HA	2.05	0.56
1:C:434:CYS:HB2	1:C:477:PHE:CZ	2.40	0.56
1:B:118:LEU:O	1:B:122:GLU:HG3	2.04	0.56
1:B:232:LYS:O	1:B:236:ILE:HG23	2.05	0.56
1:B:407:LYS:HB2	1:B:408:PRO:CD	2.35	0.56
1:B:56:LEU:CD2	1:B:65:GLU:OE2	2.52	0.56
1:C:87:ALA:O	1:C:88:LEU:HD23	2.05	0.56
1:G:339:ARG:NH1	1:G:380:ILE:HG13	2.19	0.56
1:B:153:LYS:HD3	1:B:154:TYR:CE2	2.39	0.56
1:B:30:LEU:N	1:B:30:LEU:HD12	2.19	0.56
1:C:442:LYS:HD2	1:C:449:ASP:HB3	1.87	0.56
1:C:278:VAL:HG21	1:C:763:LEU:HD23	1.87	0.56
1:D:43:ILE:O	1:D:44:LEU:HD23	2.06	0.56
1:E:178:LEU:N	1:E:179:PRO:CD	2.68	0.56
1:F:248:ARG:HH11	1:F:248:ARG:HB3	1.70	0.56
1:F:354:GLU:OE1	1:F:366:ARG:NH2	2.38	0.56
1:F:390:GLU:OE1	1:F:796:ARG:HD2	2.04	0.56
1:F:46:GLN:CB	1:F:50:ILE:HG22	2.29	0.56
1:F:48:GLN:O	1:F:51:ALA:O	2.22	0.56
1:F:66:GLY:O	1:F:68:PRO:HD2	2.05	0.56
1:G:124:LEU:HD23	1:G:124:LEU:O	2.05	0.56
1:H:224:THR:HG23	1:H:228:GLU:HG3	1.86	0.56
1:H:484:GLN:OE1	1:H:697:GLY:HA2	2.06	0.56
1:B:162:LEU:HD11	1:B:772:TRP:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LEU:HG	1:D:261:GLU:OE1	2.06	0.56
1:D:69:PHE:O	1:D:69:PHE:CD1	2.59	0.56
1:H:82:LEU:HD21	1:H:85:TRP:CB	2.31	0.56
1:A:62:LYS:C	1:A:64:LEU:H	2.09	0.56
1:B:166:LEU:HB3	1:B:268:LEU:CD2	2.35	0.56
1:B:56:LEU:CD1	1:B:65:GLU:OE2	2.53	0.56
1:B:789:MET:HB3	1:C:789:MET:HE1	1.86	0.56
1:E:441:GLU:HA	1:E:441:GLU:OE1	2.06	0.56
1:D:462:SER:HB2	1:D:507:LEU:HD21	1.87	0.56
1:F:85:TRP:CZ3	1:F:101:ARG:HG2	2.40	0.56
1:G:340:LEU:HB2	1:G:366:ARG:HB3	1.87	0.56
1:D:419:ASN:HB3	1:D:471:ALA:CB	2.36	0.56
1:D:54:GLU:CG	1:D:55:ALA:N	2.68	0.56
1:D:83:PRO:HB2	1:D:84:PRO:CD	2.34	0.56
1:E:125:VAL:CG1	1:E:126:ASP:N	2.69	0.56
1:B:354:GLU:OE1	1:B:366:ARG:NH2	2.37	0.56
1:E:79:ALA:HB2	1:E:88:LEU:CD2	2.35	0.56
1:F:83:PRO:HG2	1:F:85:TRP:CB	2.35	0.56
1:G:102:VAL:HG22	1:G:109:VAL:HG22	1.87	0.56
1:B:583:ARG:HG2	1:B:583:ARG:HH11	1.71	0.56
1:E:230:GLU:O	1:E:234:GLU:HG3	2.05	0.56
1:G:170:LEU:HD13	1:G:177:LEU:HD23	1.87	0.56
1:G:82:LEU:CB	1:G:83:PRO:HD3	2.34	0.56
1:A:145:SER:HB3	1:A:779:ASP:OD2	2.06	0.56
1:C:80:ILE:HD11	1:C:121:LYS:HG2	1.88	0.56
1:F:371:THR:OG1	1:F:373:LYS:HE3	2.06	0.56
1:G:220:LEU:H	1:G:220:LEU:CD1	2.19	0.56
1:C:302:GLY:CA	3:C:902:FRU:O1	2.54	0.56
1:E:586:ASN:HB3	1:E:671:PRO:O	2.06	0.56
1:F:609:VAL:HG22	1:F:645:ILE:HB	1.88	0.56
1:F:83:PRO:CG	1:F:85:TRP:H	2.19	0.56
1:H:224:THR:CG2	1:H:228:GLU:HG3	2.36	0.56
1:H:52:GLU:CD	1:H:53:PHE:N	2.59	0.56
1:B:48:GLN:HG2	1:B:76:THR:O	2.05	0.55
1:C:216:TYR:CD2	1:C:232:LYS:HG2	2.41	0.55
1:D:53:PHE:O	1:D:57:PRO:HG2	2.06	0.55
1:E:716:HIS:HB3	4:E:913:SO4:O2	2.06	0.55
1:F:284:LEU:HD13	1:F:337:LEU:HB2	1.86	0.55
1:F:420:LEU:HD13	1:F:420:LEU:C	2.27	0.55
1:G:81:VAL:HG22	1:G:81:VAL:O	2.06	0.55
1:C:210:LEU:CD2	1:C:253:ILE:HG23	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:GLU:CG	1:F:55:ALA:N	2.68	0.55
1:D:221:LYS:HD2	1:D:222:SER:H	1.71	0.55
1:G:54:GLU:CG	1:G:55:ALA:N	2.69	0.55
1:H:216:TYR:HE2	1:H:232:LYS:HG2	1.67	0.55
1:A:216:TYR:HD1	1:A:216:TYR:O	1.89	0.55
1:C:56:LEU:HB3	1:C:57:PRO:HD3	1.88	0.55
1:D:140:GLU:N	1:D:141:PRO:HD2	2.21	0.55
1:E:243:GLY:HA2	1:E:326:GLN:HA	1.87	0.55
1:E:45:GLN:HB3	1:E:80:ILE:HD13	1.89	0.55
1:G:216:TYR:HD1	1:G:216:TYR:O	1.89	0.55
1:B:407:LYS:HB2	1:B:408:PRO:HD2	1.88	0.55
1:D:411:ILE:CD1	1:D:431:VAL:HB	2.37	0.55
1:G:171:PHE:HD1	1:G:263:PRO:HD2	1.71	0.55
1:H:135:LEU:HD12	1:H:136:GLU:N	2.20	0.55
1:H:138:ASP:OD1	1:H:141:PRO:HD2	2.06	0.55
1:C:491:GLU:CD	1:C:491:GLU:H	2.10	0.55
1:F:348:THR:O	1:F:351:GLU:HG2	2.05	0.55
1:H:173:ASP:CB	1:H:176:SER:CB	2.85	0.55
1:C:151:LEU:HD12	1:D:261:GLU:HG2	1.89	0.55
1:F:83:PRO:HG2	1:F:85:TRP:O	2.07	0.55
1:H:304:GLN:HB3	3:H:902:FRU:O1	2.06	0.55
1:H:583:ARG:HG2	1:H:583:ARG:HH11	1.72	0.55
1:B:39:LYS:CB	1:B:104:LEU:CD1	2.82	0.55
1:D:207:GLN:OE1	1:D:211:ARG:NH2	2.40	0.55
1:G:442:LYS:HB2	7:G:860:HOH:O	2.07	0.55
1:H:80:ILE:HG12	1:H:121:LYS:HG2	1.89	0.55
1:A:298:TYR:HE1	1:A:649:MET:CE	2.19	0.55
1:E:147:PRO:HB2	1:F:172:HIS:ND1	2.22	0.55
1:H:121:LYS:HE2	1:H:450:ILE:HD11	1.88	0.55
1:B:59:GLN:HG3	1:B:60:THR:H	1.72	0.54
1:B:793:LEU:CD1	1:C:135:LEU:HD22	2.30	0.54
1:C:41:LYS:O	1:C:44:LEU:CD1	2.55	0.54
1:D:181:LEU:HD13	1:D:206:LEU:HD22	1.88	0.54
1:E:143:ASN:HB3	1:E:148:ARG:HH12	1.72	0.54
1:E:30:LEU:HD11	1:E:62:LYS:HB3	1.88	0.54
1:G:65:GLU:HB3	1:G:68:PRO:HG3	1.88	0.54
1:H:564:LEU:HD22	1:H:613:ARG:CZ	2.37	0.54
1:C:216:TYR:CD2	1:C:232:LYS:HE2	2.43	0.54
1:D:44:LEU:CD1	1:D:45:GLN:H	2.20	0.54
1:F:276:PRO:HG3	1:F:326:GLN:CG	2.37	0.54
1:D:102:VAL:HG23	1:D:108:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LEU:HG	1:D:319:MET:HE1	1.89	0.54
1:A:43:ILE:HG23	1:A:82:LEU:HD23	1.89	0.54
1:B:76:THR:O	1:B:76:THR:HG23	2.06	0.54
1:C:295:VAL:HB	1:C:301:THR:HG21	1.89	0.54
1:A:259:LEU:HD21	1:A:267:THR:HG22	1.89	0.54
1:A:704:VAL:HA	4:A:912:SO4:O3	2.08	0.54
1:B:322:ARG:HD3	1:B:763:LEU:HD13	1.90	0.54
1:C:69:PHE:HE1	1:C:73:LEU:HD11	1.72	0.54
1:E:196:LEU:HD11	1:E:206:LEU:HD13	1.90	0.54
1:G:172:HIS:CE1	1:H:147:PRO:HB2	2.42	0.54
1:H:609:VAL:HG22	1:H:645:ILE:HB	1.89	0.54
1:D:216:TYR:CE1	1:D:220:LEU:HD21	2.38	0.54
1:D:86:VAL:HG12	1:D:102:VAL:CG1	2.37	0.54
1:H:386:TRP:HH2	1:H:416:SER:HB3	1.72	0.54
1:A:420:LEU:C	1:A:420:LEU:HD13	2.28	0.54
1:D:145:SER:HB3	1:D:779:ASP:CG	2.15	0.54
1:D:160:ASP:O	1:D:164:ARG:HG3	2.08	0.54
1:F:162:LEU:HD11	1:F:772:TRP:CE2	2.43	0.54
1:F:52:GLU:O	1:F:57:PRO:CD	2.56	0.54
1:F:659:ARG:O	1:F:662:CYS:HB2	2.07	0.54
1:C:164:ARG:HD2	1:D:262:ALA:HB1	1.89	0.54
1:C:400:LEU:HD12	1:C:400:LEU:C	2.28	0.54
1:D:112:LEU:HD22	1:D:116:GLU:HB3	1.90	0.54
1:E:44:LEU:HD22	1:E:124:LEU:HD11	1.88	0.54
1:H:480:THR:HB	1:H:485:GLU:CD	2.27	0.54
1:B:232:LYS:O	1:B:235:GLU:HB2	2.07	0.54
1:B:80:ILE:CG2	1:B:87:ALA:HB3	2.37	0.54
1:D:433:GLN:O	1:D:476:ASP:HB2	2.06	0.54
1:F:276:PRO:HG3	1:F:326:GLN:CB	2.38	0.54
1:B:789:MET:CE	1:C:789:MET:CE	2.85	0.54
1:C:304:GLN:CB	3:C:902:FRU:H12	2.36	0.53
1:E:784:ARG:O	1:E:788:GLU:HG3	2.08	0.53
1:B:83:PRO:O	1:B:85:TRP:N	2.42	0.53
1:B:80:ILE:HG22	1:B:87:ALA:O	2.08	0.53
1:E:143:ASN:HB2	1:E:148:ARG:HH12	1.74	0.53
1:G:124:LEU:HD23	1:G:124:LEU:C	2.29	0.53
1:H:84:PRO:HB2	1:H:85:TRP:CD1	2.43	0.53
1:A:48:GLN:H	1:A:51:ALA:HB3	1.73	0.53
1:D:52:GLU:CD	1:D:53:PHE:N	2.62	0.53
1:E:290:PHE:O	1:E:366:ARG:NH1	2.39	0.53
1:E:545:LYS:HG2	4:E:914:SO4:O4	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:386:TRP:CH2	1:G:464:GLN:HG3	2.43	0.53
1:A:140:GLU:HB3	1:A:141:PRO:HD3	1.90	0.53
1:B:437:ALA:O	1:B:438:HIS:HB2	2.09	0.53
1:F:81:VAL:CG1	1:F:86:VAL:CG2	2.84	0.53
1:G:173:ASP:HB3	1:G:176:SER:CB	2.38	0.53
1:G:181:LEU:HD13	1:G:206:LEU:HD22	1.90	0.53
1:B:386:TRP:N	1:B:387:PRO:HD2	2.24	0.53
1:E:216:TYR:CE2	1:E:232:LYS:HG2	2.43	0.53
1:E:233:PHE:O	1:E:236:ILE:HG12	2.09	0.53
1:E:43:ILE:HG23	1:E:44:LEU:H	1.74	0.53
1:E:645:ILE:HG22	1:E:646:SER:O	2.08	0.53
1:A:156:GLY:HA3	1:A:523:ILE:HG13	1.91	0.53
1:A:61:ARG:C	1:A:63:LYS:N	2.62	0.53
1:A:796:ARG:HB2	1:A:797:PRO:HD3	1.90	0.53
1:B:53:PHE:HA	1:B:57:PRO:CG	2.33	0.53
1:C:54:GLU:O	1:C:58:GLU:CB	2.56	0.53
1:C:69:PHE:CE1	1:C:73:LEU:HD11	2.43	0.53
1:D:582:ASP:OD1	1:D:582:ASP:C	2.46	0.53
1:D:91:ARG:NH2	1:D:94:PRO:HA	2.24	0.53
1:G:264:ASP:OD1	1:G:267:THR:HB	2.09	0.53
1:G:564:LEU:HD22	1:G:613:ARG:NH2	2.24	0.53
1:H:441:GLU:OE1	1:H:444:LYS:HD3	2.09	0.53
1:B:173:ASP:HB2	1:B:176:SER:HB3	1.90	0.53
1:B:226:TYR:HB3	1:B:240:ARG:HH21	1.73	0.53
1:B:93:ARG:HB2	1:B:96:VAL:HG21	1.90	0.53
1:C:32:LEU:HD21	1:C:105:HIS:HA	1.90	0.53
1:D:538:GLU:OE1	1:D:541:ARG:HD3	2.09	0.53
1:E:304:GLN:HB2	3:E:902:FRU:H12	1.90	0.53
1:F:437:ALA:C	1:F:439:ALA:H	2.12	0.53
1:F:81:VAL:HG12	1:F:86:VAL:CA	2.36	0.53
1:H:615:LYS:HE2	1:H:616:GLU:O	2.08	0.53
1:H:670:GLN:O	1:H:670:GLN:HG3	2.08	0.53
1:A:33:LEU:O	1:A:36:VAL:HB	2.09	0.53
1:A:399:GLU:HG2	7:A:860:HOH:O	2.07	0.53
1:B:44:LEU:O	1:B:81:VAL:N	2.42	0.53
1:C:131:GLY:CA	1:C:134:THR:HG23	2.35	0.53
1:E:105:HIS:O	1:E:106:ALA:CB	2.57	0.53
1:F:357:TYR:CE2	5:F:922:MLA:HC22	2.44	0.53
1:G:609:VAL:HG22	1:G:645:ILE:HB	1.90	0.53
1:G:580:ARG:HD3	2:G:901:UDP:O3B	2.09	0.53
1:H:590:LEU:HB2	1:H:671:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLN:HE22	1:A:80:ILE:HD13	1.72	0.53
1:C:410:LEU:HD12	1:C:411:ILE:H	1.73	0.53
1:C:441:GLU:OE1	1:C:441:GLU:HA	2.08	0.53
1:D:103:ASN:CB	1:D:108:VAL:CG1	2.87	0.53
1:G:119:HIS:CE1	1:G:129:LYS:CD	2.68	0.53
1:G:518:ASP:OD1	1:G:520:LYS:HG2	2.09	0.53
1:H:534:PHE:HB2	1:H:535:PRO:CD	2.39	0.53
1:B:442:LYS:HD2	1:B:449:ASP:HB3	1.91	0.53
1:E:100:LEU:O	1:E:100:LEU:HD12	2.09	0.53
1:E:230:GLU:OE1	1:E:240:ARG:NH1	2.42	0.53
1:E:772:TRP:CH2	1:E:776:SER:HB3	2.44	0.53
1:F:216:TYR:CD1	1:F:216:TYR:C	2.82	0.53
1:F:778:LEU:N	1:F:778:LEU:CD1	2.72	0.53
1:G:226:TYR:CE2	1:G:240:ARG:HG2	2.43	0.53
1:B:216:TYR:CD2	1:B:232:LYS:HG2	2.43	0.52
1:B:63:LYS:CG	1:B:64:LEU:H	2.23	0.52
1:E:315:LEU:HG	1:E:319:MET:CE	2.38	0.52
1:G:173:ASP:HB3	1:G:176:SER:HB3	1.91	0.52
1:G:477:PHE:HA	1:G:520:LYS:HB2	1.92	0.52
1:A:146:ILE:CG1	1:A:147:PRO:CD	2.86	0.52
1:B:226:TYR:CE2	1:B:240:ARG:HG2	2.45	0.52
1:D:82:LEU:C	1:D:82:LEU:CD1	2.77	0.52
1:F:54:GLU:O	1:F:57:PRO:HD2	2.10	0.52
1:H:107:LEU:O	1:H:108:VAL:HG23	2.08	0.52
1:H:131:GLY:O	1:H:134:THR:HG23	2.09	0.52
1:H:72:LEU:CD2	1:H:90:VAL:HG11	2.39	0.52
1:A:304:GLN:HB3	3:A:902:FRU:H12	1.90	0.52
1:C:233:PHE:HE1	1:C:249:VAL:HG11	1.75	0.52
1:D:32:LEU:HD21	1:D:106:ALA:H	1.73	0.52
1:F:420:LEU:C	1:F:420:LEU:CD1	2.78	0.52
1:F:784:ARG:O	1:F:788:GLU:HG3	2.10	0.52
1:G:128:VAL:HG22	1:G:129:LYS:N	2.24	0.52
1:G:171:PHE:CD1	1:G:263:PRO:HD2	2.45	0.52
1:H:435:THR:HG23	1:H:475:THR:HB	1.91	0.52
1:H:779:ASP:N	1:H:779:ASP:OD2	2.41	0.52
1:A:386:TRP:N	1:A:387:PRO:HD2	2.25	0.52
1:G:230:GLU:O	1:G:234:GLU:HG3	2.09	0.52
1:H:187:HIS:NE2	1:H:276:PRO:O	2.41	0.52
1:H:39:LYS:HD3	1:H:39:LYS:C	2.30	0.52
1:A:298:TYR:CE1	1:A:649:MET:CE	2.92	0.52
1:D:209:THR:HG23	1:D:236:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:GLN:HA	1:D:45:GLN:NE2	2.19	0.52
1:D:479:ILE:HD11	1:D:762:LEU:HD13	1.91	0.52
1:D:616:GLU:HA	1:D:616:GLU:OE1	2.09	0.52
1:E:79:ALA:CB	1:E:88:LEU:CD2	2.87	0.52
1:E:81:VAL:HG13	1:E:86:VAL:CG2	2.40	0.52
1:H:49:ILE:O	1:H:53:PHE:CB	2.58	0.52
1:B:102:VAL:CB	1:B:109:VAL:CB	2.88	0.52
1:B:30:LEU:O	1:B:33:LEU:HB2	2.08	0.52
1:C:581:LEU:HD11	1:C:625:GLU:HG3	1.92	0.52
1:F:216:TYR:CD2	1:F:232:LYS:HG2	2.44	0.52
1:F:233:PHE:HD1	1:F:238:LEU:CB	2.22	0.52
1:F:417:ASP:O	1:F:421:VAL:HG23	2.09	0.52
1:H:242:TRP:CB	1:H:249:VAL:HG13	2.40	0.52
1:A:35:ARG:NH2	1:A:102:VAL:H	2.07	0.52
1:A:140:GLU:N	1:A:141:PRO:HD2	2.25	0.52
1:B:54:GLU:CG	1:B:55:ALA:N	2.68	0.52
1:C:354:GLU:OE1	1:C:366:ARG:NH2	2.43	0.52
1:D:333:ARG:HG2	1:D:333:ARG:HH11	1.75	0.52
1:E:35:ARG:CZ	1:E:35:ARG:HB2	2.39	0.52
1:E:73:LEU:HD13	1:E:73:LEU:O	2.09	0.52
1:G:479:ILE:CD1	1:G:762:LEU:HD13	2.39	0.52
1:A:48:GLN:H	1:A:51:ALA:CB	2.23	0.52
1:A:572:LYS:CE	1:A:605:ASN:OD1	2.57	0.52
1:B:586:ASN:HB3	1:B:671:PRO:O	2.09	0.52
1:C:47:ASN:O	1:C:51:ALA:N	2.39	0.52
1:C:72:LEU:C	1:C:72:LEU:CD1	2.76	0.52
1:E:220:LEU:HD12	1:E:220:LEU:N	2.24	0.52
1:H:564:LEU:HD22	1:H:613:ARG:NH2	2.24	0.52
1:H:566:VAL:O	1:H:640:GLY:HA2	2.09	0.52
1:A:79:ALA:HB2	1:A:88:LEU:CD2	2.40	0.52
1:C:50:ILE:C	1:C:50:ILE:HD12	2.30	0.52
1:D:796:ARG:HB2	1:D:797:PRO:HD3	1.92	0.52
1:F:103:ASN:HB3	1:F:106:ALA:O	2.10	0.52
1:F:224:THR:HG22	1:F:228:GLU:HG3	1.92	0.52
1:F:796:ARG:HB2	1:F:797:PRO:HD3	1.92	0.52
1:H:560:ASN:OD1	1:H:562:GLU:HB2	2.09	0.52
1:A:35:ARG:HH21	1:A:102:VAL:CB	2.21	0.52
1:B:209:THR:HG23	1:B:236:ILE:HG13	1.92	0.52
1:C:50:ILE:HD12	1:C:54:GLU:HG2	1.90	0.52
1:D:125:VAL:HG13	1:D:126:ASP:H	1.75	0.52
1:F:524:VAL:HG12	1:F:758:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:ASN:HB3	1:G:106:ALA:O	2.09	0.52
1:A:434:CYS:HB2	1:A:477:PHE:CZ	2.44	0.51
1:A:437:ALA:O	1:A:438:HIS:HB2	2.11	0.51
1:A:472:MET:HG2	1:A:514:ILE:HD13	1.91	0.51
1:B:55:ALA:O	1:B:59:GLN:CB	2.52	0.51
1:C:226:TYR:O	1:C:230:GLU:HB2	2.10	0.51
1:C:535:PRO:HD2	1:C:538:GLU:OE2	2.09	0.51
1:D:411:ILE:HG13	1:D:431:VAL:HG11	1.92	0.51
1:D:72:LEU:HD13	1:D:72:LEU:C	2.30	0.51
1:F:284:LEU:N	1:F:284:LEU:HD22	2.25	0.51
1:H:125:VAL:HG12	1:H:126:ASP:N	2.24	0.51
1:H:553:LEU:HG	1:H:645:ILE:HD13	1.91	0.51
1:C:86:VAL:HG12	1:C:102:VAL:HG23	1.92	0.51
1:F:143:ASN:HB3	1:F:148:ARG:HH22	1.73	0.51
1:H:164:ARG:CG	1:H:164:ARG:NH1	2.71	0.51
1:H:216:TYR:CE1	1:H:220:LEU:CD1	2.89	0.51
1:A:54:GLU:CG	1:A:55:ALA:N	2.63	0.51
1:D:82:LEU:HD12	1:D:85:TRP:H	1.74	0.51
1:E:796:ARG:O	1:E:800:GLN:HG3	2.11	0.51
1:G:243:GLY:HA2	1:G:326:GLN:HA	1.92	0.51
1:H:72:LEU:C	1:H:72:LEU:HD13	2.31	0.51
1:A:147:PRO:HB2	1:B:172:HIS:ND1	2.25	0.51
1:A:36:VAL:O	1:A:39:LYS:HG3	2.09	0.51
1:C:770:GLY:O	1:C:773:LYS:HB2	2.10	0.51
1:D:216:TYR:C	1:D:216:TYR:HD1	2.13	0.51
1:D:534:PHE:HB2	1:D:535:PRO:HD2	1.92	0.51
1:A:670:GLN:HG3	1:A:670:GLN:O	2.09	0.51
1:B:224:THR:CG2	1:B:228:GLU:HG3	2.40	0.51
1:C:105:HIS:O	1:C:106:ALA:CB	2.58	0.51
1:E:606:LEU:HD23	1:E:642:PHE:CD1	2.45	0.51
1:F:32:LEU:O	1:F:32:LEU:HD13	2.10	0.51
1:F:437:ALA:O	1:F:438:HIS:HB2	2.09	0.51
1:B:581:LEU:CD1	1:B:625:GLU:HG2	2.40	0.51
1:B:92:PRO:HD2	1:B:96:VAL:O	2.10	0.51
1:B:92:PRO:HG2	1:B:96:VAL:CG2	2.40	0.51
1:C:54:GLU:OE2	1:C:55:ALA:HA	2.10	0.51
1:E:411:ILE:HG13	1:E:431:VAL:CG1	2.39	0.51
1:F:534:PHE:HB2	1:F:535:PRO:HD2	1.92	0.51
1:A:105:HIS:O	1:A:106:ALA:HB2	2.10	0.51
1:B:789:MET:HE3	1:C:789:MET:CE	2.41	0.51
1:C:390:GLU:OE1	1:C:796:ARG:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:HB2	1:D:83:PRO:HD3	1.92	0.51
1:F:216:TYR:HD1	1:F:216:TYR:C	2.14	0.51
1:F:46:GLN:HB3	1:F:50:ILE:CG2	2.32	0.51
1:G:692:PHE:CD1	1:G:692:PHE:N	2.79	0.51
1:H:146:ILE:HG13	1:H:147:PRO:CD	2.35	0.51
1:H:468:ASP:O	1:H:472:MET:HB2	2.11	0.51
1:C:173:ASP:OD2	1:C:176:SER:HB2	2.11	0.51
1:D:82:LEU:HB2	1:D:83:PRO:CD	2.40	0.51
1:F:226:TYR:CE2	1:F:240:ARG:HG2	2.45	0.51
1:F:65:GLU:HB3	1:F:70:PHE:HB2	1.93	0.51
1:G:419:ASN:HB3	1:G:471:ALA:HB1	1.91	0.51
1:H:322:ARG:HD2	1:H:763:LEU:HD13	1.93	0.51
1:A:59:GLN:HG3	1:A:60:THR:H	1.74	0.51
1:A:682:VAL:HG13	1:A:749:ILE:HD12	1.93	0.51
1:E:173:ASP:HB3	1:E:176:SER:CB	2.40	0.51
1:F:778:LEU:CD1	1:F:778:LEU:H	2.23	0.51
1:B:445:TYR:O	1:B:448:SER:HB3	2.11	0.51
1:C:43:ILE:O	1:C:44:LEU:CG	2.59	0.51
1:C:514:ILE:HG13	1:C:515:ASP:N	2.26	0.51
1:D:354:GLU:OE1	1:D:366:ARG:NH2	2.44	0.51
1:D:80:ILE:N	1:D:80:ILE:HD12	2.26	0.51
1:E:176:SER:O	1:E:179:PRO:HD2	2.11	0.51
1:F:155:ILE:HD13	1:F:516:VAL:HG13	1.93	0.51
1:G:542:ARG:CD	1:G:659:ARG:HD2	2.41	0.51
1:H:319:MET:O	1:H:323:ILE:HG13	2.11	0.51
1:C:50:ILE:O	1:C:50:ILE:HD12	2.10	0.50
1:E:135:LEU:HD11	1:H:789:MET:HG3	1.93	0.50
1:F:233:PHE:CD1	1:F:238:LEU:CD1	2.95	0.50
1:F:83:PRO:HD2	1:F:85:TRP:O	2.11	0.50
1:G:31:ALA:HB3	1:G:35:ARG:NH2	2.26	0.50
1:G:82:LEU:CG	1:G:83:PRO:HD3	2.38	0.50
1:H:72:LEU:HD22	1:H:90:VAL:HG11	1.92	0.50
1:D:82:LEU:HG	1:D:120:PHE:CE1	2.47	0.50
1:G:437:ALA:C	1:G:439:ALA:H	2.13	0.50
1:G:682:VAL:HG13	1:G:749:ILE:HD12	1.92	0.50
1:A:279:PHE:HB2	1:A:409:ASP:OD2	2.11	0.50
1:A:52:GLU:CD	1:A:52:GLU:C	2.70	0.50
1:C:772:TRP:CZ2	1:C:776:SER:HB3	2.46	0.50
1:D:419:ASN:OD1	1:D:435:THR:HB	2.12	0.50
1:D:779:ASP:O	1:D:779:ASP:OD1	2.30	0.50
1:E:437:ALA:O	1:E:438:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:GLN:CA	3:E:902:FRU:H12	2.40	0.50
1:F:458:LYS:HD3	1:F:459:TYR:CE2	2.46	0.50
1:G:52:GLU:CD	1:G:53:PHE:N	2.65	0.50
1:G:670:GLN:O	1:G:670:GLN:HG3	2.11	0.50
1:H:46:GLN:O	1:H:78:GLU:HA	2.11	0.50
1:A:339:ARG:HD2	1:A:369:PHE:CE2	2.46	0.50
1:A:789:MET:HB3	1:D:789:MET:HE2	1.89	0.50
1:D:49:ILE:O	1:D:53:PHE:CB	2.59	0.50
1:F:575:LEU:HD21	1:F:724:LEU:HD13	1.92	0.50
1:B:91:ARG:HD2	1:B:97:TRP:CZ2	2.46	0.50
1:C:582:ASP:HB2	1:C:621:GLU:OE1	2.12	0.50
1:C:86:VAL:CG1	1:C:102:VAL:CG2	2.88	0.50
1:D:35:ARG:O	1:D:104:LEU:HD22	2.12	0.50
1:G:284:LEU:HD13	1:G:337:LEU:HB2	1.93	0.50
1:G:80:ILE:HD12	1:G:80:ILE:N	2.26	0.50
1:A:160:ASP:O	1:A:164:ARG:HG3	2.12	0.50
1:B:80:ILE:HG23	1:B:87:ALA:HB3	1.94	0.50
1:C:772:TRP:CE2	1:C:776:SER:HB3	2.46	0.50
1:D:230:GLU:OE1	1:D:240:ARG:NH1	2.45	0.50
1:H:146:ILE:CG1	1:H:147:PRO:HD2	2.33	0.50
1:H:173:ASP:HB3	1:H:176:SER:H	1.76	0.50
1:A:566:VAL:O	1:A:640:GLY:HA2	2.12	0.50
1:B:284:LEU:CD2	1:B:284:LEU:N	2.75	0.50
1:B:789:MET:HB3	1:C:789:MET:HE2	1.93	0.50
1:D:419:ASN:HB3	1:D:471:ALA:HB1	1.92	0.50
1:F:415:TYR:CG	1:F:416:SER:N	2.80	0.50
1:H:411:ILE:HG13	1:H:431:VAL:HG11	1.92	0.50
1:B:216:TYR:HE1	1:B:220:LEU:HD11	1.74	0.50
1:B:587:LEU:HD13	1:B:608:VAL:HG13	1.94	0.50
1:B:587:LEU:HD13	1:B:608:VAL:CG1	2.42	0.50
1:C:553:LEU:HG	1:C:645:ILE:HD13	1.94	0.50
1:D:437:ALA:C	1:D:439:ALA:H	2.14	0.50
1:D:55:ALA:O	1:D:59:GLN:CB	2.56	0.50
1:A:789:MET:CB	1:D:789:MET:HE3	2.41	0.50
1:G:35:ARG:HD3	1:G:102:VAL:CG1	2.41	0.50
1:H:173:ASP:HB3	1:H:176:SER:HB2	1.93	0.50
1:H:386:TRP:N	1:H:387:PRO:HD2	2.27	0.50
1:E:789:MET:CB	1:H:789:MET:CE	2.73	0.50
1:D:41:LYS:HE3	1:D:54:GLU:CG	2.42	0.50
1:B:578:MET:HG3	1:B:609:VAL:CG1	2.41	0.49
1:B:72:LEU:O	1:B:76:THR:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:HB2	1:C:179:PRO:HD3	1.92	0.49
1:D:449:ASP:O	1:D:504:LEU:HD23	2.12	0.49
1:E:259:LEU:O	1:E:263:PRO:HG3	2.12	0.49
1:F:230:GLU:OE1	1:F:240:ARG:NH1	2.46	0.49
1:F:442:LYS:HD2	1:F:449:ASP:HB3	1.93	0.49
1:C:668:PHE:HB2	1:C:689:LEU:HD21	1.94	0.49
1:D:103:ASN:CB	1:D:106:ALA:CB	2.89	0.49
1:D:333:ARG:HG2	1:D:333:ARG:NH1	2.27	0.49
1:D:452:TRP:HB3	1:D:504:LEU:HD22	1.95	0.49
1:E:154:TYR:OH	1:F:262:ALA:HB3	2.11	0.49
1:E:407:LYS:HB2	1:E:408:PRO:HD2	1.93	0.49
1:H:34:SER:HG	1:H:55:ALA:HB1	1.78	0.49
1:A:35:ARG:HH12	1:A:86:VAL:H	1.60	0.49
1:D:216:TYR:C	1:D:216:TYR:CD1	2.85	0.49
1:D:437:ALA:O	1:D:438:HIS:HB2	2.13	0.49
1:E:177:LEU:C	1:E:179:PRO:HD2	2.32	0.49
1:E:91:ARG:HD2	1:E:97:TRP:CZ2	2.48	0.49
1:F:169:LYS:HG2	1:F:176:SER:OG	2.12	0.49
1:G:81:VAL:CB	1:G:86:VAL:HG23	2.27	0.49
1:A:617:SER:O	1:A:623:LYS:HD2	2.12	0.49
1:A:83:PRO:CB	1:A:84:PRO:HD3	2.42	0.49
1:F:668:PHE:HB2	1:F:689:LEU:HD23	1.95	0.49
1:F:83:PRO:CB	1:F:85:TRP:H	2.24	0.49
1:H:32:LEU:HD22	1:H:35:ARG:HH12	1.71	0.49
1:B:52:GLU:O	1:B:57:PRO:CD	2.60	0.49
1:C:590:LEU:HB2	1:C:671:PRO:HG3	1.94	0.49
1:D:219:GLU:OE1	1:D:219:GLU:HA	2.12	0.49
1:D:242:TRP:O	1:D:252:MET:HG3	2.12	0.49
1:E:136:GLU:HG2	1:E:511:VAL:HG23	1.94	0.49
1:E:61:ARG:C	1:E:63:LYS:H	2.15	0.49
1:F:472:MET:HG2	1:F:514:ILE:HD13	1.94	0.49
1:A:56:LEU:HB3	1:A:57:PRO:CD	2.36	0.49
1:A:137:LEU:HD11	1:A:790:PHE:CE1	2.47	0.49
1:B:52:GLU:O	1:B:57:PRO:HD3	2.13	0.49
1:C:43:ILE:O	1:C:43:ILE:HG22	2.11	0.49
1:D:756:GLN:HG3	1:D:757:ILE:HG13	1.93	0.49
1:H:207:GLN:HE21	1:H:211:ARG:NH2	2.11	0.49
1:H:46:GLN:CG	1:H:79:ALA:HB3	2.41	0.49
1:A:249:VAL:O	1:A:253:ILE:HG13	2.12	0.49
1:A:166:LEU:HB3	1:A:268:LEU:HD21	1.93	0.49
1:B:46:GLN:HB2	1:B:50:ILE:CB	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:GLN:HG3	1:B:670:GLN:O	2.12	0.49
1:G:338:THR:CG2	1:G:366:ARG:HG2	2.38	0.49
1:G:410:LEU:HD12	1:G:411:ILE:H	1.75	0.49
1:G:534:PHE:HB2	1:G:535:PRO:HD2	1.95	0.49
1:G:633:ILE:HA	1:G:638:LEU:HD12	1.94	0.49
1:B:259:LEU:O	1:B:263:PRO:HG3	2.13	0.49
1:B:36:VAL:CG1	1:B:37:GLU:N	2.75	0.49
1:D:220:LEU:N	1:D:220:LEU:CD1	2.75	0.49
1:G:427:HIS:HE1	1:G:788:GLU:OE1	1.95	0.49
1:H:480:THR:HB	1:H:485:GLU:OE1	2.12	0.49
1:A:61:ARG:C	1:A:63:LYS:H	2.16	0.49
1:B:189:HIS:ND1	1:B:330:ILE:HD13	2.27	0.49
1:C:32:LEU:CD2	1:C:105:HIS:HA	2.42	0.49
1:C:681:VAL:O	1:C:685:MET:HG3	2.13	0.49
1:D:210:LEU:CD2	1:D:253:ILE:HG23	2.41	0.49
1:D:312:VAL:HG23	1:D:313:ARG:N	2.28	0.49
1:E:451:TYR:HB3	1:E:454:LYS:HE2	1.95	0.49
1:G:140:GLU:N	1:G:141:PRO:HD2	2.28	0.49
1:A:435:THR:HG23	1:A:475:THR:HB	1.94	0.48
1:B:83:PRO:CB	1:B:84:PRO:CD	2.86	0.48
1:D:468:ASP:O	1:D:472:MET:HB2	2.12	0.48
1:E:79:ALA:CB	1:E:88:LEU:HD23	2.43	0.48
1:G:178:LEU:HD23	1:G:203:LEU:HG	1.95	0.48
1:H:376:VAL:HG21	1:H:388:TYR:CE2	2.48	0.48
1:A:230:GLU:OE1	1:A:240:ARG:NH1	2.46	0.48
1:A:449:ASP:OD1	1:A:450:ILE:N	2.46	0.48
1:B:437:ALA:C	1:B:439:ALA:H	2.17	0.48
1:B:83:PRO:O	1:B:84:PRO:C	2.52	0.48
1:E:147:PRO:CB	1:F:172:HIS:ND1	2.75	0.48
1:C:101:ARG:HB3	1:C:112:LEU:HD22	1.93	0.48
1:D:284:LEU:CD2	1:D:284:LEU:N	2.76	0.48
1:F:86:VAL:HB	1:F:104:LEU:HD21	1.94	0.48
1:G:484:GLN:NE2	1:G:488:GLY:HA2	2.28	0.48
1:H:48:GLN:HG2	1:H:76:THR:O	2.13	0.48
1:G:82:LEU:CD1	1:G:83:PRO:CD	2.68	0.48
1:H:415:TYR:CG	1:H:416:SER:N	2.81	0.48
1:A:143:ASN:HB3	1:A:148:ARG:HH22	1.77	0.48
1:A:789:MET:HE3	1:D:789:MET:CB	2.41	0.48
1:B:43:ILE:HD13	1:B:43:ILE:O	2.13	0.48
1:C:242:TRP:HA	1:C:252:MET:CE	2.43	0.48
1:C:319:MET:HE1	1:C:334:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:LEU:C	1:C:420:LEU:HD13	2.34	0.48
1:C:72:LEU:O	1:C:72:LEU:HD13	2.12	0.48
1:E:434:CYS:HB2	1:E:477:PHE:CZ	2.48	0.48
1:E:53:PHE:HA	1:E:57:PRO:CG	2.44	0.48
1:F:176:SER:O	1:F:179:PRO:HD2	2.13	0.48
1:F:80:ILE:H	1:F:80:ILE:HD12	1.79	0.48
1:H:18:LEU:HD12	1:H:109:VAL:CG1	2.39	0.48
1:A:446:PRO:HA	7:A:869:HOH:O	2.14	0.48
1:A:65:GLU:C	1:A:67:GLY:H	2.16	0.48
1:B:140:GLU:N	1:B:141:PRO:CD	2.75	0.48
1:E:590:LEU:HB2	1:E:671:PRO:HG3	1.96	0.48
1:E:63:LYS:C	1:E:65:GLU:H	2.17	0.48
1:G:54:GLU:HG3	1:G:55:ALA:H	1.77	0.48
1:G:172:HIS:ND1	1:H:147:PRO:CB	2.76	0.48
1:C:407:LYS:HB2	1:C:408:PRO:HD2	1.95	0.48
1:D:72:LEU:HD13	1:D:72:LEU:O	2.14	0.48
1:E:580:ARG:HD3	2:E:901:UDP:O3B	2.14	0.48
1:F:547:HIS:O	1:F:551:GLU:HG2	2.14	0.48
1:G:48:GLN:HE21	1:G:48:GLN:C	2.17	0.48
1:H:216:TYR:CD2	1:H:232:LYS:HG2	2.48	0.48
1:A:264:ASP:OD1	1:A:267:THR:CB	2.61	0.48
1:A:47:ASN:HB2	1:A:50:ILE:HB	1.95	0.48
1:A:65:GLU:HA	1:A:65:GLU:OE2	2.13	0.48
1:C:178:LEU:N	1:C:179:PRO:CD	2.76	0.48
1:C:458:LYS:HD3	1:C:459:TYR:CE2	2.48	0.48
1:B:135:LEU:HD21	1:C:789:MET:HG3	1.95	0.48
1:D:43:ILE:O	1:D:44:LEU:CB	2.61	0.48
1:E:704:VAL:H	1:E:708:SER:HB2	1.79	0.48
1:A:35:ARG:NH2	1:A:102:VAL:CA	2.76	0.48
1:A:572:LYS:HE2	1:A:605:ASN:OD1	2.13	0.48
1:B:452:TRP:CG	1:B:453:LYS:N	2.81	0.48
1:C:261:GLU:HG2	1:D:151:LEU:HD12	1.96	0.48
1:C:386:TRP:N	1:C:387:PRO:HD2	2.29	0.48
1:D:158:GLY:HA3	1:D:519:PRO:O	2.13	0.48
1:E:182:LYS:HE2	1:E:186:LEU:CD1	2.44	0.48
1:E:518:ASP:OD1	1:E:520:LYS:HG2	2.14	0.48
1:F:444:LYS:O	1:F:446:PRO:HD3	2.14	0.48
1:H:438:HIS:O	1:H:439:ALA:HB2	2.14	0.48
1:A:415:TYR:CG	1:A:416:SER:N	2.81	0.48
1:A:536:TYR:HA	1:A:659:ARG:HG2	1.95	0.48
1:A:575:LEU:HD21	1:A:724:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASN:N	1:B:103:ASN:ND2	2.62	0.48
1:B:206:LEU:HD11	1:B:210:LEU:HD11	1.95	0.48
1:B:48:GLN:O	1:B:52:GLU:HB3	2.14	0.48
1:B:93:ARG:O	1:B:96:VAL:HG22	2.14	0.48
1:D:670:GLN:HG3	1:D:670:GLN:O	2.13	0.48
1:D:80:ILE:HD13	1:D:117:PHE:CZ	2.49	0.48
1:D:91:ARG:HD2	1:D:97:TRP:CZ2	2.49	0.48
1:E:181:LEU:HD13	1:E:206:LEU:HD22	1.95	0.48
1:F:80:ILE:N	1:F:80:ILE:HD12	2.29	0.48
1:G:207:GLN:OE1	1:G:211:ARG:NH2	2.47	0.48
1:H:17:ARG:CZ	1:H:72:LEU:HD23	2.43	0.48
1:H:514:ILE:HG13	1:H:515:ASP:N	2.29	0.48
1:A:419:ASN:OD1	1:A:435:THR:HB	2.14	0.47
1:A:41:LYS:HE3	1:A:54:GLU:OE1	2.14	0.47
1:B:30:LEU:HD22	7:B:861:HOH:O	2.13	0.47
1:B:319:MET:O	1:B:323:ILE:HG13	2.13	0.47
1:C:410:LEU:HD12	1:C:411:ILE:N	2.29	0.47
1:E:415:TYR:CG	1:E:416:SER:N	2.82	0.47
1:F:190:GLN:NE2	1:F:405:ASN:HB3	2.29	0.47
1:G:72:LEU:C	1:G:72:LEU:HD13	2.34	0.47
1:H:87:ALA:HA	1:H:100:LEU:O	2.14	0.47
1:H:43:ILE:O	1:H:43:ILE:CG2	2.61	0.47
1:B:233:PHE:HD1	1:B:238:LEU:HB2	1.79	0.47
1:B:580:ARG:NH1	2:B:901:UDP:O2B	2.48	0.47
1:C:101:ARG:HG2	1:C:110:GLU:HB3	1.95	0.47
1:F:233:PHE:CE1	1:F:238:LEU:CD1	2.97	0.47
1:G:262:ALA:HB1	1:H:164:ARG:HD2	1.95	0.47
1:H:390:GLU:OE1	1:H:796:ARG:HD2	2.14	0.47
1:B:82:LEU:C	1:B:83:PRO:O	2.52	0.47
1:D:411:ILE:HD12	1:D:431:VAL:HB	1.95	0.47
1:F:39:LYS:O	1:F:39:LYS:HD3	2.14	0.47
1:F:407:LYS:HB2	1:F:408:PRO:HD2	1.95	0.47
1:A:276:PRO:HG3	1:A:326:GLN:CB	2.45	0.47
1:B:673:LEU:HD23	1:B:714:PRO:HB2	1.96	0.47
1:C:52:GLU:CD	1:C:52:GLU:C	2.73	0.47
1:D:170:LEU:HD23	1:D:176:SER:OG	2.15	0.47
1:E:437:ALA:C	1:E:439:ALA:H	2.16	0.47
1:E:789:MET:HG3	1:H:135:LEU:CD2	2.39	0.47
1:E:302:GLY:CA	3:E:902:FRU:O1	2.63	0.47
1:F:435:THR:HG23	1:F:475:THR:HB	1.95	0.47
1:F:56:LEU:N	1:F:57:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:HD22	1:H:120:PHE:HZ	1.78	0.47
1:H:178:LEU:HB2	1:H:179:PRO:HD3	1.96	0.47
1:H:60:THR:OG1	1:H:61:ARG:N	2.47	0.47
1:A:140:GLU:HB3	1:A:141:PRO:CD	2.44	0.47
1:B:756:GLN:HG3	1:B:757:ILE:H	1.80	0.47
1:C:43:ILE:HG23	1:C:124:LEU:CD1	2.44	0.47
1:E:35:ARG:HG2	1:E:104:LEU:O	2.13	0.47
1:G:431:VAL:HG12	1:G:432:THR:N	2.28	0.47
1:H:47:ASN:O	1:H:50:ILE:N	2.41	0.47
1:B:657:LEU:O	1:B:661:ILE:HG12	2.14	0.47
1:C:154:TYR:OH	1:D:262:ALA:HB3	2.14	0.47
1:H:61:ARG:C	1:H:63:LYS:H	2.17	0.47
1:B:276:PRO:HG3	1:B:326:GLN:HG3	1.97	0.47
1:B:479:ILE:HD11	1:B:762:LEU:HD13	1.96	0.47
1:C:588:SER:OG	1:C:628:LYS:HD2	2.14	0.47
1:C:572:LYS:CE	1:C:605:ASN:OD1	2.62	0.47
1:D:245:ASN:O	1:D:249:VAL:HG23	2.15	0.47
1:D:424:LEU:CD2	5:D:922:MLA:HC22	2.45	0.47
1:E:125:VAL:HG13	1:E:126:ASP:N	2.29	0.47
1:E:137:LEU:HD11	1:E:790:PHE:CZ	2.50	0.47
1:E:140:GLU:HB3	1:E:141:PRO:HD3	1.96	0.47
1:E:536:TYR:CE1	1:E:537:THR:HG23	2.49	0.47
1:E:483:PHE:HB3	1:E:701:GLU:OE2	2.15	0.47
1:F:44:LEU:HD11	1:F:451:TYR:OH	2.15	0.47
1:G:158:GLY:HA3	1:G:519:PRO:O	2.14	0.47
1:A:339:ARG:HD2	1:A:369:PHE:CD2	2.50	0.47
1:B:166:LEU:HD13	1:B:268:LEU:HD21	1.96	0.47
1:B:290:PHE:HB3	1:B:338:THR:HG21	1.97	0.47
1:B:69:PHE:CE1	1:B:73:LEU:HD23	2.49	0.47
1:C:80:ILE:HD13	1:C:121:LYS:HG2	1.96	0.47
1:C:290:PHE:O	1:C:366:ARG:NH1	2.46	0.47
1:F:410:LEU:HD12	1:F:411:ILE:H	1.79	0.47
1:F:47:ASN:H	1:F:50:ILE:HB	1.80	0.47
1:G:437:ALA:O	1:G:438:HIS:HB2	2.13	0.47
1:G:63:LYS:O	1:G:65:GLU:CG	2.54	0.47
1:H:702:ILE:HA	1:H:753:TYR:OH	2.15	0.47
1:B:574:ILE:HG23	1:B:607:VAL:HG23	1.97	0.47
1:B:790:PHE:O	1:B:794:LYS:HB3	2.15	0.47
1:B:371:THR:HG21	1:B:804:LEU:HD13	1.97	0.47
1:C:668:PHE:HB2	1:C:689:LEU:HD23	1.96	0.47
1:E:668:PHE:HB2	1:E:689:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:659:ARG:O	1:G:662:CYS:HB2	2.15	0.47
1:H:322:ARG:HD2	1:H:763:LEU:CD1	2.44	0.47
1:C:163:ASN:O	1:C:167:SER:HB2	2.15	0.47
1:E:188:SER:HA	1:E:194:LEU:HD12	1.96	0.47
1:E:407:LYS:HB2	1:E:408:PRO:CD	2.44	0.47
1:E:284:LEU:O	1:E:414:ASN:HB2	2.14	0.47
1:E:670:GLN:O	1:E:670:GLN:HG3	2.15	0.47
1:G:284:LEU:HD22	1:G:284:LEU:N	2.30	0.47
1:B:387:PRO:HD3	1:B:802:VAL:HB	1.97	0.47
1:C:778:LEU:CD1	1:C:778:LEU:H	2.25	0.47
1:D:512:HIS:NE2	1:D:515:ASP:HB2	2.30	0.47
1:E:38:ALA:O	1:E:41:LYS:HB2	2.14	0.47
1:F:468:ASP:O	1:F:472:MET:HB2	2.15	0.47
1:G:219:GLU:OE1	1:G:219:GLU:CA	2.63	0.47
1:G:761:ARG:O	1:G:765:LEU:HG	2.15	0.47
1:B:617:SER:O	1:B:623:LYS:HD3	2.15	0.46
1:C:34:SER:N	1:C:59:GLN:HE22	2.13	0.46
1:D:99:TYR:O	1:D:100:LEU:HD23	2.15	0.46
1:E:85:TRP:HB2	1:E:102:VAL:O	2.15	0.46
1:F:441:GLU:OE1	1:F:441:GLU:HA	2.15	0.46
1:F:52:GLU:O	1:F:52:GLU:HG2	2.15	0.46
1:F:675:GLU:HA	1:F:675:GLU:OE2	2.15	0.46
1:G:407:LYS:HB2	1:G:408:PRO:HD2	1.96	0.46
1:H:366:ARG:HD3	7:H:854:HOH:O	2.16	0.46
1:A:216:TYR:CD2	1:A:232:LYS:HG2	2.51	0.46
1:A:319:MET:CE	1:A:334:ILE:CD1	2.80	0.46
1:B:84:PRO:O	1:B:103:ASN:HB2	2.15	0.46
1:B:291:ALA:HB3	1:B:295:VAL:HG11	1.97	0.46
1:C:69:PHE:O	1:C:69:PHE:CD1	2.69	0.46
1:D:54:GLU:HG3	1:D:55:ALA:H	1.73	0.46
1:E:196:LEU:CD1	1:E:206:LEU:HD13	2.45	0.46
1:E:60:THR:HG21	1:E:62:LYS:HE3	1.97	0.46
1:F:173:ASP:HB3	1:F:176:SER:CB	2.44	0.46
1:F:56:LEU:O	1:F:59:GLN:CB	2.63	0.46
1:H:17:ARG:NH2	1:H:72:LEU:CB	2.70	0.46
1:H:85:TRP:CE3	1:H:101:ARG:HG2	2.51	0.46
1:A:607:VAL:HG22	1:A:643:ARG:HB3	1.96	0.46
1:A:262:ALA:CB	1:B:164:ARG:HD3	2.30	0.46
1:D:43:ILE:O	1:D:44:LEU:CD2	2.63	0.46
1:D:609:VAL:HG22	1:D:645:ILE:HB	1.97	0.46
1:F:43:ILE:HG13	1:F:82:LEU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG12	1:A:126:ASP:OD1	2.15	0.46
1:A:702:ILE:HA	1:A:753:TYR:OH	2.16	0.46
1:A:756:GLN:HG3	1:A:757:ILE:H	1.78	0.46
1:A:46:GLN:O	1:A:78:GLU:HA	2.16	0.46
1:B:103:ASN:H	1:B:103:ASN:ND2	2.13	0.46
1:B:333:ARG:NH1	1:B:333:ARG:HG2	2.28	0.46
1:C:594:TYR:OH	1:C:641:GLN:HB3	2.15	0.46
1:G:719:GLN:HG3	4:G:913:SO4:O3	2.15	0.46
1:H:353:LEU:HD13	1:H:365:LEU:HD13	1.97	0.46
1:B:468:ASP:O	1:B:472:MET:HB2	2.16	0.46
1:D:80:ILE:HD13	1:D:117:PHE:CE2	2.51	0.46
1:D:284:LEU:HD22	1:D:284:LEU:N	2.30	0.46
1:D:44:LEU:HD13	1:D:45:GLN:H	1.79	0.46
1:F:28:GLU:HG3	1:F:29:VAL:N	2.30	0.46
1:F:35:ARG:CG	1:F:104:LEU:HA	2.46	0.46
1:G:414:ASN:O	1:G:418:GLY:HA3	2.16	0.46
1:G:445:TYR:O	1:G:448:SER:HB3	2.16	0.46
1:A:490:LYS:HE3	1:A:490:LYS:HB2	1.68	0.46
1:C:174:LYS:HD2	1:C:203:LEU:HD12	1.96	0.46
1:E:753:TYR:CD2	1:E:753:TYR:N	2.83	0.46
1:G:137:LEU:HD11	1:G:790:PHE:CE1	2.50	0.46
1:H:437:ALA:C	1:H:439:ALA:H	2.18	0.46
1:A:35:ARG:HH22	1:A:102:VAL:H	1.62	0.46
1:G:778:LEU:CD1	1:G:778:LEU:N	2.76	0.46
1:G:82:LEU:N	1:G:83:PRO:HD3	2.30	0.46
1:H:242:TRP:HB2	1:H:249:VAL:HG13	1.97	0.46
1:H:538:GLU:O	1:H:542:ARG:HG2	2.16	0.46
1:B:131:GLY:O	1:B:134:THR:HG23	2.16	0.46
1:C:177:LEU:HD22	1:C:260:LEU:HD23	1.97	0.46
1:D:415:TYR:CG	1:D:416:SER:N	2.84	0.46
1:D:82:LEU:HG	1:D:120:PHE:HE1	1.80	0.46
1:E:85:TRP:CB	1:E:103:ASN:HA	2.37	0.46
1:F:53:PHE:CA	1:F:57:PRO:CG	2.92	0.46
1:F:162:LEU:HD11	1:F:772:TRP:CD2	2.51	0.46
1:G:178:LEU:N	1:G:179:PRO:CD	2.78	0.46
1:G:178:LEU:CD2	1:G:203:LEU:HG	2.46	0.46
1:H:80:ILE:CG2	1:H:120:PHE:CE2	2.95	0.46
1:A:284:LEU:HD13	1:A:337:LEU:HB2	1.98	0.46
1:A:298:TYR:CE1	1:A:649:MET:HE1	2.49	0.46
1:C:169:LYS:HG2	1:C:176:SER:OG	2.15	0.46
1:D:128:VAL:HG12	1:D:129:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:757:ILE:HG13	1:D:757:ILE:H	1.27	0.46
1:F:279:PHE:HD1	1:F:323:ILE:HD11	1.80	0.46
1:G:210:LEU:HD11	1:G:256:LEU:HD23	1.97	0.46
1:H:48:GLN:O	1:H:52:GLU:HB3	2.16	0.46
1:A:262:ALA:HB3	1:B:154:TYR:OH	2.14	0.46
1:A:789:MET:HE1	1:D:790:PHE:N	2.31	0.46
1:B:178:LEU:N	1:B:179:PRO:CD	2.78	0.46
1:B:689:LEU:HD12	1:B:690:PRO:HD2	1.97	0.46
1:C:338:THR:HG23	1:C:366:ARG:HG2	1.98	0.46
1:C:415:TYR:CG	1:C:416:SER:N	2.83	0.46
1:C:486:ILE:HG22	1:C:516:VAL:HG22	1.97	0.46
1:E:153:LYS:HG3	1:E:154:TYR:CD2	2.51	0.46
1:E:33:LEU:HA	1:E:33:LEU:HD23	1.85	0.46
1:E:770:GLY:O	1:E:773:LYS:HB2	2.16	0.46
1:F:82:LEU:HD12	1:F:83:PRO:CG	2.46	0.46
1:H:52:GLU:OE1	1:H:53:PHE:CA	2.60	0.46
1:A:178:LEU:N	1:A:179:PRO:CD	2.79	0.45
1:B:452:TRP:CD2	1:B:453:LYS:N	2.83	0.45
1:B:583:ARG:HG2	1:B:583:ARG:NH1	2.30	0.45
1:B:593:TRP:HB3	1:B:721:ALA:HB2	1.97	0.45
1:B:322:ARG:CD	1:B:763:LEU:HD13	2.46	0.45
1:D:490:LYS:HE3	1:D:490:LYS:HB2	1.84	0.45
1:D:49:ILE:HG22	1:D:50:ILE:N	2.30	0.45
1:D:56:LEU:C	1:D:56:LEU:HD13	2.36	0.45
1:F:80:ILE:HD11	1:F:117:PHE:CZ	2.51	0.45
1:G:434:CYS:HB2	1:G:477:PHE:CZ	2.51	0.45
1:E:789:MET:HE1	1:H:790:PHE:N	2.31	0.45
1:A:582:ASP:HB2	1:A:621:GLU:OE1	2.16	0.45
1:B:322:ARG:O	1:B:326:GLN:HG2	2.16	0.45
1:B:77:GLN:HG3	1:B:97:TRP:CH2	2.51	0.45
1:B:580:ARG:HD3	2:B:901:UDP:O1B	2.14	0.45
1:B:716:HIS:HB3	4:B:913:SO4:O3	2.15	0.45
1:C:131:GLY:HA3	1:C:134:THR:CG2	2.40	0.45
1:D:659:ARG:O	1:D:662:CYS:HB2	2.17	0.45
1:E:85:TRP:N	1:E:85:TRP:CD1	2.82	0.45
1:F:319:MET:HE1	1:F:334:ILE:CD1	2.40	0.45
1:F:53:PHE:HA	1:F:57:PRO:CG	2.47	0.45
1:F:79:ALA:HB2	1:F:88:LEU:CD2	2.45	0.45
1:H:113:GLN:O	1:H:116:GLU:HG2	2.16	0.45
1:H:227:GLU:HG3	1:H:228:GLU:N	2.31	0.45
1:H:678:GLY:O	1:H:681:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:GLU:O	1:A:58:GLU:CB	2.65	0.45
1:E:33:LEU:HD12	1:E:62:LYS:HZ2	1.80	0.45
1:E:794:LYS:HE2	1:E:794:LYS:HA	1.99	0.45
1:H:243:GLY:HA2	1:H:326:GLN:HA	1.98	0.45
1:A:668:PHE:HB2	1:A:689:LEU:CD2	2.47	0.45
1:A:46:GLN:CB	1:A:79:ALA:O	2.63	0.45
1:B:716:HIS:HB3	4:B:913:SO4:O4	2.17	0.45
1:C:304:GLN:O	1:C:308:ILE:HG13	2.15	0.45
1:C:348:THR:O	1:C:351:GLU:HG2	2.15	0.45
1:C:158:GLY:HA3	1:C:519:PRO:O	2.16	0.45
1:B:789:MET:CB	1:C:789:MET:CE	2.92	0.45
1:E:789:MET:CE	1:H:789:MET:CB	2.94	0.45
1:F:259:LEU:O	1:F:263:PRO:HG3	2.16	0.45
1:H:547:HIS:O	1:H:551:GLU:CG	2.64	0.45
1:C:597:ASN:O	1:C:601:ARG:HG3	2.16	0.45
1:C:765:LEU:HD22	1:C:769:TYR:HE2	1.81	0.45
1:D:615:LYS:HB2	1:D:615:LYS:HE3	1.81	0.45
1:E:796:ARG:N	1:E:797:PRO:CD	2.79	0.45
1:G:29:VAL:O	1:G:29:VAL:HG12	2.15	0.45
1:G:564:LEU:HA	1:G:564:LEU:HD12	1.74	0.45
1:H:80:ILE:HG21	1:H:120:PHE:CD2	2.52	0.45
1:H:338:THR:OG1	1:H:339:ARG:N	2.50	0.45
1:H:414:ASN:O	1:H:418:GLY:HA3	2.17	0.45
1:A:298:TYR:CE1	1:A:649:MET:HE2	2.51	0.45
1:E:756:GLN:HG3	1:E:757:ILE:H	1.81	0.45
3:E:902:FRU:H11	7:E:852:HOH:O	2.15	0.45
1:F:39:LYS:HD3	1:F:39:LYS:C	2.37	0.45
1:H:790:PHE:O	1:H:794:LYS:HB3	2.17	0.45
1:A:483:PHE:CE1	1:A:487:ALA:HB3	2.52	0.45
1:A:716:HIS:HA	4:A:913:SO4:O4	2.16	0.45
1:B:36:VAL:O	1:B:39:LYS:N	2.49	0.45
1:B:442:LYS:HG3	1:B:465:PHE:CZ	2.51	0.45
1:B:390:GLU:OE1	1:B:796:ARG:HD2	2.17	0.45
1:C:572:LYS:HE3	1:C:605:ASN:OD1	2.16	0.45
1:D:56:LEU:O	1:D:59:GLN:HB3	2.16	0.45
1:F:790:PHE:O	1:F:794:LYS:HB3	2.17	0.45
1:G:116:GLU:O	1:G:119:HIS:HB2	2.16	0.45
1:H:84:PRO:CG	1:H:85:TRP:CD1	2.98	0.45
1:C:63:LYS:O	1:C:64:LEU:C	2.55	0.45
1:D:276:PRO:HG3	1:D:326:GLN:HG3	1.99	0.45
1:D:581:LEU:HD12	1:D:587:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HG22	1:D:86:VAL:HG23	1.98	0.45
1:F:69:PHE:HD1	1:F:69:PHE:C	2.17	0.45
1:G:339:ARG:HD2	1:G:369:PHE:CE2	2.52	0.45
1:H:102:VAL:HA	1:H:108:VAL:O	2.17	0.45
1:H:61:ARG:HA	1:H:63:LYS:HG2	1.99	0.45
1:A:536:TYR:O	1:A:542:ARG:HD3	2.17	0.45
1:B:400:LEU:HD12	1:B:401:SER:N	2.32	0.45
1:D:466:THR:HG23	1:D:790:PHE:CZ	2.52	0.45
1:E:151:LEU:HD23	1:F:211:ARG:NH2	2.32	0.45
1:F:518:ASP:HA	1:F:519:PRO:HD3	1.84	0.45
1:H:39:LYS:CG	1:H:104:LEU:CB	2.84	0.45
1:A:116:GLU:O	1:A:119:HIS:HB2	2.16	0.45
1:A:79:ALA:HA	1:A:87:ALA:O	2.16	0.45
1:B:216:TYR:CE2	1:B:232:LYS:HG2	2.52	0.45
1:B:315:LEU:O	1:B:319:MET:HE2	2.17	0.45
1:C:302:GLY:HA3	3:C:902:FRU:O1	2.17	0.45
1:D:264:ASP:OD1	1:D:267:THR:HB	2.17	0.45
1:F:146:ILE:CG1	1:F:147:PRO:CD	2.89	0.45
1:F:435:THR:HG23	1:F:475:THR:CB	2.47	0.45
1:G:364:ILE:HG21	1:G:366:ARG:NH1	2.32	0.45
1:G:41:LYS:HG2	1:G:41:LYS:H	1.55	0.45
1:G:41:LYS:O	1:G:44:LEU:HD12	2.17	0.45
1:H:128:VAL:HG12	1:H:129:LYS:N	2.32	0.45
1:H:483:PHE:CZ	1:H:487:ALA:HB3	2.51	0.45
1:H:561:LYS:HD3	1:H:613:ARG:O	2.16	0.45
1:A:102:VAL:HA	1:A:109:VAL:HA	1.98	0.44
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.73	0.44
1:B:427:HIS:HD2	1:C:133:PHE:HE1	1.64	0.44
1:B:483:PHE:CE1	1:B:487:ALA:HB3	2.52	0.44
1:B:580:ARG:NH1	3:B:902:FRU:H61	2.32	0.44
1:C:276:PRO:HG3	1:C:326:GLN:CB	2.48	0.44
1:D:105:HIS:O	1:D:106:ALA:HB2	2.17	0.44
1:E:216:TYR:CD1	1:E:220:LEU:CD1	2.98	0.44
1:E:400:LEU:C	1:E:400:LEU:HD12	2.38	0.44
1:A:92:PRO:HD2	1:A:96:VAL:O	2.17	0.44
1:B:450:ILE:HG22	1:B:451:TYR:N	2.32	0.44
1:C:85:TRP:CE3	1:C:103:ASN:N	2.85	0.44
1:C:259:LEU:HD21	1:C:268:LEU:HA	1.98	0.44
1:D:756:GLN:HG3	1:D:757:ILE:N	2.32	0.44
1:E:49:ILE:HG12	1:E:49:ILE:H	1.60	0.44
1:E:61:ARG:C	1:E:63:LYS:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:ASP:OD2	1:F:176:SER:HB2	2.17	0.44
1:F:216:TYR:HD1	1:F:216:TYR:O	1.99	0.44
1:G:327:GLY:O	1:G:328:LEU:HD23	2.17	0.44
1:A:173:ASP:HB3	1:A:176:SER:HB3	2.00	0.44
1:A:290:PHE:C	1:A:290:PHE:CD1	2.91	0.44
1:A:542:ARG:CD	1:A:659:ARG:HD2	2.46	0.44
1:A:60:THR:O	1:A:63:LYS:HG3	2.18	0.44
1:B:174:LYS:HD2	1:B:203:LEU:CD1	2.41	0.44
1:B:49:ILE:O	1:B:53:PHE:CB	2.66	0.44
1:C:50:ILE:HG13	1:C:51:ALA:N	2.31	0.44
1:D:206:LEU:HD11	1:D:210:LEU:HD11	1.99	0.44
1:A:789:MET:CE	1:D:789:MET:CG	2.85	0.44
1:E:483:PHE:CE1	1:E:487:ALA:HB3	2.52	0.44
1:E:689:LEU:HD12	1:E:690:PRO:HD2	1.99	0.44
1:F:647:SER:HB2	1:F:649:MET:HE3	1.98	0.44
1:F:83:PRO:HG2	1:F:85:TRP:C	2.37	0.44
1:F:91:ARG:NH2	1:F:94:PRO:HA	2.31	0.44
1:A:173:ASP:O	1:A:176:SER:HB3	2.17	0.44
1:A:514:ILE:HG13	1:A:515:ASP:H	1.83	0.44
1:C:315:LEU:HA	1:C:315:LEU:HD12	1.77	0.44
1:C:349:CYS:HA	1:C:366:ARG:NH1	2.31	0.44
1:D:449:ASP:HA	1:D:504:LEU:CD2	2.48	0.44
1:D:318:GLU:CD	1:D:760:GLN:HG2	2.38	0.44
1:D:73:LEU:O	1:D:76:THR:HB	2.18	0.44
1:E:217:LEU:CD1	1:E:233:PHE:HZ	2.22	0.44
1:E:53:PHE:O	1:E:57:PRO:CG	2.47	0.44
1:H:184:LEU:HD22	1:H:195:MET:HG3	1.99	0.44
1:A:85:TRP:CD2	1:A:101:ARG:HD2	2.52	0.44
1:A:534:PHE:HB2	1:A:535:PRO:CD	2.47	0.44
1:B:93:ARG:H	1:B:96:VAL:HG23	1.82	0.44
1:D:36:VAL:HG12	1:D:36:VAL:O	2.17	0.44
1:D:84:PRO:HB2	1:D:85:TRP:CD1	2.53	0.44
1:E:102:VAL:HG13	1:E:102:VAL:O	2.18	0.44
1:F:452:TRP:CD1	1:F:504:LEU:HB3	2.52	0.44
1:G:32:LEU:HD21	1:G:105:HIS:O	2.17	0.44
1:G:316:GLU:HA	1:G:319:MET:HE3	1.99	0.44
1:G:66:GLY:CA	1:G:68:PRO:CD	2.94	0.44
1:H:105:HIS:N	1:H:105:HIS:CD2	2.85	0.44
1:B:782:GLU:HG3	1:C:141:PRO:HB2	1.99	0.44
1:C:233:PHE:CE1	1:C:249:VAL:HG11	2.52	0.44
1:E:442:LYS:HD2	1:E:449:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:538:GLU:OE1	1:F:541:ARG:HD3	2.18	0.44
1:H:76:THR:HA	1:H:89:ALA:O	2.17	0.44
1:A:512:HIS:CE1	1:A:515:ASP:HB2	2.53	0.44
1:D:192:LYS:HE3	1:D:192:LYS:HB3	1.74	0.44
1:D:536:TYR:CE1	1:D:537:THR:HG23	2.53	0.44
1:E:276:PRO:HG3	1:E:326:GLN:HG3	1.99	0.44
1:E:35:ARG:HD2	1:E:104:LEU:HA	2.00	0.44
1:H:544:THR:HA	1:H:547:HIS:CD2	2.53	0.44
1:A:226:TYR:HA	1:A:229:PHE:CZ	2.52	0.44
1:A:276:PRO:HG3	1:A:326:GLN:HG3	2.00	0.44
1:A:60:THR:OG1	1:A:61:ARG:N	2.50	0.44
1:B:164:ARG:HH11	1:B:164:ARG:HG3	1.83	0.44
1:B:597:ASN:O	1:B:601:ARG:HG3	2.18	0.44
1:C:445:TYR:O	1:C:448:SER:HB3	2.18	0.44
1:D:140:GLU:HB3	1:D:141:PRO:HD3	1.99	0.44
1:E:200:ILE:HG21	1:E:206:LEU:HB2	1.99	0.44
1:G:354:GLU:OE1	1:G:366:ARG:NH2	2.43	0.44
1:H:400:LEU:C	1:H:400:LEU:HD12	2.38	0.44
1:H:458:LYS:HD3	1:H:459:TYR:CE2	2.53	0.44
1:H:83:PRO:HG2	1:H:84:PRO:CD	2.45	0.44
1:A:60:THR:HG23	1:A:62:LYS:CB	2.48	0.44
1:B:55:ALA:O	1:B:59:GLN:N	2.51	0.44
1:C:34:SER:HA	1:C:59:GLN:NE2	2.28	0.44
1:C:645:ILE:HG22	1:C:646:SER:O	2.18	0.44
1:C:83:PRO:CG	1:C:84:PRO:CD	2.92	0.44
1:D:113:GLN:HA	1:D:113:GLN:NE2	2.25	0.44
1:D:72:LEU:C	1:D:72:LEU:CD1	2.86	0.44
1:D:82:LEU:HD12	1:D:82:LEU:O	2.18	0.44
1:F:154:TYR:HA	1:F:157:ASN:HB2	2.00	0.44
1:F:47:ASN:O	1:F:51:ALA:HB3	2.18	0.44
1:G:442:LYS:HG3	1:G:465:PHE:CZ	2.53	0.44
1:H:449:ASP:HA	1:H:504:LEU:CD2	2.48	0.44
1:B:534:PHE:HB2	1:B:535:PRO:CD	2.48	0.43
1:B:534:PHE:HB2	1:B:535:PRO:HD2	2.00	0.43
1:B:59:GLN:HB3	1:B:63:LYS:HD3	2.00	0.43
1:D:451:TYR:HB3	1:D:454:LYS:NZ	2.33	0.43
1:E:72:LEU:HD22	1:E:90:VAL:CG1	2.42	0.43
1:F:264:ASP:OD1	1:F:267:THR:CB	2.60	0.43
1:F:54:GLU:N	1:F:57:PRO:HG2	2.28	0.43
1:F:79:ALA:HA	1:F:87:ALA:O	2.17	0.43
1:H:103:ASN:CB	1:H:105:HIS:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:475:THR:HG21	1:H:478:ILE:HG12	2.00	0.43
1:A:528:ALA:HB1	1:A:533:TYR:CD2	2.53	0.43
1:C:157:ASN:O	1:C:160:ASP:HB2	2.18	0.43
1:C:437:ALA:C	1:C:439:ALA:H	2.19	0.43
1:C:802:VAL:HA	1:C:803:PRO:HD3	1.91	0.43
1:D:30:LEU:O	1:D:33:LEU:CB	2.65	0.43
1:E:33:LEU:HB3	1:E:59:GLN:OE1	2.18	0.43
1:E:383:PHE:HA	7:E:849:HOH:O	2.18	0.43
1:E:400:LEU:HD12	1:E:401:SER:N	2.33	0.43
1:F:44:LEU:HA	1:F:124:LEU:HD21	2.00	0.43
1:G:570:LYS:CG	1:G:570:LYS:O	2.65	0.43
1:H:578:MET:HA	1:H:609:VAL:O	2.17	0.43
1:H:748:ARG:NH1	1:H:752:LYS:HE3	2.33	0.43
1:A:294:ASN:HA	1:A:649:MET:SD	2.59	0.43
1:A:400:LEU:HD12	1:A:401:SER:N	2.32	0.43
1:A:47:ASN:O	1:A:48:GLN:CB	2.58	0.43
1:A:62:LYS:C	1:A:64:LEU:N	2.70	0.43
1:B:72:LEU:N	1:B:72:LEU:CD1	2.82	0.43
1:C:784:ARG:O	1:C:788:GLU:HG3	2.18	0.43
1:E:46:GLN:HB3	1:E:50:ILE:CB	2.45	0.43
1:F:86:VAL:CG1	1:F:102:VAL:HB	2.49	0.43
1:F:250:LEU:O	1:F:254:ARG:HG3	2.18	0.43
1:F:452:TRP:CG	1:F:453:LYS:N	2.86	0.43
1:F:514:ILE:HD12	1:F:514:ILE:HA	1.87	0.43
1:F:583:ARG:HH11	1:F:583:ARG:HG2	1.82	0.43
1:F:734:ASP:HA	1:F:735:PRO:HD2	1.91	0.43
1:G:223:GLU:CD	1:G:223:GLU:H	2.20	0.43
1:G:49:ILE:O	1:G:53:PHE:CB	2.66	0.43
1:H:43:ILE:HA	1:H:81:VAL:O	2.18	0.43
1:H:41:LYS:HD3	1:H:54:GLU:OE1	2.19	0.43
1:A:319:MET:HE1	1:A:334:ILE:CD1	2.47	0.43
1:A:85:TRP:CE3	1:A:101:ARG:HG2	2.53	0.43
1:B:321:GLN:HB3	1:B:321:GLN:HE21	1.65	0.43
1:B:400:LEU:HD21	1:B:425:LEU:HD11	2.00	0.43
1:B:435:THR:HG23	1:B:475:THR:CB	2.49	0.43
1:B:789:MET:HE1	1:C:786:TYR:O	2.18	0.43
1:C:216:TYR:O	1:C:216:TYR:HD1	2.02	0.43
1:E:47:ASN:HB2	1:E:49:ILE:HG12	2.00	0.43
1:F:249:VAL:O	1:F:253:ILE:HG13	2.19	0.43
1:F:443:THR:HG21	1:F:495:GLN:HA	1.99	0.43
1:F:789:MET:HG3	1:G:135:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:ASN:OD1	1:G:435:THR:HB	2.18	0.43
1:H:545:LYS:HE3	1:H:546:PHE:CZ	2.54	0.43
1:A:777:ASN:HD22	1:A:778:LEU:CA	2.29	0.43
1:C:50:ILE:HD12	1:C:54:GLU:CG	2.48	0.43
1:F:327:GLY:C	1:F:328:LEU:HD23	2.37	0.43
1:F:92:PRO:HD2	1:F:96:VAL:O	2.19	0.43
1:G:145:SER:HB3	1:G:779:ASP:OD2	2.19	0.43
1:H:178:LEU:N	1:H:179:PRO:CD	2.81	0.43
1:H:17:ARG:CG	1:H:98:GLU:OE1	2.65	0.43
1:A:59:GLN:CG	1:A:60:THR:N	2.80	0.43
1:A:30:LEU:HD12	1:A:62:LYS:O	2.19	0.43
1:B:30:LEU:CD2	7:B:861:HOH:O	2.67	0.43
1:C:296:LEU:HG	7:C:828:HOH:O	2.17	0.43
1:C:761:ARG:HG3	1:C:761:ARG:HH11	1.84	0.43
1:D:579:ALA:HB2	7:D:827:HOH:O	2.18	0.43
1:E:162:LEU:HD11	1:E:772:TRP:CE3	2.54	0.43
1:E:189:HIS:CE1	1:E:190:GLN:NE2	2.86	0.43
1:E:261:GLU:OE2	1:F:149:PRO:HA	2.18	0.43
1:H:118:LEU:O	1:H:122:GLU:HG3	2.19	0.43
1:H:290:PHE:O	1:H:366:ARG:NH1	2.51	0.43
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.76	0.43
1:B:302:GLY:C	3:B:902:FRU:O1	2.56	0.43
1:C:104:LEU:N	1:C:104:LEU:HD23	2.33	0.43
1:C:468:ASP:O	1:C:472:MET:HB2	2.19	0.43
1:C:615:LYS:HZ3	1:C:618:LYS:HE2	1.81	0.43
1:E:453:LYS:HB2	1:E:453:LYS:HE2	1.76	0.43
1:F:86:VAL:HG13	1:F:102:VAL:HB	2.00	0.43
1:F:178:LEU:HB2	1:F:179:PRO:HD3	2.00	0.43
1:F:449:ASP:O	1:F:504:LEU:HD22	2.18	0.43
1:G:80:ILE:HD13	1:G:117:PHE:CE2	2.53	0.43
1:G:50:ILE:C	1:G:52:GLU:H	2.21	0.43
1:A:166:LEU:HB3	1:A:268:LEU:CD2	2.49	0.43
1:A:341:LEU:HA	1:A:342:PRO:HD3	1.86	0.43
1:A:284:LEU:O	1:A:414:ASN:HB2	2.18	0.43
1:A:468:ASP:O	1:A:472:MET:HB2	2.19	0.43
1:A:668:PHE:HB2	1:A:689:LEU:HD23	2.01	0.43
1:C:99:TYR:O	1:C:100:LEU:HD23	2.19	0.43
1:D:121:LYS:HB3	1:D:450:ILE:HD12	2.00	0.43
1:E:33:LEU:CD1	1:E:62:LYS:NZ	2.82	0.43
1:E:65:GLU:O	1:E:66:GLY:C	2.57	0.43
1:F:386:TRP:N	1:F:387:PRO:HD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:LEU:HD12	1:F:400:LEU:C	2.39	0.43
1:F:420:LEU:HD13	1:F:420:LEU:O	2.17	0.43
1:G:245:ASN:O	1:G:249:VAL:HG23	2.19	0.43
1:G:340:LEU:HD22	1:G:368:PRO:HB3	2.00	0.43
1:G:340:LEU:O	1:G:340:LEU:HD23	2.18	0.43
1:G:52:GLU:CD	1:G:52:GLU:C	2.77	0.43
1:H:582:ASP:HB2	1:H:621:GLU:OE1	2.19	0.43
1:H:802:VAL:HA	1:H:803:PRO:HD3	1.84	0.43
1:A:136:GLU:OE2	1:A:509:ARG:NH1	2.52	0.43
1:A:245:ASN:O	1:A:249:VAL:HG23	2.18	0.43
1:A:261:GLU:OE2	1:B:149:PRO:HA	2.18	0.43
1:A:459:TYR:HB3	1:A:461:PHE:CZ	2.53	0.43
1:B:226:TYR:HB3	1:B:240:ARG:NH2	2.34	0.43
1:B:415:TYR:CG	1:B:416:SER:N	2.86	0.43
1:B:414:ASN:O	1:B:418:GLY:HA3	2.18	0.43
1:B:435:THR:HG23	1:B:475:THR:HB	2.01	0.43
1:B:80:ILE:HG13	1:B:124:LEU:CD1	2.48	0.43
1:C:217:LEU:HD11	1:C:233:PHE:HZ	1.84	0.43
1:C:245:ASN:C	1:C:245:ASN:OD1	2.57	0.43
1:D:125:VAL:CG1	1:D:126:ASP:N	2.79	0.43
1:D:248:ARG:NH1	1:D:248:ARG:HB3	2.30	0.43
1:E:376:VAL:HG21	1:E:388:TYR:CE2	2.53	0.43
1:F:407:LYS:HB2	1:F:408:PRO:HD3	1.99	0.43
1:F:67:GLY:N	1:F:68:PRO:HD3	2.32	0.43
1:F:757:ILE:H	1:F:757:ILE:HG13	1.24	0.43
1:H:360:GLU:CG	1:H:361:TYR:CE2	3.02	0.43
1:A:136:GLU:HG2	1:A:509:ARG:HD2	2.01	0.43
1:B:502:PHE:CZ	1:B:510:VAL:HG21	2.53	0.43
1:C:54:GLU:CG	1:C:55:ALA:N	2.82	0.43
1:B:789:MET:C	1:C:789:MET:HE1	2.39	0.43
1:E:117:PHE:O	1:E:120:PHE:HB2	2.18	0.43
1:E:143:ASN:HB3	1:E:148:ARG:NH1	2.33	0.43
1:G:591:VAL:HG12	1:G:632:LEU:HD13	2.01	0.43
1:H:757:ILE:HD12	1:H:757:ILE:H	1.84	0.43
1:A:419:ASN:HB3	1:A:471:ALA:CB	2.49	0.42
1:A:65:GLU:C	1:A:67:GLY:N	2.71	0.42
1:B:153:LYS:CG	1:B:154:TYR:CD2	3.03	0.42
1:B:293:ASP:HB2	7:B:845:HOH:O	2.19	0.42
1:B:339:ARG:HD2	1:B:369:PHE:CZ	2.53	0.42
1:C:284:LEU:HD22	1:C:284:LEU:N	2.33	0.42
1:C:420:LEU:O	1:C:420:LEU:HD13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LEU:HD11	1:D:365:LEU:HD23	2.01	0.42
1:D:60:THR:C	1:D:62:LYS:H	2.21	0.42
1:D:678:GLY:HA2	7:D:840:HOH:O	2.19	0.42
1:E:703:ILE:CG2	1:E:704:VAL:N	2.82	0.42
1:E:749:ILE:HA	1:E:749:ILE:HD13	1.81	0.42
1:E:81:VAL:CG1	1:E:86:VAL:HG23	2.47	0.42
1:G:226:TYR:HB3	1:G:240:ARG:HH21	1.83	0.42
1:H:140:GLU:N	1:H:141:PRO:CD	2.82	0.42
1:H:17:ARG:HH21	1:H:72:LEU:CA	2.32	0.42
1:B:166:LEU:HB3	1:B:268:LEU:HD21	2.01	0.42
1:B:581:LEU:HD11	1:B:625:GLU:HG2	2.01	0.42
1:B:789:MET:HE3	1:C:789:MET:HE3	2.01	0.42
1:C:781:LEU:HD12	1:C:781:LEU:HA	1.86	0.42
1:E:146:ILE:HG13	1:E:147:PRO:HD2	2.02	0.42
1:E:316:GLU:OE1	1:E:361:TYR:N	2.39	0.42
1:F:81:VAL:HG12	1:F:86:VAL:CB	2.49	0.42
1:G:45:GLN:HE22	1:G:80:ILE:HG13	1.83	0.42
1:H:80:ILE:HG21	1:H:120:PHE:HD2	1.84	0.42
1:A:565:CYS:C	1:A:566:VAL:HG23	2.39	0.42
1:B:158:GLY:HA3	1:B:519:PRO:O	2.19	0.42
1:F:318:GLU:OE2	1:F:322:ARG:NH1	2.48	0.42
1:G:99:TYR:O	1:G:100:LEU:HD23	2.19	0.42
1:A:438:HIS:O	1:A:439:ALA:HB2	2.19	0.42
1:A:718:ASP:HA	7:A:863:HOH:O	2.20	0.42
1:B:327:GLY:O	1:B:328:LEU:HD23	2.20	0.42
1:B:615:LYS:HB2	1:B:615:LYS:HE3	1.85	0.42
1:C:178:LEU:N	1:C:179:PRO:HD2	2.34	0.42
1:C:552:GLU:O	1:C:556:SER:HB3	2.19	0.42
1:D:386:TRP:CZ2	1:D:464:GLN:HB2	2.53	0.42
1:D:469:ILE:HD13	1:D:469:ILE:HA	1.81	0.42
1:D:390:GLU:OE1	1:D:796:ARG:HD2	2.19	0.42
1:E:60:THR:OG1	1:E:61:ARG:N	2.52	0.42
1:F:226:TYR:HA	1:F:229:PHE:CZ	2.54	0.42
1:F:81:VAL:CG1	1:F:86:VAL:CB	2.97	0.42
1:G:146:ILE:HG13	1:G:147:PRO:CD	2.43	0.42
1:H:477:PHE:HA	1:H:520:LYS:HB2	2.00	0.42
1:H:724:LEU:HD23	1:H:724:LEU:HA	1.90	0.42
1:B:22:LEU:HA	1:B:22:LEU:HD23	1.90	0.42
1:B:63:LYS:HG3	1:B:64:LEU:N	2.33	0.42
1:C:491:GLU:N	1:C:491:GLU:CD	2.72	0.42
1:C:692:PHE:HZ	1:C:727:PHE:CG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:TYR:O	1:D:448:SER:HB3	2.19	0.42
1:E:163:ASN:HD21	1:E:269:GLU:HG3	1.85	0.42
1:E:294:ASN:N	7:E:844:HOH:O	2.41	0.42
1:E:419:ASN:HB3	1:E:471:ALA:CB	2.49	0.42
1:F:245:ASN:O	1:F:249:VAL:HG23	2.19	0.42
1:F:789:MET:HE3	1:G:789:MET:HG2	2.02	0.42
1:G:547:HIS:HE1	1:G:656:GLU:OE2	2.03	0.42
1:H:466:THR:HG23	1:H:790:PHE:CE2	2.54	0.42
1:A:534:PHE:HB2	1:A:535:PRO:HD2	2.00	0.42
1:A:756:GLN:HG3	1:A:757:ILE:HG13	2.01	0.42
1:C:54:GLU:HG3	1:C:55:ALA:H	1.84	0.42
1:C:78:GLU:OE2	1:C:121:LYS:CE	2.68	0.42
1:D:315:LEU:HG	1:D:319:MET:HE2	2.00	0.42
1:E:417:ASP:O	1:E:421:VAL:HG23	2.19	0.42
1:E:52:GLU:O	1:E:57:PRO:HD2	2.19	0.42
1:E:534:PHE:HB2	1:E:535:PRO:HD2	2.00	0.42
1:E:81:VAL:HG12	1:E:86:VAL:HB	2.01	0.42
1:G:130:ASN:HB3	1:G:134:THR:HG21	2.01	0.42
1:G:148:ARG:HD3	1:G:148:ARG:HA	1.82	0.42
1:G:149:PRO:O	1:G:517:PHE:CD1	2.73	0.42
1:G:490:LYS:HB2	1:G:490:LYS:HE3	1.85	0.42
1:G:54:GLU:OE2	1:G:55:ALA:CA	2.64	0.42
1:H:169:LYS:HG2	1:H:176:SER:OG	2.20	0.42
1:H:353:LEU:HA	1:H:364:ILE:O	2.19	0.42
1:H:582:ASP:OD1	1:H:582:ASP:C	2.58	0.42
1:A:56:LEU:CB	1:A:57:PRO:HD3	2.37	0.42
1:C:102:VAL:HG12	1:C:109:VAL:CG2	2.45	0.42
1:C:78:GLU:OE2	1:C:121:LYS:HE2	2.19	0.42
1:C:86:VAL:HG13	1:C:86:VAL:O	2.19	0.42
1:D:63:LYS:O	1:D:64:LEU:C	2.57	0.42
1:E:794:LYS:C	1:E:797:PRO:HD2	2.40	0.42
1:F:564:LEU:HA	1:F:564:LEU:HD12	1.86	0.42
1:H:315:LEU:HA	1:H:315:LEU:HD12	1.78	0.42
1:H:518:ASP:OD1	1:H:520:LYS:HG2	2.19	0.42
1:A:52:GLU:OE1	1:A:57:PRO:CD	2.68	0.42
1:C:116:GLU:O	1:C:119:HIS:HB2	2.19	0.42
1:C:472:MET:HG2	1:C:514:ILE:HD13	2.01	0.42
1:C:670:GLN:O	1:C:670:GLN:HG3	2.19	0.42
1:D:60:THR:C	1:D:62:LYS:N	2.73	0.42
1:E:60:THR:HG23	1:E:62:LYS:CG	2.38	0.42
1:F:452:TRP:CD2	1:F:453:LYS:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ILE:HD13	1:G:117:PHE:CZ	2.55	0.42
1:G:565:CYS:HB2	1:G:642:PHE:O	2.20	0.42
1:H:415:TYR:O	1:H:419:ASN:ND2	2.52	0.42
1:H:87:ALA:HB2	1:H:120:PHE:CE2	2.54	0.42
1:C:444:LYS:HB3	1:C:444:LYS:HE2	1.87	0.42
1:C:435:THR:HG23	1:C:475:THR:OG1	2.20	0.42
1:C:756:GLN:HG3	1:C:757:ILE:H	1.85	0.42
1:C:82:LEU:HB3	1:C:83:PRO:CD	2.46	0.42
1:E:28:GLU:O	1:E:32:LEU:HB2	2.19	0.42
1:E:156:GLY:CA	1:E:523:ILE:HG13	2.48	0.42
1:E:704:VAL:HA	4:E:912:SO4:O3	2.20	0.42
1:F:248:ARG:HB3	1:F:248:ARG:NH1	2.32	0.42
1:F:440:LEU:HD13	1:F:499:HIS:CE1	2.55	0.42
1:G:338:THR:OG1	1:G:339:ARG:N	2.53	0.42
1:H:85:TRP:HE3	1:H:101:ARG:HG2	1.85	0.42
1:H:276:PRO:HG3	1:H:326:GLN:HG3	2.01	0.42
1:A:147:PRO:CB	1:B:172:HIS:ND1	2.83	0.42
1:A:226:TYR:HB3	1:A:240:ARG:NH2	2.34	0.42
1:A:43:ILE:HD11	1:A:83:PRO:CD	2.44	0.42
1:B:319:MET:HE1	1:B:334:ILE:CD1	2.49	0.42
1:B:341:LEU:HA	1:B:342:PRO:HD3	1.85	0.42
1:C:580:ARG:NH2	1:C:582:ASP:OD2	2.52	0.42
1:D:143:ASN:HB3	1:D:148:ARG:HH22	1.80	0.42
1:E:210:LEU:HD23	1:E:253:ILE:HG23	1.98	0.42
1:G:163:ASN:O	1:G:167:SER:HB2	2.20	0.42
1:G:702:ILE:HA	1:G:753:TYR:OH	2.19	0.42
1:A:56:LEU:CD1	1:A:63:LYS:HG2	2.50	0.41
1:B:30:LEU:N	1:B:30:LEU:CD1	2.83	0.41
1:B:60:THR:C	1:B:62:LYS:H	2.23	0.41
1:C:518:ASP:OD1	1:C:520:LYS:HG2	2.19	0.41
1:D:83:PRO:CB	1:D:84:PRO:CD	2.94	0.41
1:E:140:GLU:HB3	1:E:141:PRO:CD	2.49	0.41
1:F:276:PRO:HG3	1:F:326:GLN:HB3	2.00	0.41
1:F:790:PHE:N	1:G:789:MET:HE1	2.35	0.41
1:H:21:THR:HG23	1:H:21:THR:O	2.19	0.41
1:A:680:THR:HG23	2:A:901:UDP:O1A	2.20	0.41
1:B:609:VAL:HA	1:B:645:ILE:O	2.20	0.41
1:C:490:LYS:HB2	1:C:490:LYS:HE3	1.82	0.41
1:C:527:GLY:O	1:C:755:TRP:NE1	2.52	0.41
1:C:145:SER:HB3	1:C:779:ASP:OD2	2.19	0.41
1:D:109:VAL:O	1:D:109:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:GLU:OE1	1:D:394:GLU:HA	2.19	0.41
1:D:599:ARG:O	1:D:603:LEU:HD12	2.20	0.41
1:E:366:ARG:HD3	7:E:856:HOH:O	2.20	0.41
1:E:386:TRP:N	1:E:387:PRO:HD2	2.35	0.41
1:E:44:LEU:HB3	1:E:45:GLN:H	1.45	0.41
1:E:681:VAL:O	1:E:685:MET:HG3	2.20	0.41
1:F:171:PHE:HD1	1:F:263:PRO:HD2	1.86	0.41
1:F:482:THR:HB	1:F:701:GLU:CD	2.40	0.41
1:F:512:HIS:CE1	1:F:515:ASP:HB2	2.55	0.41
1:F:796:ARG:N	1:F:797:PRO:CD	2.83	0.41
1:G:162:LEU:HD11	1:G:772:TRP:CD2	2.55	0.41
1:H:167:SER:OG	1:H:264:ASP:CA	2.67	0.41
1:H:435:THR:HG23	1:H:475:THR:CB	2.50	0.41
1:E:789:MET:CE	1:H:789:MET:CE	2.79	0.41
1:A:130:ASN:O	1:A:131:GLY:C	2.58	0.41
1:A:48:GLN:N	1:A:51:ALA:HB3	2.35	0.41
1:A:526:PRO:O	1:A:753:TYR:HB3	2.20	0.41
1:B:171:PHE:CD1	1:B:263:PRO:HD2	2.55	0.41
1:B:76:THR:O	1:B:76:THR:CG2	2.68	0.41
1:D:462:SER:HB2	1:D:507:LEU:CD2	2.50	0.41
1:E:56:LEU:HA	1:E:56:LEU:HD22	1.85	0.41
1:F:35:ARG:HG2	1:F:104:LEU:HA	2.01	0.41
1:G:590:LEU:HA	1:G:593:TRP:CD2	2.55	0.41
1:G:781:LEU:HA	1:G:781:LEU:HD12	1.76	0.41
1:A:657:LEU:O	1:A:661:ILE:HG12	2.20	0.41
1:B:167:SER:OG	1:B:264:ASP:CA	2.68	0.41
1:B:229:PHE:CD1	1:B:233:PHE:CE2	3.08	0.41
1:C:125:VAL:HG12	1:C:126:ASP:N	2.34	0.41
1:C:564:LEU:HD12	1:C:564:LEU:HA	1.81	0.41
1:C:564:LEU:HD22	1:C:613:ARG:NH2	2.36	0.41
1:C:586:ASN:HB3	1:C:671:PRO:O	2.20	0.41
1:D:140:GLU:N	1:D:141:PRO:CD	2.83	0.41
1:D:176:SER:O	1:D:179:PRO:HD2	2.21	0.41
1:D:502:PHE:CZ	1:D:510:VAL:HG21	2.56	0.41
1:D:82:LEU:CD1	1:D:85:TRP:H	2.33	0.41
1:E:572:LYS:HE3	1:E:605:ASN:OD1	2.20	0.41
1:F:224:THR:HG23	1:F:228:GLU:HG3	2.02	0.41
1:F:419:ASN:HB3	1:F:471:ALA:CB	2.50	0.41
1:F:574:ILE:HG23	1:F:607:VAL:HG23	2.02	0.41
1:G:82:LEU:H	1:G:83:PRO:HD3	1.85	0.41
1:H:31:ALA:HB1	1:H:35:ARG:HH21	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:HG22	1:A:384:GLU:HB2	2.02	0.41
1:A:474:HIS:HA	1:A:787:LEU:CD1	2.50	0.41
1:A:708:SER:HB3	1:A:748:ARG:HB2	2.03	0.41
1:A:796:ARG:N	1:A:797:PRO:CD	2.83	0.41
1:B:177:LEU:HD22	1:B:260:LEU:HD23	2.01	0.41
1:C:483:PHE:CZ	1:C:487:ALA:HB3	2.55	0.41
1:D:43:ILE:HG23	1:D:124:LEU:CD1	2.51	0.41
1:D:480:THR:HG21	1:D:486:ILE:HG12	2.02	0.41
1:E:59:GLN:HE21	1:E:59:GLN:HA	1.85	0.41
1:F:360:GLU:HB2	1:F:361:TYR:CE2	2.55	0.41
1:F:466:THR:HG23	1:F:790:PHE:CZ	2.55	0.41
1:H:283:ILE:HD12	1:H:312:VAL:HG12	2.03	0.41
1:H:17:ARG:NH2	1:H:72:LEU:CA	2.83	0.41
1:A:35:ARG:NH2	1:A:102:VAL:N	2.68	0.41
1:A:85:TRP:HB3	1:A:101:ARG:CG	2.51	0.41
1:A:89:ALA:HB2	1:A:117:PHE:CZ	2.56	0.41
1:B:424:LEU:HD22	1:C:133:PHE:CE1	2.55	0.41
1:B:555:TYR:OH	1:B:574:ILE:HD11	2.20	0.41
1:B:606:LEU:HD12	1:B:606:LEU:HA	1.93	0.41
1:B:716:HIS:HB3	4:B:913:SO4:S	2.61	0.41
1:C:272:LEU:HA	1:C:272:LEU:HD23	1.91	0.41
1:D:493:VAL:HG22	1:D:494:GLY:N	2.35	0.41
1:E:284:LEU:HD21	1:E:425:LEU:HD12	2.03	0.41
1:F:692:PHE:HZ	1:F:727:PHE:CG	2.38	0.41
1:G:178:LEU:N	1:G:179:PRO:HD2	2.35	0.41
1:G:479:ILE:HD11	1:G:762:LEU:HD13	2.01	0.41
1:H:221:LYS:HE2	1:H:221:LYS:HB3	1.88	0.41
1:H:425:LEU:HA	1:H:425:LEU:HD23	1.81	0.41
1:A:72:LEU:HD21	1:A:90:VAL:HG21	2.01	0.41
1:B:221:LYS:HE2	1:B:221:LYS:HB3	1.90	0.41
1:B:420:LEU:CD1	1:B:420:LEU:C	2.88	0.41
1:B:56:LEU:CB	1:B:57:PRO:CD	2.92	0.41
1:B:91:ARG:NH2	1:B:487:ALA:O	2.54	0.41
1:E:327:GLY:C	1:E:328:LEU:HD23	2.40	0.41
1:E:43:ILE:O	1:E:44:LEU:HB2	2.20	0.41
1:E:547:HIS:O	1:E:551:GLU:HG3	2.20	0.41
1:E:592:GLU:HG3	1:E:636:TYR:CE2	2.56	0.41
1:E:86:VAL:HG12	1:E:102:VAL:HG13	2.02	0.41
1:F:245:ASN:OD1	1:F:248:ARG:HG3	2.21	0.41
1:F:56:LEU:HD13	1:F:56:LEU:O	2.20	0.41
1:F:52:GLU:C	1:F:57:PRO:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:ASN:HB3	7:G:879:HOH:O	2.21	0.41
1:G:43:ILE:HG12	1:G:82:LEU:HA	2.03	0.41
1:H:192:LYS:HB2	1:H:192:LYS:HE3	1.78	0.41
1:H:692:PHE:N	1:H:692:PHE:CD1	2.88	0.41
1:H:804:LEU:HD23	1:H:804:LEU:HA	1.83	0.41
1:B:216:TYR:CD1	1:B:216:TYR:C	2.94	0.41
1:B:452:TRP:CD1	1:B:504:LEU:HB3	2.55	0.41
1:D:282:VAL:HG13	1:D:337:LEU:HD23	2.02	0.41
1:D:780:ARG:HD2	1:D:780:ARG:HA	1.66	0.41
1:E:390:GLU:OE1	1:E:796:ARG:HD2	2.21	0.41
1:E:459:TYR:HB3	1:E:461:PHE:CE1	2.56	0.41
1:E:673:LEU:HD23	1:E:714:PRO:HB2	2.02	0.41
1:F:56:LEU:O	1:F:59:GLN:HB3	2.19	0.41
1:F:63:LYS:O	1:F:65:GLU:N	2.53	0.41
1:G:227:GLU:HG3	1:G:228:GLU:N	2.36	0.41
1:G:290:PHE:O	1:G:366:ARG:NH1	2.54	0.41
1:H:322:ARG:O	1:H:326:GLN:HG2	2.21	0.41
1:H:43:ILE:HG22	1:H:43:ILE:O	2.21	0.41
1:H:61:ARG:C	1:H:63:LYS:N	2.74	0.41
1:H:781:LEU:HD12	1:H:781:LEU:HA	1.79	0.41
1:H:794:LYS:HA	1:H:794:LYS:HE2	2.03	0.41
1:A:219:GLU:HA	1:A:219:GLU:OE1	2.20	0.41
1:A:226:TYR:CD2	1:A:240:ARG:CZ	3.04	0.41
1:A:43:ILE:CD1	1:A:83:PRO:HD3	2.44	0.41
1:B:302:GLY:CA	3:B:902:FRU:HO1	2.31	0.41
1:B:518:ASP:HA	1:B:519:PRO:HD3	1.95	0.41
1:B:796:ARG:N	1:B:797:PRO:CD	2.83	0.41
1:B:91:ARG:HA	1:B:92:PRO:HD2	1.96	0.41
1:D:209:THR:HG23	1:D:236:ILE:CD1	2.50	0.41
1:E:483:PHE:CZ	1:E:487:ALA:HB3	2.56	0.41
1:F:370:ARG:CB	1:F:375:ILE:HA	2.51	0.41
1:F:410:LEU:HD12	1:F:411:ILE:N	2.35	0.41
1:F:561:LYS:HD3	1:F:613:ARG:O	2.21	0.41
1:F:65:GLU:OE2	1:F:68:PRO:HB2	2.20	0.41
1:F:713:ASP:OD1	1:F:713:ASP:C	2.59	0.41
1:F:789:MET:HB3	1:G:789:MET:HE2	1.86	0.41
1:G:143:ASN:HB2	1:G:148:ARG:NH2	2.36	0.41
1:G:668:PHE:CZ	1:G:680:THR:HB	2.56	0.41
1:H:230:GLU:OE1	1:H:240:ARG:NH1	2.54	0.41
1:H:419:ASN:HB3	1:H:471:ALA:HB1	2.03	0.41
1:H:784:ARG:O	1:H:788:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:C	1:A:72:LEU:CD1	2.88	0.41
1:B:307:TYR:CD1	1:B:307:TYR:C	2.94	0.41
1:B:682:VAL:HG13	1:B:749:ILE:HD12	2.01	0.41
1:C:107:LEU:C	1:C:108:VAL:HG12	2.40	0.41
1:C:360:GLU:HB2	1:C:361:TYR:CD2	2.55	0.41
1:C:85:TRP:CZ3	1:C:103:ASN:N	2.89	0.41
1:D:156:GLY:HA3	1:D:523:ILE:HG13	2.03	0.41
1:E:438:HIS:O	1:E:439:ALA:HB2	2.21	0.41
1:E:73:LEU:HD22	1:E:73:LEU:HA	1.86	0.41
1:F:668:PHE:HB2	1:F:689:LEU:CD2	2.51	0.41
1:G:452:TRP:CG	1:G:453:LYS:N	2.88	0.41
1:H:308:ILE:O	1:H:312:VAL:HG22	2.21	0.41
1:H:757:ILE:CD1	1:H:757:ILE:H	2.32	0.41
1:A:734:ASP:HA	1:A:735:PRO:HD2	1.91	0.41
1:B:348:THR:O	1:B:351:GLU:HG2	2.21	0.41
1:B:525:SER:HB3	1:B:753:TYR:HD1	1.86	0.41
1:B:60:THR:C	1:B:62:LYS:N	2.74	0.41
1:B:93:ARG:HB2	1:B:96:VAL:HG22	2.01	0.41
1:C:261:GLU:OE1	1:D:150:THR:N	2.49	0.41
1:C:433:GLN:HG2	1:C:475:THR:OG1	2.20	0.41
1:C:630:TYR:O	1:C:633:ILE:HB	2.20	0.41
1:D:77:GLN:HG2	1:D:91:ARG:HB3	2.02	0.41
1:E:124:LEU:CD1	1:E:124:LEU:O	2.57	0.41
1:E:664:THR:O	1:E:665:LYS:HB2	2.21	0.41
1:G:228:GLU:HA	1:G:228:GLU:OE1	2.21	0.41
1:G:276:PRO:HG3	1:G:326:GLN:HG3	2.02	0.41
1:H:341:LEU:HA	1:H:342:PRO:HD3	1.90	0.41
1:H:615:LYS:HE3	1:H:615:LYS:HB2	1.92	0.41
1:H:65:GLU:C	1:H:67:GLY:N	2.74	0.41
1:A:435:THR:HG23	1:A:475:THR:CB	2.52	0.40
1:B:174:LYS:CD	1:B:203:LEU:HD12	2.44	0.40
1:B:452:TRP:CE3	1:B:453:LYS:HA	2.55	0.40
1:B:756:GLN:HG3	1:B:757:ILE:N	2.35	0.40
1:C:778:LEU:HD12	1:C:778:LEU:N	2.30	0.40
1:E:216:TYR:CD1	1:E:216:TYR:C	2.94	0.40
1:E:338:THR:HG23	1:E:366:ARG:HG2	2.03	0.40
1:E:623:LYS:HB3	1:E:623:LYS:HE2	1.94	0.40
1:F:242:TRP:O	1:F:252:MET:HG3	2.21	0.40
1:F:677:PHE:CE2	1:F:702:ILE:HD11	2.57	0.40
1:G:173:ASP:HB3	1:G:176:SER:HB2	2.03	0.40
1:G:367:VAL:HG13	1:G:368:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:518:ASP:HA	1:G:519:PRO:HD3	1.85	0.40
1:G:578:MET:HA	1:G:609:VAL:O	2.20	0.40
1:H:353:LEU:CD1	1:H:365:LEU:HD13	2.51	0.40
1:A:415:TYR:HA	1:A:437:ALA:O	2.21	0.40
1:A:450:ILE:HG23	1:A:451:TYR:CD2	2.55	0.40
1:A:461:PHE:HB3	1:A:465:PHE:CE2	2.56	0.40
1:A:565:CYS:HB3	1:A:566:VAL:H	1.67	0.40
1:B:789:MET:HG2	1:C:789:MET:CE	2.49	0.40
1:B:796:ARG:HB2	1:B:797:PRO:HD3	2.03	0.40
1:C:49:ILE:N	1:C:49:ILE:HD13	2.35	0.40
1:C:560:ASN:OD1	1:C:562:GLU:HB2	2.21	0.40
1:C:91:ARG:HD2	1:C:97:TRP:CZ2	2.57	0.40
1:D:200:ILE:HG21	1:D:206:LEU:HB2	2.03	0.40
1:D:315:LEU:C	1:D:319:MET:HE2	2.41	0.40
1:E:60:THR:O	1:E:63:LYS:CD	2.69	0.40
1:G:166:LEU:HB3	1:G:268:LEU:HD21	2.03	0.40
1:G:386:TRP:CZ2	1:G:464:GLN:HG3	2.56	0.40
1:G:91:ARG:CZ	1:G:94:PRO:HA	2.50	0.40
1:H:749:ILE:HD13	1:H:753:TYR:HD2	1.86	0.40
1:A:387:PRO:HD3	1:A:802:VAL:HB	2.03	0.40
1:A:302:GLY:C	3:A:902:FRU:O1	2.60	0.40
1:B:113:GLN:CD	1:B:114:PRO:HD2	2.39	0.40
1:B:183:PHE:O	1:B:187:HIS:HB2	2.20	0.40
1:B:564:LEU:HD13	1:B:613:ARG:NH2	2.36	0.40
1:B:80:ILE:HG23	1:B:80:ILE:O	2.22	0.40
1:C:91:ARG:NH2	1:C:487:ALA:O	2.54	0.40
1:D:102:VAL:HG23	1:D:109:VAL:HG22	2.02	0.40
1:D:61:ARG:C	1:D:63:LYS:N	2.74	0.40
1:D:665:LYS:HD3	1:D:665:LYS:HA	1.80	0.40
1:E:348:THR:O	1:E:351:GLU:HG2	2.22	0.40
1:E:719:GLN:NE2	4:E:913:SO4:O2	2.53	0.40
1:G:394:GLU:O	1:G:398:VAL:HG23	2.20	0.40
1:G:470:PHE:CE1	1:G:791:TYR:HB2	2.55	0.40
1:G:491:GLU:CD	1:G:491:GLU:H	2.24	0.40
1:G:56:LEU:CB	1:G:57:PRO:CD	2.95	0.40
1:H:491:GLU:CD	1:H:491:GLU:H	2.25	0.40
1:H:566:VAL:O	1:H:640:GLY:CA	2.69	0.40
1:H:749:ILE:HD13	1:H:749:ILE:HA	1.95	0.40
1:A:256:LEU:O	1:A:260:LEU:HG	2.21	0.40
1:A:284:LEU:HD13	1:A:284:LEU:HA	1.96	0.40
1:B:233:PHE:HD1	1:B:238:LEU:CB	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:VAL:O	1:B:401:SER:HB3	2.22	0.40
1:B:52:GLU:OE1	1:B:57:PRO:CG	2.69	0.40
1:B:664:THR:O	1:B:665:LYS:HB2	2.21	0.40
1:C:276:PRO:HG3	1:C:326:GLN:HG3	2.02	0.40
1:C:338:THR:O	1:C:366:ARG:HA	2.22	0.40
1:C:662:CYS:SG	1:C:689:LEU:HB2	2.61	0.40
1:E:30:LEU:O	1:E:33:LEU:HB2	2.21	0.40
1:E:44:LEU:HD11	1:E:451:TYR:OH	2.21	0.40
1:E:60:THR:O	1:E:63:LYS:CG	2.67	0.40
1:F:789:MET:CB	1:G:789:MET:HE3	2.48	0.40
1:G:39:LYS:NZ	1:G:105:HIS:CE1	2.90	0.40
1:G:69:PHE:O	1:G:72:LEU:HB3	2.22	0.40
1:A:319:MET:O	1:A:323:ILE:HG13	2.21	0.40
1:A:566:VAL:O	1:A:640:GLY:CA	2.69	0.40
1:A:35:ARG:NH1	1:A:86:VAL:HG12	2.36	0.40
1:B:292:GLN:OE1	1:B:357:TYR:N	2.39	0.40
1:B:757:ILE:HD12	1:B:758:TYR:N	2.37	0.40
1:C:173:ASP:HB3	1:C:176:SER:HB3	2.04	0.40
1:C:46:GLN:HB3	1:C:50:ILE:HG12	2.03	0.40
1:C:795:TYR:CD2	1:C:795:TYR:C	2.95	0.40
1:E:39:LYS:HE3	1:E:105:HIS:NE2	2.37	0.40
1:E:140:GLU:N	1:E:141:PRO:CD	2.84	0.40
1:F:81:VAL:HG23	1:F:81:VAL:O	2.21	0.40
1:F:83:PRO:HB2	1:F:85:TRP:H	1.86	0.40
1:G:101:ARG:HD3	1:G:112:LEU:HD21	2.03	0.40
1:H:135:LEU:HD12	1:H:136:GLU:H	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/816 (96%)	737 (95%)	38 (5%)	4 (0%)	29	57
1	B	787/816 (96%)	732 (93%)	51 (6%)	4 (0%)	29	57
1	C	779/816 (96%)	741 (95%)	38 (5%)	0	100	100
1	D	779/816 (96%)	739 (95%)	39 (5%)	1 (0%)	51	79
1	E	779/816 (96%)	740 (95%)	38 (5%)	1 (0%)	51	79
1	F	779/816 (96%)	736 (94%)	41 (5%)	2 (0%)	41	68
1	G	779/816 (96%)	741 (95%)	36 (5%)	2 (0%)	41	68
1	H	795/816 (97%)	751 (94%)	43 (5%)	1 (0%)	51	79
All	All	6256/6528 (96%)	5917 (95%)	324 (5%)	15 (0%)	47	75

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	ALA
1	B	83	PRO
1	A	63	LYS
1	D	63	LYS
1	A	55	ALA
1	G	55	ALA
1	G	63	LYS
1	H	65	GLU
1	A	48	GLN
1	F	43	ILE
1	A	49	ILE
1	E	43	ILE
1	B	82	LEU
1	B	108	VAL
1	F	49	ILE

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	668/718 (93%)	626 (94%)	42 (6%)	18	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	668/718 (93%)	631 (94%)	37 (6%)	21	49
1	C	674/718 (94%)	646 (96%)	28 (4%)	30	60
1	D	669/718 (93%)	639 (96%)	30 (4%)	27	57
1	E	669/718 (93%)	639 (96%)	30 (4%)	27	57
1	F	674/718 (94%)	633 (94%)	41 (6%)	18	43
1	G	675/718 (94%)	641 (95%)	34 (5%)	24	53
1	H	681/718 (95%)	649 (95%)	32 (5%)	26	56
All	All	5378/5744 (94%)	5104 (95%)	274 (5%)	24	52

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	39	LYS
1	A	44	LEU
1	A	49	ILE
1	A	54	GLU
1	A	56	LEU
1	A	59	GLN
1	A	72	LEU
1	A	76	THR
1	A	100	LEU
1	A	116	GLU
1	A	119	HIS
1	A	120	PHE
1	A	128	VAL
1	A	132	ASN
1	A	140	GLU
1	A	148	ARG
1	A	153	LYS
1	A	170	LEU
1	A	197	SER
1	A	205	THR
1	A	207	GLN
1	A	216	TYR
1	A	220	LEU
1	A	248	ARG
1	A	250	LEU
1	A	258	ASP
1	A	290	PHE

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Mol	Chain	Res	Type
1	A	322	ARG
1	A	340	LEU
1	A	358	ASP
1	A	405	ASN
1	A	484	GLN
1	A	516	VAL
1	A	530	MET
1	A	556	SER
1	A	670	GLN
1	A	708	SER
1	A	743	LYS
1	A	757	ILE
1	A	777	ASN
1	A	781	LEU
1	B	32	LEU
1	B	43	ILE
1	B	45	GLN
1	B	56	LEU
1	B	59	GLN
1	B	65	GLU
1	B	70	PHE
1	B	73	LEU
1	B	103	ASN
1	B	105	HIS
1	B	132	ASN
1	B	143	ASN
1	B	148	ARG
1	B	167	SER
1	B	205	THR
1	B	216	TYR
1	B	222	SER
1	B	236	ILE
1	B	248	ARG
1	B	251	ASP
1	B	254	ARG
1	B	258	ASP
1	B	277	MET
1	B	307	TYR
1	B	358	ASP
1	B	425	LEU
1	B	456	ASP
1	B	484	GLN

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Mol	Chain	Res	Type
1	B	492	THR
1	B	545	LYS
1	B	556	SER
1	B	602	GLU
1	B	646	SER
1	B	670	GLN
1	B	708	SER
1	B	743	LYS
1	B	779	ASP
1	C	44	LEU
1	C	45	GLN
1	C	50	ILE
1	C	52	GLU
1	C	54	GLU
1	C	81	VAL
1	C	101	ARG
1	C	105	HIS
1	C	128	VAL
1	C	164	ARG
1	C	205	THR
1	C	216	TYR
1	C	240	ARG
1	C	248	ARG
1	C	251	ASP
1	C	252	MET
1	C	258	ASP
1	C	264	ASP
1	C	345	VAL
1	C	405	ASN
1	C	484	GLN
1	C	516	VAL
1	C	530	MET
1	C	556	SER
1	C	602	GLU
1	C	670	GLN
1	C	777	ASN
1	C	804	LEU
1	D	27	ASN
1	D	44	LEU
1	D	45	GLN
1	D	50	ILE
1	D	52	GLU

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Mol	Chain	Res	Type
1	D	54	GLU
1	D	72	LEU
1	D	76	THR
1	D	82	LEU
1	D	113	GLN
1	D	120	PHE
1	D	146	ILE
1	D	153	LYS
1	D	208	HIS
1	D	216	TYR
1	D	258	ASP
1	D	284	LEU
1	D	293	ASP
1	D	321	GLN
1	D	345	VAL
1	D	358	ASP
1	D	456	ASP
1	D	484	GLN
1	D	490	LYS
1	D	516	VAL
1	D	544	THR
1	D	556	SER
1	D	708	SER
1	D	743	LYS
1	D	757	ILE
1	E	30	LEU
1	E	32	LEU
1	E	45	GLN
1	E	46	GLN
1	E	50	ILE
1	E	56	LEU
1	E	59	GLN
1	E	81	VAL
1	E	85	TRP
1	E	105	HIS
1	E	125	VAL
1	E	132	ASN
1	E	146	ILE
1	E	167	SER
1	E	178	LEU
1	E	205	THR
1	E	216	TYR

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Mol	Chain	Res	Type
1	E	264	ASP
1	E	322	ARG
1	E	345	VAL
1	E	358	ASP
1	E	456	ASP
1	E	484	GLN
1	E	492	THR
1	E	516	VAL
1	E	641	GLN
1	E	646	SER
1	E	670	GLN
1	E	743	LYS
1	E	778	LEU
1	F	32	LEU
1	F	43	ILE
1	F	44	LEU
1	F	45	GLN
1	F	52	GLU
1	F	54	GLU
1	F	56	LEU
1	F	59	GLN
1	F	69	PHE
1	F	73	LEU
1	F	74	LYS
1	F	82	LEU
1	F	100	LEU
1	F	101	ARG
1	F	111	GLU
1	F	132	ASN
1	F	148	ARG
1	F	178	LEU
1	F	205	THR
1	F	216	TYR
1	F	228	GLU
1	F	253	ILE
1	F	258	ASP
1	F	285	SER
1	F	322	ARG
1	F	345	VAL
1	F	360	GLU
1	F	375	ILE
1	F	420	LEU

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Mol	Chain	Res	Type
1	F	484	GLN
1	F	516	VAL
1	F	537	THR
1	F	556	SER
1	F	616	GLU
1	F	664	THR
1	F	670	GLN
1	F	708	SER
1	F	743	LYS
1	F	750	GLU
1	F	757	ILE
1	F	777	ASN
1	G	28	GLU
1	G	32	LEU
1	G	41	LYS
1	G	45	GLN
1	G	48	GLN
1	G	50	ILE
1	G	54	GLU
1	G	56	LEU
1	G	61	ARG
1	G	65	GLU
1	G	81	VAL
1	G	82	LEU
1	G	90	VAL
1	G	125	VAL
1	G	132	ASN
1	G	146	ILE
1	G	170	LEU
1	G	205	THR
1	G	208	HIS
1	G	216	TYR
1	G	240	ARG
1	G	258	ASP
1	G	315	LEU
1	G	322	ARG
1	G	340	LEU
1	G	358	ASP
1	G	456	ASP
1	G	484	GLN
1	G	516	VAL
1	G	670	GLN

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Mol	Chain	Res	Type
1	G	692	PHE
1	G	743	LYS
1	G	781	LEU
1	G	782	GLU
1	H	18	LEU
1	H	21	THR
1	H	22	LEU
1	H	32	LEU
1	H	45	GLN
1	H	60	THR
1	H	61	ARG
1	H	73	LEU
1	H	81	VAL
1	H	105	HIS
1	H	112	LEU
1	H	113	GLN
1	H	124	LEU
1	H	143	ASN
1	H	146	ILE
1	H	148	ARG
1	H	167	SER
1	H	173	ASP
1	H	205	THR
1	H	216	TYR
1	H	222	SER
1	H	251	ASP
1	H	258	ASP
1	H	484	GLN
1	H	492	THR
1	H	545	LYS
1	H	556	SER
1	H	670	GLN
1	H	708	SER
1	H	757	ILE
1	H	759	SER
1	H	779	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	45	GLN

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Mol	Chain	Res	Type
1	A	59	GLN
1	A	189	HIS
1	A	294	ASN
1	A	414	ASN
1	A	777	ASN
1	B	46	GLN
1	B	47	ASN
1	B	59	GLN
1	B	132	ASN
1	B	208	HIS
1	B	321	GLN
1	B	547	HIS
1	C	46	GLN
1	C	48	GLN
1	C	59	GLN
1	C	119	HIS
1	C	189	HIS
1	C	311	GLN
1	D	27	ASN
1	D	45	GLN
1	D	46	GLN
1	D	48	GLN
1	D	59	GLN
1	D	113	GLN
1	D	189	HIS
1	D	304	GLN
1	D	414	ASN
1	D	427	HIS
1	E	47	ASN
1	E	189	HIS
1	E	190	GLN
1	E	405	ASN
1	E	414	ASN
1	F	59	GLN
1	F	119	HIS
1	F	190	GLN
1	F	311	GLN
1	G	45	GLN
1	G	48	GLN
1	G	59	GLN
1	G	103	ASN
1	G	105	HIS

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Mol	Chain	Res	Type
1	G	132	ASN
1	G	326	GLN
1	G	427	HIS
1	G	484	GLN
1	G	547	HIS
1	H	12	HIS
1	H	46	GLN
1	H	103	ASN
1	H	105	HIS
1	H	119	HIS
1	H	201	GLN
1	H	207	GLN
1	H	321	GLN
1	H	484	GLN
1	H	495	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 8 are monoatomic - leaving 58 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	SO4	E	913	-	4,4,4	0.18	0	6,6,6	0.12	0
5	MLA	C	921	-	0,6,6	0.00	-	0,7,7	0.00	-
3	FRU	E	902	-	11,12,12	0.79	1 (9%)	10,18,18	1.00	0
4	SO4	H	913	-	4,4,4	0.19	0	6,6,6	0.13	0
4	SO4	F	911	-	4,4,4	0.23	0	6,6,6	0.22	0
3	FRU	F	902	-	11,12,12	0.59	0	10,18,18	1.08	0
3	FRU	G	902	-	11,12,12	1.09	1 (9%)	10,18,18	1.21	1 (10%)
4	SO4	C	911	-	4,4,4	0.18	0	6,6,6	0.21	0
2	UDP	G	901	-	20,26,26	1.13	1 (5%)	25,40,40	0.98	1 (4%)
4	SO4	G	914	-	4,4,4	0.18	0	6,6,6	0.13	0
4	SO4	F	914	-	4,4,4	0.18	0	6,6,6	0.10	0
4	SO4	H	911	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	G	913	-	4,4,4	0.20	0	6,6,6	0.15	0
3	FRU	C	902	-	11,12,12	0.66	0	10,18,18	1.15	0
4	SO4	C	913	-	4,4,4	0.17	0	6,6,6	0.09	0
4	SO4	A	913	-	4,4,4	0.22	0	6,6,6	0.22	0
4	SO4	G	912	-	4,4,4	0.15	0	6,6,6	0.08	0
5	MLA	G	921	-	0,6,6	0.00	-	0,7,7	0.00	-
4	SO4	G	911	-	4,4,4	0.19	0	6,6,6	0.18	0
5	MLA	H	922	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	D	922	-	0,6,6	0.00	-	0,7,7	0.00	-
3	FRU	H	902	-	11,12,12	1.12	1 (9%)	10,18,18	1.24	0
5	MLA	E	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	F	901	-	20,26,26	1.12	1 (5%)	25,40,40	0.88	0
5	MLA	B	921	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	A	921	-	0,6,6	0.00	-	0,7,7	0.00	-
4	SO4	D	911	-	4,4,4	0.17	0	6,6,6	0.28	0
2	UDP	H	901	-	20,26,26	1.18	1 (5%)	25,40,40	1.10	1 (4%)
4	SO4	F	912	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	A	912	-	4,4,4	0.19	0	6,6,6	0.09	0
4	SO4	C	912	-	4,4,4	0.15	0	6,6,6	0.09	0
4	SO4	A	915	-	4,4,4	0.15	0	6,6,6	0.07	0
2	UDP	C	901	-	20,26,26	1.06	1 (5%)	25,40,40	0.96	1 (4%)
3	FRU	D	902	-	11,12,12	0.68	0	10,18,18	0.99	0
4	SO4	E	912	-	4,4,4	0.16	0	6,6,6	0.10	0
5	MLA	H	921	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	F	921	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	D	921	-	0,6,6	0.00	-	0,7,7	0.00	-
4	SO4	A	914	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	D	914	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	D	913	-	4,4,4	0.23	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FRU	B	902	-	11,12,12	0.68	0	10,18,18	1.22	1 (10%)
2	UDP	B	901	-	20,26,26	1.12	1 (5%)	25,40,40	1.11	2 (8%)
4	SO4	B	911	-	4,4,4	0.26	0	6,6,6	0.25	0
2	UDP	A	901	-	20,26,26	1.18	1 (5%)	25,40,40	0.96	1 (4%)
4	SO4	H	912	-	4,4,4	0.16	0	6,6,6	0.08	0
3	FRU	A	902	-	11,12,12	0.65	0	10,18,18	1.18	0
4	SO4	D	912	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	B	912	-	4,4,4	0.18	0	6,6,6	0.09	0
5	MLA	G	922	-	0,6,6	0.00	-	0,7,7	0.00	-
4	SO4	E	911	-	4,4,4	0.23	0	6,6,6	0.31	0
5	MLA	F	922	-	0,6,6	0.00	-	0,7,7	0.00	-
4	SO4	F	913	-	4,4,4	0.22	0	6,6,6	0.17	0
4	SO4	A	911	-	4,4,4	0.18	0	6,6,6	0.28	0
4	SO4	B	913	-	4,4,4	0.23	0	6,6,6	0.16	0
2	UDP	D	901	-	20,26,26	1.15	2 (10%)	25,40,40	1.08	1 (4%)
2	UDP	E	901	-	20,26,26	1.09	1 (5%)	25,40,40	1.03	2 (8%)
4	SO4	E	914	-	4,4,4	0.18	0	6,6,6	0.12	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
5	MLA	G	922	-	-	0/0/4/4	-
5	MLA	C	921	-	-	0/0/4/4	-
3	FRU	E	902	-	-	3/5/24/24	0/1/1/1
5	MLA	B	921	-	-	0/0/4/4	-
3	FRU	F	902	-	-	5/5/24/24	0/1/1/1
3	FRU	G	902	-	-	5/5/24/24	0/1/1/1
2	UDP	G	901	-	-	7/14/32/32	0/2/2/2
3	FRU	C	902	-	-	1/5/24/24	0/1/1/1
2	UDP	B	901	-	-	6/14/32/32	0/2/2/2
5	MLA	H	922	-	-	0/0/4/4	-
5	MLA	D	922	-	-	0/0/4/4	-
3	FRU	H	902	-	-	5/5/24/24	0/1/1/1
5	MLA	E	921	-	-	0/0/4/4	-
2	UDP	F	901	-	-	7/14/32/32	0/2/2/2
2	UDP	C	901	-	-	5/14/32/32	0/2/2/2
5	MLA	A	921	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	A	902	-	-	3/5/24/24	0/1/1/1
2	UDP	H	901	-	-	5/14/32/32	0/2/2/2
3	FRU	D	902	-	-	5/5/24/24	0/1/1/1
5	MLA	H	921	-	-	0/0/4/4	-
5	MLA	F	921	-	-	0/0/4/4	-
5	MLA	D	921	-	-	0/0/4/4	-
3	FRU	B	902	-	-	1/5/24/24	0/1/1/1
5	MLA	G	921	-	-	0/0/4/4	-
2	UDP	A	901	-	-	3/14/32/32	0/2/2/2
5	MLA	F	922	-	-	0/0/4/4	-
2	UDP	D	901	-	-	7/14/32/32	0/2/2/2
2	UDP	E	901	-	-	6/14/32/32	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	UDP	C4-N3	3.19	1.38	1.33
2	H	901	UDP	C4-N3	3.11	1.38	1.33
2	B	901	UDP	C4-N3	3.09	1.38	1.33
2	F	901	UDP	C4-N3	2.99	1.38	1.33
2	C	901	UDP	C4-N3	2.94	1.38	1.33
2	G	901	UDP	C4-N3	2.89	1.38	1.33
2	E	901	UDP	C4-N3	2.75	1.37	1.33
3	G	902	FRU	O5-C2	-2.58	1.39	1.43
2	D	901	UDP	C4-N3	2.53	1.37	1.33
3	E	902	FRU	O2-C2	2.32	1.44	1.40
3	H	902	FRU	O5-C2	-2.10	1.40	1.43
2	D	901	UDP	O4'-C4'	-2.01	1.40	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	UDP	PA-O3A-PB	-4.01	119.06	132.83
2	B	901	UDP	PA-O3A-PB	-3.32	121.43	132.83
2	E	901	UDP	PA-O3A-PB	-3.20	121.84	132.83
2	G	901	UDP	PA-O3A-PB	-3.18	121.93	132.83
2	H	901	UDP	PA-O3A-PB	-3.13	122.09	132.83
2	A	901	UDP	PA-O3A-PB	-3.04	122.39	132.83
2	C	901	UDP	PA-O3A-PB	-2.75	123.39	132.83
3	B	902	FRU	O4-C4-C3	-2.38	105.02	112.15
2	E	901	UDP	O2B-PB-O3A	2.29	112.31	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	UDP	C5-C4-N3	-2.09	118.72	123.31
3	G	902	FRU	O4-C4-C5	-2.06	105.09	111.05

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	902	FRU	O1-C1-C2-C3
3	E	902	FRU	O1-C1-C2-O2
3	G	902	FRU	O1-C1-C2-C3
2	G	901	UDP	C5'-O5'-PA-O1A
2	G	901	UDP	PA-O3A-PB-O2B
3	H	902	FRU	O1-C1-C2-C3
2	F	901	UDP	C5'-O5'-PA-O1A
2	F	901	UDP	C5'-O5'-PA-O3A
2	C	901	UDP	PA-O3A-PB-O2B
2	C	901	UDP	PA-O3A-PB-O3B
2	H	901	UDP	PA-O3A-PB-O2B
2	H	901	UDP	PA-O3A-PB-O3B
2	B	901	UDP	PA-O3A-PB-O2B
2	B	901	UDP	PA-O3A-PB-O3B
2	D	901	UDP	C5'-O5'-PA-O1A
2	E	901	UDP	O4'-C1'-N1-C6
2	E	901	UDP	PA-O3A-PB-O2B
3	G	902	FRU	C4-C5-C6-O6
3	H	902	FRU	O5-C5-C6-O6
3	G	902	FRU	O5-C5-C6-O6
3	H	902	FRU	C4-C5-C6-O6
2	C	901	UDP	O4'-C4'-C5'-O5'
2	H	901	UDP	O4'-C4'-C5'-O5'
2	A	901	UDP	O4'-C4'-C5'-O5'
2	E	901	UDP	C3'-C4'-C5'-O5'
2	E	901	UDP	O4'-C4'-C5'-O5'
3	F	902	FRU	C4-C5-C6-O6
2	G	901	UDP	O4'-C4'-C5'-O5'
3	F	902	FRU	O5-C5-C6-O6
3	E	902	FRU	O1-C1-C2-O5
3	F	902	FRU	O1-C1-C2-O5
2	H	901	UDP	C3'-C4'-C5'-O5'
2	A	901	UDP	C3'-C4'-C5'-O5'
2	C	901	UDP	C3'-C4'-C5'-O5'
3	F	902	FRU	O1-C1-C2-C3

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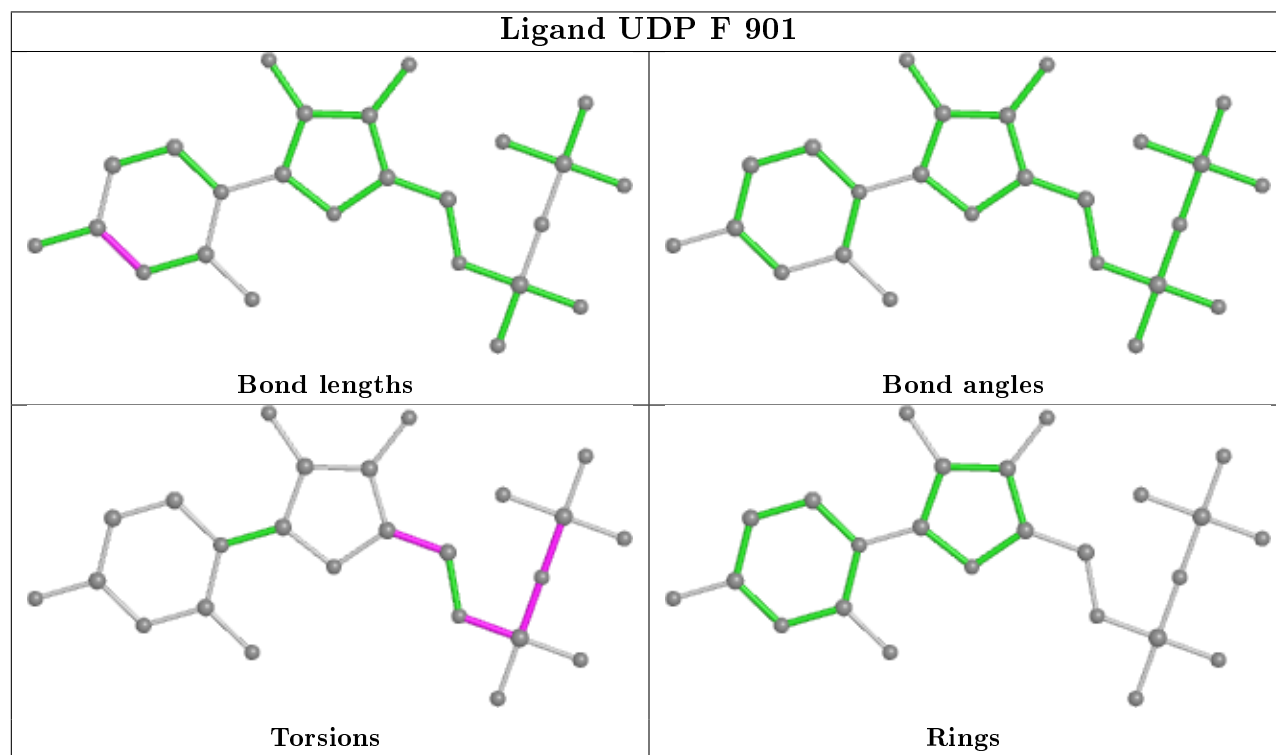
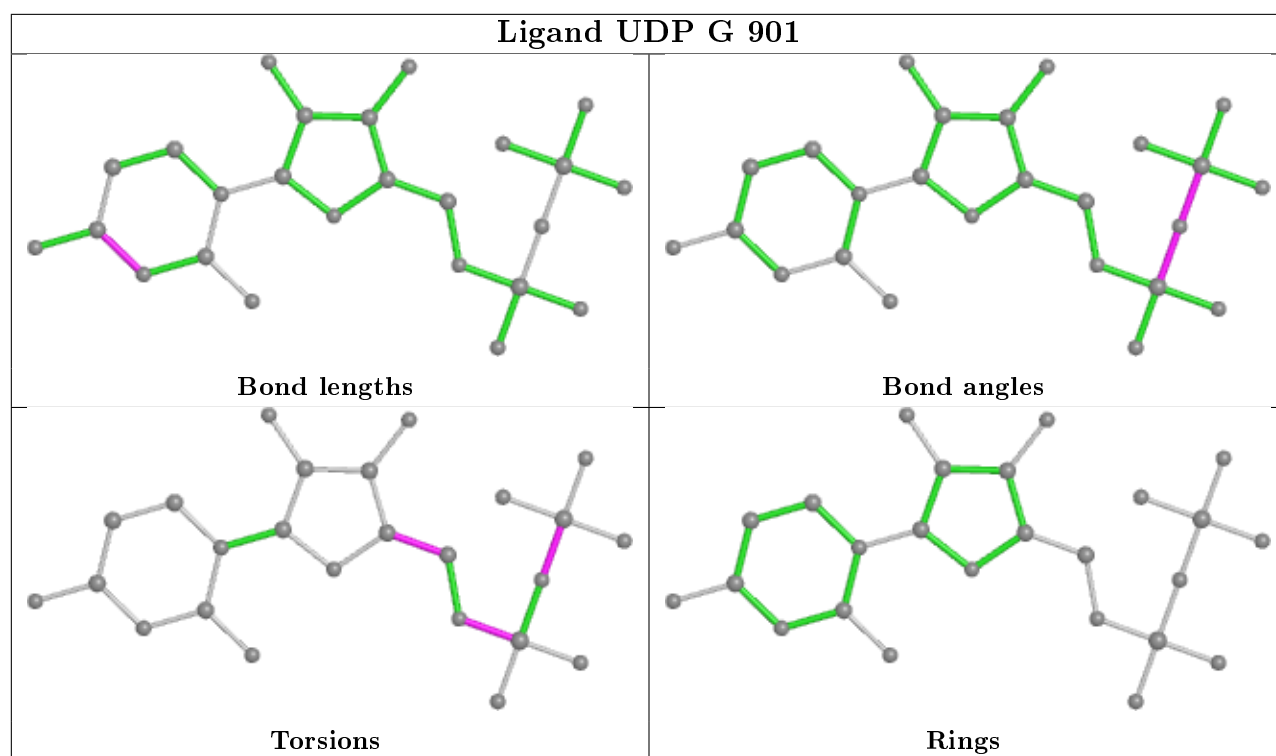
Mol	Chain	Res	Type	Atoms
3	D	902	FRU	O5-C5-C6-O6
3	F	902	FRU	O1-C1-C2-O2
2	G	901	UDP	C3'-C4'-C5'-O5'
2	B	901	UDP	O4'-C4'-C5'-O5'
3	D	902	FRU	C4-C5-C6-O6
3	C	902	FRU	O1-C1-C2-C3
3	H	902	FRU	O1-C1-C2-O5
2	H	901	UDP	PB-O3A-PA-O5'
2	A	901	UDP	PB-O3A-PA-O5'
2	E	901	UDP	PB-O3A-PA-O5'
2	F	901	UDP	PA-O3A-PB-O2B
2	G	901	UDP	C5'-O5'-PA-O3A
2	D	901	UDP	C5'-O5'-PA-O3A
3	G	902	FRU	O1-C1-C2-O2
3	H	902	FRU	O1-C1-C2-O2
3	G	902	FRU	O1-C1-C2-O5
2	D	901	UDP	O4'-C4'-C5'-O5'
2	B	901	UDP	C3'-C4'-C5'-O5'
2	D	901	UDP	PA-O3A-PB-O1B
2	E	901	UDP	PA-O3A-PB-O1B
2	F	901	UDP	PB-O3A-PA-O1A
3	A	902	FRU	O5-C5-C6-O6
3	D	902	FRU	O1-C1-C2-O2
2	G	901	UDP	PA-O3A-PB-O1B
2	G	901	UDP	PA-O3A-PB-O3B
2	F	901	UDP	PA-O3A-PB-O3B
3	A	902	FRU	C4-C5-C6-O6
2	D	901	UDP	PA-O3A-PB-O2B
2	D	901	UDP	PA-O3A-PB-O3B
3	D	902	FRU	O1-C1-C2-O5
2	F	901	UDP	O4'-C4'-C5'-O5'
2	D	901	UDP	C3'-C4'-C5'-O5'
3	A	902	FRU	O1-C1-C2-C3
3	D	902	FRU	O1-C1-C2-C3
3	B	902	FRU	O1-C1-C2-C3
2	F	901	UDP	C5'-O5'-PA-O2A
2	C	901	UDP	C5'-O5'-PA-O1A
2	B	901	UDP	C5'-O5'-PA-O1A
2	B	901	UDP	PA-O3A-PB-O1B

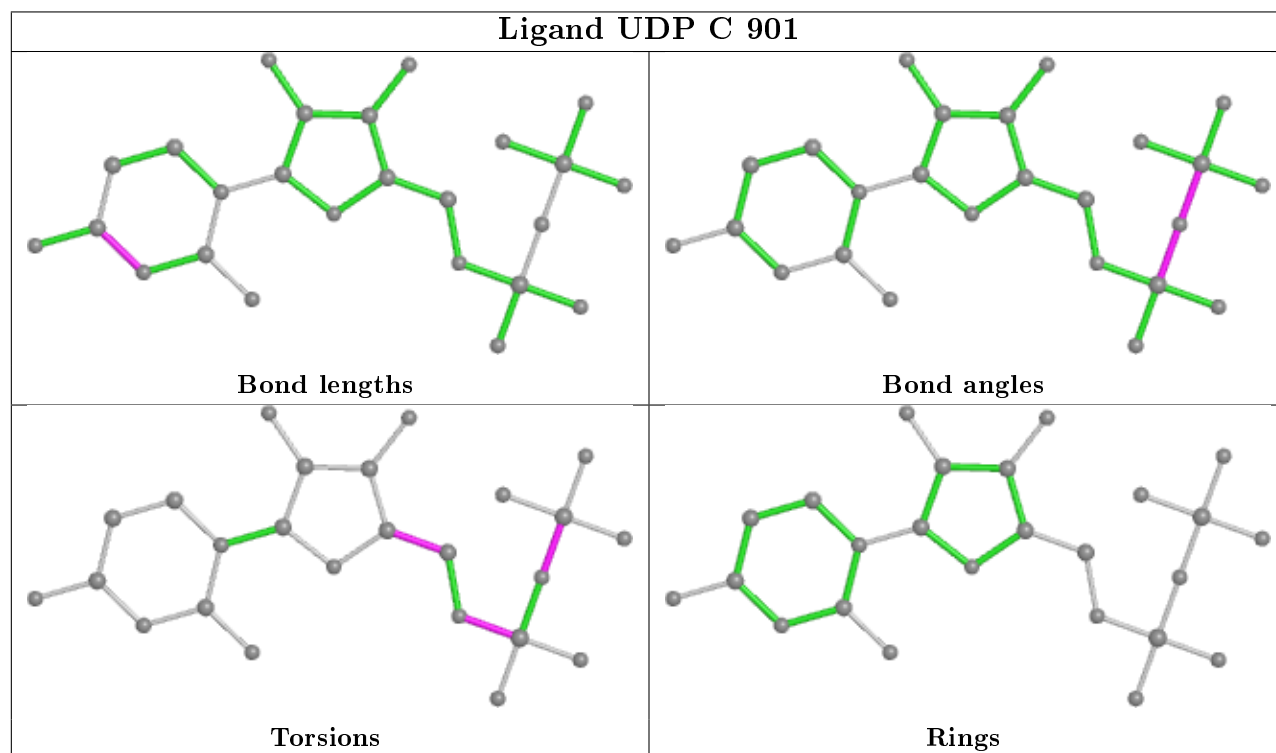
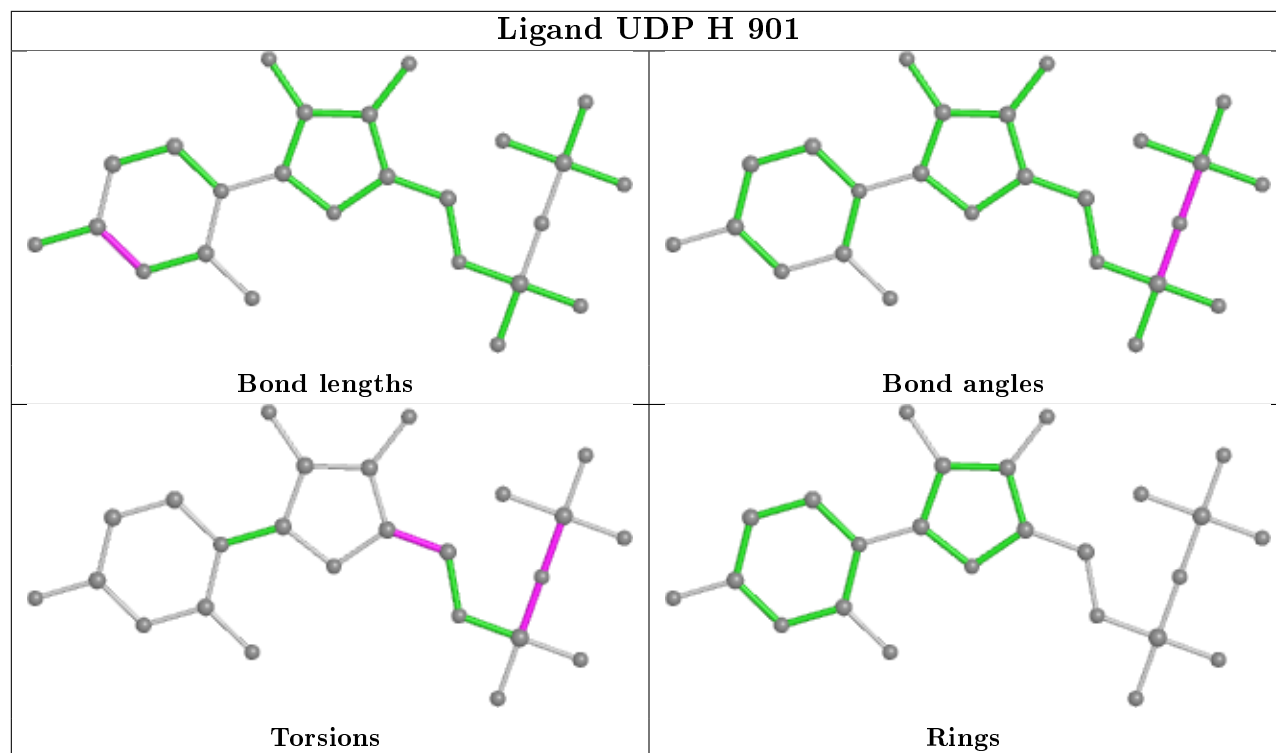
There are no ring outliers.

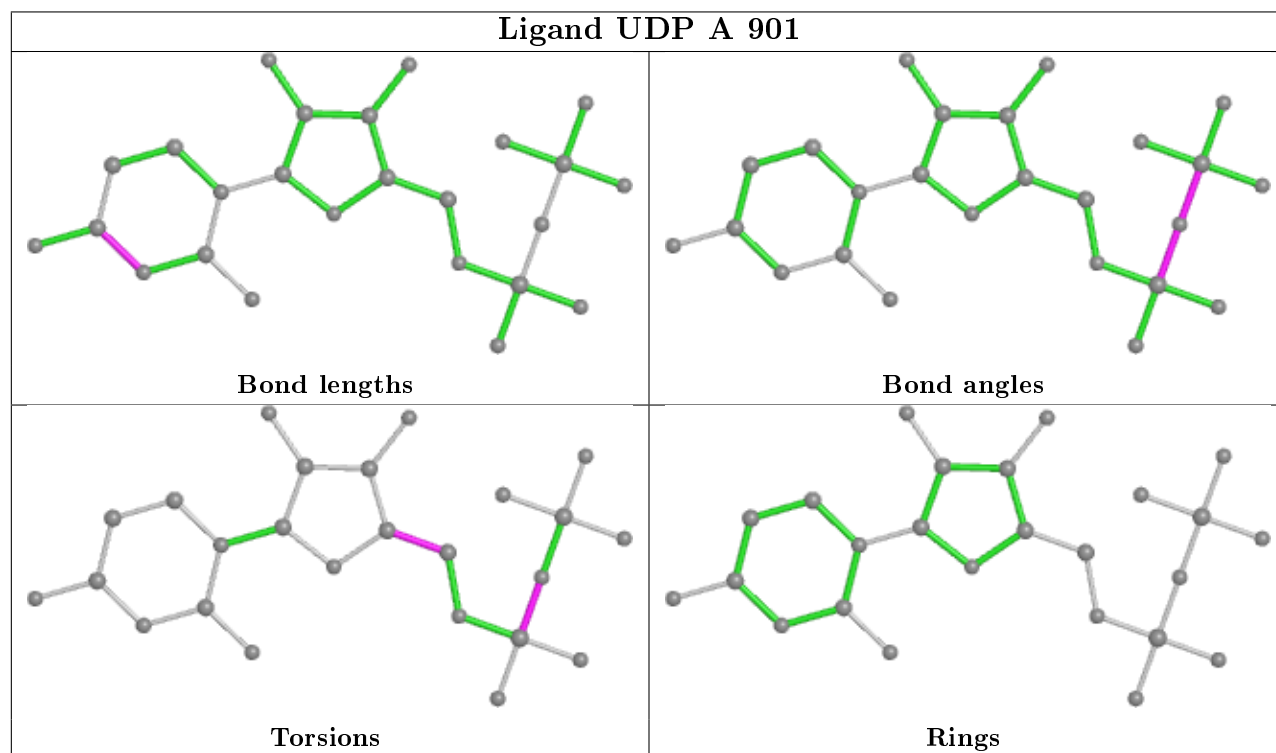
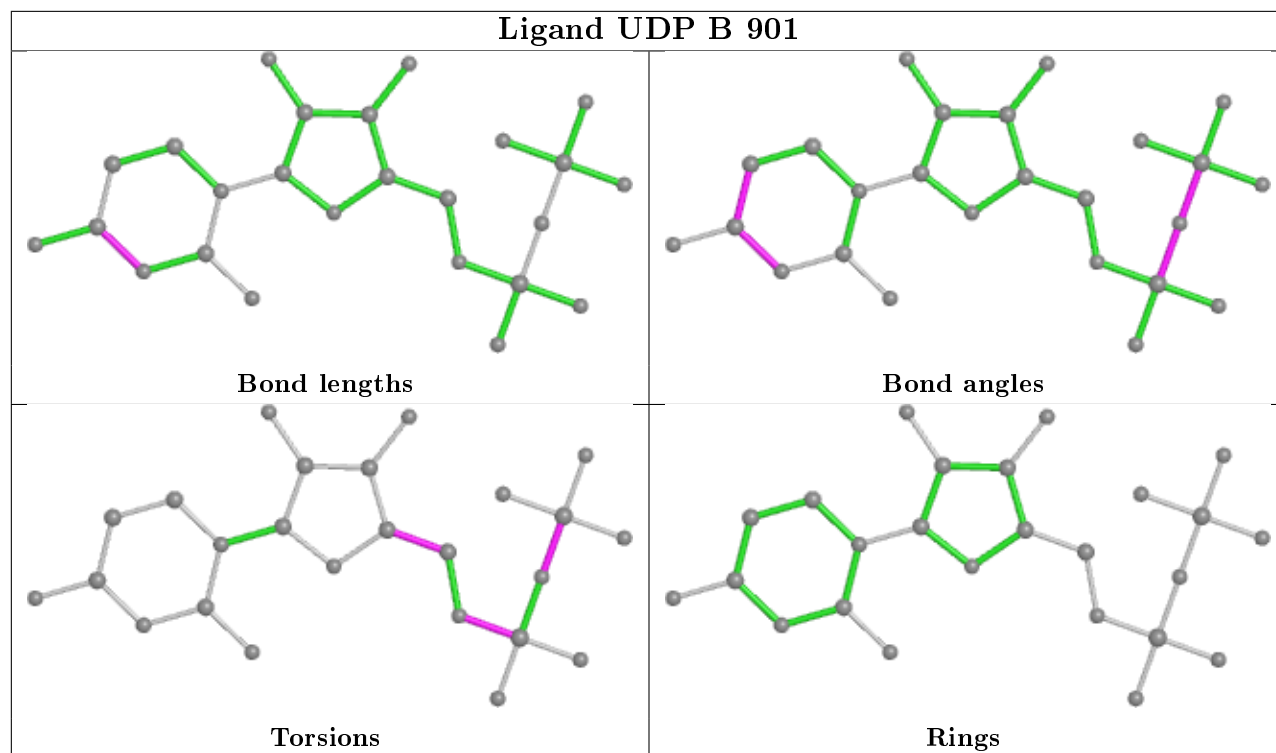
22 monomers are involved in 51 short contacts:

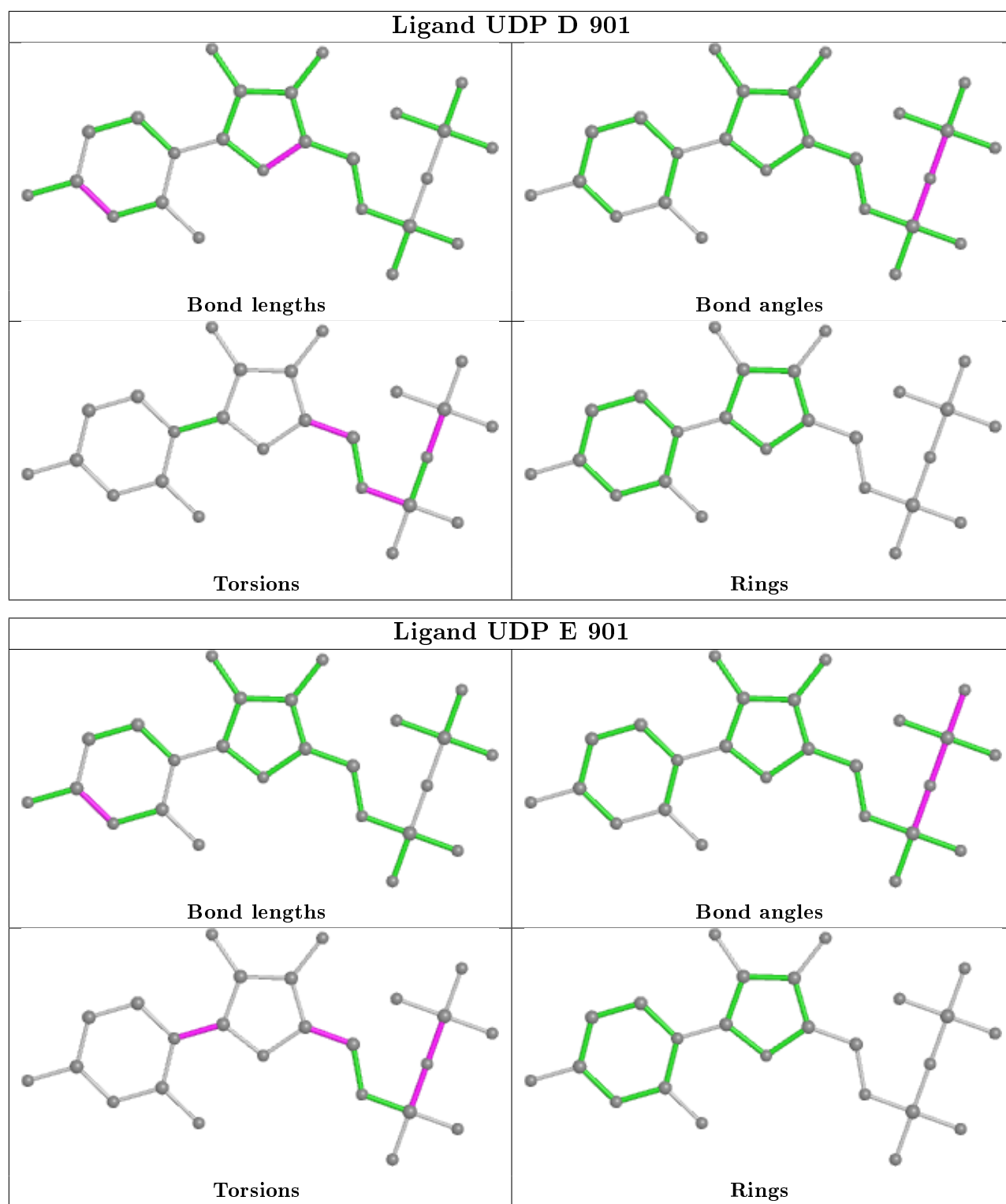
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	913	SO4	2	0
3	E	902	FRU	11	0
2	G	901	UDP	1	0
4	G	913	SO4	1	0
3	C	902	FRU	4	0
4	A	913	SO4	1	0
5	H	922	MLA	1	0
5	D	922	MLA	1	0
3	H	902	FRU	1	0
2	F	901	UDP	1	0
4	A	912	SO4	1	0
4	E	912	SO4	1	0
5	D	921	MLA	1	0
4	D	913	SO4	1	0
3	B	902	FRU	6	0
2	B	901	UDP	2	0
2	A	901	UDP	1	0
3	A	902	FRU	7	0
5	F	922	MLA	2	0
4	B	913	SO4	3	0
2	E	901	UDP	1	0
4	E	914	SO4	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	781/816 (95%)	-0.27	25 (3%)	47	42	21, 36, 99, 130	0
1	B	791/816 (96%)	-0.15	35 (4%)	34	29	24, 40, 108, 139	0
1	C	781/816 (95%)	-0.22	26 (3%)	46	41	27, 42, 89, 121	0
1	D	781/816 (95%)	-0.28	18 (2%)	60	57	23, 36, 89, 123	0
1	E	781/816 (95%)	-0.21	32 (4%)	37	31	22, 38, 109, 142	0
1	F	781/816 (95%)	-0.25	25 (3%)	47	42	21, 36, 85, 126	0
1	G	781/816 (95%)	-0.32	13 (1%)	70	68	22, 38, 83, 115	0
1	H	797/816 (97%)	-0.22	24 (3%)	50	45	24, 41, 94, 137	0
All	All	6274/6528 (96%)	-0.24	198 (3%)	47	42	21, 39, 94, 142	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	106	ALA	6.1
1	E	31	ALA	5.6
1	E	32	LEU	5.5
1	D	57	PRO	4.9
1	H	128	VAL	4.9
1	B	105	HIS	4.8
1	H	105	HIS	4.7
1	C	106	ALA	4.7
1	E	59	GLN	4.7
1	A	42	GLY	4.5
1	B	106	ALA	4.5
1	F	105	HIS	4.3
1	E	56	LEU	4.3
1	D	128	VAL	4.2
1	F	33	LEU	4.2
1	E	35	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	55	ALA	4.1
1	H	106	ALA	4.1
1	E	33	LEU	4.0
1	C	172	HIS	3.9
1	A	35	ARG	3.8
1	B	29	VAL	3.8
1	C	130	ASN	3.8
1	B	21	THR	3.8
1	D	32	LEU	3.8
1	A	128	VAL	3.7
1	G	59	GLN	3.7
1	F	59	GLN	3.7
1	E	68	PRO	3.7
1	B	128	VAL	3.7
1	H	129	LYS	3.6
1	A	68	PRO	3.6
1	B	43	ILE	3.6
1	C	59	GLN	3.6
1	B	83	PRO	3.6
1	B	84	PRO	3.6
1	H	127	GLY	3.5
1	E	83	PRO	3.5
1	F	172	HIS	3.5
1	A	59	GLN	3.5
1	C	57	PRO	3.4
1	C	128	VAL	3.4
1	H	216	TYR	3.4
1	G	128	VAL	3.4
1	E	27	ASN	3.4
1	B	109	VAL	3.3
1	A	51	ALA	3.3
1	G	29	VAL	3.3
1	E	28	GLU	3.3
1	E	44	LEU	3.3
1	E	30	LEU	3.3
1	A	57	PRO	3.3
1	F	68	PRO	3.2
1	D	46	GLN	3.2
1	A	30	LEU	3.2
1	H	83	PRO	3.2
1	B	69	PHE	3.2
1	G	130	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	31	ALA	3.1
1	D	55	ALA	3.1
1	H	59	GLN	3.1
1	H	82	LEU	3.1
1	C	104	LEU	3.1
1	E	172	HIS	3.1
1	D	130	ASN	3.1
1	A	107	LEU	3.0
1	B	102	VAL	3.0
1	C	107	LEU	3.0
1	C	127	GLY	3.0
1	E	57	PRO	3.0
1	G	107	LEU	3.0
1	A	126	ASP	3.0
1	D	42	GLY	3.0
1	C	32	LEU	3.0
1	F	67	GLY	2.9
1	H	13	SER	2.9
1	A	31	ALA	2.9
1	E	29	VAL	2.9
1	E	36	VAL	2.9
1	B	56	LEU	2.9
1	B	127	GLY	2.9
1	D	105	HIS	2.9
1	D	29	VAL	2.9
1	F	217	LEU	2.8
1	G	105	HIS	2.8
1	B	42	GLY	2.8
1	H	130	ASN	2.8
1	C	60	THR	2.8
1	B	172	HIS	2.8
1	A	46	GLN	2.7
1	E	64	LEU	2.7
1	F	36	VAL	2.7
1	E	42	GLY	2.7
1	A	43	ILE	2.7
1	D	59	GLN	2.7
1	C	42	GLY	2.7
1	D	56	LEU	2.7
1	F	30	LEU	2.7
1	C	244	ASP	2.7
1	E	58	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	110	GLU	2.7
1	B	38	ALA	2.7
1	B	107	LEU	2.6
1	B	86	VAL	2.6
1	E	244	ASP	2.6
1	G	27	ASN	2.6
1	G	32	LEU	2.6
1	B	65	GLU	2.6
1	B	191	GLY	2.6
1	B	111	GLU	2.6
1	C	105	HIS	2.6
1	B	23	VAL	2.5
1	H	126	ASP	2.5
1	C	126	ASP	2.5
1	E	245	ASN	2.5
1	F	128	VAL	2.5
1	B	62	LYS	2.5
1	D	58	GLU	2.5
1	H	236	ILE	2.5
1	A	244	ASP	2.5
1	E	127	GLY	2.5
1	A	200	ILE	2.5
1	F	104	LEU	2.5
1	D	60	THR	2.5
1	F	224	THR	2.5
1	H	103	ASN	2.5
1	C	83	PRO	2.4
1	E	67	GLY	2.4
1	B	327	GLY	2.4
1	F	40	GLY	2.4
1	E	43	ILE	2.4
1	G	129	LYS	2.4
1	H	11	VAL	2.4
1	B	126	ASP	2.4
1	F	244	ASP	2.4
1	B	54	GLU	2.4
1	A	223	GLU	2.4
1	D	220	LEU	2.4
1	H	29	VAL	2.4
1	B	59	GLN	2.3
1	A	56	LEU	2.3
1	F	42	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	44	LEU	2.3
1	C	68	PRO	2.3
1	H	58	GLU	2.3
1	A	67	GLY	2.3
1	H	733	GLU	2.3
1	D	107	LEU	2.3
1	G	30	LEU	2.3
1	H	193	ASN	2.3
1	C	220	LEU	2.3
1	E	235	GLU	2.3
1	F	220	LEU	2.3
1	E	52	GLU	2.3
1	A	32	LEU	2.3
1	E	221	LYS	2.3
1	B	537	THR	2.2
1	H	229	PHE	2.2
1	B	224	THR	2.2
1	C	245	ASN	2.2
1	E	34	SER	2.2
1	D	172	HIS	2.2
1	C	190	GLN	2.2
1	C	221	LYS	2.2
1	A	224	THR	2.2
1	B	22	LEU	2.2
1	C	31	ALA	2.2
1	B	221	LYS	2.2
1	A	83	PRO	2.2
1	B	24	SER	2.2
1	H	222	SER	2.2
1	C	108	VAL	2.2
1	D	221	LYS	2.1
1	H	80	ILE	2.1
1	G	244	ASP	2.1
1	G	42	GLY	2.1
1	E	46	GLN	2.1
1	F	249	VAL	2.1
1	C	43	ILE	2.1
1	F	221	LYS	2.1
1	A	34	SER	2.1
1	E	105	HIS	2.1
1	G	239	GLU	2.1
1	F	46	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	236	ILE	2.1
1	F	27	ASN	2.1
1	A	39	LYS	2.1
1	H	18	LEU	2.1
1	A	127	GLY	2.1
1	F	202	ASN	2.1
1	F	32	LEU	2.0
1	B	239	GLU	2.0
1	F	29	VAL	2.0
1	B	33	LEU	2.0
1	F	28	GLU	2.0
1	F	197	SER	2.0
1	C	201	GLN	2.0
1	E	38	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	K	E	931	1/1	0.80	0.18	79,79,79,79	0
6	K	B	931	1/1	0.81	0.23	99,99,99,99	0
4	SO4	H	913	5/5	0.84	0.34	70,78,93,114	0
5	MLA	G	922	7/7	0.85	0.15	69,86,100,100	0
5	MLA	F	922	7/7	0.87	0.26	49,58,70,70	0
4	SO4	A	915	5/5	0.88	0.24	120,122,135,138	0
5	MLA	H	922	7/7	0.88	0.23	70,79,84,85	0
4	SO4	G	914	5/5	0.88	0.27	62,88,97,108	0
4	SO4	H	912	5/5	0.89	0.32	66,89,99,112	0

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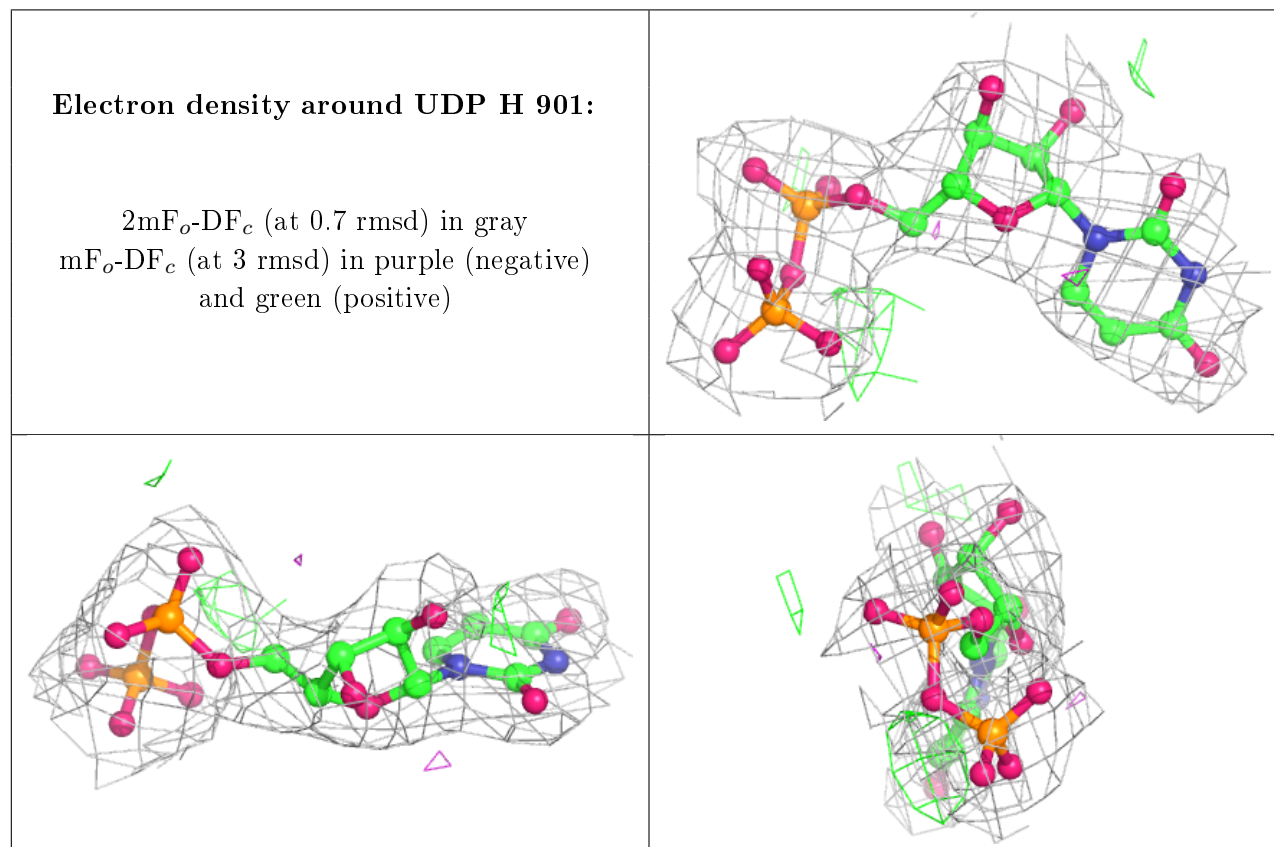
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	914	5/5	0.89	0.20	59,91,102,108	0
4	SO4	D	914	5/5	0.89	0.27	64,90,95,108	0
6	K	F	931	1/1	0.89	0.26	89,89,89,89	0
4	SO4	D	912	5/5	0.90	0.24	57,71,94,108	0
4	SO4	B	911	5/5	0.90	0.22	53,57,72,97	0
4	SO4	D	911	5/5	0.91	0.27	47,64,79,95	0
5	MLA	C	921	7/7	0.92	0.27	58,61,72,72	0
4	SO4	A	911	5/5	0.92	0.24	46,48,79,82	0
4	SO4	F	911	5/5	0.92	0.34	51,51,80,90	0
4	SO4	C	912	5/5	0.93	0.23	73,82,95,107	0
4	SO4	A	913	5/5	0.93	0.28	49,66,79,86	0
4	SO4	B	912	5/5	0.93	0.19	76,85,96,114	0
4	SO4	E	912	5/5	0.93	0.21	65,77,86,100	0
4	SO4	E	913	5/5	0.93	0.29	54,57,84,92	0
6	K	C	931	1/1	0.93	0.18	75,75,75,75	0
4	SO4	B	913	5/5	0.93	0.45	63,74,83,102	0
4	SO4	A	912	5/5	0.93	0.23	62,72,79,100	0
4	SO4	E	914	5/5	0.93	0.27	65,88,93,106	0
5	MLA	G	921	7/7	0.94	0.36	52,59,71,71	0
4	SO4	F	914	5/5	0.94	0.22	59,81,101,102	0
6	K	D	931	1/1	0.94	0.30	81,81,81,81	0
5	MLA	H	921	7/7	0.94	0.28	47,56,67,67	0
6	K	G	931	1/1	0.94	0.25	76,76,76,76	0
6	K	H	931	1/1	0.94	0.26	74,74,74,74	0
4	SO4	F	912	5/5	0.94	0.18	57,71,79,92	0
4	SO4	C	913	5/5	0.94	0.31	64,68,88,94	0
4	SO4	H	911	5/5	0.95	0.23	47,48,81,82	0
4	SO4	F	913	5/5	0.95	0.20	53,56,74,79	0
5	MLA	B	921	7/7	0.95	0.19	45,48,58,58	0
3	FRU	G	902	12/12	0.95	0.18	24,33,34,39	0
4	SO4	C	911	5/5	0.95	0.21	51,51,71,82	0
4	SO4	E	911	5/5	0.95	0.17	44,44,71,79	0
4	SO4	G	911	5/5	0.96	0.18	41,44,65,67	0
4	SO4	D	913	5/5	0.96	0.31	58,60,73,85	0
3	FRU	C	902	12/12	0.96	0.17	31,38,43,46	0
5	MLA	D	922	7/7	0.96	0.19	45,49,54,55	0
6	K	A	931	1/1	0.96	0.16	72,72,72,72	0
3	FRU	H	902	12/12	0.96	0.18	23,29,34,36	0
5	MLA	F	921	7/7	0.96	0.29	32,38,40,45	0
5	MLA	E	921	7/7	0.96	0.25	36,45,50,54	0
4	SO4	G	913	5/5	0.97	0.30	58,62,82,92	0
3	FRU	B	902	12/12	0.97	0.17	27,30,33,33	0

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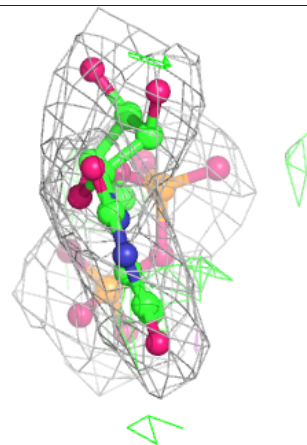
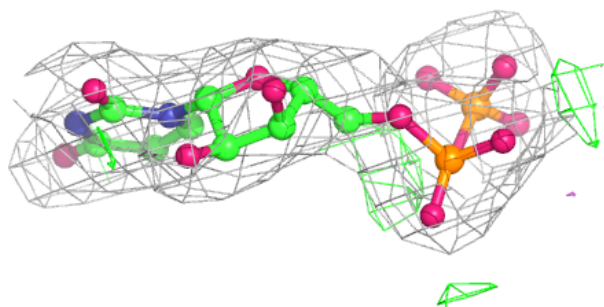
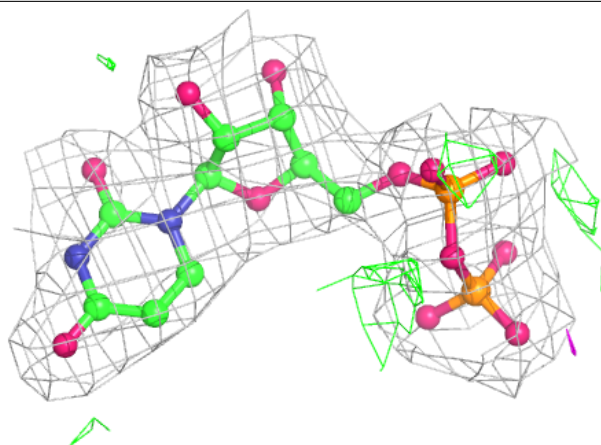
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MLA	D	921	7/7	0.97	0.24	37,44,46,48	0
4	SO4	G	912	5/5	0.97	0.20	57,74,84,97	0
3	FRU	A	902	12/12	0.97	0.21	28,29,32,34	0
5	MLA	A	921	7/7	0.98	0.20	38,41,49,49	0
3	FRU	E	902	12/12	0.98	0.16	28,30,33,33	0
2	UDP	H	901	25/25	0.98	0.18	25,28,34,37	0
3	FRU	D	902	12/12	0.98	0.17	25,28,32,32	0
3	FRU	F	902	12/12	0.98	0.17	23,26,28,28	0
2	UDP	B	901	25/25	0.99	0.18	25,29,32,32	0
2	UDP	F	901	25/25	0.99	0.17	18,25,29,33	0
2	UDP	A	901	25/25	0.99	0.16	20,26,29,33	0
2	UDP	D	901	25/25	0.99	0.17	22,25,32,35	0
2	UDP	C	901	25/25	0.99	0.16	25,31,35,39	0
2	UDP	E	901	25/25	0.99	0.18	23,26,31,33	0
2	UDP	G	901	25/25	0.99	0.16	19,26,29,31	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.



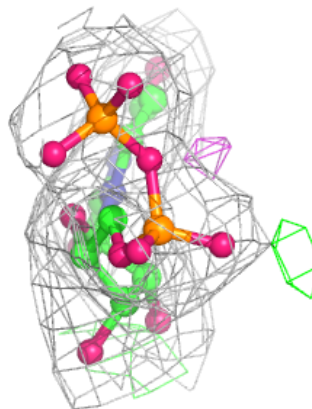
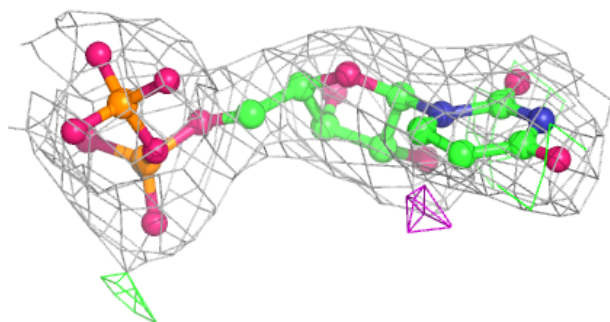
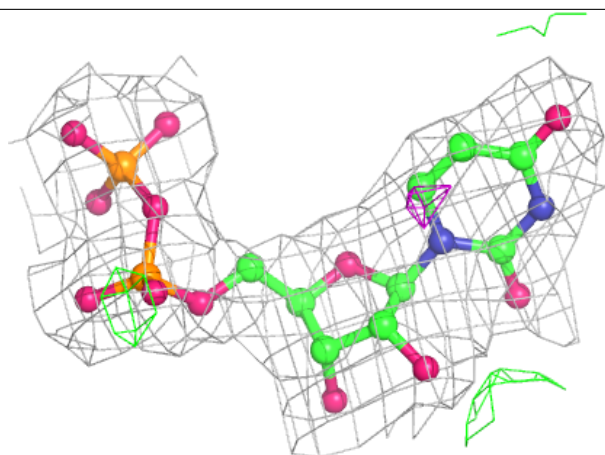
Electron density around UDP B 901:

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



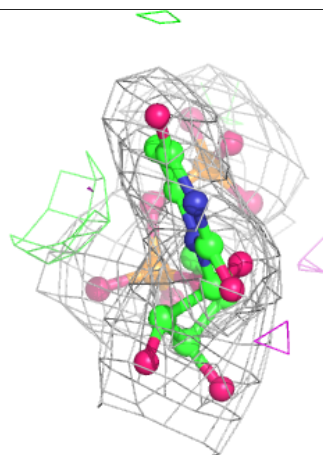
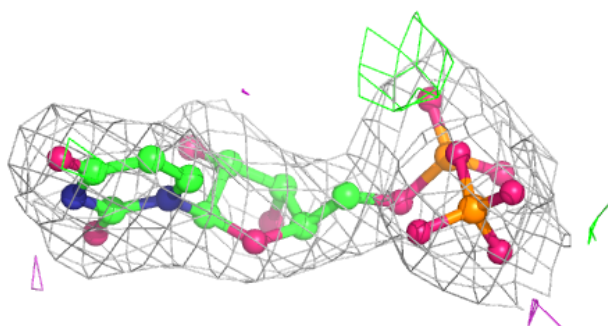
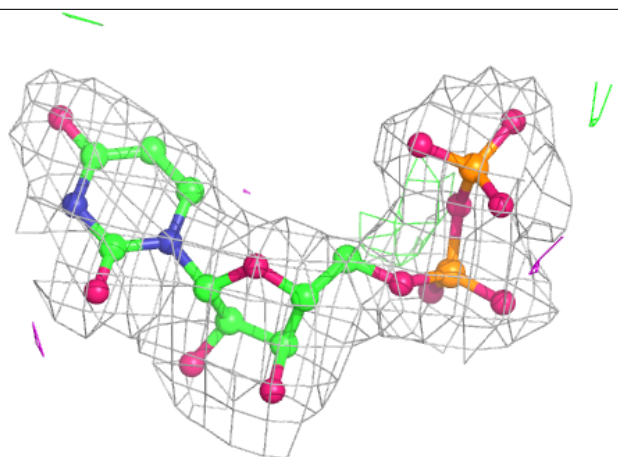
Electron density around UDP F 901:

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



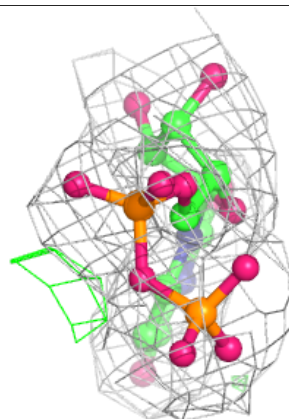
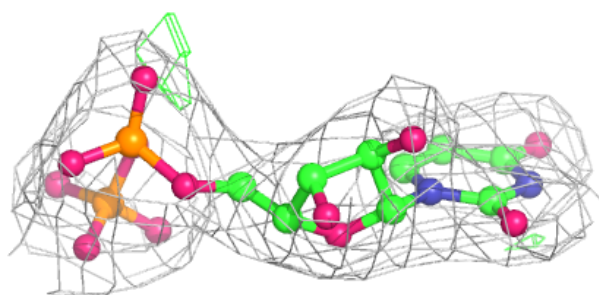
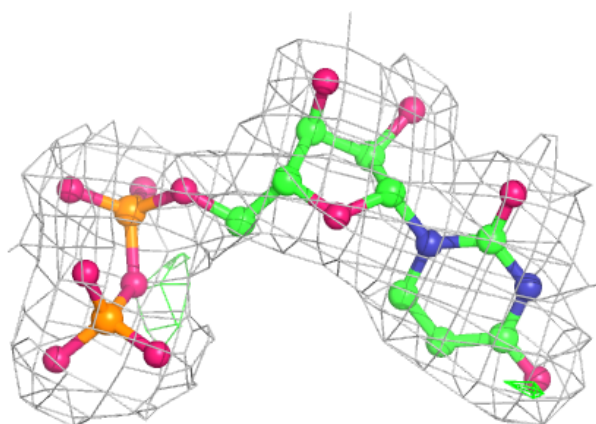
Electron density around UDP A 901:

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

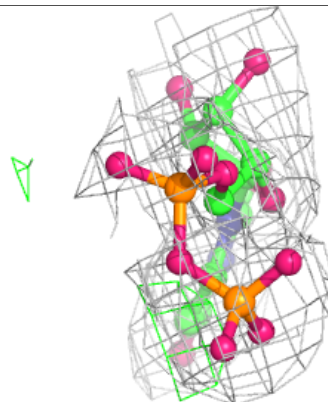
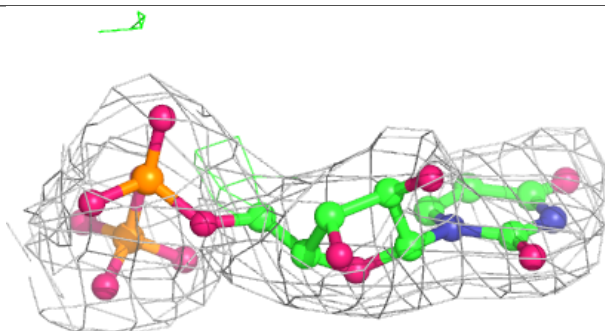
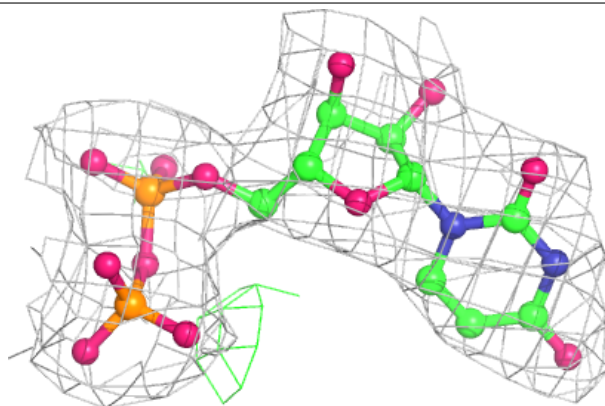


Electron density around UDP D 901:

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

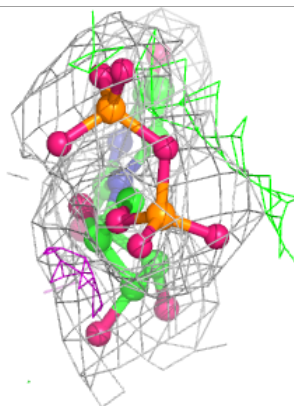
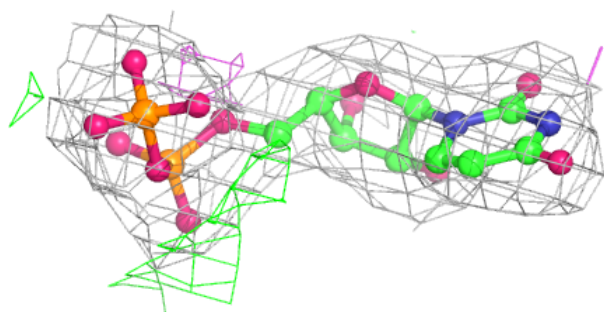
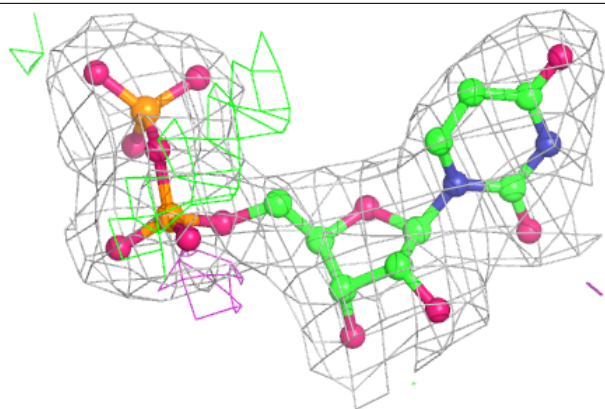
**Electron density around UDP C 901:**

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

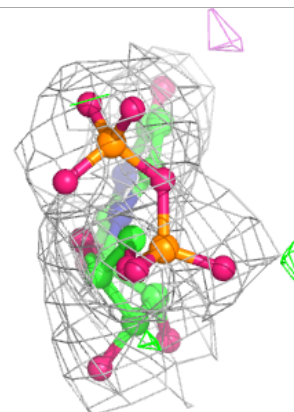
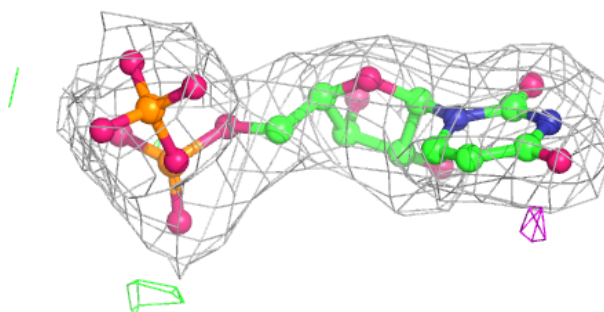
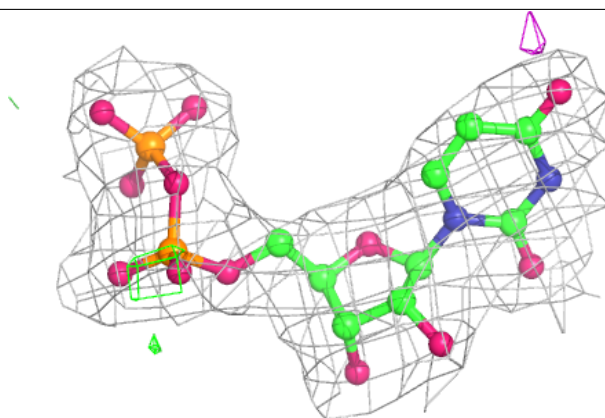


Electron density around UDP E 901:

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

**Electron density around UDP G 901:**

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



6.5 Other polymers

There are no such residues in this entry.