



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 08:28 PM EST

PDB ID : 3S27
Title : The crystal structure of sucrose synthase-1 from Arabidopsis thaliana and its functional implications.
Authors : Zheng, Y.; Garavito, R.M.
Deposited on : 2011-05-16
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

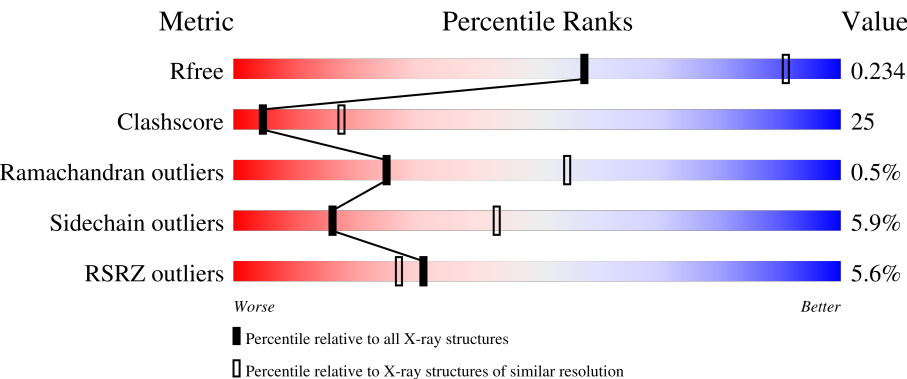
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.91 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}	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	816	<div><div>5%</div><div><div></div><div>58%</div><div>34%</div><div></div></div><div></div></div>
1	B	816	<div><div>10%</div><div><div></div><div>58%</div><div>36%</div><div></div></div><div></div></div>
1	C	816	<div><div>3%</div><div><div></div><div>54%</div><div>38%</div><div></div></div><div></div></div>
1	D	816	<div><div>4%</div><div><div></div><div>60%</div><div>34%</div><div></div></div><div></div></div>
1	E	816	<div><div>5%</div><div><div></div><div>60%</div><div>31%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	816	
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
4	SO4	B	913	-	-	X	-
4	SO4	F	913	-	-	X	-
5	MLA	E	921	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 51483 atoms, of which 200 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	Se	0	0	0
			6277	4031	1065	1159	10	12			
1	B	793	Total	C	N	O	S	Se	0	0	0
			6313	4046	1074	1171	10	12			
1	C	781	Total	C	N	O	S	Se	0	0	0
			6268	4028	1064	1154	10	12			
1	D	781	Total	C	N	O	S	Se	0	0	0
			6243	4014	1059	1148	10	12			
1	E	781	Total	C	N	O	S	Se	0	0	0
			6249	4014	1061	1152	10	12			
1	F	781	Total	C	N	O	S	Se	0	0	0
			6275	4031	1064	1158	10	12			
1	G	781	Total	C	N	O	S	Se	0	0	0
			6279	4032	1068	1157	10	12			
1	H	797	Total	C	N	O	S	Se	0	0	0
			6336	4060	1087	1167	10	12			

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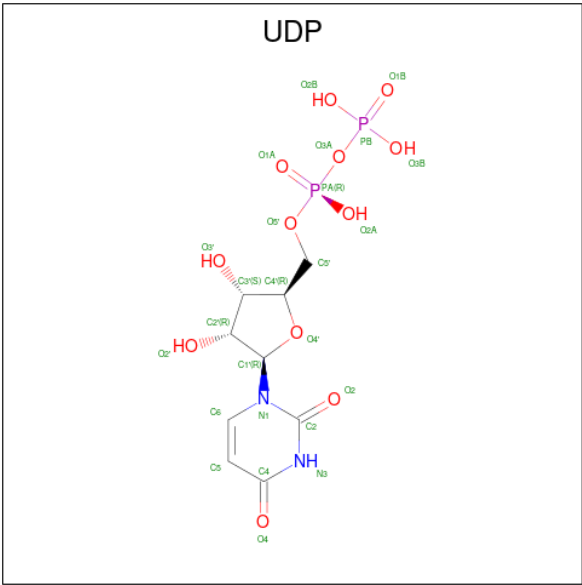
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	expression tag	UNP P49040
B	815	HIS	-	expression tag	UNP P49040
B	816	HIS	-	expression tag	UNP P49040
C	809	VAL	-	expression tag	UNP P49040
C	810	GLU	-	expression tag	UNP P49040
C	811	HIS	-	expression tag	UNP P49040
C	812	HIS	-	expression tag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



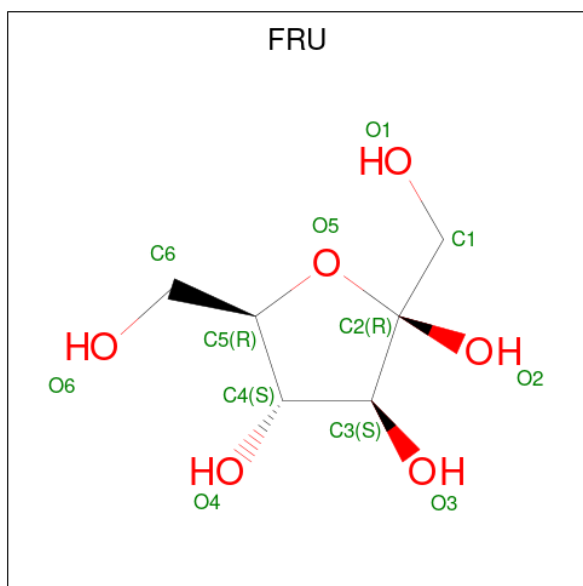
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
2	B	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
2	C	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
2	D	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
2	E	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
2	F	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
2	G	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	H	N	O	P	
			36	9	11	2	12	2	
								0	0

- Molecule 3 is beta-D-fructofuranose (three-letter code: FRU) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O		
			24	6	12	6	0	0
3	B	1	Total	C	H	O		
			24	6	12	6	0	0
3	C	1	Total	C	H	O		
			24	6	12	6	0	0
3	D	1	Total	C	H	O		
			24	6	12	6	0	0
3	E	1	Total	C	H	O		
			24	6	12	6	0	0
3	F	1	Total	C	H	O		
			24	6	12	6	0	0
3	G	1	Total	C	H	O		
			24	6	12	6	0	0
3	H	1	Total	C	H	O		
			24	6	12	6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



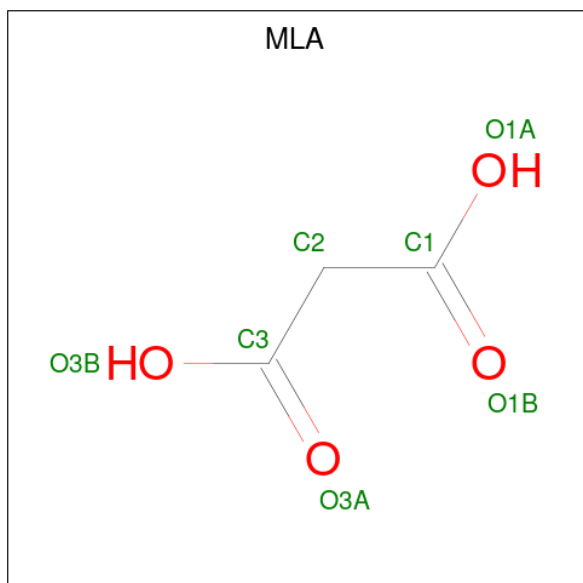
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			9	3	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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	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		

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	82	Total	O	0	0
			82	82		
7	B	72	Total	O	0	0
			72	72		

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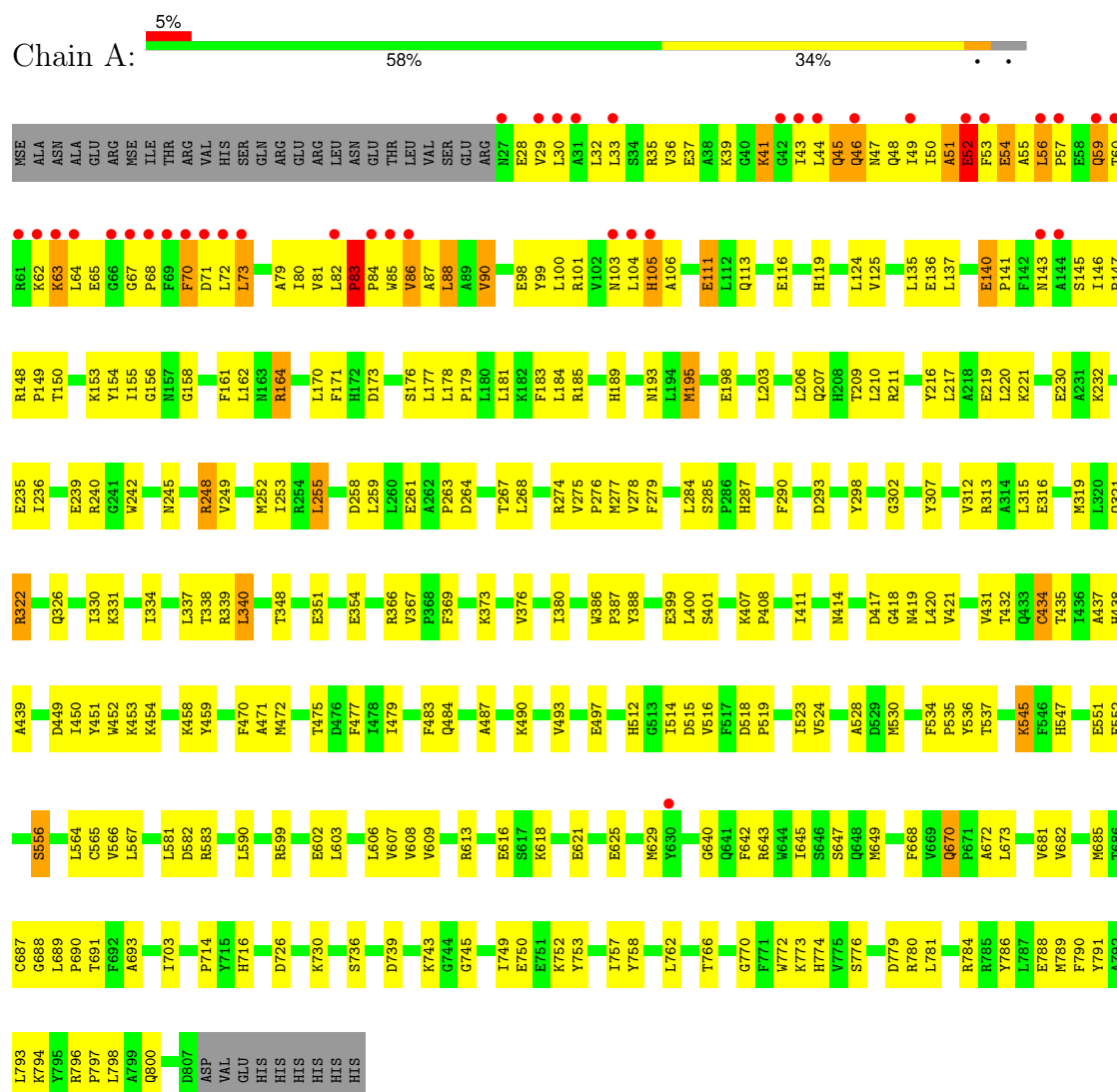
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	45	Total 45	O 45	0	0
7	D	67	Total 67	O 67	0	0
7	E	66	Total 66	O 66	0	0
7	F	90	Total 90	O 90	0	0
7	G	81	Total 81	O 81	0	0
7	H	60	Total 60	O 60	0	0

3 Residue-property plots

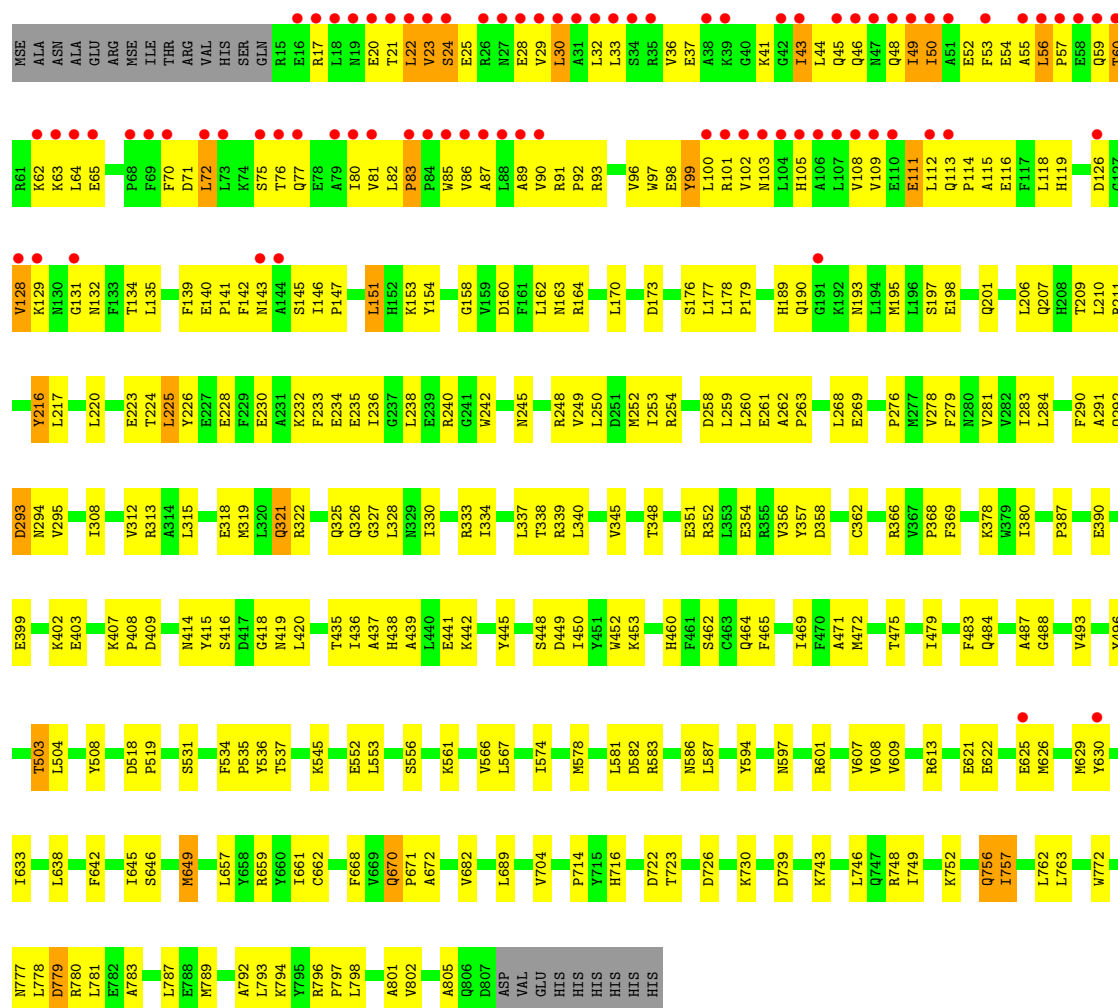
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

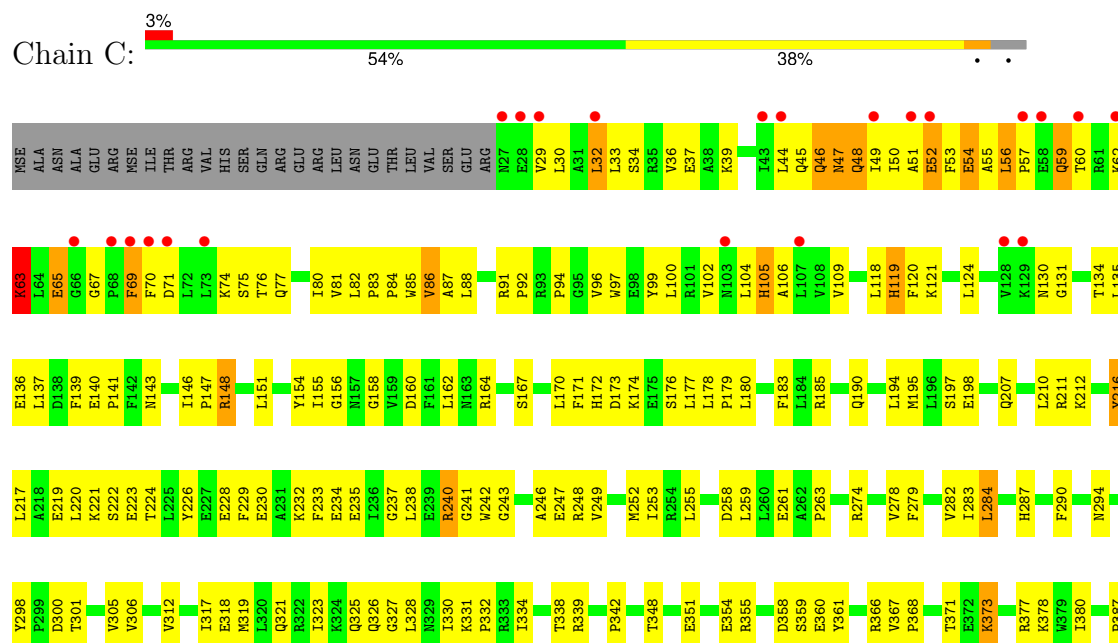


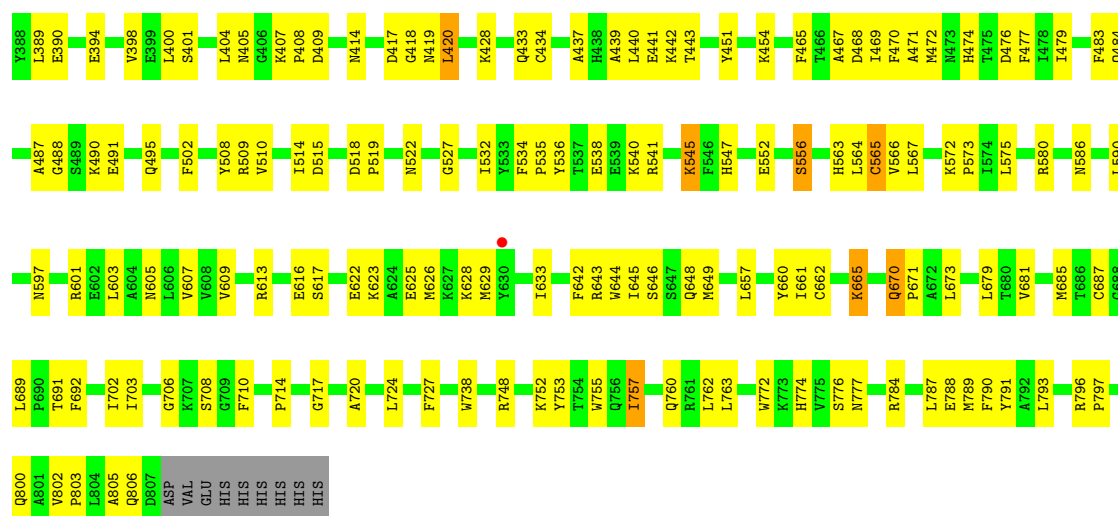
• Molecule 1: Sucrose synthase 1



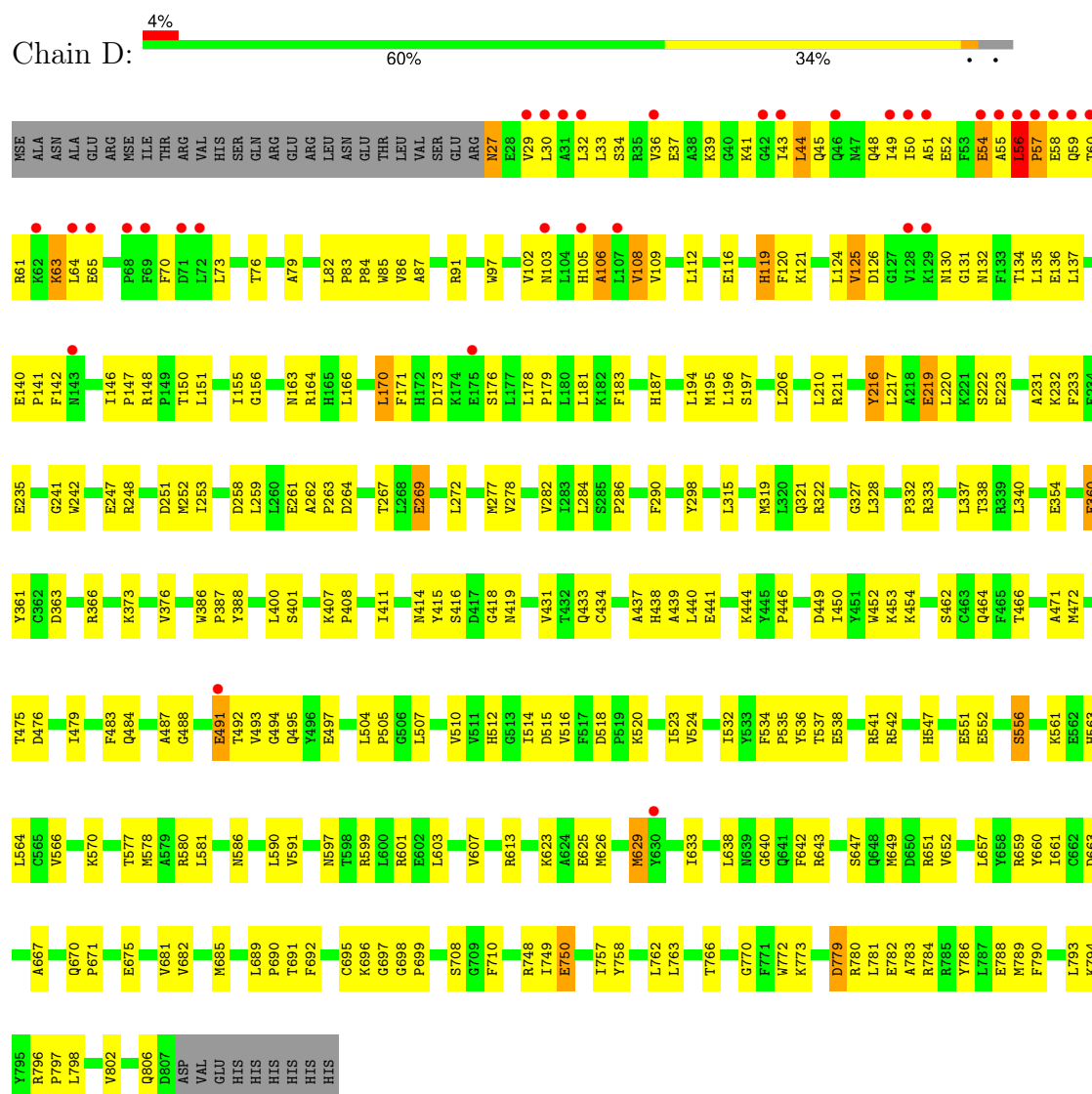


• Molecule 1: Sucrose synthase 1





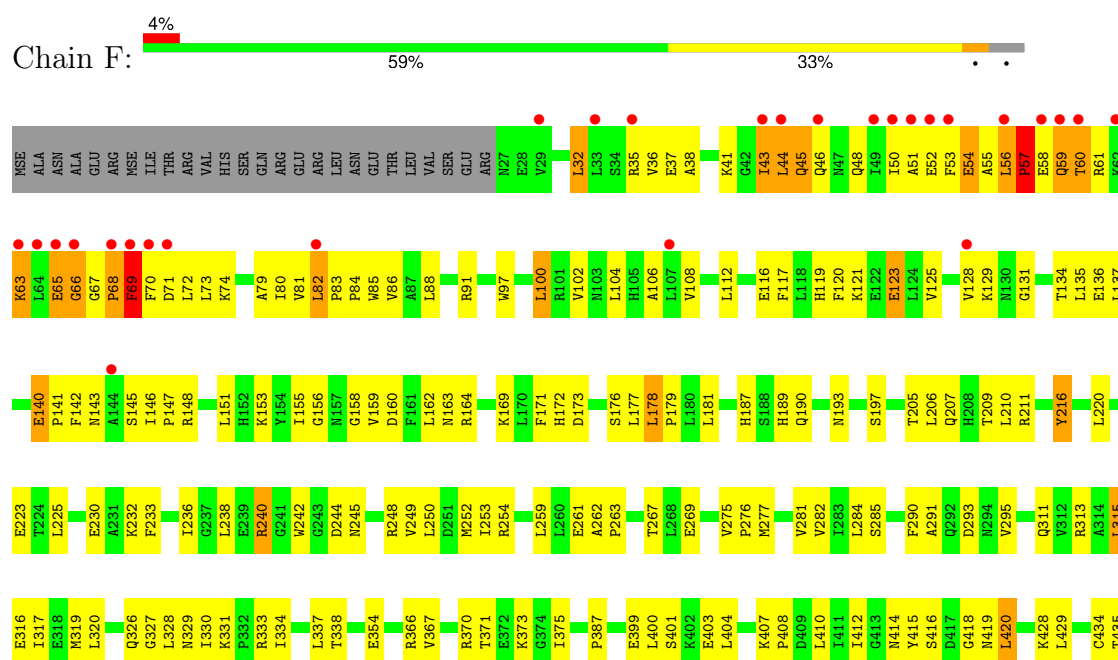
• Molecule 1: Sucrose synthase 1

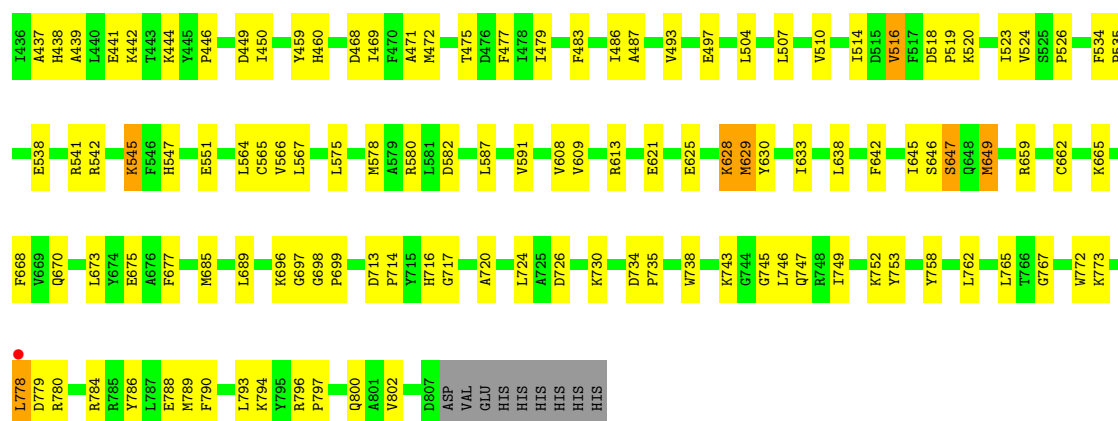


• Molecule 1: Sucrose synthase 1

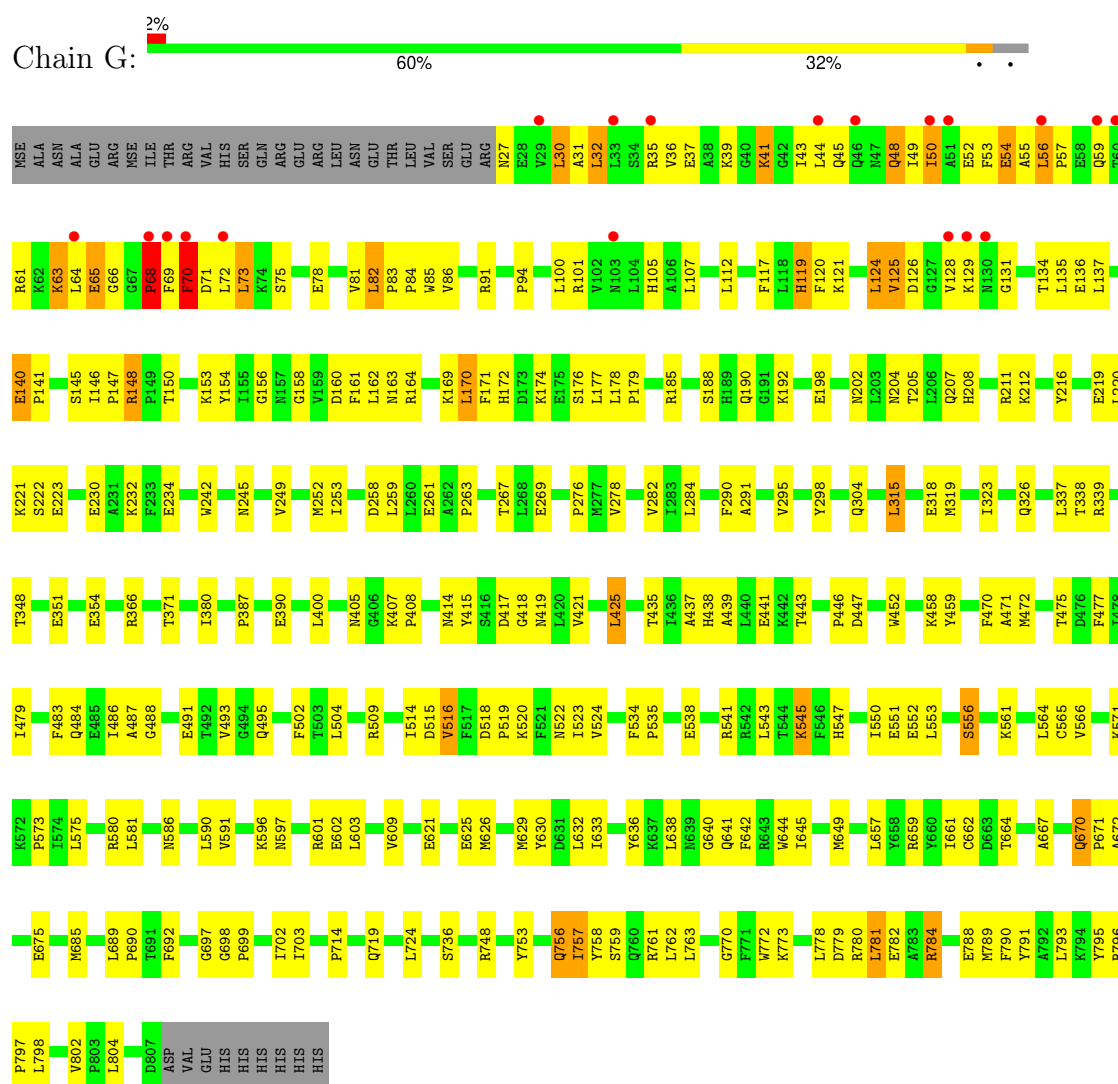


• Molecule 1: Sucrose synthase 1



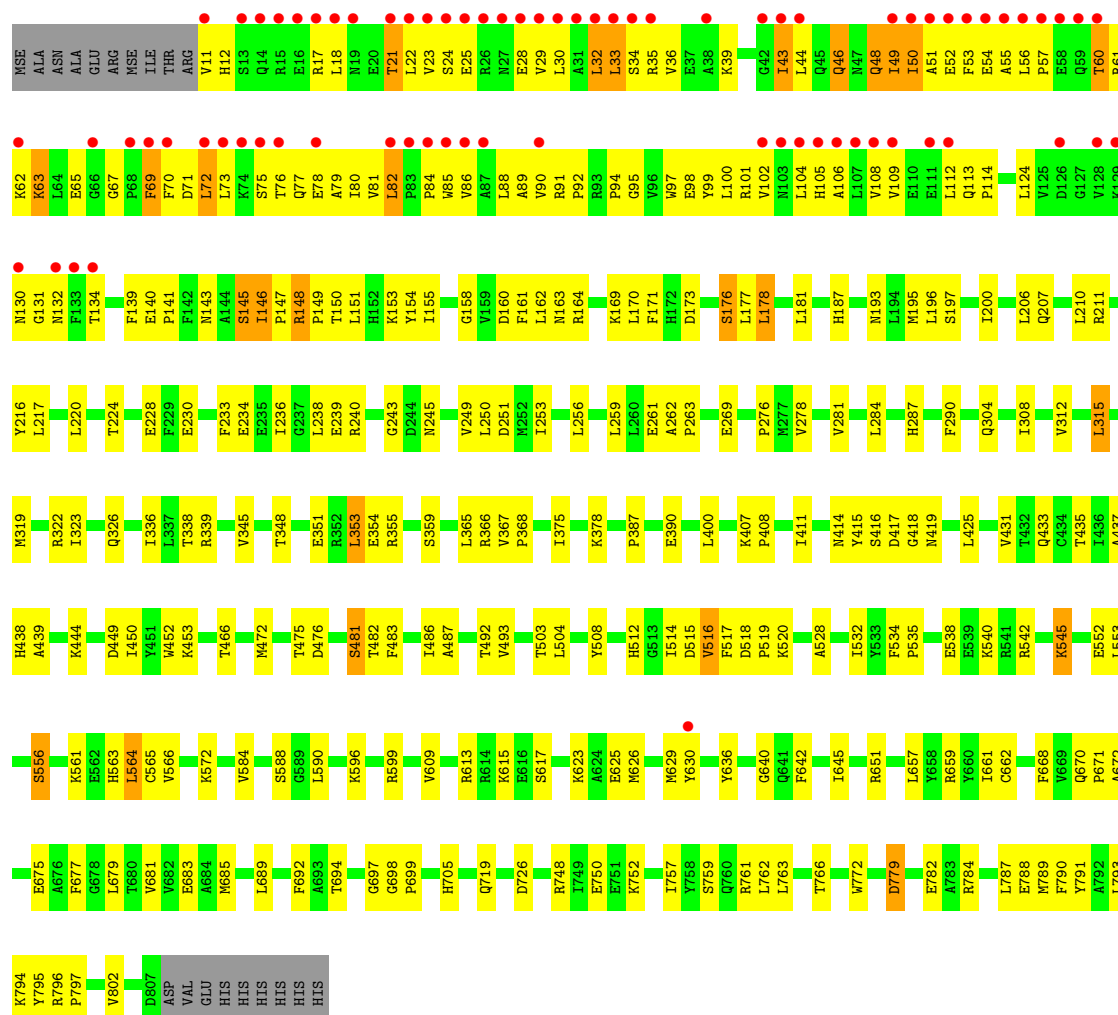


• Molecule 1: Sucrose synthase 1



• Molecule 1: Sucrose synthase 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.21Å 263.70Å 159.66Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	25.00 – 2.91 25.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.0 (25.00-2.91) 90.9 (25.00-2.91)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.186 , 0.237 0.183 , 0.234	Depositor DCC
R_{free} test set	11567 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	51483	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.21 % 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 2.7500e-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: SO4, MLA, UDP, FRU, K

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	0.40	0/6412	0.56	0/8664
1	B	0.37	0/6447	0.55	0/8717
1	C	0.36	0/6403	0.55	0/8654
1	D	0.39	0/6378	0.57	0/8624
1	E	0.39	0/6383	0.56	0/8629
1	F	0.41	0/6410	0.59	0/8663
1	G	0.38	0/6414	0.56	0/8667
1	H	0.37	0/6471	0.55	0/8749
All	All	0.38	0/51318	0.56	0/69367

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	A	0	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	3
1	G	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	C	47	ASN	Peptide
1	D	56	LEU	Peptide
1	E	70	PHE	Peptide
1	E	83	PRO	Peptide
1	F	106	ALA	Peptide
1	F	57	PRO	Peptide
1	F	66	GLY	Peptide
1	G	68	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6277	0	6191	319	0
1	B	6313	0	6170	321	0
1	C	6268	0	6189	314	0
1	D	6243	0	6143	311	0
1	E	6249	0	6158	348	0
1	F	6275	0	6195	360	0
1	G	6279	0	6201	329	0
1	H	6336	0	6196	308	0
2	A	25	11	11	0	0
2	B	25	11	11	0	0
2	C	25	11	11	1	0
2	D	25	11	11	2	0
2	E	25	11	11	4	0
2	F	25	11	11	1	0
2	G	25	11	11	1	0
2	H	25	11	11	0	0
3	A	12	12	12	1	0
3	B	12	12	12	0	0
3	C	12	12	12	1	0
3	D	12	12	12	0	0
3	E	12	12	12	1	0
3	F	12	12	12	1	0
3	G	12	12	12	4	0
3	H	12	12	12	1	0
4	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	0	3	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
4	E	15	0	0	1	0
4	F	15	0	0	2	0
4	G	15	0	0	1	0
4	H	15	0	0	1	0
5	A	7	2	2	0	0
5	B	7	2	2	1	0
5	C	7	2	2	0	0
5	D	7	2	2	0	0
5	E	7	2	2	5	0
5	F	7	2	2	0	0
5	G	7	2	2	0	0
5	H	7	2	2	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	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	82	0	0	5	0
7	B	72	0	0	7	0
7	C	45	0	0	3	0
7	D	67	0	0	3	0
7	E	66	0	0	2	0
7	F	90	0	0	10	0
7	G	81	0	0	5	0
7	H	60	0	0	6	0
All	All	51283	200	49643	2497	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 25.

All (2497) 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:C:83:PRO:HG2	1:C:84:PRO:HD3	1.22	1.19
1:G:82:LEU:HD12	1:G:83:PRO:CG	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PRO:HG2	1:B:85:TRP:HB2	1.19	1.16
1:G:65:GLU:HB3	1:G:70:PHE:CD1	1.79	1.16
1:A:789:MSE:CE	1:D:789:MSE:HB3	1.76	1.14
1:F:319:MSE:CE	1:F:334:ILE:HD11	1.78	1.14
1:G:65:GLU:HB3	1:G:70:PHE:HD1	0.96	1.13
1:C:681:VAL:HG12	1:C:685:MSE:CE	1.79	1.13
1:G:83:PRO:HG2	1:G:85:TRP:HB2	1.20	1.12
1:E:45:GLN:HB3	1:E:80:ILE:HA	1.27	1.12
1:E:315:LEU:HG	1:E:319:MSE:HE2	1.29	1.12
1:H:17:ARG:NH2	1:H:72:LEU:HB3	1.63	1.12
1:D:56:LEU:HD12	1:D:57:PRO:HD3	1.31	1.11
1:E:148:ARG:HH11	1:E:148:ARG:HG3	1.14	1.11
1:E:46:GLN:HB3	1:E:50:ILE:HB	1.16	1.10
1:B:72:LEU:HD13	1:B:90:VAL:HG11	1.26	1.09
1:C:148:ARG:HG2	1:C:148:ARG:HH11	0.93	1.09
1:C:48:GLN:HG3	1:C:76:THR:O	1.50	1.09
1:F:53:PHE:CA	1:F:57:PRO:HG2	1.81	1.09
1:F:316:GLU:HA	1:F:319:MSE:HE3	1.29	1.09
1:B:583:ARG:HA	1:B:625:GLU:OE1	1.51	1.09
1:H:146:ILE:HG12	1:H:147:PRO:HD2	1.33	1.08
1:F:469:ILE:HD13	1:F:472:MSE:HE1	1.28	1.08
1:F:469:ILE:HD13	1:F:472:MSE:CE	1.85	1.07
1:A:45:GLN:HA	1:A:45:GLN:HE21	0.91	1.07
1:A:103:ASN:CB	1:A:106:ALA:HB3	1.83	1.07
1:E:789:MSE:HE2	1:H:789:MSE:CE	1.85	1.07
1:C:681:VAL:HG12	1:C:685:MSE:HE3	1.30	1.06
1:E:789:MSE:HE2	1:H:789:MSE:HE2	1.37	1.05
1:F:53:PHE:HA	1:F:57:PRO:HG2	1.10	1.05
1:B:82:LEU:CB	1:B:83:PRO:HD2	1.86	1.05
1:G:82:LEU:HD12	1:G:83:PRO:HG3	1.13	1.05
1:H:46:GLN:HB3	1:H:51:ALA:HB2	1.39	1.05
1:C:54:GLU:HG3	1:C:55:ALA:N	1.70	1.05
1:G:276:PRO:HG3	1:G:326:GLN:HG3	1.37	1.04
1:G:82:LEU:CD1	1:G:83:PRO:HG3	1.85	1.04
1:A:45:GLN:HA	1:A:45:GLN:NE2	1.73	1.04
1:B:131:GLY:HA3	1:B:134:THR:CG2	1.87	1.04
1:F:789:MSE:CE	1:G:789:MSE:HB3	1.87	1.04
1:A:319:MSE:HE1	1:A:334:ILE:HD11	1.04	1.03
1:E:217:LEU:HD11	1:E:233:PHE:HZ	1.15	1.03
1:H:39:LYS:HB2	1:H:104:LEU:CD2	1.67	1.03
1:E:61:ARG:HH11	1:E:61:ARG:HG3	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:MSE:HE1	1:F:334:ILE:CD1	1.89	1.03
1:G:148:ARG:HG2	1:G:148:ARG:HH11	0.89	1.02
1:A:789:MSE:HE2	1:D:789:MSE:HB3	1.38	1.02
1:B:170:LEU:HD22	1:B:177:LEU:HD23	1.41	1.01
1:E:85:TRP:HB3	1:E:103:ASN:HA	1.42	1.01
1:F:82:LEU:N	1:F:83:PRO:HD3	1.73	1.01
1:C:148:ARG:HH11	1:C:148:ARG:CG	1.73	1.01
1:D:298:TYR:CE1	1:D:649:MSE:HE1	1.96	1.01
1:H:39:LYS:CB	1:H:104:LEU:HD22	1.91	1.01
1:C:50:ILE:HD12	1:C:54:GLU:HB3	1.42	1.00
1:C:50:ILE:CD1	1:C:54:GLU:HB3	1.90	1.00
1:D:146:ILE:HG23	1:D:147:PRO:HD2	1.43	1.00
1:B:92:PRO:HG2	1:B:96:VAL:HG23	1.43	1.00
1:B:80:ILE:CG1	1:B:87:ALA:HB3	1.91	0.99
1:D:552:GLU:O	1:D:556:SER:HB3	1.61	0.99
1:F:469:ILE:HA	1:F:472:MSE:HE2	1.41	0.99
1:C:32:LEU:O	1:C:36:VAL:HG23	1.63	0.99
1:H:216:TYR:CE1	1:H:220:LEU:HD11	1.97	0.99
1:D:217:LEU:HA	1:D:220:LEU:HD12	1.44	0.98
1:A:65:GLU:HB3	1:A:70:PHE:HB3	1.42	0.98
1:A:373:LYS:N	1:A:373:LYS:HD2	1.79	0.98
1:C:681:VAL:O	1:C:685:MSE:HG3	1.63	0.98
1:B:99:TYR:CE2	1:B:114:PRO:HG3	1.98	0.98
1:H:39:LYS:HB2	1:H:104:LEU:HD22	0.98	0.97
1:A:195:MSE:HE3	1:A:242:TRP:CD2	1.99	0.97
1:H:216:TYR:HE1	1:H:220:LEU:HD11	1.27	0.97
1:B:76:THR:HA	1:B:89:ALA:O	1.63	0.97
1:A:319:MSE:CE	1:A:334:ILE:HD11	1.95	0.97
1:B:327:GLY:O	1:B:328:LEU:HD23	1.64	0.97
1:E:304:GLN:HB3	3:E:902:FRU:H12	1.46	0.97
1:B:55:ALA:O	1:B:59:GLN:HB2	1.65	0.96
1:C:148:ARG:HG2	1:C:148:ARG:NH1	1.69	0.96
1:C:366:ARG:HD3	7:C:821:HOH:O	1.65	0.96
1:G:48:GLN:HA	1:G:48:GLN:HE21	1.30	0.96
1:G:148:ARG:HG2	1:G:148:ARG:NH1	1.67	0.96
1:A:124:LEU:O	1:A:124:LEU:HD23	1.64	0.95
1:F:789:MSE:HE2	1:G:789:MSE:HB3	1.44	0.95
1:A:45:GLN:HE21	1:A:45:GLN:CA	1.80	0.94
1:E:315:LEU:HD11	1:E:762:LEU:HD23	1.50	0.94
1:G:366:ARG:HD3	7:G:826:HOH:O	1.66	0.94
1:E:351:GLU:O	1:E:366:ARG:HD2	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:PHE:HA	1:F:57:PRO:CG	1.96	0.94
1:F:319:MSE:HE1	1:F:334:ILE:HD11	0.96	0.94
1:B:99:TYR:HE2	1:B:114:PRO:HG3	1.28	0.94
1:E:217:LEU:HD11	1:E:233:PHE:CZ	2.02	0.94
1:F:276:PRO:HG3	1:F:326:GLN:HG3	1.50	0.94
1:E:82:LEU:HB3	1:E:83:PRO:HD2	1.50	0.93
1:F:48:GLN:HG2	7:F:871:HOH:O	1.67	0.93
1:A:319:MSE:HE1	1:A:334:ILE:CD1	1.98	0.93
1:F:52:GLU:O	1:F:57:PRO:HD2	1.68	0.93
1:H:17:ARG:HH21	1:H:72:LEU:HB3	1.31	0.93
1:H:173:ASP:HB3	1:H:176:SER:HB2	1.49	0.93
1:A:45:GLN:HE22	1:A:80:ILE:HD13	1.31	0.93
1:D:591:VAL:HG21	1:D:629:MSE:HE1	1.48	0.92
1:E:41:LYS:HE2	1:E:54:GLU:OE1	1.68	0.92
1:G:518:ASP:OD1	1:G:520:LYS:HG2	1.70	0.92
1:C:47:ASN:O	1:C:49:ILE:N	2.02	0.92
1:E:44:LEU:HA	1:E:124:LEU:HD11	1.51	0.92
1:G:56:LEU:HB3	1:G:57:PRO:HD3	1.50	0.92
1:G:304:GLN:HB3	3:G:902:FRU:H11	1.51	0.92
1:F:37:GLU:HG2	1:F:54:GLU:OE2	1.68	0.92
1:B:72:LEU:CD1	1:B:90:VAL:HG11	1.99	0.91
1:D:163:ASN:ND2	1:D:269:GLU:HG3	1.86	0.91
1:G:148:ARG:HH11	1:G:148:ARG:CG	1.82	0.91
1:H:46:GLN:HB2	1:H:79:ALA:HB3	1.53	0.91
1:C:39:LYS:HB2	1:C:104:LEU:HD13	1.51	0.91
1:H:24:SER:O	1:H:28:GLU:HB2	1.71	0.91
1:E:789:MSE:CE	1:H:789:MSE:HE2	2.01	0.90
1:G:545:LYS:H	1:G:545:LYS:HD2	1.34	0.90
1:B:92:PRO:HG2	1:B:96:VAL:CG2	2.01	0.90
1:H:72:LEU:HA	1:H:75:SER:HB3	1.54	0.90
1:A:47:ASN:O	1:A:51:ALA:HB2	1.72	0.90
1:G:82:LEU:N	1:G:83:PRO:HD3	1.88	0.89
1:B:20:GLU:OE1	1:B:72:LEU:HD23	1.71	0.89
1:A:789:MSE:CE	1:D:789:MSE:CB	2.51	0.88
1:C:83:PRO:CG	1:C:84:PRO:HD3	2.03	0.88
1:A:56:LEU:HB3	1:A:57:PRO:HD3	1.56	0.88
1:F:45:GLN:HB3	1:F:80:ILE:HA	1.56	0.88
1:C:34:SER:HA	1:C:59:GLN:HE22	1.38	0.88
1:E:61:ARG:HH11	1:E:61:ARG:CG	1.87	0.88
1:G:31:ALA:CB	1:G:35:ARG:HH21	1.86	0.88
1:D:146:ILE:HD11	1:D:772:TRP:CZ2	2.09	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ASP:HB3	1:D:176:SER:HB3	1.56	0.88
1:G:48:GLN:HE21	1:G:48:GLN:CA	1.87	0.88
1:A:195:MSE:HE1	1:A:242:TRP:HA	1.53	0.87
1:E:45:GLN:HG2	1:E:80:ILE:CD1	2.03	0.87
1:A:316:GLU:HA	1:A:319:MSE:HE3	1.55	0.87
1:D:61:ARG:HA	1:D:63:LYS:HD3	1.56	0.87
1:E:65:GLU:HG3	1:E:70:PHE:HB3	1.56	0.87
1:G:596:LYS:HG2	1:G:636:TYR:CE1	2.10	0.87
1:D:83:PRO:HG2	1:D:84:PRO:HD3	1.55	0.87
1:D:173:ASP:HB3	1:D:176:SER:CB	2.04	0.87
1:F:143:ASN:HB3	1:F:148:ARG:NH2	1.89	0.87
1:G:216:TYR:HE1	1:G:220:LEU:HD11	1.38	0.87
1:E:789:MSE:HB3	1:H:789:MSE:CE	2.04	0.86
1:B:131:GLY:HA3	1:B:134:THR:HG21	1.56	0.86
1:D:163:ASN:HD21	1:D:269:GLU:HG3	1.40	0.86
1:D:629:MSE:HA	1:D:629:MSE:HE3	1.56	0.86
1:G:82:LEU:HD12	1:G:83:PRO:CD	2.05	0.86
1:G:83:PRO:CG	1:G:85:TRP:HB2	2.06	0.86
1:A:52:GLU:HG2	1:A:56:LEU:HB2	1.54	0.86
1:G:48:GLN:HA	1:G:48:GLN:NE2	1.90	0.85
1:F:50:ILE:O	1:F:54:GLU:HB3	1.75	0.85
1:E:35:ARG:CZ	1:E:35:ARG:HB2	2.06	0.85
1:C:748:ARG:HH11	1:C:752:LYS:HG3	1.42	0.85
1:C:796:ARG:HB2	1:C:797:PRO:HD3	1.57	0.85
1:E:45:GLN:HG2	1:E:80:ILE:HD13	1.56	0.85
1:F:789:MSE:HE2	1:G:789:MSE:CB	2.05	0.85
1:F:789:MSE:CG	1:G:789:MSE:HE3	2.07	0.85
1:G:83:PRO:HB2	1:G:85:TRP:H	1.41	0.85
1:F:82:LEU:HD12	1:F:83:PRO:HD3	1.57	0.85
1:G:83:PRO:HG2	1:G:85:TRP:CB	2.05	0.85
1:D:44:LEU:HD13	1:D:45:GLN:H	1.41	0.84
1:F:81:VAL:HG13	1:F:86:VAL:HG23	1.56	0.84
1:H:210:LEU:HD22	1:H:253:ILE:HG23	1.58	0.84
1:F:173:ASP:HB3	1:F:176:SER:HB3	1.60	0.84
1:G:304:GLN:H	3:G:902:FRU:H12	1.42	0.84
1:A:60:THR:HG23	1:A:62:LYS:H	1.40	0.84
1:F:789:MSE:HB3	1:G:789:MSE:CE	2.07	0.84
1:G:65:GLU:CB	1:G:70:PHE:HD1	1.87	0.84
1:A:32:LEU:O	1:A:36:VAL:HG23	1.77	0.84
1:D:56:LEU:CD1	1:D:57:PRO:HD3	2.07	0.84
1:G:83:PRO:HD2	1:G:85:TRP:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:O	1:A:32:LEU:HG	1.75	0.84
1:B:53:PHE:HA	1:B:57:PRO:HG2	1.59	0.84
1:E:315:LEU:CG	1:E:319:MSE:HE2	2.06	0.84
1:B:56:LEU:HB3	1:B:57:PRO:HD3	1.60	0.84
1:E:148:ARG:HH11	1:E:148:ARG:CG	1.91	0.84
1:F:43:ILE:HG23	1:F:44:LEU:N	1.92	0.83
1:E:216:TYR:HD2	1:E:232:LYS:HE2	1.41	0.83
1:F:146:ILE:HG22	1:F:147:PRO:O	1.77	0.83
1:G:298:TYR:HE1	1:G:649:MSE:HE1	1.40	0.83
1:B:668:PHE:HB2	1:B:689:LEU:HD23	1.60	0.83
1:C:143:ASN:HB3	1:C:148:ARG:NH2	1.92	0.83
1:F:59:GLN:O	1:F:60:THR:HG22	1.77	0.83
1:E:789:MSE:HE2	1:H:789:MSE:CG	2.09	0.83
1:H:72:LEU:HD12	1:H:72:LEU:O	1.77	0.83
1:D:106:ALA:HB1	1:D:108:VAL:HG23	1.59	0.83
1:B:131:GLY:HA3	1:B:134:THR:HG23	1.61	0.83
1:D:103:ASN:CB	1:D:106:ALA:HB3	2.09	0.82
1:E:789:MSE:CE	1:H:789:MSE:HG2	2.09	0.82
1:A:681:VAL:HG13	1:A:691:THR:HG21	1.60	0.82
1:F:35:ARG:HD2	1:F:104:LEU:HA	1.60	0.82
1:E:789:MSE:HG2	1:H:789:MSE:HE3	1.61	0.82
1:A:54:GLU:HG3	1:A:55:ALA:N	1.93	0.82
1:G:390:GLU:OE1	1:G:796:ARG:HD2	1.80	0.81
1:F:82:LEU:H	1:F:83:PRO:HD3	1.43	0.81
1:E:27:ASN:OD1	1:E:30:LEU:HB2	1.80	0.81
1:D:41:LYS:HG2	7:D:868:HOH:O	1.79	0.81
1:E:46:GLN:HB3	1:E:50:ILE:CB	2.06	0.81
1:B:37:GLU:HB3	1:B:55:ALA:HB2	1.63	0.81
1:C:625:GLU:O	1:C:629:MSE:HG2	1.79	0.81
1:D:83:PRO:HG2	1:D:84:PRO:CD	2.11	0.81
1:E:65:GLU:HG3	1:E:70:PHE:CB	2.10	0.81
1:D:41:LYS:HE3	1:D:54:GLU:HG2	1.62	0.81
1:E:135:LEU:HD11	1:H:789:MSE:HG3	1.62	0.81
1:G:82:LEU:H	1:G:83:PRO:HD3	1.45	0.81
1:B:146:ILE:CG2	1:B:147:PRO:HD2	2.11	0.80
1:C:48:GLN:CG	1:C:76:THR:O	2.26	0.80
1:E:315:LEU:HG	1:E:319:MSE:CE	2.09	0.80
1:F:472:MSE:HG2	1:F:514:ILE:HD13	1.63	0.80
1:C:590:LEU:HB2	1:C:671:PRO:HG3	1.63	0.80
1:D:146:ILE:CG2	1:D:147:PRO:HD2	2.11	0.80
1:E:53:PHE:O	1:E:57:PRO:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:VAL:CG1	1:F:86:VAL:HG23	2.11	0.80
1:D:360:GLU:HG3	1:D:361:TYR:CE2	2.16	0.80
1:H:82:LEU:HG	1:H:85:TRP:O	1.82	0.80
1:B:54:GLU:OE1	1:B:54:GLU:HA	1.79	0.80
1:C:319:MSE:O	1:C:323:ILE:HG13	1.81	0.80
1:G:170:LEU:HD22	1:G:176:SER:HB3	1.63	0.80
1:F:143:ASN:HA	1:F:780:ARG:HH12	1.47	0.80
1:A:789:MSE:HE2	1:D:789:MSE:CB	2.12	0.80
1:H:39:LYS:CB	1:H:104:LEU:CD2	2.57	0.80
1:D:216:TYR:CE2	1:D:232:LYS:HG2	2.15	0.79
1:B:756:GLN:HG2	1:B:757:ILE:HD13	1.62	0.79
1:E:143:ASN:HB3	1:E:148:ARG:NH2	1.98	0.79
1:A:80:ILE:O	1:A:86:VAL:HG22	1.83	0.79
1:E:217:LEU:HA	1:E:220:LEU:HD12	1.63	0.79
1:F:316:GLU:CA	1:F:319:MSE:HE3	2.12	0.79
1:F:789:MSE:HE2	1:G:789:MSE:CE	2.12	0.79
1:A:83:PRO:HB2	1:A:84:PRO:HD2	1.64	0.79
1:A:85:TRP:CE3	1:A:101:ARG:HG2	2.18	0.79
1:C:131:GLY:HA3	1:C:134:THR:HG23	1.63	0.79
1:F:173:ASP:O	1:F:177:LEU:HD12	1.82	0.79
1:F:81:VAL:HG12	1:F:86:VAL:HA	1.65	0.79
1:G:756:GLN:HG2	1:G:757:ILE:N	1.97	0.79
1:E:789:MSE:HE1	1:H:789:MSE:HB3	1.63	0.79
1:F:121:LYS:HD3	1:F:450:ILE:HD12	1.65	0.79
1:E:789:MSE:CE	1:H:789:MSE:CG	2.61	0.79
1:F:789:MSE:CE	1:G:789:MSE:CB	2.60	0.79
1:F:789:MSE:HE1	1:G:789:MSE:HB3	1.64	0.79
1:B:216:TYR:HE1	1:B:220:LEU:HD11	1.49	0.78
1:E:319:MSE:CE	1:E:334:ILE:HD11	2.12	0.78
1:H:76:THR:O	1:H:89:ALA:O	2.00	0.78
1:B:80:ILE:CD1	1:B:87:ALA:HB3	2.14	0.78
1:A:373:LYS:HD2	1:A:373:LYS:H	1.45	0.78
1:A:65:GLU:HB3	1:A:70:PHE:CB	2.12	0.78
1:B:54:GLU:O	1:B:57:PRO:HD2	1.82	0.78
1:B:80:ILE:HG13	1:B:80:ILE:O	1.83	0.78
1:C:56:LEU:HD12	7:C:842:HOH:O	1.84	0.78
1:F:35:ARG:HB2	1:F:35:ARG:CZ	2.12	0.78
1:E:162:LEU:HD11	1:E:772:TRP:CE3	2.18	0.78
1:H:39:LYS:HD3	1:H:39:LYS:C	2.04	0.78
1:E:789:MSE:HB3	1:H:789:MSE:HE1	1.65	0.78
1:F:789:MSE:HE2	1:G:789:MSE:CG	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLU:HG3	1:D:361:TYR:CD2	2.19	0.78
1:F:207:GLN:HE21	1:F:211:ARG:HH22	1.28	0.78
1:D:32:LEU:HD21	1:D:106:ALA:H	1.48	0.77
1:G:547:HIS:O	1:G:551:GLU:HG3	1.84	0.77
1:F:52:GLU:HG2	1:F:53:PHE:N	1.98	0.77
1:D:195:MSE:HE1	1:D:241:GLY:C	2.05	0.77
1:H:89:ALA:HB1	1:H:99:TYR:HD1	1.49	0.77
1:D:125:VAL:HG11	1:D:505:PRO:HG2	1.66	0.77
1:E:789:MSE:SE	1:H:789:MSE:HE2	2.35	0.77
1:F:82:LEU:CD1	1:F:83:PRO:HG3	2.15	0.77
1:G:145:SER:HB2	1:G:779:ASP:OD2	1.85	0.77
1:B:216:TYR:CE1	1:B:220:LEU:HD11	2.20	0.77
1:F:333:ARG:HH12	1:F:403:GLU:HB3	1.48	0.77
1:F:591:VAL:HG21	1:F:629:MSE:HE1	1.67	0.77
1:A:185:ARG:HD2	1:A:198:GLU:OE1	1.85	0.77
1:B:30:LEU:HG	1:B:62:LYS:O	1.85	0.77
1:C:146:ILE:HG22	1:C:147:PRO:O	1.85	0.77
1:G:276:PRO:HG3	1:G:326:GLN:CG	2.15	0.77
1:H:82:LEU:HD12	1:H:84:PRO:HG2	1.67	0.76
1:A:43:ILE:O	1:A:44:LEU:HG	1.85	0.76
1:B:553:LEU:HG	1:B:645:ILE:HD13	1.67	0.76
1:B:582:ASP:HB2	1:B:621:GLU:OE1	1.84	0.76
1:E:789:MSE:CE	1:H:789:MSE:HB3	2.14	0.76
1:B:170:LEU:HD22	1:B:177:LEU:CD2	2.15	0.76
1:G:545:LYS:H	1:G:545:LYS:CD	1.89	0.76
1:D:171:PHE:HD1	1:D:263:PRO:HD2	1.51	0.76
1:G:479:ILE:CD1	1:G:762:LEU:HD13	2.16	0.76
1:B:24:SER:O	1:B:28:GLU:CB	2.33	0.76
1:D:441:GLU:OE1	1:D:441:GLU:HA	1.86	0.76
1:E:36:VAL:HA	1:E:39:LYS:CB	2.15	0.76
1:F:538:GLU:OE1	1:F:541:ARG:HD3	1.85	0.76
1:G:131:GLY:H	1:G:134:THR:HG21	1.50	0.76
1:C:60:THR:C	1:C:62:LYS:H	1.88	0.76
1:F:210:LEU:HD22	1:F:253:ILE:HG23	1.68	0.76
1:A:146:ILE:HG23	1:A:147:PRO:HD2	1.67	0.75
1:A:29:VAL:O	1:A:33:LEU:HG	1.86	0.75
1:B:83:PRO:HG2	1:B:85:TRP:CB	2.10	0.75
1:B:460:HIS:CD2	1:B:802:VAL:HG13	2.21	0.75
1:E:210:LEU:CD2	1:E:253:ILE:HG23	2.16	0.75
1:E:796:ARG:HB2	1:E:797:PRO:HD3	1.68	0.75
1:G:298:TYR:CE1	1:G:649:MSE:HE1	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:PHE:C	1:G:70:PHE:CD2	2.56	0.75
1:F:207:GLN:HE21	1:F:211:ARG:NH2	1.84	0.75
1:G:54:GLU:HG3	1:G:55:ALA:H	1.52	0.75
1:F:70:PHE:CD2	1:F:71:ASP:N	2.55	0.75
1:G:545:LYS:HD2	1:G:545:LYS:N	2.01	0.75
1:D:146:ILE:HD11	1:D:772:TRP:CH2	2.21	0.75
1:E:230:GLU:O	1:E:234:GLU:HG3	1.86	0.75
1:G:54:GLU:HG3	1:G:55:ALA:N	2.01	0.75
1:C:119:HIS:HE1	1:C:509:ARG:NH1	1.85	0.75
1:D:264:ASP:OD1	1:D:267:THR:HB	1.87	0.75
1:D:784:ARG:O	1:D:788:GLU:HG3	1.87	0.75
1:G:216:TYR:CE1	1:G:220:LEU:HD11	2.20	0.75
1:B:82:LEU:CB	1:B:83:PRO:CD	2.63	0.74
1:F:32:LEU:O	1:F:36:VAL:HG23	1.87	0.74
1:H:48:GLN:O	1:H:52:GLU:HB3	1.86	0.74
1:H:76:THR:HA	1:H:90:VAL:HG12	1.68	0.74
1:B:210:LEU:HD22	1:B:253:ILE:HG23	1.69	0.74
1:F:82:LEU:HD21	1:F:123:GLU:HB3	1.68	0.74
1:G:31:ALA:HB1	1:G:35:ARG:HH21	1.52	0.74
1:G:692:PHE:CE2	1:G:724:LEU:HD23	2.22	0.74
1:A:46:GLN:HB2	1:A:79:ALA:O	1.87	0.74
1:B:80:ILE:HD11	1:B:87:ALA:HB3	1.67	0.74
1:B:333:ARG:HG2	1:B:333:ARG:HH11	1.52	0.74
1:E:82:LEU:HB3	1:E:83:PRO:CD	2.14	0.74
1:E:789:MSE:HE2	1:H:789:MSE:SE	2.37	0.74
1:A:81:VAL:HA	1:A:86:VAL:CG2	2.18	0.74
1:E:44:LEU:HD21	1:E:451:TYR:OH	1.87	0.74
1:F:74:LYS:HA	7:F:891:HOH:O	1.87	0.74
1:F:789:MSE:HE1	1:G:790:PHE:N	2.01	0.74
1:D:105:HIS:O	1:D:106:ALA:HB2	1.86	0.74
1:C:261:GLU:HG2	1:D:151:LEU:HD12	1.68	0.74
1:B:756:GLN:HG2	1:B:757:ILE:N	1.99	0.74
1:F:82:LEU:N	1:F:83:PRO:CD	2.50	0.74
1:F:83:PRO:HB2	1:F:85:TRP:H	1.53	0.74
1:B:93:ARG:O	1:B:96:VAL:HG22	1.88	0.73
1:D:39:LYS:HB2	1:D:39:LYS:NZ	2.02	0.73
1:A:400:LEU:C	1:A:400:LEU:HD12	2.07	0.73
1:E:789:MSE:CB	1:H:789:MSE:CE	2.66	0.73
1:A:685:MSE:HE3	1:A:745:GLY:HA2	1.71	0.73
1:D:44:LEU:CD1	1:D:45:GLN:H	2.00	0.73
1:D:217:LEU:HD11	1:D:233:PHE:HZ	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:PRO:HB2	1:E:84:PRO:HD2	1.68	0.73
1:A:786:TYR:CZ	1:D:789:MSE:HE3	2.23	0.73
1:F:59:GLN:O	1:F:60:THR:CG2	2.36	0.73
1:F:131:GLY:O	1:F:134:THR:HG23	1.89	0.73
1:A:789:MSE:HE1	1:D:789:MSE:HB3	1.71	0.73
1:B:72:LEU:HD13	1:B:90:VAL:CG1	2.15	0.73
1:B:99:TYR:O	1:B:112:LEU:HB2	1.89	0.73
1:H:131:GLY:O	1:H:134:THR:HG23	1.89	0.73
1:F:53:PHE:C	1:F:57:PRO:HG2	2.09	0.73
1:A:298:TYR:CE1	1:A:649:MSE:HE1	2.23	0.73
1:G:667:ALA:HA	1:G:689:LEU:HD11	1.71	0.73
1:B:114:PRO:HA	7:B:876:HOH:O	1.88	0.72
1:G:131:GLY:CA	1:G:134:THR:HG23	2.18	0.72
1:H:33:LEU:HA	1:H:36:VAL:HB	1.70	0.72
1:E:35:ARG:CG	1:E:104:LEU:HA	2.18	0.72
1:B:103:ASN:CB	1:B:108:VAL:CB	2.67	0.72
1:D:36:VAL:HG22	1:D:105:HIS:CE1	2.24	0.72
1:E:164:ARG:HD2	1:F:262:ALA:HB1	1.71	0.72
1:B:613:ARG:HH11	1:B:613:ARG:HG3	1.53	0.72
1:D:195:MSE:CE	1:D:241:GLY:HA3	2.19	0.72
1:G:315:LEU:HD21	1:G:762:LEU:HD23	1.72	0.72
1:E:70:PHE:C	1:E:70:PHE:CD2	2.62	0.72
1:F:69:PHE:HD1	1:F:70:PHE:N	1.87	0.72
1:C:216:TYR:HE1	1:C:220:LEU:HD11	1.55	0.72
1:E:625:GLU:HG2	7:E:839:HOH:O	1.90	0.72
1:E:789:MSE:CG	1:H:789:MSE:CE	2.67	0.72
1:A:184:LEU:HD22	1:A:195:MSE:HG2	1.72	0.72
1:E:52:GLU:OE1	1:E:57:PRO:HD3	1.89	0.72
1:E:216:TYR:CE1	1:E:220:LEU:HD21	2.25	0.72
1:E:319:MSE:HE3	1:E:334:ILE:HD11	1.72	0.72
1:H:130:ASN:HB3	1:H:134:THR:HG21	1.72	0.72
1:F:216:TYR:CE1	1:F:220:LEU:HD11	2.25	0.71
1:A:298:TYR:HE1	1:A:649:MSE:HE1	1.54	0.71
1:A:36:VAL:HA	1:A:39:LYS:HD2	1.73	0.71
1:F:789:MSE:HB3	1:G:789:MSE:HE1	1.71	0.71
1:F:575:LEU:HD21	1:F:724:LEU:HD13	1.72	0.71
1:H:89:ALA:CB	1:H:99:TYR:HD1	2.03	0.71
1:D:56:LEU:HB3	1:D:57:PRO:HD2	1.72	0.71
1:F:82:LEU:HD12	1:F:83:PRO:CD	2.21	0.71
1:A:210:LEU:HD22	1:A:253:ILE:HG23	1.72	0.71
1:F:629:MSE:HA	1:F:629:MSE:CE	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ALA:N	7:B:876:HOH:O	2.23	0.71
1:E:486:ILE:HG22	1:E:516:VAL:HG22	1.73	0.71
1:B:153:LYS:HD3	1:B:154:TYR:CE2	2.26	0.71
1:E:170:LEU:HD22	1:E:177:LEU:HD23	1.71	0.71
1:G:27:ASN:CA	1:G:30:LEU:HD12	2.21	0.70
1:H:48:GLN:OE1	1:H:492:THR:HG22	1.89	0.70
1:A:60:THR:O	1:A:63:LYS:HG3	1.91	0.70
1:D:91:ARG:HD2	1:D:97:TRP:CZ2	2.26	0.70
1:D:112:LEU:HD22	1:D:116:GLU:HB3	1.73	0.70
1:F:469:ILE:HA	1:F:472:MSE:CE	2.17	0.70
1:G:441:GLU:OE1	1:G:441:GLU:HA	1.90	0.70
1:B:83:PRO:O	1:B:85:TRP:N	2.23	0.70
1:C:216:TYR:CE1	1:C:220:LEU:HD11	2.26	0.70
1:F:400:LEU:C	1:F:400:LEU:HD12	2.12	0.70
1:E:789:MSE:CE	1:H:789:MSE:CB	2.69	0.70
1:F:83:PRO:HD2	1:F:85:TRP:O	1.91	0.70
1:A:82:LEU:HB3	1:A:83:PRO:HD2	1.72	0.70
1:C:105:HIS:O	1:C:106:ALA:HB3	1.91	0.70
1:E:35:ARG:HB2	1:E:35:ARG:NH1	2.07	0.70
1:G:284:LEU:HD13	1:G:337:LEU:HB2	1.74	0.70
1:D:479:ILE:HD11	1:D:762:LEU:CD1	2.22	0.70
1:F:789:MSE:HB3	1:G:789:MSE:HE3	1.72	0.70
1:G:479:ILE:HD11	1:G:762:LEU:HD13	1.74	0.70
1:E:789:MSE:CE	1:H:789:MSE:CE	2.61	0.70
1:F:796:ARG:O	1:F:800:GLN:HG3	1.92	0.70
1:A:198:GLU:OE1	1:A:198:GLU:HA	1.91	0.70
1:A:432:THR:OG1	1:A:773:LYS:HE2	1.92	0.70
1:A:512:HIS:CE1	1:A:515:ASP:HB2	2.27	0.70
1:F:59:GLN:HG3	1:F:60:THR:N	2.05	0.70
1:F:83:PRO:CB	1:F:84:PRO:HD2	2.22	0.70
1:F:140:GLU:N	1:F:141:PRO:HD2	2.06	0.70
1:D:34:SER:O	1:D:37:GLU:HB2	1.91	0.69
1:F:43:ILE:HG13	1:F:82:LEU:HA	1.74	0.69
1:A:47:ASN:O	1:A:51:ALA:CB	2.39	0.69
1:G:204:ASN:ND2	1:H:12:HIS:H	1.90	0.69
1:B:45:GLN:CG	1:B:80:ILE:HG22	2.22	0.69
1:B:80:ILE:HD11	1:B:87:ALA:CB	2.22	0.69
1:D:414:ASN:O	1:D:418:GLY:HA3	1.92	0.69
1:E:36:VAL:HA	1:E:39:LYS:HB2	1.74	0.69
1:E:226:TYR:CE2	1:E:240:ARG:HG2	2.27	0.69
1:F:171:PHE:HD1	1:F:263:PRO:HD2	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HG	1:A:70:PHE:CD1	2.27	0.69
1:G:543:LEU:HA	1:G:545:LYS:HE3	1.73	0.69
1:H:590:LEU:HB2	1:H:671:PRO:HG3	1.73	0.69
1:B:46:GLN:HB2	1:B:50:ILE:HB	1.73	0.69
1:D:131:GLY:CA	1:D:134:THR:HG23	2.22	0.69
1:G:207:GLN:HE21	1:G:211:ARG:HE	1.37	0.69
1:B:146:ILE:HG23	1:B:147:PRO:HD2	1.75	0.69
1:E:216:TYR:CD2	1:E:232:LYS:HE2	2.27	0.69
1:B:119:HIS:CE1	1:B:129:LYS:CB	2.76	0.69
1:B:609:VAL:HG22	1:B:645:ILE:HB	1.75	0.69
1:H:315:LEU:HB3	1:H:319:MSE:HE3	1.75	0.69
1:B:75:SER:O	1:B:90:VAL:HG12	1.92	0.69
1:A:140:GLU:HB3	1:A:141:PRO:HD3	1.73	0.68
1:H:32:LEU:HD22	1:H:35:ARG:NH1	2.07	0.68
1:A:170:LEU:HD23	1:A:176:SER:OG	1.92	0.68
1:D:54:GLU:HG3	1:D:55:ALA:H	1.59	0.68
1:E:670:GLN:HG3	1:E:670:GLN:O	1.93	0.68
1:A:56:LEU:CB	1:A:57:PRO:HD3	2.23	0.68
1:B:793:LEU:HD11	1:C:135:LEU:HD22	1.74	0.68
1:C:681:VAL:HG12	1:C:685:MSE:HE2	1.73	0.68
1:D:173:ASP:HB3	1:D:176:SER:HB2	1.75	0.68
1:D:216:TYR:CD2	1:D:232:LYS:HG2	2.28	0.68
1:F:789:MSE:CB	1:G:789:MSE:HE3	2.24	0.68
1:A:52:GLU:HA	1:A:55:ALA:HB3	1.76	0.68
1:E:315:LEU:HD12	1:E:759:SER:HB3	1.74	0.68
1:G:146:ILE:HG23	1:G:147:PRO:HD2	1.74	0.68
1:B:597:ASN:HB2	7:B:842:HOH:O	1.92	0.68
1:D:171:PHE:CD1	1:D:263:PRO:HD2	2.28	0.68
1:H:124:LEU:O	1:H:124:LEU:HD23	1.93	0.68
1:H:276:PRO:HG3	1:H:326:GLN:HG3	1.74	0.68
1:A:373:LYS:N	1:A:373:LYS:CD	2.56	0.68
1:B:583:ARG:CA	1:B:625:GLU:OE1	2.35	0.68
1:B:756:GLN:CG	1:B:757:ILE:HD13	2.23	0.68
1:E:148:ARG:HG3	1:E:148:ARG:NH1	1.95	0.68
1:B:220:LEU:HD22	1:B:224:THR:HG21	1.75	0.68
1:B:101:ARG:CB	1:B:112:LEU:HD11	2.23	0.68
1:F:649:MSE:HG3	7:F:897:HOH:O	1.92	0.68
1:E:789:MSE:HE3	1:H:789:MSE:HG2	1.76	0.67
1:H:757:ILE:HG22	1:H:761:ARG:HG2	1.75	0.67
1:F:276:PRO:HG3	1:F:326:GLN:CG	2.24	0.67
1:G:73:LEU:HD23	1:G:73:LEU:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:483:PHE:CE1	1:G:487:ALA:HB3	2.29	0.67
1:A:207:GLN:HE21	1:A:211:ARG:NH1	1.92	0.67
1:B:670:GLN:HG3	1:B:670:GLN:O	1.94	0.67
1:E:315:LEU:HB3	1:E:319:MSE:HE3	1.76	0.67
1:H:290:PHE:O	1:H:366:ARG:NH1	2.27	0.67
1:D:538:GLU:OE1	1:D:541:ARG:HD3	1.94	0.67
1:B:99:TYR:HE2	1:B:114:PRO:CG	2.04	0.67
1:C:92:PRO:HD2	1:C:96:VAL:O	1.94	0.67
1:F:52:GLU:O	1:F:55:ALA:N	2.28	0.67
1:H:160:ASP:O	1:H:164:ARG:HG3	1.95	0.67
1:B:189:HIS:ND1	1:B:330:ILE:HD13	2.10	0.67
1:D:419:ASN:HB3	1:D:471:ALA:HB1	1.75	0.67
1:A:195:MSE:HE3	1:A:242:TRP:CG	2.29	0.67
1:E:44:LEU:CA	1:E:124:LEU:HD11	2.25	0.67
1:E:45:GLN:HG3	1:E:124:LEU:CD2	2.24	0.67
1:F:69:PHE:CD1	1:F:70:PHE:N	2.62	0.67
1:G:54:GLU:CG	1:G:55:ALA:N	2.58	0.67
1:B:29:VAL:HG13	1:B:30:LEU:CD1	2.25	0.67
1:A:83:PRO:CB	1:A:84:PRO:HD2	2.25	0.66
1:D:181:LEU:HD13	1:D:206:LEU:HD22	1.78	0.66
1:E:45:GLN:HG3	1:E:124:LEU:HD21	1.77	0.66
1:E:458:LYS:HD2	1:E:459:TYR:CE2	2.28	0.66
1:B:80:ILE:HG13	1:B:87:ALA:HB3	1.75	0.66
1:E:216:TYR:HE1	1:E:220:LEU:HD21	1.60	0.66
1:H:668:PHE:HB2	1:H:689:LEU:HD23	1.77	0.66
1:F:57:PRO:O	1:F:59:GLN:N	2.28	0.66
1:A:45:GLN:HE22	1:A:80:ILE:CD1	2.06	0.66
1:D:440:LEU:HD12	1:D:495:GLN:HB3	1.78	0.66
1:F:146:ILE:HG23	1:F:147:PRO:HD2	1.76	0.66
1:F:414:ASN:ND2	1:F:438:HIS:NE2	2.43	0.66
1:F:685:MSE:CE	1:F:745:GLY:HA2	2.25	0.66
1:G:82:LEU:N	1:G:83:PRO:CD	2.58	0.66
1:B:225:LEU:N	1:B:225:LEU:HD23	2.09	0.66
1:E:209:THR:HG23	1:E:236:ILE:HB	1.77	0.66
1:H:625:GLU:O	1:H:629:MSE:HG2	1.96	0.66
1:A:52:GLU:O	1:A:57:PRO:HD2	1.96	0.66
1:B:80:ILE:HG12	1:B:87:ALA:HB3	1.77	0.66
1:C:259:LEU:O	1:C:263:PRO:HG3	1.96	0.66
1:E:210:LEU:HD23	1:E:253:ILE:HG23	1.77	0.66
1:E:315:LEU:CG	1:E:319:MSE:CE	2.71	0.66
1:H:30:LEU:HD13	1:H:62:LYS:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:SER:O	1:A:179:PRO:HD2	1.95	0.66
1:E:148:ARG:HD3	1:E:515:ASP:OD2	1.95	0.66
1:G:81:VAL:HG12	1:G:86:VAL:HB	1.78	0.66
1:A:524:VAL:HG12	1:A:758:TYR:CD2	2.31	0.65
1:F:789:MSE:SE	1:G:789:MSE:HE3	2.46	0.65
1:G:32:LEU:HD21	1:G:105:HIS:O	1.96	0.65
1:G:48:GLN:CA	1:G:48:GLN:NE2	2.54	0.65
1:H:34:SER:OG	1:H:55:ALA:HB1	1.96	0.65
1:A:124:LEU:HD23	1:A:124:LEU:C	2.16	0.65
1:A:158:GLY:HA3	1:A:519:PRO:O	1.97	0.65
1:C:53:PHE:O	1:C:57:PRO:HG2	1.96	0.65
1:E:32:LEU:HD21	1:E:107:LEU:CB	2.26	0.65
1:E:315:LEU:O	1:E:319:MSE:HG3	1.96	0.65
1:A:264:ASP:OD1	1:A:267:THR:HB	1.96	0.65
1:D:27:ASN:N	1:D:27:ASN:ND2	2.42	0.65
1:G:667:ALA:CA	1:G:689:LEU:HD11	2.26	0.65
1:A:181:LEU:HD13	1:A:206:LEU:HD22	1.78	0.65
1:B:86:VAL:O	1:B:101:ARG:HA	1.97	0.65
1:C:49:ILE:O	1:C:53:PHE:CB	2.45	0.65
1:D:216:TYR:HE2	1:D:232:LYS:HG2	1.61	0.65
1:E:45:GLN:CG	1:E:80:ILE:HD13	2.27	0.65
1:A:145:SER:HB3	1:A:779:ASP:OD2	1.96	0.65
1:B:33:LEU:O	1:B:36:VAL:HB	1.96	0.65
1:D:102:VAL:HG23	1:D:109:VAL:CG2	2.26	0.65
1:F:233:PHE:CD1	1:F:238:LEU:HD12	2.32	0.65
1:H:113:GLN:N	1:H:113:GLN:OE1	2.29	0.65
1:G:48:GLN:HG2	7:G:877:HOH:O	1.96	0.65
1:A:315:LEU:HG	1:A:319:MSE:HE2	1.77	0.65
1:C:552:GLU:O	1:C:556:SER:HB3	1.97	0.65
1:G:486:ILE:HG22	1:G:516:VAL:HG22	1.79	0.65
1:H:173:ASP:CB	1:H:176:SER:HB2	2.23	0.65
1:C:54:GLU:HG3	1:C:55:ALA:H	1.60	0.65
1:G:178:LEU:HB2	1:G:179:PRO:HD3	1.79	0.65
1:H:95:GLY:HA3	1:H:517:PHE:HE2	1.61	0.65
1:B:460:HIS:NE2	1:B:802:VAL:HG13	2.12	0.65
1:C:63:LYS:O	1:C:65:GLU:HG2	1.95	0.65
1:C:681:VAL:CG1	1:C:685:MSE:CE	2.67	0.65
1:G:66:GLY:HA2	1:G:71:ASP:OD2	1.96	0.65
1:A:36:VAL:O	1:A:39:LYS:HG3	1.98	0.64
1:C:80:ILE:HD11	1:C:121:LYS:HG3	1.80	0.64
1:G:31:ALA:HB3	1:G:35:ARG:HH21	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:ASN:ND2	1:H:12:HIS:N	2.44	0.64
1:H:281:VAL:HG21	1:H:319:MSE:HE1	1.79	0.64
1:H:353:LEU:HD12	1:H:365:LEU:HD13	1.79	0.64
1:B:442:LYS:HD2	1:B:449:ASP:HB3	1.78	0.64
1:E:564:LEU:HD22	1:E:613:ARG:NH2	2.11	0.64
1:H:169:LYS:HG2	1:H:176:SER:OG	1.98	0.64
1:B:178:LEU:HB2	1:B:179:PRO:HD3	1.79	0.64
1:C:131:GLY:CA	1:C:134:THR:HG23	2.27	0.64
1:F:37:GLU:OE1	1:F:59:GLN:HB2	1.97	0.64
1:B:552:GLU:O	1:B:556:SER:HB3	1.97	0.64
1:E:36:VAL:HA	1:E:39:LYS:HB3	1.77	0.64
1:E:282:VAL:HG13	1:E:337:LEU:HD23	1.80	0.64
1:B:146:ILE:HG22	1:B:147:PRO:HD2	1.78	0.64
1:C:69:PHE:CD1	1:C:70:PHE:N	2.66	0.64
1:C:224:THR:HG23	1:C:228:GLU:HG3	1.79	0.64
1:F:91:ARG:HD2	1:F:97:TRP:CZ2	2.33	0.64
1:B:54:GLU:HG3	1:B:55:ALA:H	1.62	0.64
1:B:668:PHE:HB2	1:B:689:LEU:CD2	2.27	0.64
1:D:131:GLY:HA3	1:D:134:THR:HG23	1.79	0.64
1:E:321:GLN:O	1:E:325:GLN:HG3	1.98	0.64
1:E:333:ARG:HG2	1:E:333:ARG:HH11	1.63	0.64
1:E:675:GLU:O	1:E:697:GLY:HA3	1.97	0.64
1:F:486:ILE:HG22	1:F:516:VAL:HG22	1.79	0.64
1:A:367:VAL:HG22	1:A:399:GLU:HG3	1.79	0.64
1:B:748:ARG:NH1	1:B:752:LYS:HD2	2.13	0.64
1:E:105:HIS:O	1:E:106:ALA:HB3	1.96	0.64
1:F:171:PHE:CD1	1:F:263:PRO:HD2	2.33	0.64
1:F:315:LEU:HB3	1:F:319:MSE:HE2	1.78	0.64
1:H:139:PHE:CE1	1:H:787:LEU:HD21	2.33	0.64
1:H:171:PHE:CD1	1:H:263:PRO:HD2	2.33	0.64
1:B:190:GLN:OE1	1:B:190:GLN:HA	1.97	0.63
1:B:224:THR:HG23	1:B:228:GLU:HG3	1.80	0.63
1:C:207:GLN:HE21	1:C:211:ARG:HH21	1.46	0.63
1:E:45:GLN:CB	1:E:80:ILE:HA	2.17	0.63
1:F:158:GLY:HA3	1:F:519:PRO:O	1.98	0.63
1:G:667:ALA:HA	1:G:689:LEU:CD1	2.27	0.63
1:A:149:PRO:HB3	1:A:161:PHE:CE1	2.32	0.63
1:E:243:GLY:HA2	1:E:326:GLN:HA	1.80	0.63
1:A:647:SER:HB2	1:A:649:MSE:HE3	1.80	0.63
1:B:250:LEU:O	1:B:254:ARG:HG3	1.98	0.63
1:F:59:GLN:HG3	1:F:60:THR:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:ALA:HB3	1:G:35:ARG:NH2	2.13	0.63
1:G:212:LYS:HE3	1:G:232:LYS:HZ2	1.64	0.63
1:G:538:GLU:OE1	1:G:541:ARG:HD3	1.97	0.63
1:A:70:PHE:C	1:A:70:PHE:CD2	2.71	0.63
1:B:366:ARG:HD3	7:B:837:HOH:O	1.97	0.63
1:C:796:ARG:O	1:C:800:GLN:HG3	1.98	0.63
1:E:400:LEU:C	1:E:400:LEU:HD12	2.19	0.63
1:E:789:MSE:HG2	1:H:789:MSE:CE	2.27	0.63
1:G:83:PRO:CB	1:G:84:PRO:HD2	2.27	0.63
1:A:90:VAL:HG23	1:A:98:GLU:O	1.98	0.63
1:C:224:THR:CG2	1:C:228:GLU:HG3	2.28	0.63
1:H:35:ARG:O	1:H:104:LEU:HD22	1.99	0.63
1:D:561:LYS:HD2	1:D:613:ARG:O	1.99	0.63
1:E:315:LEU:CD1	1:E:762:LEU:HD23	2.27	0.63
1:E:588:SER:HB3	1:E:625:GLU:OE2	1.99	0.63
1:G:692:PHE:CD2	1:G:724:LEU:HD23	2.34	0.63
1:C:173:ASP:HB3	1:C:176:SER:HB3	1.81	0.63
1:F:387:PRO:HD3	1:F:802:VAL:HB	1.81	0.63
1:G:156:GLY:O	1:G:522:ASN:HA	1.98	0.63
1:G:477:PHE:HA	1:G:520:LYS:HB2	1.81	0.63
1:H:211:ARG:HD2	7:H:867:HOH:O	1.98	0.63
1:G:304:GLN:CB	3:G:902:FRU:H11	2.26	0.63
1:G:596:LYS:HG2	1:G:636:TYR:HE1	1.59	0.63
1:B:348:THR:O	1:B:351:GLU:HG2	1.99	0.63
1:C:207:GLN:NE2	1:C:211:ARG:HH21	1.95	0.63
1:C:371:THR:OG1	1:C:373:LYS:HG3	1.99	0.63
1:A:420:LEU:HD13	1:A:420:LEU:C	2.20	0.62
1:B:142:PHE:HB3	1:B:783:ALA:HB2	1.79	0.62
1:D:195:MSE:HE1	1:D:241:GLY:HA3	1.81	0.62
1:E:61:ARG:HG3	1:E:61:ARG:NH1	1.98	0.62
1:E:85:TRP:CD1	1:E:85:TRP:N	2.64	0.62
1:E:146:ILE:HD11	1:E:772:TRP:CZ2	2.34	0.62
1:E:230:GLU:OE1	1:E:240:ARG:NH1	2.32	0.62
1:H:90:VAL:N	1:H:98:GLU:O	2.32	0.62
1:C:217:LEU:HD11	1:C:249:VAL:HG12	1.81	0.62
1:H:17:ARG:NH2	1:H:72:LEU:CB	2.52	0.62
1:F:65:GLU:HG3	1:F:70:PHE:CB	2.28	0.62
1:H:552:GLU:O	1:H:556:SER:HB3	1.98	0.62
1:H:719:GLN:HG3	4:H:913:SO4:O4	1.98	0.62
1:C:772:TRP:CZ2	1:C:776:SER:HB3	2.34	0.62
1:D:298:TYR:CE1	1:D:649:MSE:CE	2.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:GLU:N	1:H:141:PRO:HD2	2.14	0.62
1:A:52:GLU:CG	1:A:56:LEU:HB2	2.28	0.62
1:A:682:VAL:HG13	1:A:749:ILE:HD12	1.81	0.62
1:D:105:HIS:O	1:D:106:ALA:CB	2.46	0.62
1:H:784:ARG:O	1:H:788:GLU:HG3	1.98	0.62
1:D:56:LEU:HB3	1:D:57:PRO:CD	2.30	0.62
1:H:82:LEU:HD12	1:H:84:PRO:CG	2.29	0.62
1:A:400:LEU:HD12	1:A:401:SER:N	2.15	0.62
1:E:45:GLN:HG2	1:E:80:ILE:HD12	1.82	0.62
1:E:756:GLN:HG2	1:E:757:ILE:N	2.15	0.62
1:G:702:ILE:HA	1:G:753:TYR:OH	2.00	0.62
1:H:281:VAL:HG21	1:H:319:MSE:CE	2.30	0.62
1:D:536:TYR:CE1	1:D:537:THR:HG23	2.34	0.62
1:E:159:VAL:HG13	1:E:160:ASP:N	2.15	0.62
1:A:178:LEU:HB2	1:A:179:PRO:HD3	1.82	0.62
1:B:50:ILE:O	1:B:54:GLU:HB2	2.00	0.62
1:D:146:ILE:CD1	1:D:772:TRP:CZ2	2.82	0.62
1:E:789:MSE:HE1	1:H:789:MSE:CB	2.30	0.62
1:G:230:GLU:O	1:G:234:GLU:HG3	2.00	0.62
1:D:340:LEU:HB2	1:D:366:ARG:HB3	1.82	0.62
1:E:61:ARG:CG	1:E:61:ARG:NH1	2.55	0.62
1:G:65:GLU:CB	1:G:70:PHE:CD1	2.71	0.62
1:A:46:GLN:OE1	1:A:46:GLN:HA	1.99	0.61
1:A:51:ALA:O	1:A:53:PHE:N	2.33	0.61
1:A:83:PRO:CB	1:A:84:PRO:CD	2.77	0.61
1:A:84:PRO:O	1:A:104:LEU:N	2.25	0.61
1:D:231:ALA:O	1:D:235:GLU:HG2	2.00	0.61
1:G:53:PHE:O	1:G:57:PRO:HD2	2.00	0.61
1:A:140:GLU:HB3	1:A:141:PRO:CD	2.30	0.61
1:A:255:LEU:HD23	1:A:267:THR:HG23	1.82	0.61
1:A:483:PHE:CE1	1:A:487:ALA:HB3	2.34	0.61
1:B:293:ASP:HB2	7:B:847:HOH:O	2.00	0.61
1:C:54:GLU:CG	1:C:55:ALA:N	2.55	0.61
1:B:230:GLU:O	1:B:234:GLU:HG3	2.00	0.61
1:C:354:GLU:OE1	1:C:366:ARG:NH2	2.34	0.61
1:E:321:GLN:HE21	1:E:325:GLN:NE2	1.99	0.61
1:G:146:ILE:HD11	1:G:772:TRP:CZ2	2.35	0.61
1:C:748:ARG:NH1	1:C:752:LYS:HG3	2.14	0.61
1:D:590:LEU:HB2	1:D:671:PRO:HG3	1.82	0.61
1:G:39:LYS:HZ3	1:G:105:HIS:CD2	2.19	0.61
1:H:46:GLN:O	1:H:78:GLU:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:O	1:B:312:VAL:HG22	2.00	0.61
1:C:414:ASN:O	1:C:418:GLY:HA3	2.01	0.61
1:D:327:GLY:O	1:D:328:LEU:HD23	2.00	0.61
1:E:789:MSE:HE1	1:H:790:PHE:N	2.16	0.61
1:G:245:ASN:O	1:G:249:VAL:HG23	2.00	0.61
1:C:119:HIS:CE1	1:C:509:ARG:NH1	2.68	0.61
1:G:414:ASN:O	1:G:418:GLY:HA3	2.01	0.61
1:B:163:ASN:HD21	1:B:269:GLU:HG3	1.66	0.61
1:D:216:TYR:CE1	1:D:220:LEU:HD11	2.35	0.61
1:E:43:ILE:HG12	1:E:44:LEU:H	1.66	0.61
1:F:69:PHE:CD1	1:F:69:PHE:C	2.72	0.61
1:F:685:MSE:HE3	1:F:745:GLY:HA2	1.81	0.61
1:B:333:ARG:HG2	1:B:333:ARG:NH1	2.15	0.61
1:D:211:ARG:HG3	1:D:211:ARG:HH11	1.66	0.61
1:F:65:GLU:HG3	1:F:70:PHE:HB2	1.81	0.61
1:F:420:LEU:C	1:F:420:LEU:HD13	2.21	0.61
1:C:33:LEU:O	1:C:36:VAL:HB	2.01	0.61
1:F:547:HIS:O	1:F:551:GLU:HG2	2.00	0.61
1:H:46:GLN:CB	1:H:79:ALA:HB3	2.27	0.61
1:A:30:LEU:HD12	1:A:62:LYS:O	2.01	0.61
1:D:524:VAL:HG12	1:D:758:TYR:CD2	2.36	0.61
1:E:60:THR:HG23	1:E:62:LYS:H	1.65	0.61
1:C:483:PHE:CE1	1:C:487:ALA:HB3	2.35	0.60
1:F:675:GLU:O	1:F:697:GLY:HA3	2.01	0.60
1:G:70:PHE:C	1:G:70:PHE:HD2	2.04	0.60
1:A:164:ARG:HD2	1:B:262:ALA:HB1	1.83	0.60
1:E:60:THR:O	1:E:63:LYS:HG3	2.01	0.60
1:F:82:LEU:HD13	1:F:83:PRO:HG3	1.82	0.60
1:G:419:ASN:HB3	1:G:471:ALA:CB	2.31	0.60
1:H:419:ASN:OD1	1:H:435:THR:HB	2.01	0.60
1:A:39:LYS:NZ	1:A:105:HIS:HD2	1.99	0.60
1:A:373:LYS:H	1:A:373:LYS:CD	2.13	0.60
1:B:43:ILE:O	1:B:43:ILE:HG23	2.00	0.60
1:F:789:MSE:HG2	1:G:789:MSE:HE3	1.81	0.60
1:H:89:ALA:HB1	1:H:99:TYR:CD1	2.35	0.60
1:B:245:ASN:O	1:B:249:VAL:HG23	2.02	0.60
1:C:83:PRO:O	1:C:104:LEU:HD12	2.01	0.60
1:D:43:ILE:HG23	1:D:124:LEU:HD12	1.82	0.60
1:D:411:ILE:HG13	1:D:431:VAL:HG11	1.82	0.60
1:D:750:GLU:HA	1:D:750:GLU:OE2	2.00	0.60
1:H:259:LEU:O	1:H:263:PRO:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:HG3	1:A:59:GLN:HE22	1.65	0.60
1:A:794:LYS:O	1:A:797:PRO:HD2	2.02	0.60
1:C:60:THR:C	1:C:62:LYS:N	2.54	0.60
1:C:80:ILE:HD11	1:C:121:LYS:CG	2.30	0.60
1:C:534:PHE:HB2	1:C:535:PRO:CD	2.31	0.60
1:C:586:ASN:HB3	1:C:671:PRO:O	2.01	0.60
1:C:597:ASN:O	1:C:601:ARG:HG3	2.02	0.60
1:D:32:LEU:O	1:D:36:VAL:HG23	2.01	0.60
1:D:564:LEU:HG	1:D:613:ARG:NH2	2.16	0.60
1:F:668:PHE:HB2	1:F:689:LEU:HD23	1.83	0.60
1:H:158:GLY:HA3	1:H:519:PRO:O	2.01	0.60
1:C:140:GLU:N	1:C:141:PRO:HD2	2.15	0.60
1:D:116:GLU:O	1:D:119:HIS:HB2	2.02	0.60
1:B:441:GLU:HA	1:B:441:GLU:OE1	2.01	0.60
1:E:547:HIS:O	1:E:551:GLU:HG3	2.00	0.60
1:F:43:ILE:HG23	1:F:44:LEU:H	1.66	0.60
1:G:158:GLY:HA3	1:G:519:PRO:O	2.01	0.60
1:H:145:SER:HB3	1:H:779:ASP:CG	2.21	0.60
1:B:32:LEU:O	1:B:36:VAL:HG23	2.02	0.60
1:B:659:ARG:O	1:B:662:CYS:HB2	2.02	0.60
1:B:716:HIS:HB3	4:B:913:SO4:O4	2.02	0.60
1:C:217:LEU:CD1	1:C:249:VAL:HG12	2.32	0.60
1:D:43:ILE:O	1:D:44:LEU:HB2	2.01	0.60
1:G:56:LEU:HB3	1:G:57:PRO:CD	2.30	0.60
1:H:545:LYS:H	1:H:545:LYS:HD3	1.66	0.60
1:B:131:GLY:CA	1:B:134:THR:HG21	2.29	0.60
1:D:629:MSE:HA	1:D:629:MSE:CE	2.29	0.60
1:F:647:SER:HB2	1:F:649:MSE:HE2	1.84	0.60
1:H:668:PHE:HB2	1:H:689:LEU:CD2	2.31	0.60
1:B:210:LEU:CD2	1:B:253:ILE:HG23	2.31	0.60
1:D:54:GLU:HG3	1:D:55:ALA:N	2.16	0.60
1:F:629:MSE:HA	1:F:629:MSE:HE2	1.84	0.60
1:H:17:ARG:HH21	1:H:72:LEU:CB	2.11	0.60
1:H:564:LEU:HD22	1:H:613:ARG:NH2	2.17	0.60
1:C:83:PRO:HG2	1:C:84:PRO:CD	2.15	0.59
1:D:137:LEU:HD12	1:D:510:VAL:HG22	1.84	0.59
1:E:789:MSE:HB3	1:H:789:MSE:HE2	1.84	0.59
1:G:597:ASN:O	1:G:601:ARG:HG3	2.02	0.59
1:A:73:LEU:N	1:A:73:LEU:HD23	2.16	0.59
1:A:193:ASN:HB3	1:A:239:GLU:HG3	1.84	0.59
1:D:195:MSE:HE1	1:D:241:GLY:CA	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:ILE:HD13	1:F:516:VAL:CG1	2.32	0.59
1:F:789:MSE:CE	1:G:790:PHE:N	2.65	0.59
1:H:670:GLN:HG3	1:H:670:GLN:O	2.02	0.59
1:C:56:LEU:HB3	1:C:57:PRO:HD3	1.84	0.59
1:C:170:LEU:HD22	1:C:177:LEU:HD23	1.83	0.59
1:A:739:ASP:O	1:A:743:LYS:HG2	2.02	0.59
1:C:290:PHE:O	1:C:366:ARG:NH1	2.35	0.59
1:C:622:GLU:O	1:C:626:MSE:HG3	2.03	0.59
1:D:146:ILE:CG2	1:D:147:PRO:CD	2.79	0.59
1:E:210:LEU:HD22	1:E:253:ILE:HG23	1.82	0.59
1:G:48:GLN:HE21	1:G:48:GLN:C	2.05	0.59
1:G:146:ILE:CG2	1:G:147:PRO:HD2	2.33	0.59
1:G:419:ASN:HB3	1:G:471:ALA:HB1	1.84	0.59
1:D:48:GLN:HE22	1:D:492:THR:HG22	1.66	0.59
1:D:187:HIS:HD2	1:D:194:LEU:HB2	1.67	0.59
1:E:65:GLU:HB3	1:E:70:PHE:HD1	1.67	0.59
1:E:67:GLY:O	1:E:71:ASP:HB2	2.03	0.59
1:F:82:LEU:HD12	1:F:83:PRO:HG3	1.81	0.59
1:A:56:LEU:HG	1:A:70:PHE:HD1	1.66	0.59
1:A:146:ILE:CG2	1:A:147:PRO:HD2	2.33	0.59
1:E:586:ASN:HB3	1:E:671:PRO:O	2.03	0.59
1:F:668:PHE:HB2	1:F:689:LEU:CD2	2.32	0.59
1:H:82:LEU:CD1	1:H:84:PRO:HG2	2.31	0.59
1:A:65:GLU:HA	1:A:65:GLU:OE2	2.03	0.59
1:A:249:VAL:O	1:A:253:ILE:HG13	2.02	0.59
1:B:30:LEU:CD1	1:B:30:LEU:N	2.66	0.59
1:B:209:THR:HG23	1:B:236:ILE:HB	1.83	0.59
1:B:518:ASP:OD1	1:B:519:PRO:HD2	2.03	0.59
1:F:65:GLU:HA	1:F:65:GLU:OE2	2.03	0.59
1:C:378:LYS:HD3	1:C:805:ALA:HB1	1.84	0.59
1:D:248:ARG:HH11	1:D:248:ARG:HB3	1.67	0.59
1:E:83:PRO:O	1:E:85:TRP:N	2.36	0.59
1:F:54:GLU:HG3	1:F:55:ALA:N	2.17	0.59
1:G:675:GLU:O	1:G:697:GLY:HA3	2.03	0.59
1:H:187:HIS:HD2	1:H:195:MSE:HG2	1.68	0.59
1:H:564:LEU:HD22	1:H:613:ARG:CZ	2.33	0.59
1:A:80:ILE:N	1:A:87:ALA:O	2.34	0.59
1:F:647:SER:HB2	1:F:649:MSE:CE	2.33	0.59
1:B:43:ILE:O	1:B:43:ILE:HD13	2.03	0.59
1:B:217:LEU:HD11	1:B:233:PHE:HZ	1.67	0.59
1:B:249:VAL:O	1:B:253:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LYS:HB2	1:D:39:LYS:HZ2	1.66	0.59
1:F:316:GLU:HA	1:F:319:MSE:CE	2.20	0.59
1:A:195:MSE:HE3	1:A:242:TRP:CE2	2.38	0.58
1:A:547:HIS:O	1:A:551:GLU:HG3	2.03	0.58
1:C:146:ILE:HG23	1:C:147:PRO:HD2	1.85	0.58
1:C:564:LEU:HG	1:C:613:ARG:NH2	2.17	0.58
1:E:60:THR:HG23	1:E:62:LYS:CB	2.33	0.58
1:F:81:VAL:O	1:F:81:VAL:HG23	2.03	0.58
1:H:171:PHE:HD1	1:H:263:PRO:HD2	1.68	0.58
1:A:772:TRP:CZ2	1:A:776:SER:HB3	2.38	0.58
1:B:146:ILE:HD11	1:B:772:TRP:CZ2	2.38	0.58
1:D:102:VAL:HG23	1:D:109:VAL:HG23	1.85	0.58
1:E:100:LEU:HD12	1:E:100:LEU:O	2.03	0.58
1:F:545:LYS:H	1:F:545:LYS:CD	2.16	0.58
1:G:83:PRO:HB2	1:G:84:PRO:HD2	1.85	0.58
1:H:131:GLY:CA	1:H:134:THR:HG23	2.33	0.58
1:A:81:VAL:HA	1:A:86:VAL:HG23	1.85	0.58
1:A:435:THR:HG23	1:A:475:THR:HB	1.84	0.58
1:D:41:LYS:N	7:D:868:HOH:O	2.36	0.58
1:F:284:LEU:O	1:F:414:ASN:HB2	2.04	0.58
1:G:586:ASN:HB3	1:G:671:PRO:O	2.03	0.58
1:A:789:MSE:HE2	1:D:789:MSE:CG	2.33	0.58
1:B:83:PRO:C	1:B:85:TRP:N	2.57	0.58
1:C:121:LYS:O	1:C:124:LEU:HB3	2.02	0.58
1:C:156:GLY:O	1:C:522:ASN:HA	2.03	0.58
1:D:187:HIS:CD2	1:D:194:LEU:HB2	2.39	0.58
1:D:387:PRO:HD3	1:D:802:VAL:HB	1.85	0.58
1:F:582:ASP:HB2	1:F:621:GLU:OE1	2.04	0.58
1:G:170:LEU:HD13	1:G:177:LEU:HD23	1.85	0.58
1:B:796:ARG:HB2	1:B:797:PRO:HD3	1.85	0.58
1:C:50:ILE:CD1	1:C:54:GLU:CB	2.75	0.58
1:C:221:LYS:HE3	1:C:223:GLU:OE2	2.04	0.58
1:E:207:GLN:HE21	1:E:211:ARG:NH2	2.01	0.58
1:E:593:TRP:HB3	1:E:721:ALA:HB2	1.84	0.58
1:F:162:LEU:HD11	1:F:772:TRP:CD2	2.38	0.58
1:G:56:LEU:HD13	1:G:63:LYS:HG2	1.85	0.58
1:G:698:GLY:N	1:G:699:PRO:CD	2.67	0.58
1:H:82:LEU:HD12	1:H:84:PRO:HD2	1.85	0.58
1:E:148:ARG:CG	1:E:148:ARG:NH1	2.57	0.58
1:C:80:ILE:CD1	1:C:121:LYS:HG3	2.34	0.58
1:D:39:LYS:HZ2	1:D:39:LYS:CB	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:GLY:HA3	1:G:134:THR:HG23	1.84	0.58
1:G:249:VAL:O	1:G:253:ILE:HG12	2.03	0.58
1:G:591:VAL:HG12	1:G:632:LEU:HD13	1.86	0.58
1:D:48:GLN:HA	1:D:51:ALA:HB3	1.84	0.58
1:F:244:ASP:OD2	1:F:248:ARG:HD2	2.04	0.58
1:G:407:LYS:HB2	1:G:408:PRO:CD	2.33	0.58
1:G:479:ILE:HD11	1:G:762:LEU:CD1	2.34	0.58
1:H:681:VAL:HG12	1:H:685:MSE:SE	2.54	0.58
1:A:796:ARG:O	1:A:800:GLN:HG3	2.03	0.58
1:E:65:GLU:CG	1:E:70:PHE:HB2	2.33	0.58
1:E:207:GLN:HE21	1:E:211:ARG:HH22	1.52	0.58
1:G:65:GLU:CG	1:G:70:PHE:HB2	2.34	0.58
1:G:338:THR:HG23	1:G:366:ARG:HG2	1.84	0.58
1:H:113:GLN:N	1:H:113:GLN:CD	2.57	0.58
1:B:259:LEU:HD21	1:B:268:LEU:HA	1.85	0.57
1:C:564:LEU:HG	1:C:613:ARG:HH22	1.70	0.57
1:D:27:ASN:N	1:D:27:ASN:HD22	2.01	0.57
1:F:173:ASP:HB3	1:F:176:SER:CB	2.33	0.57
1:H:217:LEU:HD23	1:H:220:LEU:HD12	1.85	0.57
1:B:160:ASP:O	1:B:164:ARG:HG3	2.03	0.57
1:C:772:TRP:CH2	1:C:776:SER:HB3	2.39	0.57
1:E:53:PHE:O	1:E:57:PRO:CG	2.50	0.57
1:E:156:GLY:O	1:E:522:ASN:HA	2.03	0.57
1:E:158:GLY:HA3	1:E:519:PRO:O	2.04	0.57
1:H:143:ASN:HB3	1:H:148:ARG:HH12	1.69	0.57
1:B:338:THR:HG23	1:B:366:ARG:HG2	1.84	0.57
1:B:622:GLU:HG2	1:B:626:MSE:HE3	1.86	0.57
1:F:65:GLU:CG	1:F:70:PHE:HB2	2.34	0.57
1:F:70:PHE:CG	1:F:71:ASP:N	2.72	0.57
1:B:278:VAL:HG12	1:B:319:MSE:HE3	1.87	0.57
1:D:83:PRO:CG	1:D:84:PRO:CD	2.82	0.57
1:F:145:SER:HB2	1:F:779:ASP:OD2	2.04	0.57
1:F:633:ILE:HA	1:F:638:LEU:HD12	1.86	0.57
1:G:124:LEU:HD23	1:G:124:LEU:O	2.05	0.57
1:G:659:ARG:O	1:G:662:CYS:HB2	2.04	0.57
1:A:407:LYS:HB2	1:A:408:PRO:HD2	1.87	0.57
1:A:789:MSE:HE1	1:D:790:PHE:N	2.19	0.57
1:E:442:LYS:HD2	1:E:449:ASP:HB3	1.85	0.57
1:E:756:GLN:HG2	1:E:757:ILE:H	1.69	0.57
1:H:131:GLY:N	1:H:134:THR:HG23	2.19	0.57
1:B:140:GLU:N	1:B:141:PRO:HD2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LYS:CB	1:C:104:LEU:HD13	2.29	0.57
1:C:217:LEU:HD11	1:C:249:VAL:CG1	2.34	0.57
1:C:407:LYS:HB2	1:C:408:PRO:CD	2.35	0.57
1:D:37:GLU:HG3	1:D:59:GLN:HE21	1.68	0.57
1:B:52:GLU:O	1:B:57:PRO:HD2	2.04	0.57
1:F:315:LEU:O	1:F:319:MSE:HG3	2.05	0.57
1:C:566:VAL:HG12	1:C:567:LEU:N	2.19	0.57
1:B:17:ARG:CB	1:B:72:LEU:HD21	2.34	0.57
1:C:80:ILE:CD1	1:C:121:LYS:CG	2.83	0.57
1:E:73:LEU:N	1:E:73:LEU:CD2	2.67	0.57
1:F:52:GLU:CG	1:F:53:PHE:N	2.66	0.57
1:H:95:GLY:HA3	1:H:517:PHE:CE2	2.38	0.57
1:F:56:LEU:N	1:F:57:PRO:CD	2.68	0.57
1:F:59:GLN:CG	1:F:60:THR:H	2.17	0.57
1:G:784:ARG:O	1:G:788:GLU:HG3	2.04	0.57
1:D:322:ARG:HD2	1:D:763:LEU:HD12	1.86	0.56
1:F:628:LYS:CA	1:F:628:LYS:HE2	2.35	0.56
1:F:726:ASP:O	1:F:730:LYS:HG3	2.04	0.56
1:G:32:LEU:O	1:G:32:LEU:HD13	2.05	0.56
1:G:119:HIS:CE1	1:G:129:LYS:CB	2.88	0.56
1:G:472:MSE:SE	1:G:514:ILE:HB	2.55	0.56
1:A:668:PHE:HB2	1:A:689:LEU:HD23	1.87	0.56
1:A:784:ARG:O	1:A:788:GLU:HG3	2.05	0.56
1:C:70:PHE:O	1:C:71:ASP:CB	2.52	0.56
1:E:44:LEU:O	1:E:81:VAL:HG12	2.04	0.56
1:E:173:ASP:HB3	1:E:176:SER:HB2	1.87	0.56
1:F:82:LEU:HD12	1:F:82:LEU:H	1.71	0.56
1:F:479:ILE:CD1	1:F:762:LEU:HD13	2.35	0.56
1:A:470:PHE:CE1	1:A:791:TYR:HB2	2.40	0.56
1:B:682:VAL:HG13	1:B:749:ILE:HD12	1.87	0.56
1:C:119:HIS:HE1	1:C:509:ARG:HH12	1.50	0.56
1:C:171:PHE:CD1	1:C:263:PRO:HD2	2.40	0.56
1:C:348:THR:O	1:C:351:GLU:HG2	2.05	0.56
1:D:166:LEU:O	1:D:170:LEU:HB2	2.05	0.56
1:D:259:LEU:O	1:D:263:PRO:HG3	2.06	0.56
1:D:491:GLU:CD	1:D:491:GLU:H	2.09	0.56
1:E:565:CYS:C	1:E:566:VAL:CG2	2.73	0.56
1:F:83:PRO:HG2	1:F:85:TRP:HB2	1.88	0.56
1:G:54:GLU:OE2	1:G:55:ALA:HA	2.05	0.56
1:G:565:CYS:HB2	1:G:642:PHE:O	2.05	0.56
1:G:625:GLU:O	1:G:629:MSE:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:657:LEU:O	1:G:661:ILE:HG12	2.05	0.56
1:H:407:LYS:HB2	1:H:408:PRO:HD2	1.86	0.56
1:A:195:MSE:HE1	1:A:242:TRP:CA	2.31	0.56
1:B:63:LYS:HG3	1:B:64:LEU:H	1.70	0.56
1:C:670:GLN:O	1:C:670:GLN:HG3	2.05	0.56
1:D:44:LEU:HA	1:D:124:LEU:HD11	1.87	0.56
1:E:435:THR:HG23	1:E:475:THR:CB	2.36	0.56
1:E:447:ASP:HB3	1:E:451:TYR:CD2	2.40	0.56
1:E:565:CYS:C	1:E:566:VAL:HG23	2.26	0.56
1:F:56:LEU:N	1:F:57:PRO:HD2	2.20	0.56
1:F:534:PHE:HB2	1:F:535:PRO:CD	2.36	0.56
1:A:72:LEU:C	1:A:73:LEU:HD23	2.26	0.56
1:B:83:PRO:C	1:B:85:TRP:H	2.08	0.56
1:B:102:VAL:HA	1:B:109:VAL:HA	1.88	0.56
1:B:206:LEU:HD11	1:B:210:LEU:HD11	1.87	0.56
1:B:407:LYS:HB2	1:B:408:PRO:HD2	1.86	0.56
1:B:420:LEU:C	1:B:420:LEU:HD13	2.25	0.56
1:D:39:LYS:NZ	1:D:39:LYS:CB	2.68	0.56
1:D:400:LEU:HD12	1:D:400:LEU:C	2.25	0.56
1:E:156:GLY:HA3	1:E:523:ILE:HG13	1.86	0.56
1:F:189:HIS:ND1	1:F:330:ILE:HD13	2.21	0.56
1:F:717:GLY:O	1:F:720:ALA:HB3	2.05	0.56
1:H:56:LEU:O	1:H:63:LYS:HD2	2.06	0.56
1:H:63:LYS:O	1:H:65:GLU:HG2	2.05	0.56
1:A:338:THR:HG23	1:A:366:ARG:HG2	1.88	0.56
1:B:56:LEU:CB	1:B:57:PRO:HD3	2.32	0.56
1:D:532:ILE:HD12	1:D:652:VAL:HG22	1.88	0.56
1:E:217:LEU:HD23	1:E:220:LEU:CD1	2.36	0.56
1:E:224:THR:HG23	1:E:228:GLU:HG3	1.87	0.56
1:E:659:ARG:O	1:E:662:CYS:HB2	2.05	0.56
1:F:51:ALA:O	1:F:52:GLU:HB3	2.05	0.56
1:F:469:ILE:CD1	1:F:472:MSE:HE1	2.19	0.56
1:B:794:LYS:O	1:B:798:LEU:HD12	2.05	0.56
1:D:131:GLY:C	1:D:134:THR:HG23	2.26	0.56
1:D:181:LEU:HD12	1:D:196:LEU:HD12	1.86	0.56
1:E:44:LEU:HA	1:E:124:LEU:HD21	1.88	0.56
1:E:101:ARG:H	1:E:112:LEU:HD21	1.70	0.56
1:G:390:GLU:HG3	1:G:791:TYR:OH	2.06	0.56
1:A:536:TYR:CE1	1:A:537:THR:HG23	2.41	0.56
1:A:789:MSE:HE2	1:D:789:MSE:SE	2.56	0.56
1:C:172:HIS:CD2	1:D:147:PRO:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:ASN:HB3	1:E:239:GLU:HG3	1.88	0.56
1:E:789:MSE:HE1	1:H:789:MSE:C	2.26	0.56
1:A:232:LYS:HE3	1:A:236:ILE:HD13	1.87	0.56
1:B:63:LYS:CG	1:B:64:LEU:H	2.19	0.56
1:B:232:LYS:O	1:B:235:GLU:HB2	2.06	0.56
1:B:449:ASP:O	1:B:504:LEU:HD22	2.06	0.56
1:E:83:PRO:CB	1:E:84:PRO:CD	2.84	0.56
1:E:116:GLU:O	1:E:119:HIS:HB2	2.05	0.56
1:F:315:LEU:HD11	1:F:762:LEU:HD23	1.87	0.56
1:G:65:GLU:HG2	1:G:70:PHE:HB2	1.88	0.56
1:G:131:GLY:H	1:G:134:THR:CG2	2.18	0.56
1:D:216:TYR:CD1	1:D:216:TYR:C	2.80	0.56
1:G:670:GLN:HG3	1:G:670:GLN:O	2.06	0.56
1:A:153:LYS:HD3	1:A:154:TYR:CE2	2.41	0.55
1:B:99:TYR:CZ	1:B:114:PRO:HG3	2.40	0.55
1:C:623:LYS:HA	1:C:626:MSE:HE2	1.87	0.55
1:F:778:LEU:HD12	1:F:779:ASP:H	1.70	0.55
1:A:146:ILE:HG22	1:A:147:PRO:O	2.06	0.55
1:A:170:LEU:HD22	1:A:177:LEU:HD23	1.88	0.55
1:C:278:VAL:HG21	1:C:763:LEU:HD23	1.87	0.55
1:A:135:LEU:HD22	1:D:793:LEU:HD11	1.88	0.55
1:B:146:ILE:HG22	1:B:147:PRO:CD	2.35	0.55
1:C:146:ILE:HD11	1:C:162:LEU:HD13	1.87	0.55
1:C:665:LYS:HD3	1:C:665:LYS:N	2.21	0.55
1:D:223:GLU:HG3	1:D:223:GLU:O	2.05	0.55
1:E:125:VAL:HG22	1:E:126:ASP:OD2	2.05	0.55
1:E:414:ASN:O	1:E:418:GLY:HA3	2.07	0.55
1:F:591:VAL:CG2	1:F:629:MSE:HE1	2.35	0.55
1:A:681:VAL:O	1:A:685:MSE:HG3	2.06	0.55
1:D:146:ILE:HG22	1:D:147:PRO:N	2.21	0.55
1:E:48:GLN:HB3	7:E:875:HOH:O	2.06	0.55
1:F:68:PRO:O	1:F:70:PHE:N	2.39	0.55
1:F:82:LEU:HD12	1:F:83:PRO:CG	2.36	0.55
1:F:137:LEU:HD12	1:F:510:VAL:HG22	1.89	0.55
1:C:52:GLU:OE2	1:C:53:PHE:N	2.39	0.55
1:D:222:SER:HB3	1:D:247:GLU:HB2	1.88	0.55
1:E:249:VAL:O	1:E:253:ILE:HG12	2.05	0.55
1:E:680:THR:HG23	2:E:901:UDP:O1A	2.07	0.55
1:F:70:PHE:CD2	1:F:71:ASP:HB2	2.41	0.55
1:F:210:LEU:CD2	1:F:253:ILE:HG23	2.35	0.55
1:F:250:LEU:HG	1:F:254:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLY:HA3	1:A:523:ILE:HG13	1.89	0.55
1:D:106:ALA:CB	1:D:108:VAL:HG23	2.32	0.55
1:D:131:GLY:O	1:D:134:THR:HG23	2.06	0.55
1:D:532:ILE:HG13	1:D:651:ARG:HD2	1.88	0.55
1:F:419:ASN:HB3	1:F:471:ALA:HB1	1.89	0.55
1:F:789:MSE:HE2	1:G:789:MSE:HE3	1.89	0.55
1:B:318:GLU:HG3	1:B:322:ARG:HD2	1.89	0.55
1:F:32:LEU:O	1:F:35:ARG:HB3	2.07	0.55
1:F:629:MSE:HA	1:F:629:MSE:HE3	1.88	0.55
1:H:143:ASN:HB3	1:H:148:ARG:NH1	2.22	0.55
1:H:216:TYR:CD1	1:H:220:LEU:HD11	2.40	0.55
1:C:298:TYR:CE1	1:C:649:MSE:HE1	2.42	0.55
1:E:367:VAL:HG22	1:E:399:GLU:HG3	1.88	0.55
1:F:35:ARG:CD	1:F:104:LEU:HA	2.32	0.55
1:F:81:VAL:HG12	1:F:86:VAL:CA	2.35	0.55
1:F:233:PHE:CE1	1:F:238:LEU:HD12	2.42	0.55
1:E:333:ARG:HG2	1:E:333:ARG:NH1	2.22	0.55
1:A:82:LEU:HB3	1:A:83:PRO:CD	2.35	0.55
1:A:230:GLU:OE1	1:A:240:ARG:NH1	2.40	0.55
1:A:789:MSE:CE	1:D:789:MSE:CG	2.84	0.55
1:A:140:GLU:N	1:A:141:PRO:HD2	2.21	0.54
1:F:141:PRO:HB2	1:G:782:GLU:HG3	1.90	0.54
1:H:33:LEU:HA	1:H:36:VAL:CB	2.37	0.54
1:H:91:ARG:HD2	1:H:97:TRP:CZ2	2.42	0.54
1:H:400:LEU:C	1:H:400:LEU:HD12	2.27	0.54
1:A:56:LEU:HB3	1:A:57:PRO:CD	2.34	0.54
1:A:154:TYR:OH	1:B:262:ALA:HB3	2.06	0.54
1:A:316:GLU:CA	1:A:319:MSE:HE3	2.32	0.54
1:A:419:ASN:HB3	1:A:471:ALA:HB1	1.89	0.54
1:A:458:LYS:HE2	1:A:459:TYR:CZ	2.42	0.54
1:F:216:TYR:CE2	1:F:232:LYS:HG2	2.41	0.54
1:F:793:LEU:HB3	1:G:793:LEU:HB3	1.89	0.54
1:A:786:TYR:CE1	1:D:789:MSE:HE3	2.41	0.54
1:C:692:PHE:CG	1:C:724:LEU:HD21	2.42	0.54
1:C:757:ILE:HD13	1:C:757:ILE:N	2.23	0.54
1:D:56:LEU:CD1	1:D:57:PRO:CD	2.84	0.54
1:F:428:LYS:HG2	1:F:429:LEU:HD23	1.90	0.54
1:H:210:LEU:CD2	1:H:253:ILE:HG23	2.34	0.54
1:B:225:LEU:O	1:B:228:GLU:HG2	2.08	0.54
1:B:354:GLU:OE1	1:B:366:ARG:NH2	2.40	0.54
1:B:777:ASN:OD1	1:B:778:LEU:HD23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LYS:O	1:C:65:GLU:CG	2.55	0.54
1:C:681:VAL:HG13	1:C:691:THR:HG21	1.89	0.54
1:D:41:LYS:HE3	1:D:54:GLU:CG	2.37	0.54
1:D:518:ASP:OD1	1:D:520:LYS:HG2	2.07	0.54
1:A:232:LYS:O	1:A:235:GLU:HB2	2.07	0.54
1:A:245:ASN:O	1:A:249:VAL:HG23	2.07	0.54
1:A:793:LEU:HB3	1:D:793:LEU:HB3	1.88	0.54
1:B:41:LYS:HD2	1:B:46:GLN:HE22	1.73	0.54
1:B:534:PHE:HB2	1:B:535:PRO:CD	2.38	0.54
1:C:158:GLY:HA3	1:C:519:PRO:O	2.07	0.54
1:D:210:LEU:HD22	1:D:253:ILE:HG23	1.89	0.54
1:E:534:PHE:HB2	1:E:535:PRO:CD	2.37	0.54
1:F:434:CYS:SG	1:F:479:ILE:HG13	2.47	0.54
1:G:73:LEU:N	1:G:73:LEU:CD2	2.70	0.54
1:G:315:LEU:HD21	1:G:762:LEU:CD2	2.36	0.54
1:H:39:LYS:HD3	1:H:39:LYS:O	2.08	0.54
1:H:657:LEU:O	1:H:661:ILE:HG12	2.08	0.54
1:C:87:ALA:O	1:C:88:LEU:HD23	2.08	0.54
1:C:483:PHE:CZ	1:C:487:ALA:HB3	2.43	0.54
1:C:607:VAL:HG22	1:C:643:ARG:HB3	1.89	0.54
1:E:189:HIS:ND1	1:E:330:ILE:HD13	2.22	0.54
1:E:790:PHE:O	1:E:794:LYS:HB3	2.07	0.54
1:G:164:ARG:HD2	1:H:262:ALA:HB1	1.89	0.54
1:G:259:LEU:HD21	1:G:267:THR:HG22	1.89	0.54
1:H:82:LEU:HD11	1:H:85:TRP:HB2	1.89	0.54
1:A:195:MSE:CE	1:A:242:TRP:HA	2.32	0.54
1:A:609:VAL:HG22	1:A:645:ILE:HB	1.90	0.54
1:C:692:PHE:CE2	1:C:724:LEU:HD23	2.42	0.54
1:E:137:LEU:HD11	1:E:790:PHE:CE1	2.42	0.54
1:F:716:HIS:HB3	4:F:913:SO4:O2	2.08	0.54
1:G:278:VAL:HG12	1:G:319:MSE:HE3	1.89	0.54
1:B:131:GLY:CA	1:B:134:THR:CG2	2.76	0.54
1:B:322:ARG:CD	1:B:763:LEU:HD13	2.37	0.54
1:B:672:ALA:O	1:B:714:PRO:HG3	2.07	0.54
1:D:112:LEU:CD2	1:D:116:GLU:HB3	2.38	0.54
1:D:131:GLY:HA3	1:D:134:THR:CG2	2.37	0.54
1:D:176:SER:O	1:D:179:PRO:HD2	2.08	0.54
1:D:770:GLY:O	1:D:773:LYS:HG2	2.08	0.54
1:E:65:GLU:CG	1:E:70:PHE:CB	2.83	0.54
1:G:443:THR:HG21	1:G:495:GLN:HA	1.88	0.54
1:H:33:LEU:HD23	1:H:33:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:PRO:HB3	1:H:487:ALA:HB1	1.90	0.54
1:H:308:ILE:O	1:H:312:VAL:HG22	2.08	0.54
1:H:407:LYS:HB2	1:H:408:PRO:CD	2.38	0.54
1:A:354:GLU:OE1	1:A:366:ARG:NH2	2.41	0.54
1:A:685:MSE:HE3	1:A:745:GLY:CA	2.36	0.54
1:C:216:TYR:HE2	1:C:232:LYS:CD	2.21	0.54
1:D:298:TYR:HE1	1:D:649:MSE:HE1	1.62	0.54
1:F:315:LEU:C	1:F:319:MSE:HE2	2.28	0.54
1:A:116:GLU:O	1:A:119:HIS:HB2	2.08	0.54
1:B:633:ILE:HA	1:B:638:LEU:HD12	1.90	0.54
1:C:86:VAL:HB	1:C:104:LEU:HD21	1.90	0.54
1:F:181:LEU:HD13	1:F:206:LEU:HD22	1.90	0.54
1:G:27:ASN:C	1:G:30:LEU:HD12	2.29	0.54
1:H:163:ASN:ND2	1:H:269:GLU:HB2	2.23	0.54
1:H:553:LEU:CD2	1:H:645:ILE:HD13	2.38	0.54
1:A:35:ARG:O	1:A:39:LYS:HG3	2.08	0.53
1:B:30:LEU:CG	1:B:62:LYS:O	2.56	0.53
1:B:43:ILE:N	1:B:81:VAL:CB	2.71	0.53
1:B:153:LYS:HG2	1:B:154:TYR:CD2	2.43	0.53
1:B:259:LEU:O	1:B:263:PRO:HG3	2.07	0.53
1:C:207:GLN:NE2	1:C:211:ARG:NH2	2.56	0.53
1:C:242:TRP:HB2	1:C:249:VAL:HG22	1.91	0.53
1:C:243:GLY:HA2	1:C:326:GLN:HA	1.89	0.53
1:D:140:GLU:N	1:D:141:PRO:HD2	2.22	0.53
1:F:789:MSE:CE	1:G:789:MSE:C	2.77	0.53
1:G:146:ILE:HG22	1:G:147:PRO:O	2.08	0.53
1:B:91:ARG:HD2	1:B:97:TRP:CZ2	2.43	0.53
1:B:789:MSE:HE2	1:C:135:LEU:HD21	1.90	0.53
1:E:35:ARG:CG	1:E:35:ARG:HH11	2.19	0.53
1:E:140:GLU:N	1:E:141:PRO:HD2	2.23	0.53
1:F:789:MSE:SE	1:G:789:MSE:CE	3.06	0.53
1:G:126:ASP:C	1:G:128:VAL:H	2.10	0.53
1:F:53:PHE:O	1:F:57:PRO:HB2	2.08	0.53
1:F:88:LEU:HB2	1:F:100:LEU:HD12	1.89	0.53
1:G:49:ILE:HD12	1:G:49:ILE:N	2.23	0.53
1:G:117:PHE:O	1:G:120:PHE:HB2	2.08	0.53
1:G:692:PHE:CD2	1:G:724:LEU:CD2	2.91	0.53
1:H:131:GLY:N	1:H:134:THR:CG2	2.72	0.53
1:C:222:SER:HB3	1:C:247:GLU:HB2	1.91	0.53
1:C:443:THR:HG21	1:C:495:GLN:HA	1.89	0.53
1:E:35:ARG:HH11	1:E:35:ARG:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:HIS:O	1:E:106:ALA:CB	2.57	0.53
1:E:178:LEU:N	1:E:179:PRO:HD2	2.22	0.53
1:E:441:GLU:HA	1:E:441:GLU:OE1	2.08	0.53
1:G:458:LYS:HD3	1:G:459:TYR:CE2	2.43	0.53
1:C:420:LEU:C	1:C:420:LEU:HD13	2.29	0.53
1:E:178:LEU:HB2	1:E:179:PRO:HD3	1.89	0.53
1:F:178:LEU:HB2	1:F:179:PRO:HD3	1.89	0.53
1:G:131:GLY:N	1:G:134:THR:CG2	2.71	0.53
1:H:486:ILE:HG22	1:H:516:VAL:HG22	1.90	0.53
1:B:45:GLN:HG3	1:B:80:ILE:HG22	1.89	0.53
1:B:793:LEU:HB3	1:C:793:LEU:HB3	1.89	0.53
1:C:195:MSE:HE1	1:C:241:GLY:HA3	1.90	0.53
1:E:181:LEU:HD13	1:E:206:LEU:HD22	1.91	0.53
1:F:277:MSE:HE1	1:F:767:GLY:HA2	1.89	0.53
1:G:137:LEU:HD11	1:G:790:PHE:CE1	2.43	0.53
1:D:48:GLN:NE2	1:D:492:THR:HG22	2.24	0.53
1:E:536:TYR:CE1	1:E:537:THR:HG23	2.44	0.53
1:F:789:MSE:CE	1:G:789:MSE:CE	2.86	0.53
1:A:36:VAL:HA	1:A:39:LYS:CD	2.38	0.53
1:F:59:GLN:CG	1:F:60:THR:N	2.70	0.53
1:G:27:ASN:HA	1:G:30:LEU:HD12	1.90	0.53
1:G:534:PHE:HB2	1:G:535:PRO:CD	2.39	0.53
1:H:43:ILE:HG22	1:H:43:ILE:O	2.09	0.53
1:A:290:PHE:O	1:A:366:ARG:NH1	2.40	0.53
1:C:565:CYS:HB2	1:C:642:PHE:O	2.07	0.53
1:D:102:VAL:HG23	1:D:109:VAL:HG22	1.91	0.53
1:D:354:GLU:OE1	1:D:366:ARG:NH2	2.41	0.53
1:G:91:ARG:NH2	1:G:94:PRO:HA	2.23	0.53
1:G:131:GLY:N	1:G:134:THR:HG21	2.22	0.53
1:H:12:HIS:CE1	1:H:150:THR:HG21	2.43	0.53
1:C:394:GLU:OE1	1:C:428:LYS:HE3	2.09	0.53
1:D:248:ARG:HB3	1:D:248:ARG:NH1	2.24	0.53
1:E:217:LEU:HD23	1:E:220:LEU:HD12	1.91	0.53
1:E:394:GLU:OE2	1:H:132:ASN:OD1	2.27	0.53
1:E:629:MSE:HG2	1:E:644:TRP:CZ2	2.44	0.53
1:F:160:ASP:O	1:F:164:ARG:HG3	2.08	0.53
1:H:72:LEU:CA	1:H:75:SER:HB3	2.33	0.53
1:H:82:LEU:HD12	1:H:84:PRO:CD	2.39	0.53
1:B:792:ALA:HA	1:B:796:ARG:HG3	1.91	0.52
1:D:685:MSE:HE1	1:D:748:ARG:HG2	1.91	0.52
1:F:35:ARG:HG2	1:F:104:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:GLU:HG2	1:G:54:GLU:OE2	2.09	0.52
1:G:298:TYR:CE1	1:G:649:MSE:CE	2.92	0.52
1:H:84:PRO:O	1:H:85:TRP:HD1	1.92	0.52
1:A:171:PHE:CD1	1:A:263:PRO:HD2	2.44	0.52
1:A:451:TYR:HB3	1:A:454:LYS:HE2	1.91	0.52
1:B:59:GLN:CG	1:B:60:THR:H	2.22	0.52
1:C:69:PHE:CD1	1:C:69:PHE:C	2.82	0.52
1:C:451:TYR:HB3	1:C:454:LYS:HE2	1.90	0.52
1:D:131:GLY:CA	1:D:134:THR:CG2	2.87	0.52
1:E:170:LEU:HD23	1:E:176:SER:HB3	1.90	0.52
1:F:46:GLN:HB3	1:F:50:ILE:HB	1.91	0.52
1:G:150:THR:N	1:H:261:GLU:OE1	2.40	0.52
1:G:761:ARG:HD2	7:G:835:HOH:O	2.07	0.52
1:A:83:PRO:O	1:A:85:TRP:N	2.42	0.52
1:B:173:ASP:HB3	1:B:176:SER:HB3	1.90	0.52
1:D:607:VAL:HG22	1:D:643:ARG:HB3	1.91	0.52
1:F:116:GLU:O	1:F:119:HIS:HB2	2.08	0.52
1:F:155:ILE:HB	1:F:483:PHE:HE2	1.73	0.52
1:G:580:ARG:HD3	2:G:901:UDP:O3B	2.08	0.52
1:A:49:ILE:HG22	1:A:50:ILE:N	2.25	0.52
1:D:472:MSE:SE	1:D:514:ILE:HB	2.60	0.52
1:E:44:LEU:HA	1:E:124:LEU:CD1	2.33	0.52
1:E:94:PRO:HB3	1:E:487:ALA:HB1	1.91	0.52
1:F:547:HIS:O	1:F:551:GLU:CG	2.56	0.52
1:F:789:MSE:HE2	1:G:789:MSE:HE2	1.89	0.52
1:G:48:GLN:NE2	1:G:48:GLN:O	2.43	0.52
1:G:49:ILE:O	1:G:53:PHE:CB	2.58	0.52
1:G:82:LEU:CG	1:G:83:PRO:HD3	2.39	0.52
1:H:411:ILE:HG13	1:H:431:VAL:HG11	1.91	0.52
1:A:340:LEU:HB2	1:A:366:ARG:HB3	1.92	0.52
1:F:83:PRO:CB	1:F:84:PRO:CD	2.88	0.52
1:A:103:ASN:CB	1:A:106:ALA:CB	2.74	0.52
1:A:143:ASN:HA	1:A:780:ARG:HH12	1.73	0.52
1:B:100:LEU:C	1:B:112:LEU:HD12	2.30	0.52
1:C:538:GLU:OE1	1:C:541:ARG:HD3	2.10	0.52
1:C:545:LYS:H	1:C:545:LYS:CD	2.22	0.52
1:D:56:LEU:HD12	1:D:57:PRO:CD	2.21	0.52
1:F:190:GLN:OE1	1:F:190:GLN:HA	2.09	0.52
1:F:414:ASN:O	1:F:418:GLY:HA3	2.09	0.52
1:G:407:LYS:HB2	1:G:408:PRO:HD2	1.91	0.52
1:G:609:VAL:HG22	1:G:645:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:675:GLU:O	1:H:697:GLY:HA3	2.09	0.52
1:B:92:PRO:HD2	1:B:96:VAL:O	2.10	0.52
1:B:723:THR:O	1:B:726:ASP:HB2	2.09	0.52
1:C:479:ILE:CD1	1:C:762:LEU:HD13	2.39	0.52
1:C:536:TYR:HH	1:C:738:TRP:HZ3	1.58	0.52
1:D:86:VAL:CG1	1:D:102:VAL:HG12	2.39	0.52
1:E:72:LEU:C	1:E:73:LEU:HD22	2.29	0.52
1:F:81:VAL:CG1	1:F:86:VAL:CG2	2.85	0.52
1:F:145:SER:HB2	1:F:779:ASP:CG	2.31	0.52
1:F:407:LYS:HB2	1:F:408:PRO:CD	2.40	0.52
1:A:434:CYS:HB2	1:A:477:PHE:CZ	2.45	0.52
1:A:716:HIS:HB3	4:A:913:SO4:O2	2.09	0.52
1:C:645:ILE:HG22	1:C:648:GLN:HE21	1.75	0.52
1:D:400:LEU:HD12	1:D:401:SER:N	2.25	0.52
1:E:35:ARG:HG2	1:E:104:LEU:HA	1.90	0.52
1:G:259:LEU:O	1:G:263:PRO:HG3	2.10	0.52
1:B:153:LYS:CG	1:B:154:TYR:CD2	2.93	0.52
1:B:162:LEU:HD11	1:B:772:TRP:CD2	2.45	0.52
1:B:291:ALA:HB3	1:B:295:VAL:HG11	1.91	0.52
1:C:226:TYR:HA	1:C:229:PHE:CZ	2.45	0.52
1:C:784:ARG:O	1:C:788:GLU:HG3	2.10	0.52
1:D:682:VAL:HG13	1:D:749:ILE:HD12	1.91	0.52
1:G:83:PRO:HB2	1:G:84:PRO:CD	2.40	0.52
1:H:33:LEU:HA	1:H:36:VAL:CG2	2.39	0.52
1:C:195:MSE:HE2	1:C:195:MSE:H	1.73	0.52
1:F:524:VAL:HG12	1:F:758:TYR:CD2	2.45	0.52
1:A:28:GLU:O	1:A:32:LEU:CG	2.53	0.51
1:A:105:HIS:O	1:A:106:ALA:HB2	2.10	0.51
1:A:386:TRP:N	1:A:387:PRO:HD2	2.25	0.51
1:A:607:VAL:HG22	1:A:643:ARG:HB3	1.91	0.51
1:B:284:LEU:HD13	1:B:337:LEU:HB2	1.92	0.51
1:B:315:LEU:O	1:B:319:MSE:HG3	2.09	0.51
1:C:437:ALA:C	1:C:439:ALA:H	2.13	0.51
1:F:207:GLN:NE2	1:F:211:ARG:NH2	2.56	0.51
1:G:31:ALA:CB	1:G:35:ARG:NH2	2.64	0.51
1:A:264:ASP:OD1	1:A:267:THR:CB	2.58	0.51
1:A:435:THR:HG23	1:A:475:THR:CB	2.40	0.51
1:B:90:VAL:HG23	1:B:98:GLU:CB	2.40	0.51
1:C:197:SER:OG	1:C:237:GLY:HA2	2.10	0.51
1:E:32:LEU:CD2	1:E:107:LEU:CB	2.87	0.51
1:E:518:ASP:OD1	1:E:520:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:737:HIS:HE1	5:E:921:MLA:O3A	1.93	0.51
1:B:44:LEU:O	1:B:80:ILE:HA	2.10	0.51
1:B:793:LEU:HD11	1:C:135:LEU:CD2	2.40	0.51
1:C:32:LEU:HD11	1:C:105:HIS:HA	1.92	0.51
1:E:319:MSE:HE1	1:E:334:ILE:CD1	2.41	0.51
1:F:479:ILE:HD11	1:F:762:LEU:HD13	1.92	0.51
1:G:470:PHE:CE1	1:G:791:TYR:HB2	2.46	0.51
1:A:284:LEU:HD13	1:A:337:LEU:HB2	1.91	0.51
1:A:608:VAL:HG11	1:A:629:MSE:HE1	1.91	0.51
1:E:43:ILE:HG23	1:E:44:LEU:N	2.24	0.51
1:E:784:ARG:O	1:E:788:GLU:HG3	2.10	0.51
1:H:146:ILE:HG21	1:H:519:PRO:HG2	1.90	0.51
1:C:105:HIS:O	1:C:106:ALA:CB	2.55	0.51
1:F:230:GLU:OE1	1:F:240:ARG:NH1	2.44	0.51
1:H:145:SER:HB3	1:H:779:ASP:OD1	2.11	0.51
1:D:625:GLU:O	1:D:629:MSE:HG2	2.10	0.51
1:E:789:MSE:CG	1:H:789:MSE:HE2	2.41	0.51
1:F:112:LEU:HD22	1:F:116:GLU:HB3	1.92	0.51
1:G:31:ALA:O	1:G:35:ARG:HB2	2.10	0.51
1:G:72:LEU:C	1:G:73:LEU:HD23	2.31	0.51
1:G:703:ILE:HG22	1:G:703:ILE:O	2.10	0.51
1:H:105:HIS:CG	1:H:106:ALA:H	2.28	0.51
1:H:545:LYS:H	1:H:545:LYS:CD	2.21	0.51
1:A:248:ARG:NH2	7:A:836:HOH:O	2.44	0.51
1:B:224:THR:CG2	1:B:228:GLU:HG3	2.41	0.51
1:B:566:VAL:CG1	1:B:567:LEU:N	2.74	0.51
1:D:479:ILE:CD1	1:D:762:LEU:CD1	2.88	0.51
1:D:577:THR:HG21	1:D:590:LEU:HD23	1.92	0.51
1:D:647:SER:HB2	1:D:649:MSE:HE3	1.92	0.51
1:E:65:GLU:HG3	1:E:70:PHE:HB2	1.86	0.51
1:G:63:LYS:O	1:G:64:LEU:C	2.48	0.51
1:G:692:PHE:CG	1:G:724:LEU:HD21	2.46	0.51
1:H:146:ILE:HG12	1:H:147:PRO:CD	2.22	0.51
1:H:170:LEU:HD22	1:H:177:LEU:HD23	1.93	0.51
1:B:113:GLN:O	1:B:116:GLU:HB2	2.11	0.51
1:B:198:GLU:O	1:B:201:GLN:NE2	2.44	0.51
1:B:789:MSE:HG3	1:B:793:LEU:HD12	1.91	0.51
1:C:261:GLU:OE1	1:D:150:THR:N	2.44	0.51
1:G:135:LEU:HD12	1:G:136:GLU:N	2.25	0.51
1:G:148:ARG:NH1	1:G:148:ARG:CG	2.51	0.51
1:A:670:GLN:HG3	1:A:670:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:CD1	1:C:105:HIS:HA	2.40	0.51
1:D:54:GLU:CG	1:D:55:ALA:N	2.73	0.51
1:F:789:MSE:HE2	1:G:789:MSE:HG2	1.92	0.51
1:H:224:THR:HG23	1:H:228:GLU:HG3	1.93	0.51
1:H:483:PHE:CZ	1:H:487:ALA:HB3	2.46	0.51
1:B:54:GLU:O	1:B:56:LEU:N	2.44	0.51
1:B:290:PHE:O	1:B:366:ARG:NH1	2.44	0.51
1:B:415:TYR:CG	1:B:416:SER:N	2.80	0.51
1:G:52:GLU:OE1	1:G:53:PHE:HA	2.10	0.51
1:G:689:LEU:HD12	1:G:690:PRO:HD2	1.91	0.51
1:B:322:ARG:HD3	1:B:763:LEU:HD13	1.93	0.50
1:C:56:LEU:HD13	1:C:63:LYS:HG2	1.94	0.50
1:C:287:HIS:HD2	1:C:300:ASP:HB3	1.75	0.50
1:D:30:LEU:N	1:D:30:LEU:HD22	2.25	0.50
1:D:444:LYS:O	1:D:446:PRO:HD3	2.11	0.50
1:E:730:LYS:NZ	5:E:921:MLA:C2	2.74	0.50
1:F:242:TRP:O	1:F:252:MSE:HG3	2.10	0.50
1:F:477:PHE:HA	1:F:520:LYS:HB2	1.91	0.50
1:G:140:GLU:N	1:G:141:PRO:HD2	2.26	0.50
1:G:172:HIS:CD2	1:H:147:PRO:HB2	2.46	0.50
1:H:56:LEU:HG	1:H:70:PHE:HE1	1.75	0.50
1:H:193:ASN:ND2	1:H:197:SER:HA	2.25	0.50
1:H:217:LEU:HB2	1:H:250:LEU:HD13	1.92	0.50
1:B:56:LEU:HB3	1:B:57:PRO:CD	2.39	0.50
1:B:195:MSE:HE1	1:B:252:MSE:CE	2.41	0.50
1:C:216:TYR:CE2	1:C:232:LYS:HD3	2.46	0.50
1:C:294:ASN:C	1:C:649:MSE:SE	3.00	0.50
1:C:342:PRO:HD2	1:C:377:ARG:O	2.10	0.50
1:C:692:PHE:CD2	1:C:724:LEU:CD2	2.94	0.50
1:D:670:GLN:HG3	1:D:670:GLN:O	2.11	0.50
1:H:72:LEU:HD12	1:H:72:LEU:C	2.31	0.50
1:A:564:LEU:HD22	1:A:613:ARG:NH2	2.25	0.50
1:A:794:LYS:C	1:A:797:PRO:HD2	2.32	0.50
1:C:190:GLN:O	1:C:190:GLN:HG3	2.11	0.50
1:C:387:PRO:HD3	1:C:802:VAL:HB	1.93	0.50
1:C:394:GLU:O	1:C:398:VAL:HG23	2.12	0.50
1:C:532:ILE:HD13	1:C:532:ILE:N	2.26	0.50
1:C:673:LEU:HD23	1:C:714:PRO:HB2	1.94	0.50
1:C:692:PHE:HZ	1:C:727:PHE:CG	2.30	0.50
1:E:82:LEU:C	1:E:83:PRO:O	2.49	0.50
1:H:53:PHE:O	1:H:57:PRO:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PRO:CG	1:B:96:VAL:HG23	2.30	0.50
1:B:173:ASP:HB3	1:B:176:SER:CB	2.40	0.50
1:C:420:LEU:HD23	1:C:467:ALA:CB	2.41	0.50
1:E:160:ASP:O	1:E:164:ARG:HG3	2.10	0.50
1:E:190:GLN:NE2	1:E:405:ASN:HB3	2.26	0.50
1:F:483:PHE:CZ	1:F:487:ALA:HB3	2.46	0.50
1:F:609:VAL:HG22	1:F:645:ILE:HB	1.92	0.50
1:F:784:ARG:O	1:F:788:GLU:HG3	2.11	0.50
1:G:52:GLU:CD	1:G:53:PHE:N	2.65	0.50
1:D:56:LEU:O	1:D:59:GLN:N	2.41	0.50
1:E:143:ASN:HB3	1:E:148:ARG:CZ	2.41	0.50
1:E:319:MSE:CE	1:E:334:ILE:CD1	2.87	0.50
1:E:790:PHE:N	1:H:789:MSE:HE1	2.27	0.50
1:G:154:TYR:CD1	1:G:161:PHE:HB2	2.46	0.50
1:B:789:MSE:HG2	1:C:789:MSE:SE	2.61	0.50
1:E:150:THR:N	1:F:261:GLU:OE1	2.42	0.50
1:G:81:VAL:HG23	1:G:81:VAL:O	2.12	0.50
1:H:43:ILE:HG23	1:H:124:LEU:HD21	1.93	0.50
1:H:211:ARG:NE	7:H:867:HOH:O	2.44	0.50
1:C:195:MSE:CE	1:C:241:GLY:HA3	2.42	0.50
1:D:56:LEU:O	1:D:58:GLU:N	2.44	0.50
1:D:146:ILE:HG22	1:D:147:PRO:O	2.12	0.50
1:E:70:PHE:C	1:E:70:PHE:HD2	2.12	0.50
1:E:178:LEU:N	1:E:179:PRO:CD	2.75	0.50
1:F:80:ILE:HD12	1:F:80:ILE:N	2.27	0.50
1:F:119:HIS:HD2	1:F:129:LYS:CB	2.24	0.50
1:G:185:ARG:HD2	1:G:198:GLU:OE2	2.12	0.50
1:G:188:SER:HB2	1:G:192:LYS:O	2.12	0.50
1:G:685:MSE:HE1	1:G:748:ARG:HG2	1.93	0.50
1:H:338:THR:HG23	1:H:366:ARG:HG2	1.94	0.50
1:A:113:GLN:HB2	1:A:116:GLU:OE1	2.11	0.50
1:A:367:VAL:CG2	1:A:399:GLU:HG3	2.42	0.50
1:D:483:PHE:CZ	1:D:487:ALA:HB3	2.47	0.50
1:E:37:GLU:OE1	1:E:59:GLN:NE2	2.45	0.50
1:E:437:ALA:O	1:E:438:HIS:HB2	2.11	0.50
1:G:242:TRP:O	1:G:252:MSE:HG3	2.11	0.50
1:H:211:ARG:CD	7:H:867:HOH:O	2.59	0.50
1:D:259:LEU:HD21	1:D:267:THR:HG22	1.94	0.50
1:D:779:ASP:N	1:D:779:ASP:OD1	2.44	0.50
1:F:146:ILE:HD11	1:F:772:TRP:CZ2	2.47	0.50
1:F:206:LEU:HD11	1:F:210:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:LEU:HD22	1:F:613:ARG:NH2	2.26	0.50
1:H:65:GLU:O	1:H:70:PHE:HB2	2.11	0.50
1:H:366:ARG:HD3	7:H:857:HOH:O	2.12	0.50
1:A:210:LEU:CD2	1:A:253:ILE:HG23	2.41	0.49
1:A:552:GLU:O	1:A:556:SER:HB3	2.12	0.49
1:B:415:TYR:HA	1:B:437:ALA:O	2.12	0.49
1:B:552:GLU:O	1:B:556:SER:CB	2.59	0.49
1:C:283:ILE:HG23	1:C:414:ASN:HD21	1.76	0.49
1:E:162:LEU:HD11	1:E:772:TRP:CD2	2.46	0.49
1:F:146:ILE:HG22	1:F:147:PRO:N	2.27	0.49
1:H:145:SER:HB3	1:H:779:ASP:OD2	2.12	0.49
1:H:155:ILE:HB	1:H:483:PHE:HE2	1.76	0.49
1:H:596:LYS:HE3	1:H:636:TYR:OH	2.12	0.49
1:A:100:LEU:HD23	1:A:111:GLU:HA	1.93	0.49
1:B:613:ARG:HG3	1:B:613:ARG:NH1	2.24	0.49
1:C:702:ILE:HA	1:C:753:TYR:OH	2.13	0.49
1:E:82:LEU:CB	1:E:83:PRO:HD2	2.35	0.49
1:F:420:LEU:HD13	1:F:420:LEU:O	2.11	0.49
1:G:282:VAL:HG21	1:G:400:LEU:HD22	1.94	0.49
1:H:315:LEU:HG	1:H:319:MSE:CE	2.42	0.49
1:A:56:LEU:HG	1:A:70:PHE:CE1	2.47	0.49
1:B:226:TYR:CE2	1:B:240:ARG:HG2	2.47	0.49
1:C:46:GLN:HB2	1:C:50:ILE:HG23	1.93	0.49
1:G:437:ALA:O	1:G:438:HIS:HB2	2.12	0.49
1:D:57:PRO:HA	1:D:63:LYS:HE3	1.93	0.49
1:D:462:SER:HB2	1:D:507:LEU:HD21	1.93	0.49
1:E:28:GLU:O	1:E:32:LEU:HD23	2.13	0.49
1:E:56:LEU:HB3	1:E:57:PRO:HD3	1.94	0.49
1:F:665:LYS:HD2	1:F:738:TRP:CD2	2.47	0.49
1:G:575:LEU:HD21	1:G:724:LEU:HD13	1.93	0.49
1:H:82:LEU:CG	1:H:85:TRP:O	2.57	0.49
1:A:37:GLU:HG3	1:A:59:GLN:NE2	2.27	0.49
1:B:437:ALA:C	1:B:439:ALA:H	2.15	0.49
1:B:657:LEU:O	1:B:661:ILE:HG12	2.13	0.49
1:C:772:TRP:CZ2	1:C:776:SER:CB	2.95	0.49
1:D:65:GLU:HB3	1:D:70:PHE:HB2	1.94	0.49
1:D:121:LYS:O	1:D:124:LEU:HB3	2.12	0.49
1:D:407:LYS:HB2	1:D:408:PRO:CD	2.42	0.49
1:D:479:ILE:HD11	1:D:762:LEU:HD12	1.94	0.49
1:D:578:MSE:HE3	2:D:901:UDP:O2'	2.12	0.49
1:E:137:LEU:HD11	1:E:790:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:TRP:O	1:E:252:MSE:HG3	2.13	0.49
1:E:419:ASN:HB3	1:E:471:ALA:CB	2.43	0.49
1:F:414:ASN:HD22	1:F:438:HIS:CD2	2.30	0.49
1:H:99:TYR:HB2	1:H:112:LEU:O	2.11	0.49
1:H:162:LEU:HD21	1:H:772:TRP:CG	2.47	0.49
1:A:331:LYS:NZ	1:F:61:ARG:HH12	2.11	0.49
1:C:48:GLN:HA	1:C:51:ALA:HB3	1.93	0.49
1:C:312:VAL:HG12	1:C:334:ILE:HG21	1.93	0.49
1:C:567:LEU:HD21	1:C:643:ARG:HB2	1.94	0.49
1:D:79:ALA:HA	1:D:87:ALA:O	2.13	0.49
1:D:195:MSE:HE2	1:D:241:GLY:HA3	1.93	0.49
1:D:419:ASN:HB3	1:D:471:ALA:CB	2.42	0.49
1:D:512:HIS:CE1	1:D:515:ASP:HB2	2.47	0.49
1:F:659:ARG:O	1:F:662:CYS:HB2	2.12	0.49
1:H:387:PRO:HD3	1:H:802:VAL:HB	1.93	0.49
1:A:63:LYS:O	1:A:65:GLU:N	2.46	0.49
1:A:207:GLN:HE21	1:A:211:ARG:HH12	1.59	0.49
1:C:185:ARG:HD2	1:C:198:GLU:OE1	2.13	0.49
1:D:264:ASP:OD1	1:D:267:THR:CB	2.57	0.49
1:D:535:PRO:O	1:D:538:GLU:HG3	2.12	0.49
1:E:375:ILE:HG13	1:E:375:ILE:O	2.11	0.49
1:E:432:THR:OG1	1:E:773:LYS:HE3	2.13	0.49
1:F:80:ILE:HD12	1:F:80:ILE:H	1.78	0.49
1:A:124:LEU:C	1:A:124:LEU:CD2	2.81	0.49
1:B:52:GLU:O	1:B:57:PRO:CD	2.60	0.49
1:B:313:ARG:HD3	1:B:357:TYR:O	2.12	0.49
1:C:34:SER:CA	1:C:59:GLN:HE22	2.17	0.49
1:C:173:ASP:OD2	1:C:176:SER:HB2	2.12	0.49
1:E:35:ARG:NH1	1:E:35:ARG:CB	2.74	0.49
1:B:21:THR:C	1:B:23:VAL:H	2.15	0.49
1:D:82:LEU:O	1:D:85:TRP:O	2.31	0.49
1:D:166:LEU:HD21	1:D:772:TRP:CE3	2.47	0.49
1:E:32:LEU:O	1:E:36:VAL:HG23	2.13	0.49
1:F:102:VAL:HA	1:F:108:VAL:O	2.12	0.49
1:B:30:LEU:N	1:B:30:LEU:HD12	2.28	0.49
1:B:55:ALA:O	1:B:59:GLN:CB	2.50	0.49
1:E:216:TYR:CD1	1:E:216:TYR:C	2.85	0.49
1:B:739:ASP:O	1:B:743:LYS:HG2	2.12	0.48
1:C:210:LEU:HD22	1:C:253:ILE:HG23	1.95	0.48
1:C:474:HIS:HB2	1:C:787:LEU:HD13	1.95	0.48
1:E:141:PRO:HB2	1:H:782:GLU:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:GLY:HA3	2:E:901:UDP:O2B	2.12	0.48
1:F:367:VAL:HG22	1:F:399:GLU:HG3	1.94	0.48
1:C:226:TYR:CE2	1:C:240:ARG:HG2	2.48	0.48
1:D:599:ARG:O	1:D:603:LEU:HD12	2.13	0.48
1:F:420:LEU:C	1:F:420:LEU:CD1	2.80	0.48
1:G:178:LEU:N	1:G:179:PRO:CD	2.76	0.48
1:H:561:LYS:HD3	1:H:613:ARG:O	2.13	0.48
1:A:417:ASP:OD1	1:A:418:GLY:N	2.45	0.48
1:B:41:LYS:HD2	1:B:46:GLN:NE2	2.28	0.48
1:B:44:LEU:O	1:B:81:VAL:N	2.46	0.48
1:C:69:PHE:HD1	1:C:70:PHE:N	2.10	0.48
1:C:160:ASP:O	1:C:164:ARG:HG3	2.13	0.48
1:C:617:SER:O	1:C:623:LYS:HD3	2.14	0.48
1:D:319:MSE:HE2	1:D:332:PRO:CB	2.43	0.48
1:F:223:GLU:N	1:F:223:GLU:OE2	2.46	0.48
1:G:137:LEU:HD11	1:G:790:PHE:CZ	2.48	0.48
1:A:789:MSE:HE3	1:D:789:MSE:C	2.33	0.48
1:C:573:PRO:HD2	1:C:603:LEU:O	2.13	0.48
1:D:146:ILE:CD1	1:D:772:TRP:CH2	2.95	0.48
1:E:34:SER:O	1:E:37:GLU:HB3	2.12	0.48
1:G:685:MSE:HE1	1:G:748:ARG:CG	2.43	0.48
1:A:48:GLN:O	1:A:51:ALA:HB3	2.14	0.48
1:A:312:VAL:HG23	1:A:313:ARG:N	2.28	0.48
1:B:59:GLN:HG2	1:B:60:THR:H	1.79	0.48
1:B:250:LEU:HG	1:B:254:ARG:NH1	2.29	0.48
1:D:83:PRO:HG2	1:D:84:PRO:HD2	1.93	0.48
1:D:211:ARG:HG3	1:D:211:ARG:NH1	2.29	0.48
1:D:493:VAL:CG2	1:D:494:GLY:N	2.77	0.48
1:E:52:GLU:CD	1:E:52:GLU:C	2.72	0.48
1:E:146:ILE:HG12	1:E:772:TRP:CH2	2.48	0.48
1:E:447:ASP:HB3	1:E:451:TYR:HD2	1.78	0.48
1:F:72:LEU:C	1:F:73:LEU:HD12	2.34	0.48
1:H:143:ASN:HD22	1:H:148:ARG:HH22	1.60	0.48
1:H:367:VAL:HG13	1:H:368:PRO:HD2	1.94	0.48
1:B:177:LEU:HD13	1:B:260:LEU:HD23	1.95	0.48
1:B:574:ILE:HG23	1:B:607:VAL:HG23	1.96	0.48
1:D:140:GLU:HB3	1:D:141:PRO:CD	2.42	0.48
1:F:74:LYS:CA	7:F:891:HOH:O	2.54	0.48
1:G:45:GLN:NE2	1:G:45:GLN:HA	2.28	0.48
1:G:81:VAL:CG1	1:G:86:VAL:HB	2.43	0.48
1:G:354:GLU:OE1	1:G:366:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:566:VAL:O	1:G:640:GLY:HA2	2.13	0.48
1:H:65:GLU:C	1:H:67:GLY:H	2.17	0.48
1:H:197:SER:HB3	1:H:239:GLU:OE1	2.13	0.48
1:H:791:TYR:CE1	1:H:795:TYR:CD2	3.01	0.48
1:A:259:LEU:O	1:A:263:PRO:HG3	2.14	0.48
1:A:449:ASP:OD1	1:A:450:ILE:N	2.46	0.48
1:B:20:GLU:CD	1:B:72:LEU:HD23	2.34	0.48
1:B:483:PHE:CZ	1:B:487:ALA:HB3	2.48	0.48
1:C:360:GLU:HB2	1:C:361:TYR:CD2	2.49	0.48
1:D:466:THR:HG23	1:D:790:PHE:CZ	2.49	0.48
1:E:387:PRO:HD3	1:E:802:VAL:HB	1.94	0.48
1:E:647:SER:HB2	1:E:649:MSE:HE3	1.95	0.48
1:E:789:MSE:CB	1:H:789:MSE:HE1	2.36	0.48
1:G:387:PRO:HD3	1:G:802:VAL:HB	1.95	0.48
1:A:419:ASN:HB3	1:A:471:ALA:CB	2.43	0.48
1:B:83:PRO:CG	1:B:85:TRP:HB2	2.13	0.48
1:B:233:PHE:HB3	1:B:238:LEU:HB2	1.95	0.48
1:B:242:TRP:O	1:B:252:MSE:HG3	2.14	0.48
1:C:355:ARG:HD2	1:C:359:SER:O	2.13	0.48
1:C:534:PHE:HB2	1:C:535:PRO:HD2	1.96	0.48
1:D:86:VAL:HG13	1:D:102:VAL:HG12	1.95	0.48
1:E:42:GLY:O	1:E:81:VAL:CG1	2.62	0.48
1:E:789:MSE:HE2	1:H:789:MSE:HB3	1.94	0.48
1:F:293:ASP:HB2	7:F:849:HOH:O	2.14	0.48
1:F:333:ARG:NH1	1:F:403:GLU:HB3	2.21	0.48
1:F:354:GLU:OE1	1:F:366:ARG:NH2	2.46	0.48
1:F:786:TYR:O	1:G:789:MSE:HE1	2.13	0.48
1:H:196:LEU:HD22	1:H:200:ILE:HD12	1.94	0.48
1:A:206:LEU:HD11	1:A:210:LEU:HD11	1.96	0.48
1:B:139:PHE:CE1	1:B:787:LEU:HD21	2.49	0.48
1:C:82:LEU:O	1:C:85:TRP:O	2.32	0.48
1:C:338:THR:OG1	1:C:339:ARG:N	2.47	0.48
1:D:577:THR:HG21	1:D:590:LEU:CD2	2.44	0.48
1:E:419:ASN:HB3	1:E:471:ALA:HB1	1.94	0.48
1:F:143:ASN:HA	1:F:780:ARG:NH1	2.25	0.48
1:F:282:VAL:HG13	1:F:337:LEU:HD23	1.96	0.48
1:G:348:THR:O	1:G:351:GLU:HG2	2.14	0.48
1:G:553:LEU:HG	1:G:645:ILE:HD13	1.96	0.48
1:H:433:GLN:O	1:H:476:ASP:HB2	2.14	0.48
1:A:414:ASN:O	1:A:418:GLY:HA3	2.14	0.47
1:B:779:ASP:OD1	1:B:779:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:VAL:CG1	1:D:102:VAL:CG1	2.92	0.47
1:F:437:ALA:C	1:F:439:ALA:H	2.17	0.47
1:B:145:SER:HB3	7:B:877:HOH:O	2.13	0.47
1:D:284:LEU:HD22	1:D:284:LEU:N	2.29	0.47
1:D:449:ASP:OD1	1:D:450:ILE:N	2.46	0.47
1:G:83:PRO:CB	1:G:85:TRP:H	2.17	0.47
1:G:160:ASP:O	1:G:164:ARG:HG3	2.14	0.47
1:G:290:PHE:O	1:G:366:ARG:NH1	2.47	0.47
1:G:484:GLN:HG2	1:G:488:GLY:HA2	1.94	0.47
1:B:462:SER:HB2	1:B:798:LEU:HD22	1.96	0.47
1:C:82:LEU:O	1:C:85:TRP:N	2.47	0.47
1:C:195:MSE:HE1	1:C:241:GLY:C	2.35	0.47
1:D:140:GLU:HB3	1:D:141:PRO:HD3	1.95	0.47
1:D:479:ILE:CD1	1:D:762:LEU:HD13	2.44	0.47
1:F:415:TYR:CG	1:F:416:SER:N	2.82	0.47
1:F:444:LYS:O	1:F:446:PRO:HD3	2.14	0.47
1:H:34:SER:OG	1:H:55:ALA:CB	2.61	0.47
1:H:354:GLU:OE1	1:H:366:ARG:NH2	2.46	0.47
1:H:553:LEU:HD21	1:H:645:ILE:HG21	1.96	0.47
1:D:166:LEU:HD21	1:D:772:TRP:HE3	1.79	0.47
1:D:319:MSE:HE2	1:D:332:PRO:HB2	1.95	0.47
1:D:781:LEU:O	1:D:784:ARG:HB3	2.14	0.47
1:E:794:LYS:O	1:E:794:LYS:HD3	2.15	0.47
1:G:162:LEU:HD11	1:G:772:TRP:CD2	2.50	0.47
1:G:483:PHE:CZ	1:G:487:ALA:HB3	2.49	0.47
1:H:23:VAL:C	1:H:25:GLU:N	2.68	0.47
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.15	0.47
1:A:673:LEU:HD23	1:A:714:PRO:HB2	1.97	0.47
1:A:789:MSE:CE	1:D:790:PHE:N	2.78	0.47
1:B:126:ASP:HB2	1:B:128:VAL:O	2.14	0.47
1:B:483:PHE:CE1	1:B:487:ALA:HB3	2.49	0.47
1:C:319:MSE:HE2	1:C:332:PRO:HB3	1.95	0.47
1:C:367:VAL:HG13	1:C:368:PRO:HD2	1.96	0.47
1:C:796:ARG:HB2	1:C:797:PRO:CD	2.39	0.47
1:D:282:VAL:HG13	1:D:337:LEU:HD23	1.97	0.47
1:D:484:GLN:HG2	1:D:488:GLY:HA2	1.97	0.47
1:D:657:LEU:O	1:D:661:ILE:HG12	2.14	0.47
1:E:474:HIS:HA	1:E:787:LEU:HD13	1.97	0.47
1:E:704:VAL:HA	4:E:912:SO4:O3	2.13	0.47
1:F:276:PRO:HG3	1:F:326:GLN:CB	2.44	0.47
1:F:290:PHE:HD2	7:F:894:HOH:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LEU:HG	1:G:83:PRO:HD3	1.96	0.47
1:G:178:LEU:N	1:G:179:PRO:HD2	2.29	0.47
1:G:212:LYS:NZ	1:G:232:LYS:HZ1	2.13	0.47
1:G:276:PRO:HG3	1:G:326:GLN:CB	2.45	0.47
1:H:315:LEU:HD21	1:H:762:LEU:HD23	1.95	0.47
1:H:390:GLU:OE2	1:H:796:ARG:NH1	2.47	0.47
1:A:143:ASN:O	1:A:145:SER:N	2.48	0.47
1:A:189:HIS:ND1	1:A:330:ILE:HD13	2.30	0.47
1:B:90:VAL:N	1:B:98:GLU:O	2.40	0.47
1:C:172:HIS:CD2	1:D:147:PRO:CB	2.97	0.47
1:E:159:VAL:CG1	1:E:160:ASP:N	2.77	0.47
1:E:588:SER:CB	1:E:625:GLU:OE2	2.63	0.47
1:A:772:TRP:CH2	1:A:776:SER:HB3	2.49	0.47
1:B:30:LEU:CD2	7:B:863:HOH:O	2.63	0.47
1:B:91:ARG:HD2	1:B:97:TRP:CH2	2.50	0.47
1:B:479:ILE:CD1	1:B:762:LEU:HD13	2.45	0.47
1:B:561:LYS:HD3	1:B:613:ARG:O	2.15	0.47
1:C:50:ILE:C	1:C:52:GLU:N	2.67	0.47
1:C:566:VAL:CG1	1:C:567:LEU:N	2.78	0.47
1:D:125:VAL:HG13	1:D:126:ASP:H	1.80	0.47
1:E:46:GLN:HA	1:E:50:ILE:HD12	1.97	0.47
1:E:212:LYS:HD2	1:E:236:ILE:HG21	1.96	0.47
1:E:572:LYS:HE2	1:E:602:GLU:O	2.15	0.47
1:E:665:LYS:HD3	1:E:665:LYS:HA	1.70	0.47
1:E:680:THR:HG22	2:E:901:UDP:H3'	1.96	0.47
1:F:35:ARG:O	1:F:38:ALA:N	2.47	0.47
1:F:52:GLU:O	1:F:57:PRO:CD	2.52	0.47
1:G:39:LYS:NZ	1:G:105:HIS:CD2	2.83	0.47
1:G:81:VAL:HG12	1:G:86:VAL:CB	2.43	0.47
1:G:573:PRO:HD2	1:G:603:LEU:O	2.14	0.47
1:H:105:HIS:CG	1:H:106:ALA:N	2.82	0.47
1:H:319:MSE:O	1:H:323:ILE:HG13	2.14	0.47
1:H:355:ARG:HD2	1:H:359:SER:O	2.15	0.47
1:H:415:TYR:CG	1:H:416:SER:N	2.81	0.47
1:H:437:ALA:C	1:H:439:ALA:H	2.18	0.47
1:H:626:MSE:O	1:H:630:TYR:HD2	1.97	0.47
1:A:81:VAL:HA	1:A:86:VAL:HG22	1.95	0.47
1:A:137:LEU:CD2	1:D:789:MSE:HE2	2.45	0.47
1:C:662:CYS:SG	1:C:689:LEU:HB2	2.54	0.47
1:E:315:LEU:CB	1:E:319:MSE:HE3	2.44	0.47
1:G:35:ARG:HH12	1:G:107:LEU:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LEU:HD12	1:G:83:PRO:HD3	1.92	0.47
1:G:633:ILE:HA	1:G:638:LEU:HD12	1.97	0.47
1:H:245:ASN:O	1:H:249:VAL:HG23	2.14	0.47
1:C:56:LEU:HB3	1:C:57:PRO:CD	2.45	0.47
1:C:216:TYR:HD1	1:C:216:TYR:C	2.18	0.47
1:C:389:LEU:HD11	1:C:417:ASP:CB	2.45	0.47
1:C:419:ASN:HB3	1:C:471:ALA:CB	2.45	0.47
1:C:420:LEU:C	1:C:420:LEU:CD1	2.83	0.47
1:C:440:LEU:HD12	1:C:495:GLN:HB3	1.97	0.47
1:D:681:VAL:HG13	1:D:691:THR:HG21	1.96	0.47
1:F:159:VAL:HB	1:F:765:LEU:CD2	2.45	0.47
1:G:319:MSE:O	1:G:323:ILE:HG13	2.15	0.47
1:G:590:LEU:HB2	1:G:671:PRO:HG3	1.97	0.47
1:H:153:LYS:HG3	1:H:154:TYR:CD2	2.50	0.47
1:A:68:PRO:O	1:A:72:LEU:HD12	2.14	0.47
1:A:490:LYS:HE3	1:A:490:LYS:HB2	1.72	0.47
1:B:472:MSE:HG2	1:B:496:TYR:HE1	1.80	0.47
1:C:130:ASN:HB3	1:C:134:THR:OG1	2.15	0.47
1:C:434:CYS:HB2	1:C:477:PHE:CZ	2.50	0.47
1:E:552:GLU:O	1:E:556:SER:HB2	2.15	0.47
1:E:582:ASP:C	1:E:582:ASP:OD1	2.52	0.47
1:F:53:PHE:O	1:F:57:PRO:HG2	2.13	0.47
1:F:209:THR:CG2	1:F:236:ILE:HG13	2.45	0.47
1:G:78:GLU:OE2	1:G:121:LYS:CE	2.63	0.47
1:C:48:GLN:HB2	1:C:77:GLN:O	2.15	0.46
1:C:99:TYR:C	1:C:100:LEU:HD23	2.36	0.46
1:D:690:PRO:HA	7:D:866:HOH:O	2.14	0.46
1:H:76:THR:O	1:H:77:GLN:CB	2.63	0.46
1:A:339:ARG:HD2	1:A:369:PHE:CE2	2.51	0.46
1:B:292:GLN:HE22	1:B:356:VAL:HA	1.80	0.46
1:D:433:GLN:O	1:D:476:ASP:HB2	2.14	0.46
1:F:79:ALA:HB2	1:F:88:LEU:CD2	2.44	0.46
1:H:32:LEU:CD2	1:H:35:ARG:NH1	2.75	0.46
1:C:94:PRO:HB3	1:C:487:ALA:HB1	1.97	0.46
1:C:146:ILE:HD11	1:C:162:LEU:CD1	2.45	0.46
1:C:717:GLY:O	1:C:720:ALA:HB3	2.15	0.46
1:E:193:ASN:O	1:E:194:LEU:HD23	2.15	0.46
1:E:566:VAL:O	1:E:567:LEU:HD23	2.15	0.46
1:F:125:VAL:HG21	1:F:450:ILE:O	2.14	0.46
1:G:54:GLU:OE2	1:G:55:ALA:CA	2.62	0.46
1:H:90:VAL:O	1:H:98:GLU:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:PHE:HE1	1:H:787:LEU:HD21	1.78	0.46
1:H:210:LEU:HD11	1:H:256:LEU:HD23	1.97	0.46
1:A:259:LEU:HD21	1:A:268:LEU:HA	1.98	0.46
1:A:770:GLY:O	1:A:773:LYS:HB2	2.15	0.46
1:B:292:GLN:NE2	1:B:356:VAL:HA	2.30	0.46
1:B:387:PRO:HD3	1:B:802:VAL:HB	1.97	0.46
1:B:798:LEU:O	1:B:801:ALA:HB3	2.16	0.46
1:C:563:HIS:HA	1:C:644:TRP:O	2.16	0.46
1:C:575:LEU:HD21	1:C:724:LEU:HD13	1.96	0.46
1:C:692:PHE:CD2	1:C:724:LEU:HD23	2.51	0.46
1:D:146:ILE:CG1	1:D:772:TRP:CZ2	2.99	0.46
1:D:216:TYR:C	1:D:216:TYR:HD1	2.17	0.46
1:E:92:PRO:HD2	1:E:96:VAL:O	2.16	0.46
1:F:73:LEU:CD1	1:F:73:LEU:N	2.78	0.46
1:F:142:PHE:CE2	1:F:786:TYR:CD2	3.04	0.46
1:G:171:PHE:CD1	1:G:263:PRO:HD2	2.51	0.46
1:H:449:ASP:O	1:H:504:LEU:HD22	2.16	0.46
1:A:479:ILE:HD11	1:A:762:LEU:HD13	1.97	0.46
1:B:414:ASN:O	1:B:418:GLY:HA3	2.16	0.46
1:C:284:LEU:CD2	1:C:284:LEU:N	2.79	0.46
1:D:796:ARG:HB2	1:D:797:PRO:HD3	1.96	0.46
1:E:73:LEU:N	1:E:73:LEU:HD22	2.30	0.46
1:G:39:LYS:O	1:G:39:LYS:HG2	2.15	0.46
1:G:65:GLU:HG3	1:G:70:PHE:CB	2.45	0.46
1:H:52:GLU:OE1	1:H:53:PHE:HA	2.15	0.46
1:A:189:HIS:CD2	1:A:279:PHE:HD2	2.33	0.46
1:B:781:LEU:HD12	1:B:781:LEU:HA	1.74	0.46
1:B:789:MSE:HE3	1:B:789:MSE:HB2	1.81	0.46
1:B:789:MSE:SE	1:C:789:MSE:HG2	2.66	0.46
1:C:137:LEU:HD11	1:C:790:PHE:CZ	2.51	0.46
1:C:151:LEU:N	1:D:261:GLU:OE1	2.49	0.46
1:C:216:TYR:C	1:C:216:TYR:CD1	2.88	0.46
1:C:319:MSE:HE2	1:C:332:PRO:CB	2.45	0.46
1:F:580:ARG:HG3	7:F:839:HOH:O	2.15	0.46
1:G:49:ILE:N	1:G:49:ILE:CD1	2.79	0.46
1:G:204:ASN:HD21	1:H:12:HIS:N	2.12	0.46
1:A:195:MSE:HE2	1:A:252:MSE:CE	2.45	0.46
1:B:581:LEU:HD13	1:B:587:LEU:HD12	1.98	0.46
1:C:400:LEU:C	1:C:400:LEU:HD12	2.36	0.46
1:C:657:LEU:O	1:C:661:ILE:HG12	2.16	0.46
1:D:195:MSE:HE1	1:D:241:GLY:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ILE:CG2	1:E:147:PRO:HD2	2.45	0.46
1:F:38:ALA:O	1:F:41:LYS:HB2	2.16	0.46
1:F:163:ASN:ND2	1:F:269:GLU:HB2	2.31	0.46
1:F:169:LYS:HG2	1:F:176:SER:OG	2.16	0.46
1:F:545:LYS:H	1:F:545:LYS:HD3	1.80	0.46
1:F:675:GLU:HA	1:F:675:GLU:OE2	2.15	0.46
1:F:789:MSE:CE	1:G:789:MSE:HE3	2.45	0.46
1:G:56:LEU:CB	1:G:57:PRO:HD3	2.33	0.46
1:G:190:GLN:HG2	1:G:405:ASN:HD22	1.80	0.46
1:A:366:ARG:HD3	7:A:898:HOH:O	2.14	0.46
1:B:193:ASN:ND2	1:B:197:SER:HA	2.30	0.46
1:B:704:VAL:HA	4:B:912:SO4:O1	2.16	0.46
1:C:155:ILE:CG2	1:C:483:PHE:CE2	2.98	0.46
1:C:278:VAL:HG21	1:C:763:LEU:CD2	2.45	0.46
1:C:540:LYS:H	1:C:540:LYS:HG3	1.54	0.46
1:D:43:ILE:CG2	1:D:124:LEU:HD12	2.45	0.46
1:D:698:GLY:N	1:D:699:PRO:CD	2.79	0.46
1:F:81:VAL:HG12	1:F:86:VAL:CB	2.45	0.46
1:F:435:THR:HG23	1:F:475:THR:CB	2.46	0.46
1:G:756:GLN:HG2	1:G:757:ILE:H	1.80	0.46
1:G:757:ILE:HA	1:G:757:ILE:HD13	1.59	0.46
1:H:49:ILE:O	1:H:53:PHE:CB	2.64	0.46
1:H:466:THR:HG23	1:H:790:PHE:CZ	2.50	0.46
1:A:45:GLN:NE2	1:A:80:ILE:HD13	2.13	0.46
1:C:80:ILE:CD1	1:C:121:LYS:HG2	2.45	0.46
1:C:400:LEU:HD12	1:C:401:SER:N	2.31	0.46
1:D:37:GLU:HG3	1:D:59:GLN:NE2	2.31	0.46
1:D:146:ILE:CG1	1:D:772:TRP:CH2	2.99	0.46
1:E:45:GLN:CB	1:E:80:ILE:HD13	2.46	0.46
1:E:348:THR:O	1:E:351:GLU:HG2	2.16	0.46
1:F:176:SER:O	1:F:179:PRO:HD2	2.16	0.46
1:F:244:ASP:OD2	1:F:248:ARG:CD	2.63	0.46
1:F:400:LEU:HD12	1:F:401:SER:N	2.31	0.46
1:G:163:ASN:ND2	1:G:269:GLU:OE1	2.49	0.46
1:G:452:TRP:CD1	1:G:504:LEU:HB3	2.51	0.46
1:H:33:LEU:HD23	1:H:33:LEU:N	2.29	0.46
1:A:155:ILE:HB	1:A:483:PHE:CE2	2.51	0.46
1:B:452:TRP:CG	1:B:453:LYS:N	2.83	0.46
1:C:220:LEU:N	1:C:220:LEU:HD12	2.31	0.46
1:C:360:GLU:HB2	1:C:361:TYR:CE2	2.50	0.46
1:C:706:GLY:HA2	1:C:710:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:TRP:H	1:E:85:TRP:HD1	1.62	0.46
1:F:538:GLU:O	1:F:542:ARG:HG2	2.15	0.46
1:A:63:LYS:O	1:A:65:GLU:HG2	2.15	0.45
1:A:155:ILE:HB	1:A:483:PHE:HE2	1.81	0.45
1:B:140:GLU:O	1:B:143:ASN:HB2	2.16	0.45
1:B:223:GLU:O	1:B:225:LEU:HD23	2.16	0.45
1:C:194:LEU:HD22	1:C:328:LEU:HD11	1.98	0.45
1:D:86:VAL:HG12	1:D:102:VAL:CG1	2.46	0.45
1:D:675:GLU:O	1:D:697:GLY:HA3	2.16	0.45
1:E:83:PRO:CB	1:E:84:PRO:HD2	2.38	0.45
1:E:434:CYS:HB2	1:E:477:PHE:CZ	2.51	0.45
1:E:552:GLU:O	1:E:556:SER:CB	2.64	0.45
1:F:128:VAL:HG22	1:F:129:LYS:N	2.31	0.45
1:F:277:MSE:CE	1:F:767:GLY:HA2	2.47	0.45
1:G:140:GLU:HB3	1:G:141:PRO:HD3	1.97	0.45
1:H:438:HIS:O	1:H:439:ALA:HB2	2.16	0.45
1:H:508:TYR:HD2	1:H:794:LYS:HE3	1.81	0.45
1:A:794:LYS:HD2	1:A:798:LEU:HD11	1.97	0.45
1:B:54:GLU:HG3	1:B:55:ALA:N	2.30	0.45
1:B:146:ILE:CG2	1:B:147:PRO:CD	2.87	0.45
1:B:437:ALA:O	1:B:438:HIS:HB2	2.16	0.45
1:C:99:TYR:O	1:C:100:LEU:HD23	2.16	0.45
1:C:572:LYS:HE3	1:C:605:ASN:OD1	2.17	0.45
1:C:692:PHE:CD2	1:C:724:LEU:HD21	2.51	0.45
1:E:133:PHE:HB3	1:H:791:TYR:HE2	1.79	0.45
1:E:154:TYR:OH	1:F:262:ALA:HB3	2.16	0.45
1:F:56:LEU:HD22	1:F:56:LEU:HA	1.69	0.45
1:F:59:GLN:C	1:F:60:THR:CG2	2.84	0.45
1:G:101:ARG:HB3	1:G:112:LEU:HD11	1.99	0.45
1:H:230:GLU:O	1:H:234:GLU:HG3	2.15	0.45
1:A:275:VAL:O	1:A:277:MSE:HG3	2.16	0.45
1:A:287:HIS:C	1:A:287:HIS:CD2	2.89	0.45
1:B:76:THR:CA	1:B:89:ALA:O	2.51	0.45
1:B:93:ARG:HB2	1:B:96:VAL:CG2	2.46	0.45
1:B:334:ILE:HD12	1:B:362:CYS:SG	2.55	0.45
1:D:55:ALA:O	1:D:56:LEU:CB	2.64	0.45
1:D:566:VAL:O	1:D:640:GLY:HA2	2.16	0.45
1:D:667:ALA:CA	1:D:689:LEU:HD11	2.47	0.45
1:E:124:LEU:HD12	1:E:124:LEU:O	2.16	0.45
1:E:534:PHE:HB2	1:E:535:PRO:HD2	1.98	0.45
1:F:628:LYS:CE	1:F:628:LYS:HA	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:628:LYS:HA	1:F:628:LYS:HD2	1.86	0.45
1:H:28:GLU:HG2	1:H:32:LEU:HD23	1.98	0.45
1:H:60:THR:O	1:H:63:LYS:HD3	2.16	0.45
1:H:224:THR:CG2	1:H:228:GLU:HG3	2.46	0.45
1:A:407:LYS:HB2	1:A:408:PRO:CD	2.45	0.45
1:C:420:LEU:HD23	1:C:467:ALA:HB1	1.97	0.45
1:C:491:GLU:H	1:C:491:GLU:CD	2.19	0.45
1:D:130:ASN:HB3	1:D:134:THR:OG1	2.16	0.45
1:D:178:LEU:N	1:D:179:PRO:CD	2.80	0.45
1:G:140:GLU:HB3	1:G:141:PRO:CD	2.46	0.45
1:G:221:LYS:HE2	1:G:221:LYS:HB3	1.62	0.45
1:G:261:GLU:HG2	1:H:151:LEU:HD12	1.98	0.45
1:G:291:ALA:HB3	1:G:295:VAL:HG11	1.99	0.45
1:G:672:ALA:O	1:G:714:PRO:HG3	2.16	0.45
1:A:150:THR:N	1:B:261:GLU:OE1	2.47	0.45
1:C:178:LEU:N	1:C:179:PRO:CD	2.80	0.45
1:C:442:LYS:HG3	1:C:465:PHE:CZ	2.51	0.45
1:C:609:VAL:HG22	1:C:645:ILE:HB	1.98	0.45
1:D:146:ILE:CG2	1:D:147:PRO:N	2.78	0.45
1:D:216:TYR:HD1	1:D:216:TYR:O	2.00	0.45
1:E:42:GLY:O	1:E:81:VAL:HG13	2.16	0.45
1:E:52:GLU:CD	1:E:53:PHE:N	2.70	0.45
1:E:55:ALA:O	1:E:59:GLN:HB2	2.16	0.45
1:E:80:ILE:HG23	1:E:124:LEU:HD22	1.99	0.45
1:E:82:LEU:CB	1:E:83:PRO:CD	2.87	0.45
1:E:85:TRP:HB2	1:E:102:VAL:O	2.17	0.45
1:E:135:LEU:CD1	1:H:789:MSE:HG3	2.42	0.45
1:F:70:PHE:CD2	1:F:71:ASP:CA	3.00	0.45
1:H:187:HIS:NE2	1:H:276:PRO:O	2.48	0.45
1:A:302:GLY:N	3:A:902:FRU:O1	2.50	0.45
1:B:508:TYR:CD2	1:B:794:LYS:HE2	2.52	0.45
1:C:50:ILE:C	1:C:52:GLU:H	2.20	0.45
1:E:187:HIS:NE2	1:E:276:PRO:O	2.50	0.45
1:G:169:LYS:O	1:G:169:LYS:HG2	2.17	0.45
1:G:550:ILE:O	1:G:553:LEU:HB3	2.16	0.45
1:H:29:VAL:O	1:H:33:LEU:HD21	2.17	0.45
1:H:140:GLU:HB2	1:H:512:HIS:CD2	2.51	0.45
1:A:43:ILE:HG23	1:A:82:LEU:HD23	1.99	0.45
1:A:518:ASP:OD1	1:A:519:PRO:HD2	2.17	0.45
1:A:566:VAL:O	1:A:640:GLY:HA2	2.17	0.45
1:B:206:LEU:HD11	1:B:210:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LYS:HB2	1:B:408:PRO:CD	2.46	0.45
1:C:143:ASN:HB3	1:C:148:ARG:HH22	1.79	0.45
1:C:216:TYR:HD1	1:C:216:TYR:O	2.00	0.45
1:D:103:ASN:CB	1:D:106:ALA:CB	2.89	0.45
1:E:315:LEU:CD2	1:E:319:MSE:HE2	2.46	0.45
1:E:319:MSE:HE1	1:E:334:ILE:HD11	1.94	0.45
1:E:407:LYS:HB2	1:E:408:PRO:HD2	1.97	0.45
1:F:435:THR:HG23	1:F:475:THR:OG1	2.17	0.45
1:F:673:LEU:HD23	1:F:714:PRO:HB2	1.98	0.45
1:H:33:LEU:CA	1:H:36:VAL:HB	2.45	0.45
1:H:243:GLY:HA2	1:H:326:GLN:HA	1.99	0.45
1:H:453:LYS:HB2	1:H:453:LYS:HE2	1.76	0.45
1:H:698:GLY:N	1:H:699:PRO:CD	2.79	0.45
1:H:794:LYS:HA	1:H:794:LYS:HD3	1.62	0.45
1:A:30:LEU:HA	1:A:33:LEU:HD12	1.98	0.45
1:A:56:LEU:CB	1:A:57:PRO:CD	2.92	0.45
1:A:189:HIS:CD2	1:A:279:PHE:CD2	3.05	0.45
1:A:452:TRP:CG	1:A:453:LYS:N	2.84	0.45
1:A:472:MSE:HG2	1:A:514:ILE:HD13	1.99	0.45
1:B:114:PRO:O	1:B:115:ALA:HB3	2.16	0.45
1:C:53:PHE:O	1:C:57:PRO:CG	2.64	0.45
1:C:216:TYR:HE2	1:C:232:LYS:HE2	1.81	0.45
1:C:628:LYS:HA	1:C:628:LYS:HD2	1.80	0.45
1:D:181:LEU:HD12	1:D:196:LEU:CD1	2.47	0.45
1:D:437:ALA:C	1:D:439:ALA:H	2.20	0.45
1:E:35:ARG:CG	1:E:35:ARG:NH1	2.77	0.45
1:E:730:LYS:CE	5:E:921:MLA:HC22	2.46	0.45
1:G:581:LEU:CD2	1:G:626:MSE:HG3	2.46	0.45
1:H:146:ILE:CG1	1:H:147:PRO:HD2	2.24	0.45
1:A:41:LYS:HA	1:A:41:LYS:HD2	1.56	0.45
1:C:137:LEU:HD11	1:C:790:PHE:CE1	2.52	0.45
1:C:681:VAL:CG1	1:C:685:MSE:HE2	2.42	0.45
1:D:135:LEU:HD12	1:D:136:GLU:N	2.32	0.45
1:E:153:LYS:HD3	1:E:154:TYR:CE2	2.52	0.45
1:E:723:THR:O	1:E:726:ASP:HB2	2.17	0.45
1:F:146:ILE:CG2	1:F:147:PRO:HD2	2.46	0.45
1:F:587:LEU:HD13	1:F:608:VAL:HG13	1.98	0.45
1:G:78:GLU:OE2	1:G:121:LYS:HE3	2.17	0.45
1:A:217:LEU:CD2	1:A:220:LEU:HD12	2.47	0.45
1:A:261:GLU:HG2	1:B:151:LEU:HB2	1.98	0.45
1:C:321:GLN:HG2	1:C:325:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:565:CYS:O	1:E:566:VAL:HG22	2.17	0.45
1:F:63:LYS:C	1:F:65:GLU:N	2.68	0.45
1:F:338:THR:HG23	1:F:366:ARG:HG2	1.98	0.45
1:G:425:LEU:HD23	1:G:425:LEU:HA	1.79	0.45
1:G:596:LYS:CG	1:G:636:TYR:CE1	2.92	0.45
1:H:28:GLU:CG	1:H:32:LEU:HD23	2.47	0.45
1:H:538:GLU:O	1:H:542:ARG:HG2	2.16	0.45
1:A:217:LEU:HD23	1:A:220:LEU:HD12	1.98	0.44
1:B:45:GLN:CB	1:B:80:ILE:HG22	2.47	0.44
1:B:449:ASP:OD1	1:B:450:ILE:HG22	2.17	0.44
1:C:148:ARG:CG	1:C:148:ARG:NH1	2.44	0.44
1:C:419:ASN:HB3	1:C:471:ALA:HB1	1.99	0.44
1:C:420:LEU:HD13	1:C:420:LEU:O	2.16	0.44
1:C:490:LYS:HD2	1:C:490:LYS:O	2.17	0.44
1:D:73:LEU:N	1:D:73:LEU:CD1	2.79	0.44
1:D:290:PHE:O	1:D:366:ARG:NH1	2.38	0.44
1:E:44:LEU:HD11	1:E:451:TYR:OH	2.17	0.44
1:E:117:PHE:C	1:E:117:PHE:CD1	2.90	0.44
1:F:135:LEU:HD12	1:F:136:GLU:N	2.32	0.44
1:F:313:ARG:O	1:F:317:ILE:HG13	2.17	0.44
1:F:566:VAL:CG1	1:F:567:LEU:N	2.80	0.44
1:G:212:LYS:HE3	1:G:232:LYS:NZ	2.32	0.44
1:H:748:ARG:NH1	1:H:752:LYS:HG3	2.32	0.44
1:A:125:VAL:HG21	1:A:450:ILE:HG12	1.99	0.44
1:A:534:PHE:HB2	1:A:535:PRO:CD	2.46	0.44
1:B:93:ARG:O	1:B:96:VAL:CG2	2.62	0.44
1:B:340:LEU:HD23	1:B:368:PRO:HB3	1.99	0.44
1:C:252:MSE:O	1:C:255:LEU:HB2	2.17	0.44
3:C:902:FRU:H61	7:C:841:HOH:O	2.16	0.44
1:D:242:TRP:O	1:D:252:MSE:HG3	2.17	0.44
1:D:415:TYR:CG	1:D:416:SER:N	2.85	0.44
1:D:497:GLU:HB2	1:D:516:VAL:HG11	1.99	0.44
1:F:53:PHE:O	1:F:57:PRO:CB	2.64	0.44
1:F:73:LEU:HD12	1:F:73:LEU:N	2.33	0.44
1:F:172:HIS:CE1	1:F:261:GLU:O	2.71	0.44
1:F:207:GLN:NE2	1:F:211:ARG:HH22	2.07	0.44
1:F:796:ARG:N	1:F:797:PRO:CD	2.79	0.44
1:G:437:ALA:C	1:G:439:ALA:H	2.20	0.44
1:G:770:GLY:O	1:G:773:LYS:HB2	2.17	0.44
1:A:153:LYS:HG3	1:A:154:TYR:N	2.31	0.44
1:B:76:THR:C	1:B:77:GLN:HG2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:LEU:HD23	1:C:404:LEU:HA	1.79	0.44
1:D:33:LEU:O	1:D:37:GLU:CG	2.66	0.44
1:E:400:LEU:HD12	1:E:401:SER:N	2.31	0.44
1:E:419:ASN:OD1	1:E:435:THR:HB	2.18	0.44
1:F:80:ILE:HD11	1:F:117:PHE:CZ	2.52	0.44
1:G:41:LYS:HE2	1:G:41:LYS:HB3	1.77	0.44
1:G:43:ILE:HA	1:G:81:VAL:O	2.17	0.44
1:G:796:ARG:N	1:G:797:PRO:CD	2.81	0.44
1:H:43:ILE:HA	1:H:81:VAL:O	2.17	0.44
1:H:149:PRO:HB3	1:H:161:PHE:CE1	2.52	0.44
1:H:178:LEU:HD22	1:H:178:LEU:HA	1.70	0.44
1:H:481:SER:O	1:H:482:THR:CG2	2.66	0.44
1:H:534:PHE:HB2	1:H:535:PRO:CD	2.48	0.44
1:H:790:PHE:O	1:H:794:LYS:HB3	2.18	0.44
1:A:56:LEU:HD22	1:A:56:LEU:HA	1.78	0.44
1:A:417:ASP:O	1:A:421:VAL:HG23	2.18	0.44
1:C:178:LEU:HB2	1:C:179:PRO:HD3	2.00	0.44
1:C:219:GLU:OE1	1:C:219:GLU:HA	2.17	0.44
1:C:692:PHE:N	1:C:692:PHE:CD1	2.86	0.44
1:D:56:LEU:CB	1:D:57:PRO:CD	2.96	0.44
1:D:327:GLY:C	1:D:328:LEU:HD23	2.37	0.44
1:F:82:LEU:CD1	1:F:83:PRO:CG	2.91	0.44
1:G:32:LEU:O	1:G:36:VAL:HG23	2.17	0.44
1:H:425:LEU:HA	1:H:425:LEU:HD23	1.60	0.44
1:H:481:SER:HB2	1:H:677:PHE:CD2	2.52	0.44
1:B:756:GLN:HG2	1:B:757:ILE:CD1	2.40	0.44
1:C:178:LEU:N	1:C:179:PRO:HD2	2.33	0.44
1:C:221:LYS:HE3	1:C:223:GLU:HB2	1.99	0.44
1:C:232:LYS:O	1:C:235:GLU:HB2	2.17	0.44
1:D:219:GLU:HG3	1:D:220:LEU:N	2.32	0.44
1:D:407:LYS:HB2	1:D:408:PRO:HD2	1.99	0.44
1:D:780:ARG:HA	1:D:780:ARG:HD2	1.70	0.44
1:E:143:ASN:O	1:E:145:SER:N	2.51	0.44
1:E:590:LEU:HB2	1:E:671:PRO:HG3	1.99	0.44
1:F:56:LEU:CB	1:F:57:PRO:HD3	2.47	0.44
1:F:79:ALA:CB	1:F:88:LEU:HD23	2.48	0.44
1:F:143:ASN:HB3	1:F:148:ARG:HH21	1.79	0.44
1:F:245:ASN:O	1:F:249:VAL:HG23	2.18	0.44
1:F:259:LEU:HD21	1:F:267:THR:HG22	1.99	0.44
1:G:32:LEU:O	1:G:32:LEU:CD1	2.65	0.44
1:H:65:GLU:C	1:H:67:GLY:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:278:VAL:CG2	1:H:766:THR:HG21	2.47	0.44
1:A:583:ARG:HG2	1:A:583:ARG:HH11	1.81	0.44
1:B:93:ARG:H	1:B:96:VAL:CG2	2.30	0.44
1:B:484:GLN:HG2	1:B:488:GLY:HA2	2.00	0.44
1:B:587:LEU:HD13	1:B:608:VAL:CG1	2.47	0.44
1:C:527:GLY:O	1:C:755:TRP:NE1	2.51	0.44
1:D:315:LEU:HD12	1:D:315:LEU:HA	1.77	0.44
1:D:434:CYS:SG	1:D:479:ILE:HG13	2.58	0.44
1:D:695:CYS:SG	1:D:696:LYS:HD3	2.57	0.44
1:F:225:LEU:HD12	1:F:225:LEU:N	2.32	0.44
1:F:370:ARG:CB	1:F:375:ILE:HA	2.48	0.44
1:G:400:LEU:C	1:G:400:LEU:HD12	2.38	0.44
1:H:483:PHE:CE1	1:H:487:ALA:HB3	2.53	0.44
1:A:195:MSE:CE	1:A:242:TRP:CD2	2.88	0.44
1:A:419:ASN:OD1	1:A:435:THR:HB	2.18	0.44
1:B:80:ILE:HG12	1:B:87:ALA:O	2.18	0.44
1:B:135:LEU:HD21	1:C:789:MSE:HE2	2.00	0.44
1:B:594:TYR:CE1	1:B:601:ARG:HG2	2.53	0.44
1:C:327:GLY:O	1:C:328:LEU:HD23	2.17	0.44
1:C:390:GLU:OE1	1:C:796:ARG:HD2	2.17	0.44
1:C:534:PHE:O	1:C:687:CYS:HA	2.18	0.44
1:E:315:LEU:HD23	1:E:319:MSE:CE	2.48	0.44
1:F:43:ILE:CG1	1:F:82:LEU:HA	2.46	0.44
1:F:65:GLU:HG3	1:F:70:PHE:HB3	2.00	0.44
1:F:140:GLU:N	1:F:141:PRO:CD	2.76	0.44
1:F:284:LEU:HD22	1:F:284:LEU:N	2.33	0.44
1:F:526:PRO:HG2	1:F:677:PHE:CE1	2.53	0.44
1:H:304:GLN:HB3	3:H:902:FRU:O1	2.17	0.44
1:H:514:ILE:HG13	1:H:515:ASP:N	2.33	0.44
1:A:63:LYS:O	1:A:64:LEU:C	2.55	0.44
1:B:142:PHE:O	1:B:780:ARG:NH1	2.51	0.44
1:B:416:SER:CB	1:B:464:GLN:HE21	2.30	0.44
1:C:441:GLU:OE1	1:C:441:GLU:HA	2.17	0.44
1:C:484:GLN:HA	1:C:488:GLY:HA2	1.98	0.44
1:D:59:GLN:O	1:D:63:LYS:HD2	2.17	0.44
1:E:66:GLY:HA2	1:E:71:ASP:OD1	2.18	0.44
1:F:67:GLY:HA3	1:F:68:PRO:HD2	1.53	0.44
1:F:159:VAL:HG13	1:F:160:ASP:N	2.33	0.44
1:G:131:GLY:CA	1:G:134:THR:CG2	2.93	0.44
1:G:136:GLU:HG2	1:G:509:ARG:HD2	1.99	0.44
1:G:169:LYS:HG2	1:G:176:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:HB3	1:A:221:LYS:HE2	1.67	0.44
1:D:43:ILE:O	1:D:44:LEU:CB	2.64	0.44
1:D:73:LEU:N	1:D:73:LEU:HD12	2.33	0.44
1:E:245:ASN:O	1:E:249:VAL:HG23	2.17	0.44
1:E:277:MSE:HE3	1:E:277:MSE:HB3	1.83	0.44
1:E:415:TYR:HA	1:E:437:ALA:O	2.18	0.44
1:E:730:LYS:HE3	5:E:921:MLA:HC22	1.99	0.44
1:E:789:MSE:CE	1:H:789:MSE:C	2.87	0.44
1:F:137:LEU:HD11	1:F:790:PHE:CZ	2.53	0.44
1:F:789:MSE:CE	1:G:789:MSE:CG	2.91	0.44
1:G:65:GLU:HG3	1:G:70:PHE:HB2	1.98	0.44
1:G:70:PHE:CZ	1:G:71:ASP:OD1	2.71	0.44
1:G:692:PHE:N	1:G:692:PHE:CD1	2.86	0.44
1:H:50:ILE:O	1:H:54:GLU:HB3	2.18	0.44
1:H:65:GLU:HA	1:H:65:GLU:OE2	2.17	0.44
1:H:444:LYS:HE3	1:H:584:VAL:HG11	1.99	0.44
1:H:679:LEU:O	1:H:683:GLU:HG3	2.18	0.44
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.80	0.43
1:A:315:LEU:C	1:A:319:MSE:CE	2.86	0.43
1:A:789:MSE:HE1	1:D:786:TYR:O	2.18	0.43
1:B:89:ALA:HA	1:B:99:TYR:HA	1.99	0.43
1:C:71:ASP:HA	1:C:74:LYS:CB	2.48	0.43
1:C:279:PHE:HB2	1:C:409:ASP:OD2	2.17	0.43
1:C:597:ASN:C	1:C:597:ASN:OD1	2.57	0.43
1:D:376:VAL:HG21	1:D:388:TYR:CE2	2.53	0.43
1:D:452:TRP:CG	1:D:453:LYS:N	2.86	0.43
1:E:35:ARG:CD	1:E:104:LEU:HA	2.46	0.43
1:E:112:LEU:N	1:E:112:LEU:HD23	2.32	0.43
1:E:693:ALA:HB3	1:E:703:ILE:HD12	2.00	0.43
1:E:789:MSE:SE	1:H:789:MSE:CE	3.14	0.43
1:F:580:ARG:NH1	2:F:901:UDP:O1B	2.51	0.43
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.18	0.43
1:G:223:GLU:H	1:G:223:GLU:CD	2.22	0.43
1:G:435:THR:HG23	1:G:475:THR:CB	2.48	0.43
1:H:99:TYR:HE2	1:H:114:PRO:HB3	1.83	0.43
1:H:284:LEU:HD22	1:H:284:LEU:N	2.33	0.43
1:B:281:VAL:HB	1:B:334:ILE:HG23	2.00	0.43
1:C:685:MSE:HE1	1:C:703:ILE:HG13	2.00	0.43
1:D:102:VAL:CG2	1:D:109:VAL:HG22	2.47	0.43
1:F:83:PRO:HB2	1:F:84:PRO:CD	2.48	0.43
1:G:70:PHE:HD2	1:G:70:PHE:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:524:VAL:HG12	1:G:758:TYR:CD2	2.53	0.43
1:H:315:LEU:CB	1:H:319:MSE:HE3	2.44	0.43
1:A:528:ALA:HA	7:A:827:HOH:O	2.17	0.43
1:B:586:ASN:HB3	1:B:671:PRO:O	2.18	0.43
1:C:91:ARG:HD2	1:C:97:TRP:CZ2	2.52	0.43
1:C:306:VAL:HG21	2:C:901:UDP:H4'	2.00	0.43
1:E:60:THR:OG1	1:E:61:ARG:N	2.52	0.43
1:E:135:LEU:HD22	1:H:793:LEU:HD11	1.99	0.43
1:F:187:HIS:NE2	1:F:276:PRO:O	2.49	0.43
1:F:442:LYS:HB2	7:F:872:HOH:O	2.17	0.43
1:G:63:LYS:O	1:G:65:GLU:N	2.51	0.43
1:G:295:VAL:HG23	7:G:892:HOH:O	2.18	0.43
1:H:86:VAL:O	1:H:101:ARG:HA	2.18	0.43
1:H:545:LYS:NZ	1:H:545:LYS:HB2	2.33	0.43
1:A:70:PHE:CD2	1:A:71:ASP:HA	2.53	0.43
1:A:599:ARG:O	1:A:603:LEU:HD12	2.17	0.43
1:C:86:VAL:HG12	1:C:102:VAL:HB	2.00	0.43
1:D:156:GLY:HA3	1:D:523:ILE:HG13	2.01	0.43
1:E:340:LEU:HB2	1:E:366:ARG:HB3	1.99	0.43
1:E:415:TYR:CG	1:E:416:SER:N	2.87	0.43
1:F:734:ASP:HA	1:F:735:PRO:HD2	1.89	0.43
1:G:156:GLY:HA3	1:G:523:ILE:HG13	2.00	0.43
1:G:524:VAL:HA	7:G:820:HOH:O	2.18	0.43
1:H:56:LEU:HG	1:H:70:PHE:CE1	2.53	0.43
1:H:102:VAL:HA	1:H:109:VAL:HA	2.01	0.43
1:H:131:GLY:C	1:H:134:THR:HG23	2.39	0.43
1:H:757:ILE:HG22	1:H:761:ARG:CG	2.46	0.43
1:A:39:LYS:HZ1	1:A:105:HIS:HD2	1.65	0.43
1:A:43:ILE:C	1:A:44:LEU:HG	2.37	0.43
1:B:22:LEU:HD13	1:B:25:GLU:OE2	2.19	0.43
1:B:419:ASN:HB3	1:B:471:ALA:HB1	1.99	0.43
1:D:61:ARG:HB3	1:G:405:ASN:OD1	2.19	0.43
1:D:373:LYS:HE3	1:D:373:LYS:HB2	1.90	0.43
1:G:68:PRO:O	1:G:70:PHE:N	2.52	0.43
1:G:131:GLY:C	1:G:134:THR:HG23	2.39	0.43
1:G:552:GLU:O	1:G:556:SER:HB3	2.19	0.43
1:H:217:LEU:HD11	1:H:233:PHE:HZ	1.84	0.43
1:A:278:VAL:HG22	1:A:766:THR:HG21	1.99	0.43
1:A:565:CYS:HB3	1:A:566:VAL:H	1.66	0.43
1:A:673:LEU:HD23	1:A:673:LEU:HA	1.74	0.43
1:B:49:ILE:O	1:B:53:PHE:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ILE:HG22	1:C:318:GLU:N	2.32	0.43
1:F:794:LYS:C	1:F:797:PRO:HD2	2.39	0.43
1:A:56:LEU:HD13	1:A:63:LYS:HD2	2.01	0.43
1:A:209:THR:HG23	1:A:236:ILE:HB	2.01	0.43
1:B:178:LEU:N	1:B:179:PRO:CD	2.81	0.43
1:B:293:ASP:O	1:B:294:ASN:HB2	2.19	0.43
1:C:183:PHE:HD1	1:C:774:HIS:ND1	2.16	0.43
1:E:216:TYR:O	1:E:216:TYR:HD1	2.01	0.43
1:E:433:GLN:O	1:E:476:ASP:HB2	2.18	0.43
1:F:143:ASN:HB3	1:F:148:ARG:HH22	1.77	0.43
1:F:156:GLY:HA3	1:F:523:ILE:HG13	1.99	0.43
1:F:178:LEU:CB	1:F:179:PRO:HD3	2.48	0.43
1:F:419:ASN:HB3	1:F:471:ALA:CB	2.49	0.43
1:F:713:ASP:C	1:F:713:ASP:OD1	2.57	0.43
1:H:71:ASP:O	1:H:75:SER:HB3	2.18	0.43
1:H:315:LEU:HD12	1:H:315:LEU:HA	1.51	0.43
1:H:348:THR:O	1:H:351:GLU:HG2	2.19	0.43
1:A:564:LEU:HD22	1:A:613:ARG:CZ	2.49	0.43
1:B:45:GLN:HA	1:B:80:ILE:HA	2.01	0.43
1:B:63:LYS:CG	1:B:64:LEU:N	2.81	0.43
1:B:583:ARG:HG2	1:B:583:ARG:HH11	1.84	0.43
1:E:340:LEU:O	1:E:342:PRO:HD3	2.19	0.43
1:F:479:ILE:HD11	1:F:762:LEU:CD1	2.49	0.43
1:G:131:GLY:O	1:G:134:THR:HG23	2.18	0.43
1:G:435:THR:HG23	1:G:475:THR:HB	2.00	0.43
1:G:781:LEU:HD12	1:G:781:LEU:HA	1.68	0.43
1:H:518:ASP:OD1	1:H:520:LYS:HG2	2.19	0.43
1:A:41:LYS:O	1:A:44:LEU:HD12	2.18	0.43
1:B:48:GLN:O	1:B:52:GLU:N	2.51	0.43
1:B:352:ARG:NH2	1:B:403:GLU:OE2	2.43	0.43
1:B:534:PHE:HB2	1:B:535:PRO:HD2	2.00	0.43
1:C:139:PHE:CE1	1:C:787:LEU:HD21	2.54	0.43
1:C:230:GLU:O	1:C:234:GLU:HG3	2.18	0.43
1:D:170:LEU:HA	1:D:170:LEU:HD12	1.78	0.43
1:D:462:SER:O	1:D:798:LEU:HD13	2.19	0.43
1:E:125:VAL:HG22	1:E:126:ASP:N	2.33	0.43
1:E:571:LYS:HD2	1:E:571:LYS:H	1.82	0.43
1:F:131:GLY:O	1:F:134:THR:CG2	2.64	0.43
1:F:146:ILE:CG2	1:F:147:PRO:N	2.82	0.43
1:F:193:ASN:ND2	1:F:197:SER:HA	2.34	0.43
1:H:143:ASN:CB	1:H:148:ARG:HH22	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:236:ILE:HD11	1:H:238:LEU:HD12	2.01	0.43
1:A:39:LYS:HZ3	1:A:105:HIS:HD2	1.65	0.43
1:A:65:GLU:C	1:A:67:GLY:N	2.71	0.43
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.47	0.43
1:A:581:LEU:HD11	1:A:625:GLU:HG3	2.01	0.43
1:B:339:ARG:HD2	1:B:369:PHE:CE2	2.53	0.43
1:C:514:ILE:HG13	1:C:515:ASP:N	2.34	0.43
1:D:142:PHE:HB3	1:D:783:ALA:HB2	2.01	0.43
1:D:586:ASN:HB3	1:D:671:PRO:O	2.19	0.43
1:D:638:LEU:HD23	1:D:638:LEU:HA	1.78	0.43
1:E:44:LEU:CD1	1:E:45:GLN:H	2.32	0.43
1:E:292:GLN:OE1	1:E:356:VAL:HA	2.19	0.43
1:E:629:MSE:HG2	1:E:644:TRP:CH2	2.54	0.43
1:E:680:THR:CG2	2:E:901:UDP:H3'	2.48	0.43
1:F:80:ILE:CD1	1:F:117:PHE:CE2	3.02	0.43
1:F:83:PRO:CB	1:F:85:TRP:H	2.25	0.43
1:F:459:TYR:O	1:F:460:HIS:HB2	2.19	0.43
1:G:43:ILE:O	1:G:44:LEU:HG	2.18	0.43
1:H:163:ASN:HD21	1:H:269:GLU:HB2	1.84	0.43
1:A:173:ASP:HB3	1:A:176:SER:HB3	2.00	0.42
1:A:582:ASP:HB2	1:A:621:GLU:OE1	2.18	0.42
1:A:583:ARG:HG2	1:A:583:ARG:NH1	2.34	0.42
1:B:29:VAL:HG11	1:E:405:ASN:OD1	2.18	0.42
1:B:131:GLY:CA	1:B:134:THR:HG23	2.43	0.42
1:D:30:LEU:O	1:D:33:LEU:N	2.52	0.42
1:D:125:VAL:CG1	1:D:505:PRO:HG2	2.44	0.42
1:D:449:ASP:HB2	1:D:504:LEU:CD2	2.49	0.42
1:E:321:GLN:HA	1:E:321:GLN:OE1	2.19	0.42
1:F:320:LEU:HD23	1:F:320:LEU:HA	1.68	0.42
1:F:493:VAL:HG23	1:F:497:GLU:HG2	2.00	0.42
1:F:685:MSE:HE2	1:F:745:GLY:HA2	2.00	0.42
1:G:339:ARG:HH12	1:G:380:ILE:HG13	1.83	0.42
1:G:780:ARG:HA	1:G:780:ARG:HD2	1.81	0.42
1:H:88:LEU:N	1:H:100:LEU:O	2.46	0.42
1:A:39:LYS:NZ	1:A:105:HIS:CD2	2.84	0.42
1:B:63:LYS:HG3	1:B:64:LEU:N	2.33	0.42
1:C:226:TYR:O	1:C:230:GLU:HB2	2.19	0.42
1:C:298:TYR:CE1	1:C:649:MSE:CE	3.02	0.42
1:D:333:ARG:NH2	1:D:363:ASP:OD1	2.51	0.42
1:D:542:ARG:HD2	1:D:659:ARG:HD2	2.00	0.42
1:E:301:THR:HG23	1:E:305:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:556:SER:HB3	1:E:643:ARG:NH2	2.35	0.42
1:E:730:LYS:NZ	5:E:921:MLA:HC22	2.33	0.42
1:F:497:GLU:HB2	1:F:516:VAL:CG2	2.49	0.42
1:F:630:TYR:O	1:F:633:ILE:HB	2.20	0.42
1:G:146:ILE:HG22	1:G:147:PRO:N	2.34	0.42
1:H:415:TYR:O	1:H:419:ASN:ND2	2.52	0.42
1:H:435:THR:HG23	1:H:475:THR:HB	2.01	0.42
1:H:553:LEU:HD23	1:H:645:ILE:HD13	2.01	0.42
1:B:82:LEU:C	1:B:83:PRO:O	2.58	0.42
1:B:113:GLN:HA	1:B:114:PRO:HD3	1.92	0.42
1:B:230:GLU:OE1	1:B:240:ARG:NH1	2.52	0.42
1:C:46:GLN:HB2	1:C:50:ILE:CG2	2.50	0.42
1:C:60:THR:O	1:C:62:LYS:N	2.53	0.42
1:C:284:LEU:N	1:C:284:LEU:HD22	2.34	0.42
1:C:470:PHE:CE1	1:C:791:TYR:HB2	2.54	0.42
1:D:61:ARG:HA	1:D:63:LYS:CD	2.38	0.42
1:D:278:VAL:CG2	1:D:766:THR:HG21	2.48	0.42
1:D:441:GLU:HG2	1:D:464:GLN:NE2	2.34	0.42
1:F:145:SER:CB	1:F:779:ASP:OD2	2.65	0.42
1:G:125:VAL:HG12	1:G:126:ASP:N	2.34	0.42
1:G:371:THR:HG21	1:G:804:LEU:HD13	2.00	0.42
1:H:565:CYS:HB2	1:H:642:PHE:O	2.19	0.42
1:A:41:LYS:HE3	1:A:54:GLU:OE1	2.18	0.42
1:A:216:TYR:CE2	1:A:232:LYS:HG2	2.53	0.42
1:A:688:GLY:O	1:A:690:PRO:HD3	2.20	0.42
1:A:693:ALA:HB3	1:A:703:ILE:HD12	2.00	0.42
1:A:752:LYS:HB2	1:A:753:TYR:CE2	2.54	0.42
1:B:20:GLU:OE1	1:B:71:ASP:CB	2.67	0.42
1:B:730:LYS:HE3	5:B:921:MLA:O1A	2.20	0.42
1:C:71:ASP:O	1:C:75:SER:HB2	2.20	0.42
1:D:386:TRP:N	1:D:387:PRO:HD2	2.34	0.42
1:D:580:ARG:HD3	2:D:901:UDP:O2B	2.19	0.42
1:E:45:GLN:CB	1:E:79:ALA:O	2.68	0.42
1:E:491:GLU:H	1:E:491:GLU:CD	2.22	0.42
1:E:794:LYS:HA	1:E:794:LYS:HE2	2.01	0.42
1:F:400:LEU:C	1:F:400:LEU:CD1	2.85	0.42
1:F:752:LYS:HB2	1:F:753:TYR:CE2	2.55	0.42
1:G:86:VAL:O	1:G:101:ARG:HA	2.20	0.42
1:G:148:ARG:HD2	1:G:515:ASP:OD2	2.20	0.42
1:H:89:ALA:HA	1:H:99:TYR:HA	2.01	0.42
1:H:322:ARG:HD2	1:H:763:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:O	1:B:33:LEU:HB2	2.19	0.42
1:C:547:HIS:HD2	1:C:660:TYR:CE2	2.37	0.42
1:D:566:VAL:O	1:D:640:GLY:CA	2.68	0.42
1:E:60:THR:O	1:E:63:LYS:CD	2.68	0.42
1:E:119:HIS:HE1	1:E:509:ARG:NH2	2.18	0.42
1:F:216:TYR:CD2	1:F:232:LYS:HG2	2.55	0.42
1:F:645:ILE:HG22	1:F:646:SER:O	2.19	0.42
1:F:794:LYS:O	1:F:797:PRO:HD2	2.19	0.42
3:F:902:FRU:H61	7:F:888:HOH:O	2.19	0.42
1:G:65:GLU:HA	1:G:65:GLU:OE2	2.19	0.42
1:G:82:LEU:CD1	1:G:83:PRO:HD3	2.49	0.42
1:H:72:LEU:HA	1:H:75:SER:CB	2.37	0.42
1:H:528:ALA:HA	7:H:834:HOH:O	2.18	0.42
1:H:609:VAL:HG22	1:H:645:ILE:HB	2.00	0.42
1:A:52:GLU:O	1:A:53:PHE:C	2.56	0.42
1:B:56:LEU:HD22	1:B:56:LEU:HA	1.93	0.42
1:B:321:GLN:O	1:B:325:GLN:HG3	2.20	0.42
1:B:420:LEU:HD13	1:B:420:LEU:O	2.19	0.42
1:B:629:MSE:HE1	1:B:642:PHE:HZ	1.85	0.42
1:E:155:ILE:HB	1:E:483:PHE:HE2	1.85	0.42
1:G:65:GLU:CG	1:G:70:PHE:CB	2.97	0.42
1:H:339:ARG:NH2	1:H:378:LYS:O	2.52	0.42
1:A:322:ARG:O	1:A:326:GLN:HG2	2.20	0.42
1:A:773:LYS:HB2	1:A:773:LYS:HE3	1.81	0.42
1:D:60:THR:O	1:D:63:LYS:CD	2.68	0.42
1:D:183:PHE:HZ	1:D:277:MSE:SE	2.52	0.42
1:E:216:TYR:C	1:E:216:TYR:HD1	2.23	0.42
1:F:135:LEU:HD22	1:G:793:LEU:HD11	2.01	0.42
1:F:468:ASP:O	1:F:472:MSE:HB2	2.18	0.42
1:F:507:LEU:HD12	1:F:507:LEU:HA	1.75	0.42
1:F:794:LYS:HD2	1:F:794:LYS:HA	1.66	0.42
1:H:76:THR:O	1:H:77:GLN:HB2	2.20	0.42
1:A:99:TYR:CD2	1:A:99:TYR:N	2.88	0.42
1:A:203:LEU:O	1:A:207:GLN:HB3	2.20	0.42
1:A:287:HIS:HB3	1:A:417:ASP:OD2	2.20	0.42
1:B:56:LEU:HD21	1:B:65:GLU:CD	2.40	0.42
1:B:435:THR:HG23	1:B:475:THR:HB	2.02	0.42
1:C:301:THR:HG23	1:C:305:VAL:HG21	2.02	0.42
1:D:43:ILE:HG23	1:D:124:LEU:CD1	2.49	0.42
1:D:63:LYS:O	1:D:64:LEU:C	2.58	0.42
1:E:99:TYR:CD2	1:E:99:TYR:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:TYR:CE2	1:E:240:ARG:CG	3.02	0.42
1:E:315:LEU:CD2	1:E:319:MSE:CE	2.98	0.42
1:E:796:ARG:HB2	1:E:797:PRO:CD	2.46	0.42
1:F:63:LYS:H	1:F:63:LYS:HG3	1.59	0.42
1:F:441:GLU:OE1	1:F:441:GLU:HA	2.19	0.42
1:H:596:LYS:CE	1:H:636:TYR:OH	2.68	0.42
1:H:617:SER:HB3	1:H:623:LYS:HG3	2.01	0.42
1:H:796:ARG:HB2	1:H:797:PRO:HD3	2.00	0.42
1:A:146:ILE:HD11	1:A:162:LEU:CD1	2.50	0.42
1:A:348:THR:O	1:A:351:GLU:HG2	2.20	0.42
1:B:33:LEU:O	1:B:36:VAL:N	2.43	0.42
1:B:99:TYR:OH	1:B:114:PRO:HG3	2.20	0.42
1:C:50:ILE:O	1:C:52:GLU:N	2.52	0.42
1:C:119:HIS:CE1	1:C:509:ARG:CZ	3.02	0.42
1:C:339:ARG:HH12	1:C:380:ILE:N	2.18	0.42
1:C:540:LYS:HE3	1:C:540:LYS:HB2	1.91	0.42
1:C:572:LYS:HE3	1:C:605:ASN:CG	2.40	0.42
1:D:629:MSE:CE	1:D:629:MSE:CA	2.95	0.42
1:E:462:SER:HB2	1:E:507:LEU:HD21	2.01	0.42
1:E:789:MSE:HE2	1:H:789:MSE:CB	2.40	0.42
1:F:43:ILE:CG2	1:F:44:LEU:N	2.63	0.42
1:G:50:ILE:O	1:G:52:GLU:N	2.53	0.42
1:G:417:ASP:O	1:G:421:VAL:HG23	2.19	0.42
1:H:140:GLU:N	1:H:141:PRO:CD	2.82	0.42
1:A:141:PRO:HB2	1:D:782:GLU:HG3	2.01	0.42
1:A:252:MSE:SE	1:A:274:ARG:HD2	2.70	0.42
1:A:290:PHE:HD2	7:A:882:HOH:O	2.03	0.42
1:A:437:ALA:O	1:A:438:HIS:HB2	2.20	0.42
1:A:545:LYS:H	1:A:545:LYS:CD	2.32	0.42
1:B:91:ARG:HA	1:B:92:PRO:HD2	1.86	0.42
1:B:162:LEU:HD11	1:B:772:TRP:CE3	2.55	0.42
1:B:465:PHE:HD2	1:B:504:LEU:HD11	1.84	0.42
1:C:81:VAL:HB	1:C:86:VAL:HG23	2.02	0.42
1:C:136:GLU:OE2	1:C:509:ARG:NH1	2.53	0.42
1:C:238:LEU:HA	1:C:238:LEU:HD23	1.81	0.42
1:D:206:LEU:O	1:D:210:LEU:HG	2.19	0.42
1:E:435:THR:HG23	1:E:475:THR:HB	2.00	0.42
1:E:743:LYS:HA	1:E:746:LEU:HD12	2.02	0.42
1:F:46:GLN:HG2	1:F:50:ILE:HG22	2.02	0.42
1:F:371:THR:OG1	1:F:373:LYS:HE3	2.19	0.42
1:F:434:CYS:HG	1:F:479:ILE:HG13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:716:HIS:HB3	4:F:913:SO4:S	2.59	0.42
1:G:446:PRO:O	1:G:447:ASP:HB2	2.20	0.42
1:A:339:ARG:HD2	1:A:369:PHE:CD2	2.55	0.41
1:A:582:ASP:C	1:A:582:ASP:OD1	2.58	0.41
1:A:726:ASP:O	1:A:730:LYS:HG3	2.20	0.41
1:A:789:MSE:CE	1:D:789:MSE:C	2.89	0.41
1:B:62:LYS:HE3	1:B:62:LYS:HB2	1.83	0.41
1:B:276:PRO:HG3	1:B:326:GLN:HB3	2.02	0.41
1:C:83:PRO:CG	1:C:84:PRO:CD	2.88	0.41
1:C:180:LEU:HD12	1:C:180:LEU:O	2.20	0.41
1:C:216:TYR:CE2	1:C:232:LYS:HE2	2.55	0.41
1:C:752:LYS:HB2	1:C:753:TYR:CE2	2.55	0.41
1:D:433:GLN:HG2	1:D:475:THR:OG1	2.20	0.41
1:E:63:LYS:O	1:E:64:LEU:C	2.59	0.41
1:F:749:ILE:HD13	1:F:749:ILE:HA	1.86	0.41
1:G:55:ALA:O	1:G:59:GLN:HB2	2.20	0.41
1:H:46:GLN:HB3	1:H:51:ALA:CB	2.29	0.41
1:H:73:LEU:O	1:H:76:THR:HG23	2.19	0.41
1:H:308:ILE:HG22	1:H:336:ILE:HD13	2.01	0.41
1:H:375:ILE:O	1:H:375:ILE:HG13	2.16	0.41
1:H:659:ARG:O	1:H:662:CYS:HB2	2.20	0.41
1:A:606:LEU:HD23	1:A:642:PHE:CD1	2.55	0.41
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.91	0.41
1:C:217:LEU:HD22	1:C:246:ALA:HB1	2.03	0.41
1:C:468:ASP:O	1:C:472:MSE:HB2	2.20	0.41
1:D:173:ASP:CB	1:D:176:SER:HB2	2.46	0.41
1:E:65:GLU:HG2	1:E:70:PHE:HB2	2.02	0.41
1:F:65:GLU:O	1:F:66:GLY:C	2.57	0.41
1:F:81:VAL:CG1	1:F:86:VAL:CB	2.98	0.41
1:F:404:LEU:HD23	1:F:404:LEU:HA	1.86	0.41
1:F:743:LYS:O	1:F:747:GLN:HG3	2.20	0.41
1:G:82:LEU:CD1	1:G:83:PRO:CD	2.88	0.41
1:G:641:GLN:CD	1:G:641:GLN:N	2.73	0.41
1:G:778:LEU:HD12	1:G:778:LEU:N	2.35	0.41
1:H:113:GLN:HB3	1:H:114:PRO:HD2	2.02	0.41
1:H:672:ALA:HB3	1:H:694:THR:HG21	2.03	0.41
1:B:438:HIS:O	1:B:439:ALA:HB2	2.20	0.41
1:C:67:GLY:O	1:C:70:PHE:HB3	2.20	0.41
1:C:287:HIS:HB3	1:C:417:ASP:OD2	2.20	0.41
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.76	0.41
1:C:433:GLN:O	1:C:476:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:ILE:HD11	1:D:642:PHE:HE2	1.85	0.41
1:E:44:LEU:O	1:E:81:VAL:CG1	2.68	0.41
1:E:664:THR:O	1:E:665:LYS:HB2	2.19	0.41
1:F:275:VAL:O	1:F:277:MSE:HG3	2.20	0.41
1:F:291:ALA:HB3	1:F:295:VAL:HG11	2.02	0.41
1:F:327:GLY:O	1:F:328:LEU:HD23	2.20	0.41
1:F:789:MSE:HE3	1:G:789:MSE:C	2.40	0.41
1:G:502:PHE:N	1:G:502:PHE:CD2	2.88	0.41
1:G:798:LEU:HD23	1:G:798:LEU:HA	1.88	0.41
1:H:21:THR:O	1:H:21:THR:HG23	2.19	0.41
1:A:146:ILE:CD1	1:A:162:LEU:HD13	2.50	0.41
1:A:149:PRO:HB3	1:A:161:PHE:CD1	2.55	0.41
1:B:283:ILE:HD12	1:B:312:VAL:CG1	2.50	0.41
1:C:52:GLU:O	1:C:57:PRO:HD2	2.19	0.41
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.83	0.41
1:C:146:ILE:CD1	1:C:162:LEU:HD13	2.51	0.41
1:E:177:LEU:HD23	1:E:177:LEU:HA	1.92	0.41
1:E:298:TYR:CE1	1:E:649:MSE:HE1	2.56	0.41
1:E:452:TRP:CG	1:E:453:LYS:N	2.88	0.41
1:H:599:ARG:NH2	1:H:726:ASP:OD1	2.53	0.41
1:A:39:LYS:HG3	1:A:39:LYS:H	1.61	0.41
1:A:479:ILE:CD1	1:A:762:LEU:HD13	2.51	0.41
1:B:399:GLU:O	1:B:402:LYS:HB2	2.20	0.41
1:D:449:ASP:HA	1:D:504:LEU:HD22	2.03	0.41
1:D:536:TYR:CD1	1:D:537:THR:HG23	2.55	0.41
1:D:660:TYR:O	1:D:663:ASP:HB2	2.19	0.41
1:E:564:LEU:HD22	1:E:613:ARG:CZ	2.49	0.41
1:F:315:LEU:CD1	1:F:762:LEU:HD23	2.50	0.41
1:G:415:TYR:HA	1:G:437:ALA:O	2.21	0.41
1:G:621:GLU:O	1:G:625:GLU:HB2	2.21	0.41
1:H:615:LYS:HG3	7:H:865:HOH:O	2.20	0.41
1:B:158:GLY:HA3	1:B:519:PRO:O	2.19	0.41
1:B:207:GLN:HG3	1:B:211:ARG:NH2	2.35	0.41
1:B:378:LYS:HD3	1:B:805:ALA:HB1	2.03	0.41
1:B:449:ASP:OD1	1:B:450:ILE:N	2.48	0.41
1:B:536:TYR:CE1	1:B:537:THR:HG23	2.55	0.41
1:C:518:ASP:OD1	1:C:519:PRO:HD2	2.20	0.41
1:C:802:VAL:HA	1:C:803:PRO:HD3	1.93	0.41
1:D:27:ASN:HB2	1:D:30:LEU:HD23	2.03	0.41
1:D:102:VAL:O	1:D:102:VAL:HG13	2.20	0.41
1:D:272:LEU:HD23	1:D:272:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:HIS:O	1:D:439:ALA:HB2	2.20	0.41
1:E:44:LEU:C	1:E:124:LEU:HD21	2.41	0.41
1:E:223:GLU:CD	1:E:223:GLU:N	2.74	0.41
1:E:284:LEU:HD21	1:E:425:LEU:HD12	2.02	0.41
1:E:438:HIS:O	1:E:439:ALA:HB2	2.20	0.41
1:E:583:ARG:HH11	1:E:583:ARG:HG2	1.85	0.41
1:F:329:ASN:O	1:F:331:LYS:NZ	2.45	0.41
1:H:503:THR:O	1:H:504:LEU:HD23	2.20	0.41
1:A:73:LEU:HD22	1:A:90:VAL:HG11	2.03	0.41
1:A:276:PRO:HG3	1:A:326:GLN:CB	2.51	0.41
1:A:497:GLU:HB2	1:A:516:VAL:CG2	2.51	0.41
1:B:23:VAL:O	1:B:23:VAL:HG13	2.19	0.41
1:B:93:ARG:H	1:B:96:VAL:HG23	1.86	0.41
1:B:111:GLU:O	1:B:112:LEU:HD23	2.21	0.41
1:B:146:ILE:HG22	1:B:147:PRO:N	2.34	0.41
1:C:212:LYS:HE2	1:C:212:LYS:HB3	1.97	0.41
1:C:233:PHE:HE1	1:C:249:VAL:HG11	1.85	0.41
1:D:581:LEU:CD2	1:D:626:MSE:HG3	2.51	0.41
1:E:272:LEU:HA	1:E:272:LEU:HD23	1.75	0.41
1:G:284:LEU:HD22	1:G:284:LEU:N	2.36	0.41
1:G:795:TYR:CD2	1:G:795:TYR:C	2.94	0.41
1:H:44:LEU:O	1:H:80:ILE:HA	2.21	0.41
1:A:411:ILE:HG13	1:A:431:VAL:HG11	2.03	0.41
1:A:590:LEU:HD21	1:A:606:LEU:HD11	2.03	0.41
1:A:670:GLN:OE1	1:A:672:ALA:HB2	2.20	0.41
1:C:194:LEU:CD2	1:C:328:LEU:HD11	2.51	0.41
1:D:532:ILE:CD1	1:D:652:VAL:HG22	2.49	0.41
1:E:295:VAL:HB	1:E:301:THR:HG21	2.03	0.41
1:E:469:ILE:HD13	1:E:469:ILE:HA	1.93	0.41
1:F:86:VAL:HG12	1:F:102:VAL:O	2.21	0.41
1:F:284:LEU:HD13	1:F:337:LEU:HB2	2.03	0.41
1:G:259:LEU:CD2	1:G:267:THR:HG22	2.50	0.41
1:G:630:TYR:CE1	1:G:644:TRP:HZ3	2.39	0.41
1:H:532:ILE:HG13	1:H:651:ARG:NH1	2.36	0.41
1:A:82:LEU:C	1:A:83:PRO:O	2.59	0.41
1:A:137:LEU:HD11	1:A:790:PHE:CZ	2.56	0.41
1:A:149:PRO:HD3	1:A:161:PHE:CE2	2.56	0.41
1:A:420:LEU:C	1:A:420:LEU:CD1	2.88	0.41
1:A:437:ALA:C	1:A:439:ALA:H	2.23	0.41
1:A:682:VAL:HG13	1:A:749:ILE:CD1	2.50	0.41
1:A:793:LEU:HB3	1:D:793:LEU:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.81	0.41
1:B:436:ILE:HG12	1:B:479:ILE:HB	2.03	0.41
1:B:469:ILE:HD13	1:B:469:ILE:HA	1.96	0.41
1:B:578:MSE:HA	1:B:609:VAL:O	2.20	0.41
1:C:195:MSE:HE1	1:C:241:GLY:CA	2.50	0.41
1:C:330:ILE:HG22	1:C:331:LYS:N	2.36	0.41
1:C:502:PHE:CZ	1:C:510:VAL:HG21	2.55	0.41
1:C:629:MSE:O	1:C:633:ILE:HG13	2.21	0.41
1:D:155:ILE:HG21	1:D:487:ALA:HB2	2.03	0.41
1:D:178:LEU:N	1:D:179:PRO:HD2	2.35	0.41
1:D:284:LEU:N	1:D:284:LEU:CD2	2.84	0.41
1:D:534:PHE:HB2	1:D:535:PRO:CD	2.50	0.41
1:D:597:ASN:O	1:D:601:ARG:HG3	2.20	0.41
1:D:623:LYS:HE3	1:D:623:LYS:HB2	1.80	0.41
1:D:692:PHE:CD2	1:D:710:PHE:HB2	2.55	0.41
1:E:102:VAL:O	1:E:102:VAL:HG12	2.19	0.41
1:E:386:TRP:HH2	1:E:416:SER:HB3	1.86	0.41
1:F:151:LEU:HA	1:F:151:LEU:HD23	1.77	0.41
1:F:497:GLU:HB2	1:F:516:VAL:HG21	2.03	0.41
1:F:518:ASP:OD1	1:F:520:LYS:HG2	2.21	0.41
1:F:565:CYS:HB2	1:F:642:PHE:O	2.21	0.41
1:G:73:LEU:C	1:G:75:SER:N	2.75	0.41
1:G:174:LYS:N	1:G:174:LYS:HD2	2.36	0.41
1:G:208:HIS:CE1	1:G:211:ARG:HH22	2.38	0.41
1:G:438:HIS:O	1:G:439:ALA:HB2	2.21	0.41
1:H:89:ALA:HB2	1:H:99:TYR:HD1	1.85	0.41
1:H:91:ARG:HA	1:H:92:PRO:HD2	1.93	0.41
1:H:452:TRP:CG	1:H:453:LYS:N	2.89	0.41
1:H:472:MSE:HG3	1:H:514:ILE:HD13	2.02	0.41
1:A:30:LEU:CD1	1:A:62:LYS:O	2.68	0.41
1:A:298:TYR:CE1	1:A:649:MSE:CE	3.01	0.41
1:A:315:LEU:CG	1:A:319:MSE:HE2	2.48	0.41
1:B:445:TYR:O	1:B:448:SER:HB3	2.21	0.41
1:D:148:ARG:HA	1:D:148:ARG:HD3	1.87	0.41
1:D:547:HIS:O	1:D:551:GLU:HG3	2.21	0.41
1:E:206:LEU:HD11	1:E:210:LEU:HD11	2.01	0.41
1:E:431:VAL:CG1	1:E:432:THR:N	2.83	0.41
1:F:117:PHE:O	1:F:120:PHE:HB2	2.21	0.41
1:F:746:LEU:HD23	1:F:746:LEU:HA	1.94	0.41
1:G:304:GLN:HB3	3:G:902:FRU:C1	2.37	0.41
1:G:564:LEU:HA	1:G:564:LEU:HD12	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:HIS:CD2	1:H:287:HIS:C	2.94	0.41
1:H:315:LEU:HG	1:H:319:MSE:HE2	2.02	0.41
1:H:588:SER:HB3	1:H:625:GLU:OE2	2.21	0.41
1:A:88:LEU:N	1:A:88:LEU:CD2	2.84	0.40
1:A:88:LEU:O	1:A:88:LEU:HD23	2.20	0.40
1:A:183:PHE:HD1	1:A:774:HIS:ND1	2.19	0.40
1:A:512:HIS:NE2	1:A:515:ASP:HB2	2.36	0.40
1:A:567:LEU:HD23	1:A:567:LEU:HA	1.87	0.40
1:B:380:ILE:HD11	1:B:805:ALA:CB	2.51	0.40
1:D:34:SER:HA	1:D:59:GLN:HE22	1.86	0.40
1:D:564:LEU:HD23	1:D:564:LEU:HA	1.81	0.40
1:E:48:GLN:HG3	1:E:76:THR:O	2.21	0.40
1:E:448:SER:HB2	1:E:461:PHE:CD2	2.56	0.40
1:H:69:PHE:O	1:H:69:PHE:CG	2.74	0.40
1:H:414:ASN:O	1:H:418:GLY:HA3	2.21	0.40
1:H:692:PHE:CD1	1:H:692:PHE:N	2.89	0.40
1:A:135:LEU:HD12	1:A:136:GLU:H	1.86	0.40
1:B:390:GLU:OE1	1:B:796:ARG:HD2	2.21	0.40
1:C:645:ILE:CG2	1:C:648:GLN:NE2	2.84	0.40
1:D:50:ILE:H	1:D:50:ILE:HG13	1.60	0.40
1:E:316:GLU:OE1	1:E:361:TYR:N	2.42	0.40
1:E:322:ARG:HD2	1:E:763:LEU:HD13	2.02	0.40
1:E:514:ILE:HG13	1:E:515:ASP:N	2.36	0.40
1:F:86:VAL:CG1	1:F:102:VAL:HB	2.51	0.40
1:F:281:VAL:HG22	1:F:410:LEU:HB3	2.02	0.40
1:F:370:ARG:HB3	1:F:375:ILE:HA	2.04	0.40
1:F:449:ASP:HA	1:F:504:LEU:CD2	2.52	0.40
1:G:172:HIS:CE1	1:G:261:GLU:O	2.75	0.40
1:G:318:GLU:HG3	1:G:763:LEU:HD12	2.03	0.40
1:G:719:GLN:HG3	4:G:913:SO4:O3	2.21	0.40
1:H:131:GLY:O	1:H:134:THR:CG2	2.65	0.40
1:H:155:ILE:HB	1:H:483:PHE:CE2	2.56	0.40
1:H:705:HIS:CD2	1:H:705:HIS:C	2.95	0.40
1:A:70:PHE:HD2	1:A:71:ASP:HA	1.87	0.40
1:A:376:VAL:HG21	1:A:388:TYR:CE2	2.57	0.40
1:A:534:PHE:O	1:A:687:CYS:HA	2.22	0.40
1:B:279:PHE:HB2	1:B:409:ASP:OD2	2.21	0.40
1:C:252:MSE:SE	1:C:274:ARG:HG2	2.71	0.40
1:C:282:VAL:HG21	1:C:400:LEU:HD22	2.03	0.40
1:D:61:ARG:C	1:D:63:LYS:N	2.73	0.40
1:D:462:SER:HB2	1:D:507:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:VAL:HG22	1:D:494:GLY:N	2.35	0.40
1:E:252:MSE:SE	1:E:274:ARG:HB3	2.72	0.40
1:E:545:LYS:HE3	1:E:545:LYS:HB2	1.95	0.40
1:F:578:MSE:HG3	1:F:609:VAL:HB	2.03	0.40
1:F:625:GLU:HG2	7:F:827:HOH:O	2.21	0.40
1:H:566:VAL:O	1:H:640:GLY:HA2	2.21	0.40
1:A:70:PHE:HD2	1:A:71:ASP:N	2.20	0.40
1:A:137:LEU:HD11	1:A:790:PHE:CE1	2.56	0.40
1:A:339:ARG:HH12	1:A:380:ILE:HG13	1.85	0.40
1:B:49:ILE:H	1:B:49:ILE:HG13	1.39	0.40
1:B:163:ASN:HD21	1:B:269:GLU:CG	2.33	0.40
1:B:716:HIS:CB	4:B:913:SO4:O4	2.66	0.40
1:B:746:LEU:HD23	1:B:746:LEU:HA	1.93	0.40
1:C:469:ILE:HD13	1:C:469:ILE:HA	1.92	0.40
1:D:146:ILE:HG13	1:D:772:TRP:CZ2	2.57	0.40
1:D:338:THR:HG23	1:D:366:ARG:HG2	2.02	0.40
1:E:386:TRP:N	1:E:387:PRO:HD2	2.36	0.40
1:E:591:VAL:HG13	1:E:638:LEU:CD1	2.51	0.40
1:E:591:VAL:CG1	1:E:638:LEU:HD11	2.51	0.40
1:F:316:GLU:N	1:F:319:MSE:CE	2.85	0.40
1:F:698:GLY:N	1:F:699:PRO:CD	2.84	0.40
1:H:181:LEU:HD13	1:H:206:LEU:HD22	2.02	0.40
1:A:146:ILE:HD11	1:A:772:TRP:CZ2	2.57	0.40
1:A:315:LEU:C	1:A:319:MSE:HE2	2.41	0.40
1:A:670:GLN:NE2	7:A:849:HOH:O	2.53	0.40
1:B:92:PRO:HG2	1:B:96:VAL:HG21	1.93	0.40
1:B:118:LEU:HD22	1:B:503:THR:HG22	2.02	0.40
1:B:479:ILE:HD11	1:B:762:LEU:CD1	2.52	0.40
1:B:649:MSE:H	1:B:649:MSE:HG2	1.59	0.40
1:C:34:SER:OG	1:C:55:ALA:HB1	2.21	0.40
1:C:154:TYR:OH	1:D:262:ALA:HB3	2.22	0.40
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.89	0.40
1:E:148:ARG:HA	1:E:149:PRO:HD2	1.89	0.40
1:E:444:LYS:HB3	1:E:444:LYS:HE2	1.97	0.40
1:F:441:GLU:OE1	1:F:444:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/816 (96%)	730 (94%)	45 (6%)	4 (0%)	25	55
1	B	791/816 (97%)	734 (93%)	56 (7%)	1 (0%)	48	76
1	C	779/816 (96%)	734 (94%)	42 (5%)	3 (0%)	30	59
1	D	779/816 (96%)	736 (94%)	38 (5%)	5 (1%)	22	51
1	E	779/816 (96%)	737 (95%)	38 (5%)	4 (0%)	25	55
1	F	779/816 (96%)	734 (94%)	39 (5%)	6 (1%)	16	44
1	G	779/816 (96%)	736 (94%)	39 (5%)	4 (0%)	25	55
1	H	795/816 (97%)	750 (94%)	42 (5%)	3 (0%)	30	59
All	All	6260/6528 (96%)	5891 (94%)	339 (5%)	30 (0%)	25	55

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	GLN
1	D	106	ALA
1	E	83	PRO
1	A	52	GLU
1	A	83	PRO
1	F	58	GLU
1	G	68	PRO
1	G	69	PHE
1	H	108	VAL
1	B	83	PRO
1	E	63	LYS
1	F	57	PRO
1	F	63	LYS
1	F	68	PRO
1	F	69	PHE
1	A	51	ALA
1	A	63	LYS

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Mol	Chain	Res	Type
1	C	63	LYS
1	C	565	CYS
1	D	63	LYS
1	D	56	LEU
1	G	63	LYS
1	G	70	PHE
1	H	63	LYS
1	D	57	PRO
1	E	84	PRO
1	H	145	SER
1	F	43	ILE
1	D	49	ILE
1	E	82	LEU

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	667/704 (95%)	626 (94%)	41 (6%)	15	42
1	B	663/704 (94%)	626 (94%)	37 (6%)	17	46
1	C	666/704 (95%)	622 (93%)	44 (7%)	14	38
1	D	659/704 (94%)	624 (95%)	35 (5%)	19	48
1	E	662/704 (94%)	620 (94%)	42 (6%)	15	40
1	F	668/704 (95%)	635 (95%)	33 (5%)	21	51
1	G	668/704 (95%)	626 (94%)	42 (6%)	15	40
1	H	663/704 (94%)	623 (94%)	40 (6%)	16	42
All	All	5316/5632 (94%)	5002 (94%)	314 (6%)	16	43

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	45	GLN

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Mol	Chain	Res	Type
1	A	46	GLN
1	A	52	GLU
1	A	54	GLU
1	A	56	LEU
1	A	59	GLN
1	A	70	PHE
1	A	73	LEU
1	A	86	VAL
1	A	88	LEU
1	A	90	VAL
1	A	105	HIS
1	A	111	GLU
1	A	140	GLU
1	A	148	ARG
1	A	164	ARG
1	A	195	MSE
1	A	248	ARG
1	A	255	LEU
1	A	258	ASP
1	A	285	SER
1	A	293	ASP
1	A	307	TYR
1	A	321	GLN
1	A	322	ARG
1	A	340	LEU
1	A	434	CYS
1	A	484	GLN
1	A	493	VAL
1	A	530	MSE
1	A	545	LYS
1	A	556	SER
1	A	602	GLU
1	A	616	GLU
1	A	618	LYS
1	A	670	GLN
1	A	736	SER
1	A	750	GLU
1	A	757	ILE
1	A	781	LEU
1	B	22	LEU
1	B	23	VAL
1	B	24	SER

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	43	ILE
1	B	49	ILE
1	B	50	ILE
1	B	56	LEU
1	B	60	THR
1	B	70	PHE
1	B	72	LEU
1	B	99	TYR
1	B	105	HIS
1	B	111	GLU
1	B	128	VAL
1	B	132	ASN
1	B	151	LEU
1	B	216	TYR
1	B	225	LEU
1	B	248	ARG
1	B	258	ASP
1	B	293	ASP
1	B	321	GLN
1	B	345	VAL
1	B	358	ASP
1	B	493	VAL
1	B	503	THR
1	B	531	SER
1	B	545	LYS
1	B	630	TYR
1	B	646	SER
1	B	649	MSE
1	B	670	GLN
1	B	722	ASP
1	B	756	GLN
1	B	757	ILE
1	B	779	ASP
1	C	29	VAL
1	C	30	LEU
1	C	32	LEU
1	C	37	GLU
1	C	44	LEU
1	C	45	GLN
1	C	46	GLN
1	C	52	GLU

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Mol	Chain	Res	Type
1	C	54	GLU
1	C	56	LEU
1	C	59	GLN
1	C	63	LYS
1	C	65	GLU
1	C	69	PHE
1	C	86	VAL
1	C	105	HIS
1	C	109	VAL
1	C	119	HIS
1	C	120	PHE
1	C	148	ARG
1	C	167	SER
1	C	174	LYS
1	C	216	TYR
1	C	240	ARG
1	C	248	ARG
1	C	258	ASP
1	C	284	LEU
1	C	358	ASP
1	C	373	LYS
1	C	405	ASN
1	C	420	LEU
1	C	508	TYR
1	C	545	LYS
1	C	556	SER
1	C	580	ARG
1	C	616	GLU
1	C	646	SER
1	C	665	LYS
1	C	670	GLN
1	C	708	SER
1	C	757	ILE
1	C	760	GLN
1	C	777	ASN
1	C	806	GLN
1	D	27	ASN
1	D	29	VAL
1	D	44	LEU
1	D	52	GLU
1	D	54	GLU
1	D	56	LEU

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Mol	Chain	Res	Type
1	D	76	THR
1	D	108	VAL
1	D	119	HIS
1	D	120	PHE
1	D	125	VAL
1	D	132	ASN
1	D	164	ARG
1	D	170	LEU
1	D	197	SER
1	D	216	TYR
1	D	219	GLU
1	D	251	ASP
1	D	258	ASP
1	D	269	GLU
1	D	286	PRO
1	D	321	GLN
1	D	360	GLU
1	D	454	LYS
1	D	491	GLU
1	D	556	SER
1	D	563	HIS
1	D	570	LYS
1	D	629	MSE
1	D	708	SER
1	D	750	GLU
1	D	757	ILE
1	D	779	ASP
1	D	794	LYS
1	D	806	GLN
1	E	30	LEU
1	E	32	LEU
1	E	35	ARG
1	E	44	LEU
1	E	45	GLN
1	E	54	GLU
1	E	56	LEU
1	E	59	GLN
1	E	61	ARG
1	E	70	PHE
1	E	73	LEU
1	E	85	TRP
1	E	102	VAL

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Mol	Chain	Res	Type
1	E	105	HIS
1	E	112	LEU
1	E	125	VAL
1	E	148	ARG
1	E	153	LYS
1	E	167	SER
1	E	193	ASN
1	E	216	TYR
1	E	235	GLU
1	E	240	ARG
1	E	293	ASP
1	E	340	LEU
1	E	358	ASP
1	E	375	ILE
1	E	401	SER
1	E	457	ASP
1	E	463	CYS
1	E	491	GLU
1	E	492	THR
1	E	493	VAL
1	E	516	VAL
1	E	530	MSE
1	E	572	LYS
1	E	653	ARG
1	E	670	GLN
1	E	750	GLU
1	E	759	SER
1	E	777	ASN
1	E	781	LEU
1	F	32	LEU
1	F	44	LEU
1	F	45	GLN
1	F	54	GLU
1	F	56	LEU
1	F	59	GLN
1	F	60	THR
1	F	65	GLU
1	F	69	PHE
1	F	82	LEU
1	F	100	LEU
1	F	123	GLU
1	F	140	GLU

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Mol	Chain	Res	Type
1	F	153	LYS
1	F	178	LEU
1	F	205	THR
1	F	216	TYR
1	F	240	ARG
1	F	285	SER
1	F	311	GLN
1	F	315	LEU
1	F	412	ILE
1	F	420	LEU
1	F	516	VAL
1	F	545	LYS
1	F	628	LYS
1	F	629	MSE
1	F	647	SER
1	F	649	MSE
1	F	670	GLN
1	F	696	LYS
1	F	773	LYS
1	F	778	LEU
1	G	30	LEU
1	G	32	LEU
1	G	41	LYS
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	70	PHE
1	G	73	LEU
1	G	82	LEU
1	G	100	LEU
1	G	119	HIS
1	G	124	LEU
1	G	125	VAL
1	G	140	GLU
1	G	148	ARG
1	G	153	LYS
1	G	170	LEU
1	G	202	ASN
1	G	205	THR

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Mol	Chain	Res	Type
1	G	222	SER
1	G	258	ASP
1	G	315	LEU
1	G	425	LEU
1	G	491	GLU
1	G	493	VAL
1	G	516	VAL
1	G	545	LYS
1	G	556	SER
1	G	561	LYS
1	G	571	LYS
1	G	602	GLU
1	G	664	THR
1	G	670	GLN
1	G	736	SER
1	G	756	GLN
1	G	757	ILE
1	G	759	SER
1	G	781	LEU
1	G	784	ARG
1	H	11	VAL
1	H	18	LEU
1	H	21	THR
1	H	22	LEU
1	H	32	LEU
1	H	33	LEU
1	H	43	ILE
1	H	46	GLN
1	H	48	GLN
1	H	49	ILE
1	H	50	ILE
1	H	60	THR
1	H	61	ARG
1	H	69	PHE
1	H	72	LEU
1	H	82	LEU
1	H	146	ILE
1	H	148	ARG
1	H	176	SER
1	H	178	LEU
1	H	207	GLN
1	H	240	ARG

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Mol	Chain	Res	Type
1	H	251	ASP
1	H	315	LEU
1	H	345	VAL
1	H	353	LEU
1	H	417	ASP
1	H	450	ILE
1	H	481	SER
1	H	493	VAL
1	H	516	VAL
1	H	540	LYS
1	H	545	LYS
1	H	556	SER
1	H	563	HIS
1	H	564	LEU
1	H	572	LYS
1	H	750	GLU
1	H	759	SER
1	H	779	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	59	GLN
1	A	105	HIS
1	A	172	HIS
1	A	189	HIS
1	A	207	GLN
1	A	287	HIS
1	A	294	ASN
1	A	414	ASN
1	A	711	HIS
1	B	48	GLN
1	B	119	HIS
1	B	163	ASN
1	B	311	GLN
1	C	59	GLN
1	C	119	HIS
1	C	172	HIS
1	C	207	GLN
1	C	287	HIS
1	C	311	GLN

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Mol	Chain	Res	Type
1	C	414	ASN
1	C	512	HIS
1	D	48	GLN
1	D	59	GLN
1	D	163	ASN
1	D	207	GLN
1	D	208	HIS
1	D	719	GLN
1	D	806	GLN
1	E	119	HIS
1	E	193	ASN
1	E	207	GLN
1	E	325	GLN
1	E	737	HIS
1	E	774	HIS
1	F	59	GLN
1	F	172	HIS
1	F	207	GLN
1	F	414	ASN
1	F	747	GLN
1	G	27	ASN
1	G	45	GLN
1	G	46	GLN
1	G	48	GLN
1	G	172	HIS
1	G	190	GLN
1	G	202	ASN
1	G	204	ASN
1	G	207	GLN
1	G	321	GLN
1	G	414	ASN
1	H	12	HIS
1	H	45	GLN
1	H	130	ASN
1	H	189	HIS
1	H	204	ASN
1	H	207	GLN
1	H	321	GLN
1	H	325	GLN
1	H	705	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FRU	B	902	-	11,12,12	0.79	1 (9%)	10,18,18	0.86	0
2	UDP	H	901	-	25,26,26	1.02	0	38,40,40	1.75	6 (15%)
2	UDP	A	901	-	25,26,26	1.04	0	38,40,40	1.71	6 (15%)
2	UDP	E	901	-	25,26,26	1.03	1 (4%)	38,40,40	1.56	6 (15%)
2	UDP	C	901	-	25,26,26	1.06	1 (4%)	38,40,40	1.63	7 (18%)
4	SO4	H	912	-	4,4,4	0.30	0	6,6,6	0.13	0
4	SO4	A	912	-	4,4,4	0.31	0	6,6,6	0.18	0
5	MLA	F	921	-	6,6,6	1.34	0	7,7,7	1.11	0
4	SO4	C	912	-	4,4,4	0.27	0	6,6,6	0.15	0
3	FRU	F	902	-	11,12,12	0.73	0	10,18,18	0.75	0
2	UDP	G	901	-	25,26,26	0.97	0	38,40,40	1.57	6 (15%)
4	SO4	C	911	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	D	912	-	4,4,4	0.28	0	6,6,6	0.09	0
3	FRU	D	902	-	11,12,12	0.91	0	10,18,18	1.19	2 (20%)
5	MLA	G	921	-	6,6,6	1.08	0	7,7,7	1.52	1 (14%)
2	UDP	D	901	-	25,26,26	1.03	0	38,40,40	1.81	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	F	913	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	F	912	-	4,4,4	0.31	0	6,6,6	0.30	0
4	SO4	D	913	-	4,4,4	0.33	0	6,6,6	0.10	0
5	MLA	E	921	-	6,6,6	1.27	0	7,7,7	0.94	0
4	SO4	G	911	-	4,4,4	0.36	0	6,6,6	0.17	0
3	FRU	H	902	-	11,12,12	0.85	1 (9%)	10,18,18	1.06	0
4	SO4	E	911	-	4,4,4	0.33	0	6,6,6	0.41	0
3	FRU	A	902	-	11,12,12	0.74	0	10,18,18	0.79	0
4	SO4	E	912	-	4,4,4	0.33	0	6,6,6	0.14	0
4	SO4	B	911	-	4,4,4	0.39	0	6,6,6	0.25	0
5	MLA	A	921	-	6,6,6	1.14	0	7,7,7	1.38	1 (14%)
3	FRU	E	902	-	11,12,12	0.73	0	10,18,18	0.84	0
5	MLA	C	921	-	6,6,6	1.15	0	7,7,7	1.42	1 (14%)
2	UDP	F	901	-	25,26,26	1.00	1 (4%)	38,40,40	1.81	8 (21%)
3	FRU	C	902	-	11,12,12	0.70	1 (9%)	10,18,18	0.91	0
5	MLA	B	921	-	6,6,6	1.31	0	7,7,7	1.06	0
4	SO4	A	911	-	4,4,4	0.33	0	6,6,6	0.19	0
3	FRU	G	902	-	11,12,12	0.70	0	10,18,18	0.76	0
5	MLA	H	921	-	6,6,6	1.14	0	7,7,7	1.32	0
4	SO4	C	913	-	4,4,4	0.30	0	6,6,6	0.14	0
4	SO4	F	911	-	4,4,4	0.37	0	6,6,6	0.41	0
4	SO4	B	912	-	4,4,4	0.33	0	6,6,6	0.24	0
4	SO4	G	913	-	4,4,4	0.29	0	6,6,6	0.13	0
4	SO4	G	912	-	4,4,4	0.29	0	6,6,6	0.08	0
4	SO4	D	911	-	4,4,4	0.32	0	6,6,6	0.28	0
4	SO4	E	913	-	4,4,4	0.36	0	6,6,6	0.19	0
4	SO4	H	911	-	4,4,4	0.36	0	6,6,6	0.25	0
5	MLA	D	921	-	6,6,6	1.12	0	7,7,7	1.23	0
4	SO4	H	913	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	A	913	-	4,4,4	0.30	0	6,6,6	0.31	0
2	UDP	B	901	-	25,26,26	1.02	1 (4%)	38,40,40	1.82	7 (18%)
4	SO4	B	913	-	4,4,4	0.36	0	6,6,6	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	B	902	-	-	2/5/24/24	0/1/1/1
2	UDP	H	901	-	-	6/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	A	901	-	-	3/16/32/32	0/2/2/2
2	UDP	E	901	-	-	5/16/32/32	0/2/2/2
2	UDP	C	901	-	-	6/16/32/32	0/2/2/2
5	MLA	F	921	-	-	0/4/4/4	-
3	FRU	F	902	-	-	5/5/24/24	0/1/1/1
2	UDP	G	901	-	-	7/16/32/32	0/2/2/2
3	FRU	D	902	-	-	5/5/24/24	0/1/1/1
5	MLA	G	921	-	-	0/4/4/4	-
2	UDP	D	901	-	-	3/16/32/32	0/2/2/2
5	MLA	E	921	-	-	0/4/4/4	-
3	FRU	H	902	-	-	5/5/24/24	0/1/1/1
3	FRU	A	902	-	-	2/5/24/24	0/1/1/1
5	MLA	A	921	-	-	2/4/4/4	-
3	FRU	E	902	-	-	1/5/24/24	0/1/1/1
5	MLA	C	921	-	-	2/4/4/4	-
2	UDP	F	901	-	-	4/16/32/32	0/2/2/2
3	FRU	C	902	-	-	2/5/24/24	0/1/1/1
5	MLA	B	921	-	-	0/4/4/4	-
3	FRU	G	902	-	-	3/5/24/24	0/1/1/1
5	MLA	H	921	-	-	0/4/4/4	-
5	MLA	D	921	-	-	2/4/4/4	-
2	UDP	B	901	-	-	5/16/32/32	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	UDP	PA-O3A	2.90	1.62	1.59
2	B	901	UDP	PA-O3A	2.59	1.62	1.59
3	B	902	FRU	O2-C2	2.35	1.44	1.40
3	H	902	FRU	O2-C2	2.24	1.44	1.40
2	F	901	UDP	PA-O3A	2.11	1.61	1.59
3	C	902	FRU	O2-C2	2.04	1.44	1.40
2	E	901	UDP	C5-C4	-2.03	1.39	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	UDP	C4-N3-C2	-7.01	117.90	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	UDP	C4-N3-C2	-6.77	118.20	126.61
2	D	901	UDP	C4-N3-C2	-6.74	118.25	126.61
2	H	901	UDP	C4-N3-C2	-6.47	118.58	126.61
2	A	901	UDP	C4-N3-C2	-6.41	118.65	126.61
2	C	901	UDP	C4-N3-C2	-5.64	119.61	126.61
2	G	901	UDP	C4-N3-C2	-5.56	119.71	126.61
2	E	901	UDP	C4-N3-C2	-5.10	120.29	126.61
2	B	901	UDP	N3-C2-N1	4.96	121.35	114.89
2	F	901	UDP	N3-C2-N1	4.91	121.28	114.89
2	D	901	UDP	N3-C2-N1	4.73	121.05	114.89
2	A	901	UDP	N3-C2-N1	4.50	120.75	114.89
2	C	901	UDP	N3-C2-N1	4.22	120.39	114.89
2	G	901	UDP	N3-C2-N1	4.14	120.29	114.89
2	D	901	UDP	C5-C4-N3	4.14	120.59	114.80
2	A	901	UDP	C5-C4-N3	4.07	120.50	114.80
2	H	901	UDP	N3-C2-N1	4.07	120.19	114.89
2	E	901	UDP	N3-C2-N1	4.06	120.18	114.89
2	F	901	UDP	C5-C4-N3	4.03	120.45	114.80
2	B	901	UDP	C5-C4-N3	3.82	120.15	114.80
2	E	901	UDP	O2-C2-N1	-3.62	118.08	122.80
2	G	901	UDP	C5-C4-N3	3.53	119.74	114.80
2	H	901	UDP	C5-C4-N3	3.51	119.71	114.80
2	C	901	UDP	C5-C4-N3	3.18	119.26	114.80
2	E	901	UDP	C5-C4-N3	3.11	119.16	114.80
2	H	901	UDP	O4-C4-C5	-3.11	119.81	125.16
2	D	901	UDP	O2-C2-N1	-3.10	118.76	122.80
2	G	901	UDP	O2-C2-N1	-2.92	118.99	122.80
2	C	901	UDP	O2-C2-N1	-2.87	119.06	122.80
2	A	901	UDP	O2-C2-N1	-2.84	119.10	122.80
2	G	901	UDP	O4-C4-C5	-2.83	120.27	125.16
2	C	901	UDP	O4-C4-C5	-2.79	120.36	125.16
2	B	901	UDP	C5-C6-N1	-2.78	117.31	121.84
2	D	901	UDP	O4-C4-C5	-2.69	120.53	125.16
2	F	901	UDP	O2-C2-N1	-2.67	119.32	122.80
2	H	901	UDP	O2-C2-N1	-2.61	119.40	122.80
2	H	901	UDP	C5-C6-N1	-2.57	117.66	121.84
2	B	901	UDP	O2-C2-N1	-2.55	119.47	122.80
2	B	901	UDP	O4-C4-C5	-2.45	120.93	125.16
2	F	901	UDP	O2A-PA-O3A	2.45	113.89	107.27
2	F	901	UDP	C5-C6-N1	-2.43	117.88	121.84
2	E	901	UDP	O4-C4-C5	-2.39	121.05	125.16
2	E	901	UDP	O2A-PA-O3A	2.24	113.33	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	UDP	O4-C4-C5	-2.21	121.36	125.16
3	D	902	FRU	O2-C2-O5	-2.20	105.11	109.33
2	C	901	UDP	O2A-PA-O3A	2.19	113.19	107.27
2	D	901	UDP	O2A-PA-O3A	2.17	113.14	107.27
2	C	901	UDP	O3B-PB-O3A	2.17	111.91	104.64
2	A	901	UDP	C5-C6-N1	-2.17	118.32	121.84
2	A	901	UDP	O4-C4-C5	-2.15	121.45	125.16
5	G	921	MLA	O3B-C3-C2	2.11	121.05	114.51
2	F	901	UDP	O2B-PB-O3A	2.10	111.69	104.64
5	C	921	MLA	O3B-C3-C2	2.08	120.95	114.51
2	G	901	UDP	O2A-PA-O3A	2.06	112.83	107.27
5	A	921	MLA	O1A-C1-C2	2.04	120.83	114.51
3	D	902	FRU	O1-C1-C2	2.04	116.18	111.67
2	B	901	UDP	O2B-PB-O3A	2.03	111.46	104.64

There are no chirality outliers.

All (70) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	F	901	UDP	O4'-C4'-C5'-O5'
2	E	901	UDP	O4'-C4'-C5'-O5'
2	F	901	UDP	C3'-C4'-C5'-O5'
3	B	902	FRU	O1-C1-C2-O5
2	E	901	UDP	PA-O3A-PB-O1B
2	E	901	UDP	C3'-C4'-C5'-O5'
5	C	921	MLA	O1A-C1-C2-C3
5	D	921	MLA	O1B-C1-C2-C3
3	A	902	FRU	O1-C1-C2-C3
3	G	902	FRU	O1-C1-C2-C3
2	D	901	UDP	O4'-C4'-C5'-O5'
2	A	901	UDP	PB-O3A-PA-O5'
2	E	901	UDP	PB-O3A-PA-O5'
2	C	901	UDP	PA-O3A-PB-O2B
2	D	901	UDP	PA-O3A-PB-O3B
2	E	901	UDP	PA-O3A-PB-O2B
5	C	921	MLA	O1B-C1-C2-C3
3	H	902	FRU	O5-C5-C6-O6
2	G	901	UDP	PB-O3A-PA-O2A
2	H	901	UDP	O4'-C4'-C5'-O5'
3	H	902	FRU	C4-C5-C6-O6
3	B	902	FRU	O1-C1-C2-C3
3	E	902	FRU	O1-C1-C2-C3
2	B	901	UDP	C5'-O5'-PA-O1A
2	C	901	UDP	C5'-O5'-PA-O1A
2	G	901	UDP	C5'-O5'-PA-O2A
2	G	901	UDP	C5'-O5'-PA-O3A
2	H	901	UDP	C5'-O5'-PA-O1A
2	D	901	UDP	C3'-C4'-C5'-O5'
2	G	901	UDP	O4'-C4'-C5'-O5'
5	D	921	MLA	O1A-C1-C2-C3
2	H	901	UDP	C3'-C4'-C5'-O5'
3	C	902	FRU	O5-C5-C6-O6
2	B	901	UDP	PA-O3A-PB-O1B
2	C	901	UDP	PA-O3A-PB-O1B
2	H	901	UDP	PA-O3A-PB-O1B
2	B	901	UDP	PA-O3A-PB-O2B
2	H	901	UDP	PA-O3A-PB-O2B
2	G	901	UDP	PB-O3A-PA-O1A
3	D	902	FRU	C4-C5-C6-O6
2	G	901	UDP	C3'-C4'-C5'-O5'
5	A	921	MLA	C1-C2-C3-O3B

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Mol	Chain	Res	Type	Atoms
2	F	901	UDP	PA-O3A-PB-O1B
5	A	921	MLA	C1-C2-C3-O3A
2	B	901	UDP	O4'-C4'-C5'-O5'
3	D	902	FRU	O5-C5-C6-O6
3	C	902	FRU	C4-C5-C6-O6

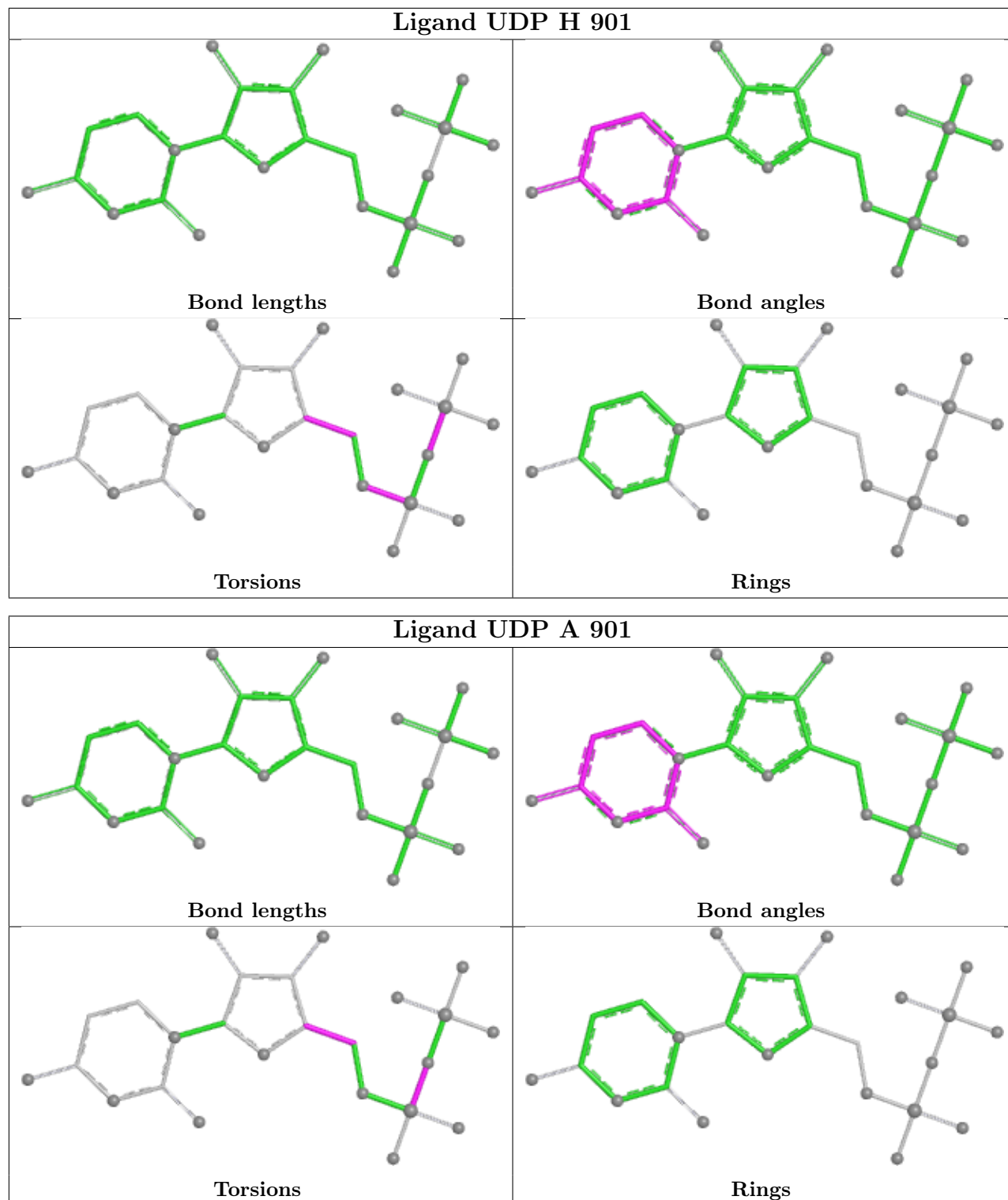
There are no ring outliers.

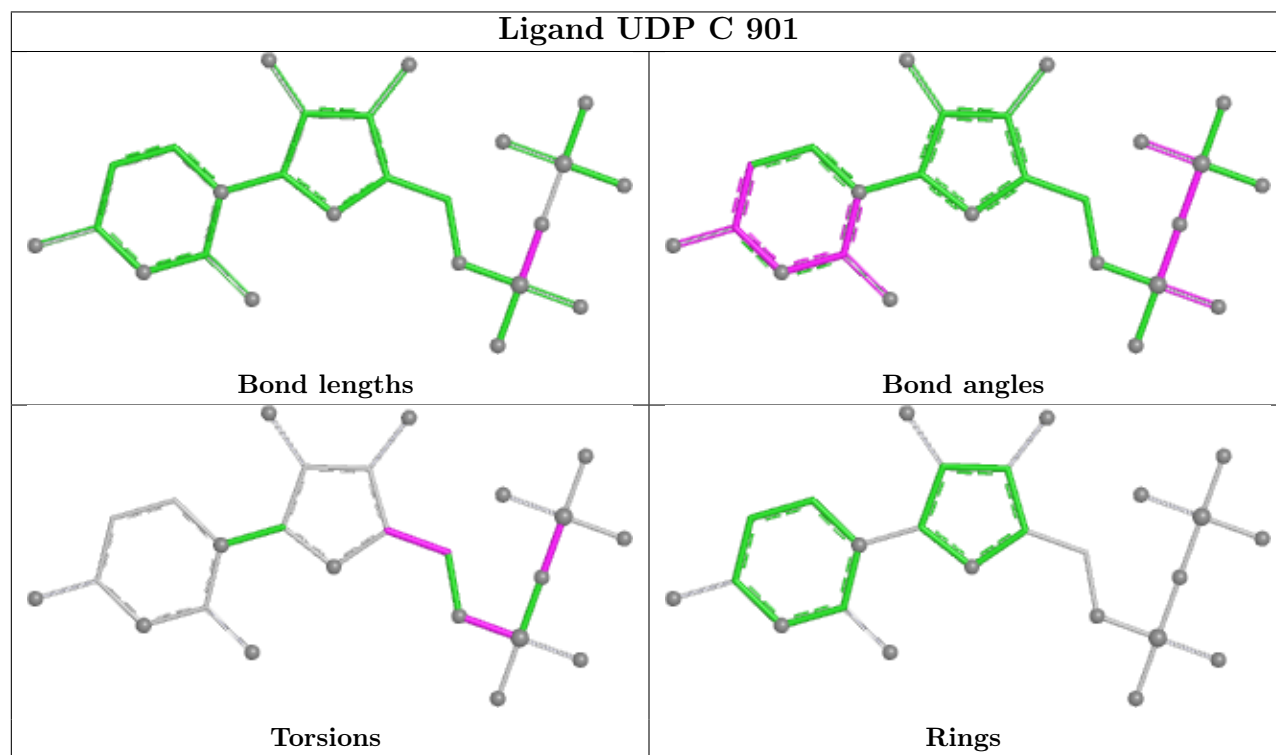
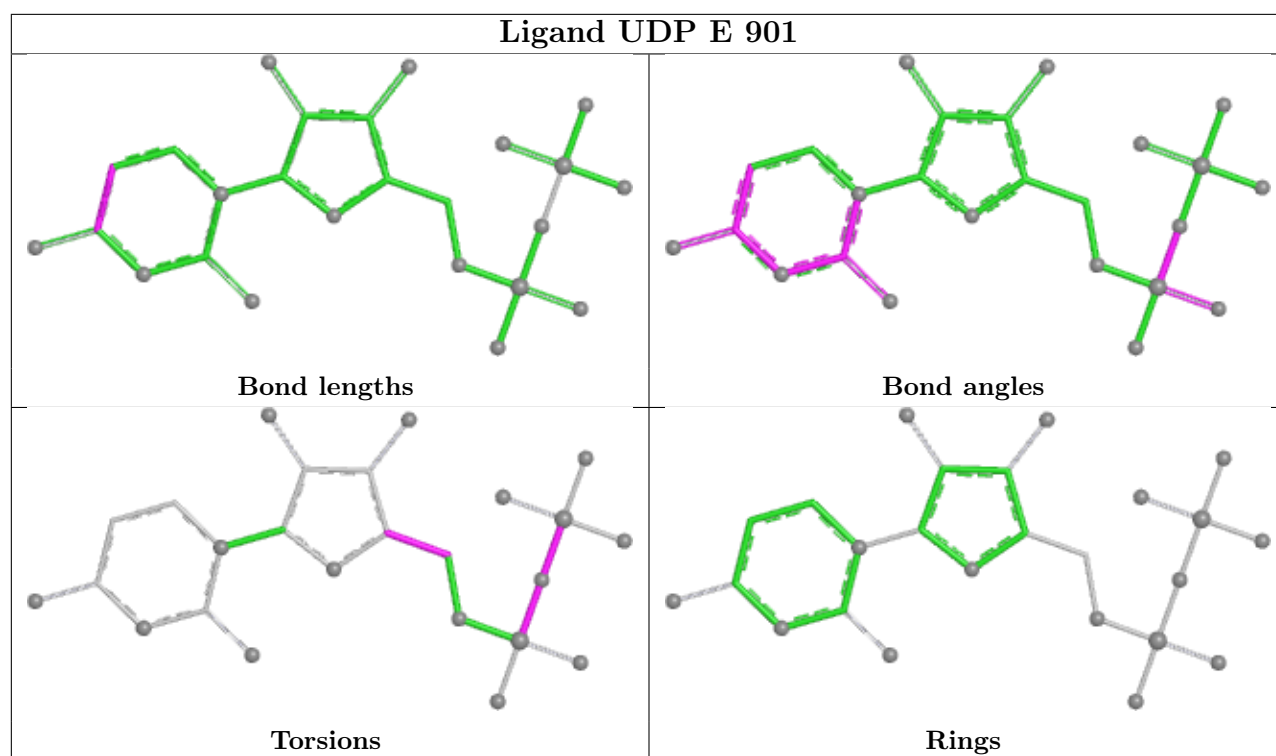
20 monomers are involved in 33 short contacts:

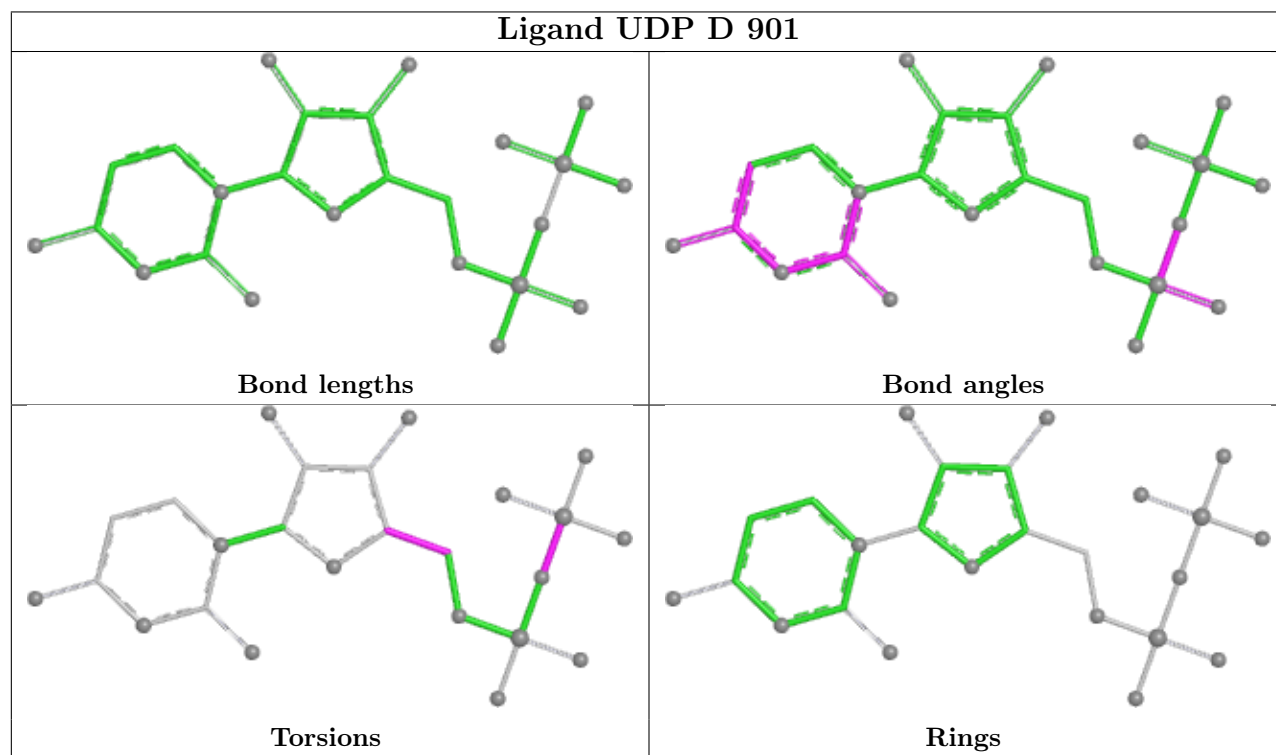
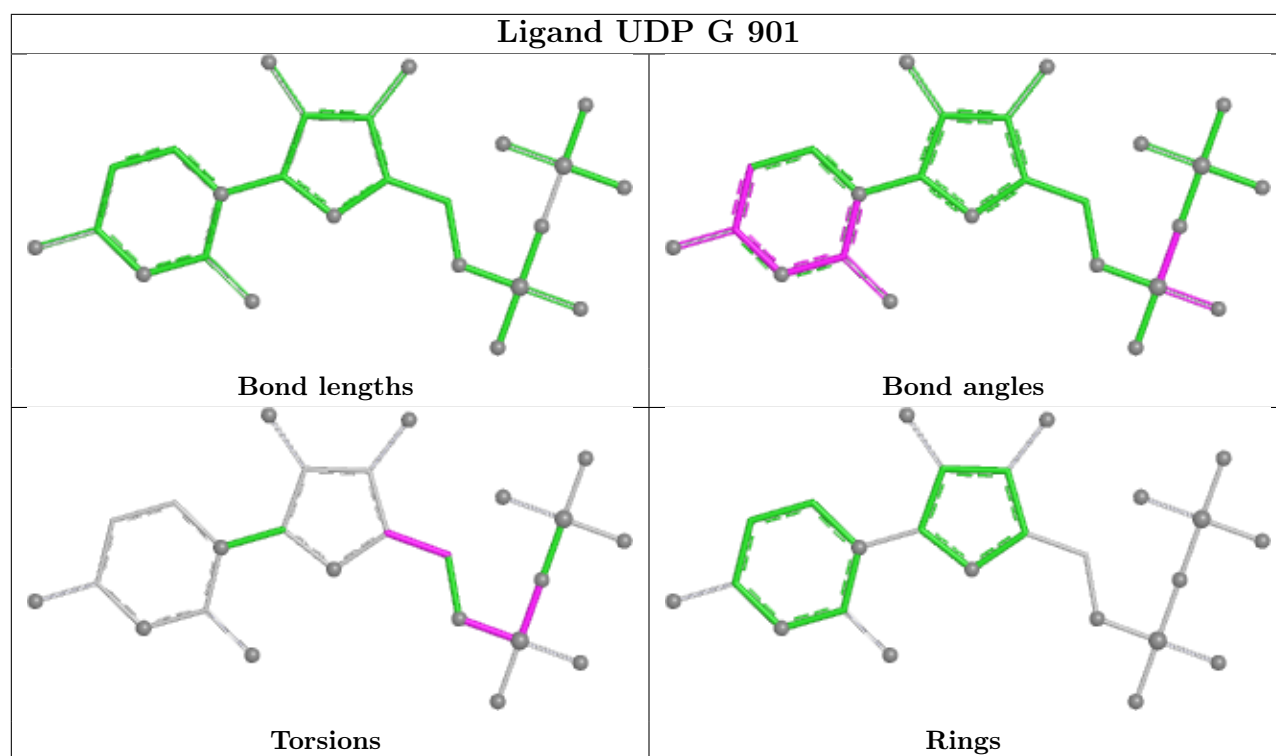
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	901	UDP	4	0
2	C	901	UDP	1	0
3	F	902	FRU	1	0
2	G	901	UDP	1	0
2	D	901	UDP	2	0
4	F	913	SO4	2	0
5	E	921	MLA	5	0
3	H	902	FRU	1	0
3	A	902	FRU	1	0
4	E	912	SO4	1	0
3	E	902	FRU	1	0
2	F	901	UDP	1	0
3	C	902	FRU	1	0
5	B	921	MLA	1	0
3	G	902	FRU	4	0
4	B	912	SO4	1	0
4	G	913	SO4	1	0
4	H	913	SO4	1	0
4	A	913	SO4	1	0
4	B	913	SO4	2	0

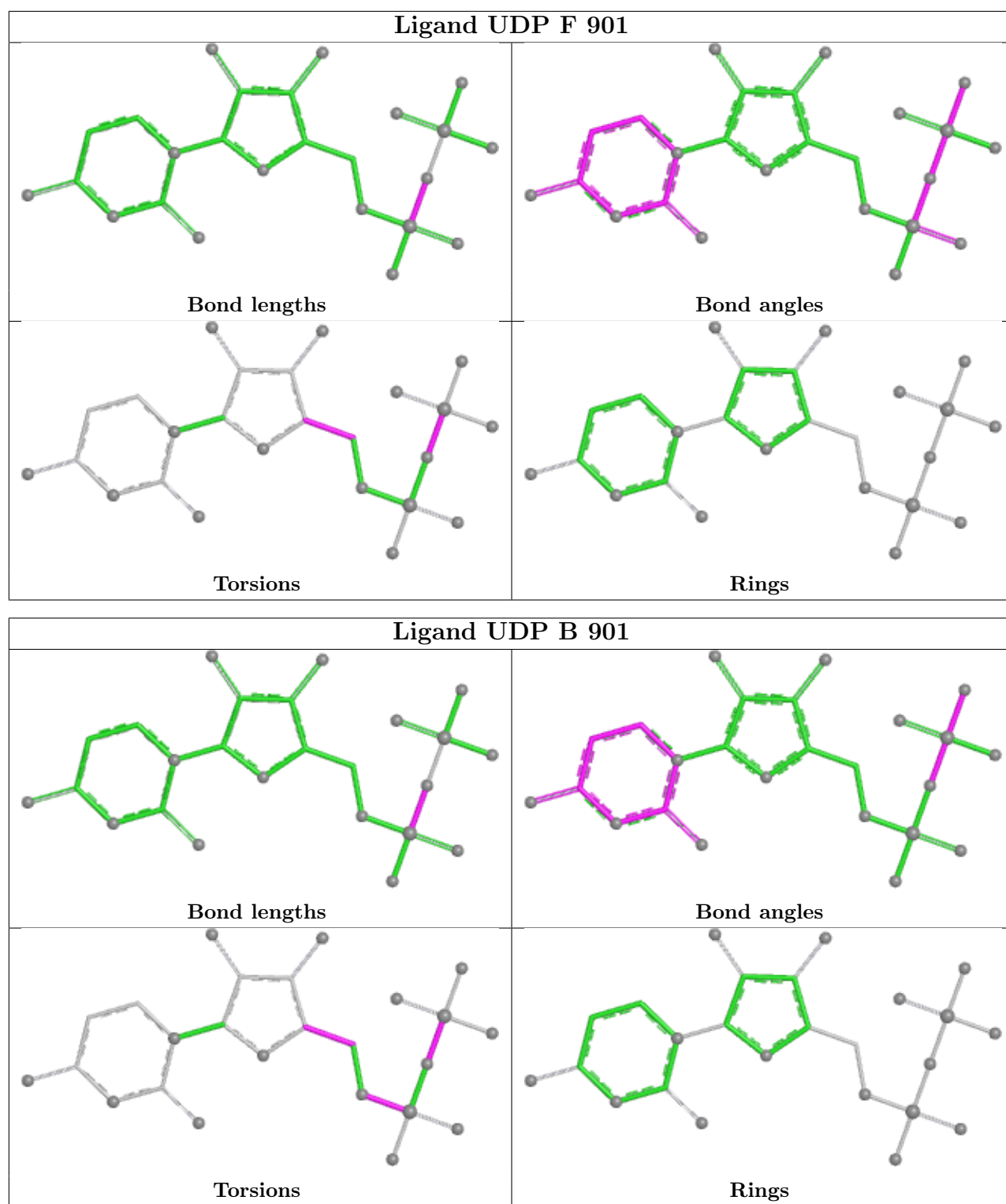
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	769/816 (94%)	-0.34	38 (4%) 36 31	13, 27, 90, 116	0
1	B	781/816 (95%)	0.01	82 (10%) 13 12	16, 33, 98, 131	0
1	C	769/816 (94%)	-0.20	24 (3%) 51 46	20, 38, 83, 122	0
1	D	769/816 (94%)	-0.36	34 (4%) 39 34	14, 28, 80, 111	0
1	E	769/816 (94%)	-0.28	42 (5%) 32 28	14, 30, 95, 118	0
1	F	769/816 (94%)	-0.38	29 (3%) 44 38	10, 26, 73, 111	0
1	G	769/816 (94%)	-0.39	19 (2%) 58 52	14, 30, 70, 108	0
1	H	785/816 (96%)	-0.04	75 (9%) 15 13	17, 35, 92, 117	0
All	All	6180/6528 (94%)	-0.25	343 (5%) 31 27	10, 31, 87, 131	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	VAL	7.0
1	B	86	VAL	6.7
1	H	23	VAL	6.4
1	H	103	ASN	6.3
1	H	86	VAL	6.1
1	A	30	LEU	6.0
1	H	18	LEU	6.0
1	H	56	LEU	5.5
1	B	51	ALA	5.5
1	E	29	VAL	5.3
1	D	71	ASP	5.3
1	B	104	LEU	5.3
1	H	21	THR	5.2
1	B	35	ARG	5.2
1	H	84	PRO	5.1
1	B	34	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	109	VAL	4.9
1	H	104	LEU	4.9
1	B	50	ILE	4.9
1	B	21	THR	4.9
1	E	35	ARG	4.9
1	H	68	PRO	4.9
1	E	44	LEU	4.8
1	H	85	TRP	4.8
1	H	57	PRO	4.8
1	B	68	PRO	4.8
1	H	130	ASN	4.7
1	G	69	PHE	4.7
1	D	42	GLY	4.6
1	H	29	VAL	4.6
1	B	56	LEU	4.6
1	E	33	LEU	4.6
1	H	22	LEU	4.5
1	E	56	LEU	4.5
1	H	59	GLN	4.5
1	C	29	VAL	4.5
1	B	22	LEU	4.5
1	H	108	VAL	4.4
1	A	29	VAL	4.4
1	B	83	PRO	4.4
1	B	85	TRP	4.4
1	A	44	LEU	4.4
1	B	26	ARG	4.4
1	H	69	PHE	4.4
1	E	30	LEU	4.3
1	H	74	LYS	4.3
1	B	84	PRO	4.2
1	H	34	SER	4.2
1	E	50	ILE	4.1
1	B	87	ALA	4.1
1	E	71	ASP	4.1
1	E	49	ILE	4.1
1	D	49	ILE	4.0
1	B	102	VAL	4.0
1	H	55	ALA	4.0
1	C	52	GLU	4.0
1	H	102	VAL	4.0
1	H	129	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	68	PRO	4.0
1	B	45	GLN	4.0
1	H	70	PHE	4.0
1	B	60	THR	3.9
1	B	28	GLU	3.9
1	E	51	ALA	3.9
1	F	29	VAL	3.9
1	H	51	ALA	3.9
1	B	73	LEU	3.9
1	H	82	LEU	3.9
1	H	60	THR	3.9
1	B	69	PHE	3.9
1	B	27	ASN	3.9
1	D	51	ALA	3.8
1	C	44	LEU	3.8
1	C	49	ILE	3.8
1	H	26	ARG	3.8
1	E	43	ILE	3.8
1	H	83	PRO	3.8
1	D	72	LEU	3.8
1	H	30	LEU	3.8
1	G	129	LYS	3.7
1	H	11	VAL	3.7
1	A	62	LYS	3.7
1	A	64	LEU	3.7
1	A	31	ALA	3.7
1	C	69	PHE	3.6
1	D	107	LEU	3.6
1	F	46	GLN	3.6
1	B	49	ILE	3.6
1	H	49	ILE	3.6
1	H	17	ARG	3.6
1	G	70	PHE	3.6
1	C	58	GLU	3.6
1	B	18	LEU	3.6
1	G	29	VAL	3.6
1	B	32	LEU	3.6
1	B	29	VAL	3.5
1	C	60	THR	3.5
1	G	51	ALA	3.5
1	B	16	GLU	3.5
1	B	65	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	71	ASP	3.5
1	E	59	GLN	3.5
1	E	31	ALA	3.5
1	E	57	PRO	3.5
1	B	17	ARG	3.5
1	B	48	GLN	3.4
1	D	46	GLN	3.4
1	B	43	ILE	3.4
1	F	66	GLY	3.4
1	C	73	LEU	3.4
1	D	30	LEU	3.4
1	E	32	LEU	3.4
1	G	44	LEU	3.4
1	A	57	PRO	3.4
1	B	38	ALA	3.4
1	B	57	PRO	3.4
1	E	72	LEU	3.4
1	F	144	ALA	3.4
1	E	70	PHE	3.4
1	D	29	VAL	3.4
1	A	104	LEU	3.3
1	C	70	PHE	3.3
1	F	65	GLU	3.3
1	B	24	SER	3.3
1	C	68	PRO	3.3
1	D	57	PRO	3.3
1	B	55	ALA	3.2
1	D	59	GLN	3.2
1	F	58	GLU	3.2
1	D	69	PHE	3.2
1	H	73	LEU	3.2
1	B	58	GLU	3.2
1	H	78	GLU	3.2
1	H	87	ALA	3.2
1	H	128	VAL	3.2
1	E	103	ASN	3.2
1	E	60	THR	3.2
1	H	58	GLU	3.2
1	B	89	ALA	3.1
1	A	72	LEU	3.1
1	B	90	VAL	3.1
1	D	32	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	64	LEU	3.1
1	E	46	GLN	3.1
1	D	55	ALA	3.1
1	B	30	LEU	3.1
1	F	128	VAL	3.1
1	D	175	GLU	3.1
1	D	31	ALA	3.1
1	F	56	LEU	3.1
1	A	82	LEU	3.1
1	E	63	LYS	3.1
1	B	101	ARG	3.0
1	H	52	GLU	3.0
1	H	35	ARG	3.0
1	A	49	ILE	3.0
1	D	128	VAL	3.0
1	G	59	GLN	3.0
1	H	66	GLY	3.0
1	H	27	ASN	3.0
1	A	56	LEU	3.0
1	F	33	LEU	3.0
1	E	52	GLU	3.0
1	E	62	LYS	3.0
1	A	69	PHE	3.0
1	F	70	PHE	3.0
1	B	88	LEU	3.0
1	B	112	LEU	3.0
1	H	90	VAL	3.0
1	E	68	PRO	2.9
1	G	68	PRO	2.9
1	H	50	ILE	2.9
1	B	106	ALA	2.9
1	F	63	LYS	2.9
1	H	109	VAL	2.9
1	B	39	LYS	2.9
1	B	625	GLU	2.9
1	H	16	GLU	2.9
1	A	67	GLY	2.8
1	E	64	LEU	2.8
1	B	20	GLU	2.8
1	A	70	PHE	2.8
1	B	191	GLY	2.8
1	D	65	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	52	GLU	2.8
1	A	66	GLY	2.8
1	A	46	GLN	2.8
1	B	113	GLN	2.8
1	F	59	GLN	2.8
1	H	106	ALA	2.8
1	A	143	ASN	2.8
1	G	103	ASN	2.8
1	A	63	LYS	2.8
1	C	62	LYS	2.8
1	B	103	ASN	2.7
1	B	59	GLN	2.7
1	A	86	VAL	2.7
1	B	81	VAL	2.7
1	B	108	VAL	2.7
1	H	630	TYR	2.7
1	D	56	LEU	2.7
1	G	56	LEU	2.7
1	G	130	ASN	2.7
1	E	190	GLN	2.7
1	A	71	ASP	2.7
1	B	105	HIS	2.7
1	A	84	PRO	2.7
1	B	46	GLN	2.7
1	D	62	LYS	2.7
1	F	44	LEU	2.7
1	A	68	PRO	2.7
1	E	104	LEU	2.6
1	H	72	LEU	2.6
1	B	53	PHE	2.6
1	D	60	THR	2.6
1	E	61	ARG	2.6
1	E	36	VAL	2.6
1	E	106	ALA	2.6
1	A	59	GLN	2.6
1	D	105	HIS	2.6
1	H	15	ARG	2.6
1	A	43	ILE	2.6
1	C	43	ILE	2.6
1	F	53	PHE	2.6
1	B	107	LEU	2.6
1	E	66	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	35	ARG	2.6
1	B	75	SER	2.6
1	B	64	LEU	2.6
1	H	43	ILE	2.5
1	B	77	GLN	2.5
1	H	14	GLN	2.5
1	B	47	ASN	2.5
1	F	62	LYS	2.5
1	D	54	GLU	2.5
1	C	107	LEU	2.5
1	B	126	ASP	2.5
1	B	143	ASN	2.5
1	C	28	GLU	2.5
1	B	76	THR	2.5
1	H	112	LEU	2.5
1	D	143	ASN	2.5
1	B	79	ALA	2.5
1	C	129	LYS	2.5
1	F	778	LEU	2.5
1	G	128	VAL	2.5
1	H	13	SER	2.4
1	B	72	LEU	2.4
1	D	64	LEU	2.4
1	F	82	LEU	2.4
1	C	128	VAL	2.4
1	A	103	ASN	2.4
1	H	19	ASN	2.4
1	G	50	ILE	2.4
1	F	69	PHE	2.4
1	G	46	GLN	2.4
1	C	32	LEU	2.4
1	H	105	HIS	2.4
1	E	58	GLU	2.4
1	B	144	ALA	2.4
1	D	103	ASN	2.4
1	B	70	PHE	2.4
1	D	68	PRO	2.4
1	H	24	SER	2.4
1	A	33	LEU	2.4
1	B	19	ASN	2.4
1	B	33	LEU	2.4
1	B	131	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	50	ILE	2.4
1	F	60	THR	2.4
1	F	107	LEU	2.3
1	G	72	LEU	2.3
1	B	42	GLY	2.3
1	H	53	PHE	2.3
1	G	60	THR	2.3
1	E	65	GLU	2.3
1	A	53	PHE	2.3
1	H	38	ALA	2.3
1	A	60	THR	2.3
1	D	129	LYS	2.3
1	D	43	ILE	2.3
1	F	49	ILE	2.3
1	H	25	GLU	2.3
1	H	31	ALA	2.3
1	H	75	SER	2.3
1	A	73	LEU	2.3
1	E	74	LYS	2.3
1	A	85	TRP	2.3
1	D	491	GLU	2.3
1	E	28	GLU	2.3
1	H	54	GLU	2.3
1	F	35	ARG	2.3
1	H	32	LEU	2.3
1	H	44	LEU	2.3
1	H	76	THR	2.3
1	H	134	THR	2.3
1	F	43	ILE	2.2
1	H	133	PHE	2.2
1	B	62	LYS	2.2
1	C	57	PRO	2.2
1	A	27	ASN	2.2
1	A	42	GLY	2.2
1	C	66	GLY	2.2
1	C	103	ASN	2.2
1	E	105	HIS	2.2
1	B	110	GLU	2.2
1	F	51	ALA	2.2
1	E	82	LEU	2.2
1	G	33	LEU	2.2
1	H	33	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	129	LYS	2.2
1	E	84	PRO	2.2
1	B	63	LYS	2.2
1	H	62	LYS	2.2
1	A	61	ARG	2.2
1	D	630	TYR	2.2
1	H	126	ASP	2.2
1	B	31	ALA	2.1
1	B	100	LEU	2.1
1	F	50	ILE	2.1
1	B	128	VAL	2.1
1	A	105	HIS	2.1
1	C	71	ASP	2.1
1	E	73	LEU	2.1
1	H	107	LEU	2.1
1	A	144	ALA	2.1
1	C	51	ALA	2.1
1	E	55	ALA	2.1
1	B	630	TYR	2.1
1	A	52	GLU	2.1
1	H	132	ASN	2.1
1	C	630	TYR	2.1
1	D	58	GLU	2.1
1	D	36	VAL	2.1
1	E	40	GLY	2.1
1	E	69	PHE	2.1
1	F	64	LEU	2.0
1	B	80	ILE	2.0
1	C	27	ASN	2.0
1	A	630	TYR	2.0
1	H	28	GLU	2.0
1	H	111	GLU	2.0
1	H	42	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	K	F	931	1/1	0.79	0.11	69,69,69,69	0
4	SO4	C	913	5/5	0.80	0.24	63,74,75,89	0
4	SO4	C	912	5/5	0.81	0.26	71,74,96,104	0
4	SO4	B	913	5/5	0.83	0.28	53,54,65,78	0
4	SO4	H	913	5/5	0.83	0.33	64,70,86,101	0
4	SO4	B	912	5/5	0.83	0.24	49,67,79,88	0
4	SO4	H	912	5/5	0.85	0.25	63,66,76,94	0
6	K	E	931	1/1	0.86	0.11	64,64,64,64	0
5	MLA	G	921	7/7	0.86	0.14	46,49,59,59	0
5	MLA	C	921	7/7	0.87	0.19	56,60,68,77	0
4	SO4	D	912	5/5	0.88	0.20	54,74,96,98	0
4	SO4	E	912	5/5	0.88	0.23	47,55,63,84	0
6	K	C	931	1/1	0.89	0.10	69,69,69,69	0
4	SO4	G	912	5/5	0.89	0.24	48,67,72,86	0
4	SO4	G	913	5/5	0.89	0.16	52,58,68,74	0
6	K	B	931	1/1	0.90	0.09	74,74,74,74	0
3	FRU	C	902	12/12	0.90	0.18	30,36,44,50	0
4	SO4	F	911	5/5	0.91	0.21	32,36,45,64	0
4	SO4	F	912	5/5	0.91	0.16	46,50,62,76	0
4	SO4	A	912	5/5	0.92	0.15	47,55,59,81	0
5	MLA	H	921	7/7	0.92	0.17	53,58,69,69	0
3	FRU	H	902	12/12	0.92	0.12	22,29,34,37	0
5	MLA	D	921	7/7	0.92	0.18	33,40,44,47	0
5	MLA	E	921	7/7	0.92	0.17	34,38,43,43	0
5	MLA	F	921	7/7	0.92	0.13	30,35,36,36	0
4	SO4	E	911	5/5	0.93	0.17	31,35,59,60	0
6	K	A	931	1/1	0.93	0.08	61,61,61,61	0
4	SO4	B	911	5/5	0.93	0.15	37,42,50,70	0
3	FRU	B	902	12/12	0.93	0.12	25,30,35,35	0
3	FRU	D	902	12/12	0.93	0.10	18,25,31,32	0
5	MLA	A	921	7/7	0.93	0.12	27,31,34,36	0
4	SO4	A	913	5/5	0.94	0.20	42,44,52,59	0
3	FRU	E	902	12/12	0.94	0.10	18,25,30,32	0
4	SO4	F	913	5/5	0.94	0.20	40,44,61,64	0
4	SO4	D	911	5/5	0.94	0.17	38,41,56,67	0
4	SO4	A	911	5/5	0.94	0.20	31,35,46,58	0
4	SO4	D	913	5/5	0.94	0.16	44,46,53,63	0

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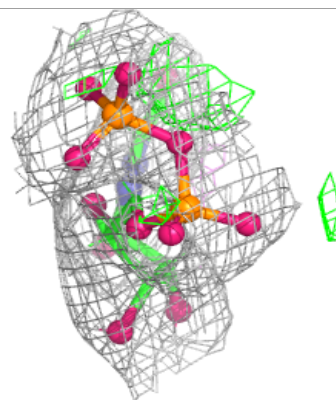
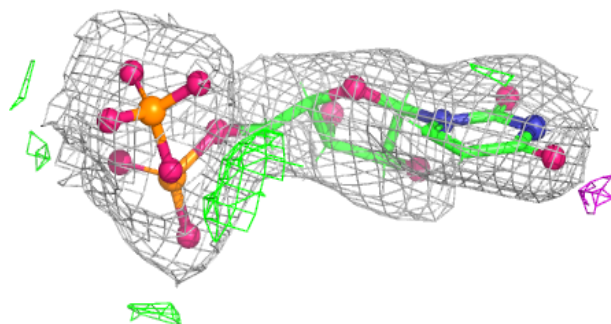
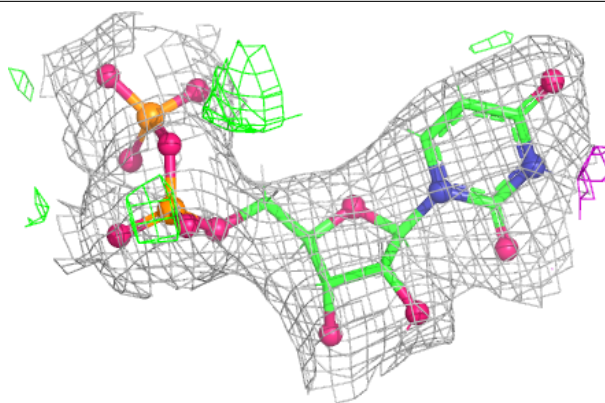
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FRU	G	902	12/12	0.94	0.11	18,25,34,34	0
4	SO4	C	911	5/5	0.94	0.16	44,46,57,63	0
6	K	D	931	1/1	0.94	0.10	61,61,61,61	0
5	MLA	B	921	7/7	0.94	0.12	38,45,50,53	0
4	SO4	E	913	5/5	0.94	0.20	44,47,62,71	0
4	SO4	G	911	5/5	0.95	0.20	32,40,56,64	0
4	SO4	H	911	5/5	0.95	0.16	37,38,69,70	0
6	K	H	931	1/1	0.95	0.07	61,61,61,61	0
3	FRU	F	902	12/12	0.96	0.12	17,22,28,35	0
6	K	G	931	1/1	0.96	0.08	57,57,57,57	0
3	FRU	A	902	12/12	0.96	0.10	16,22,27,28	0
2	UDP	B	901	25/25	0.98	0.06	19,25,30,34	0
2	UDP	C	901	25/25	0.98	0.05	21,31,40,42	0
2	UDP	F	901	25/25	0.98	0.05	14,18,23,25	0
2	UDP	H	901	25/25	0.98	0.06	22,28,36,38	0
2	UDP	E	901	25/25	0.99	0.04	17,21,27,29	0
2	UDP	A	901	25/25	0.99	0.04	14,17,21,24	0
2	UDP	G	901	25/25	0.99	0.05	14,21,25,35	0
2	UDP	D	901	25/25	0.99	0.04	17,21,25,30	0

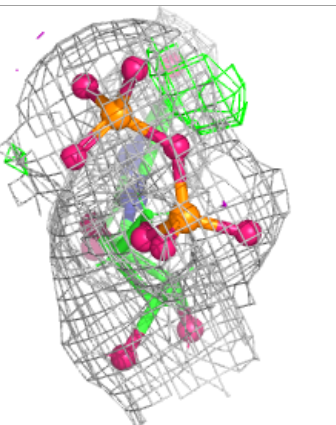
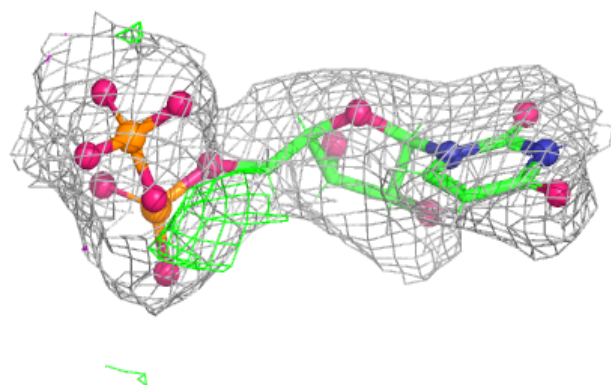
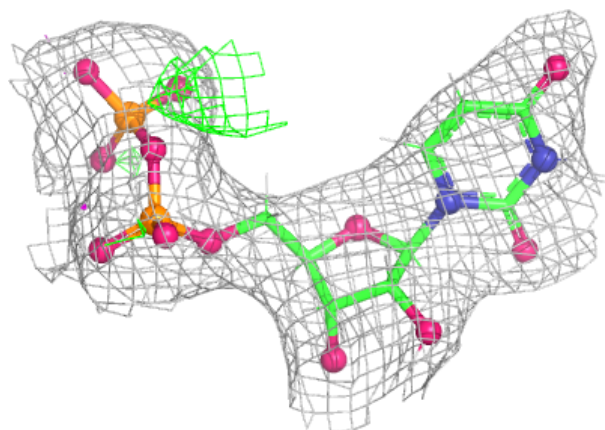
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

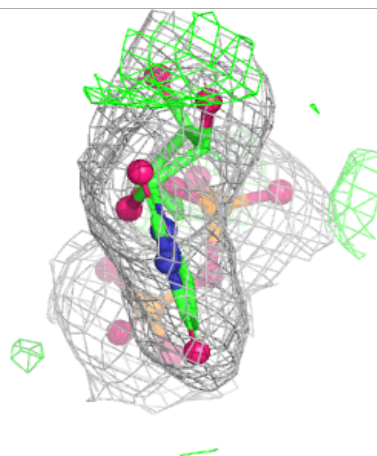
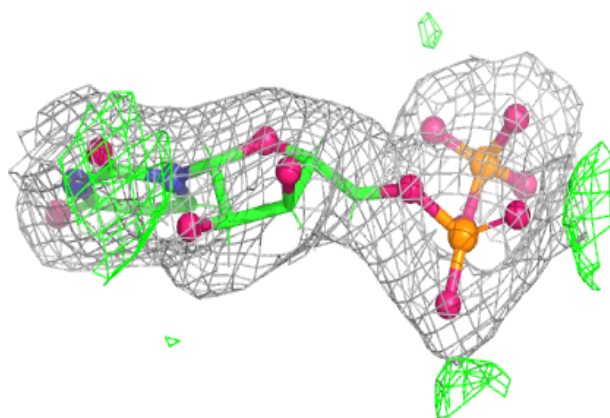
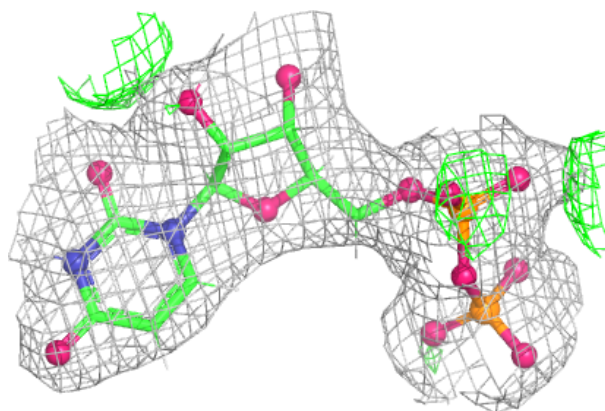
**Electron density around UDP C 901:**

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



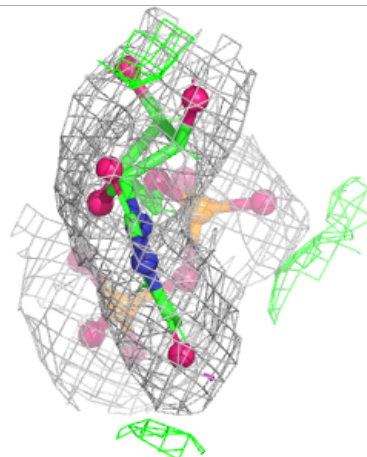
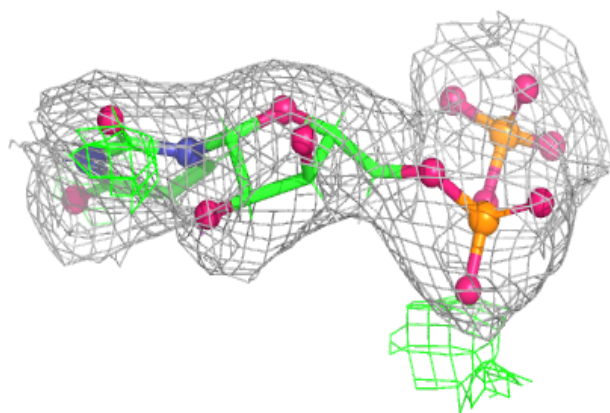
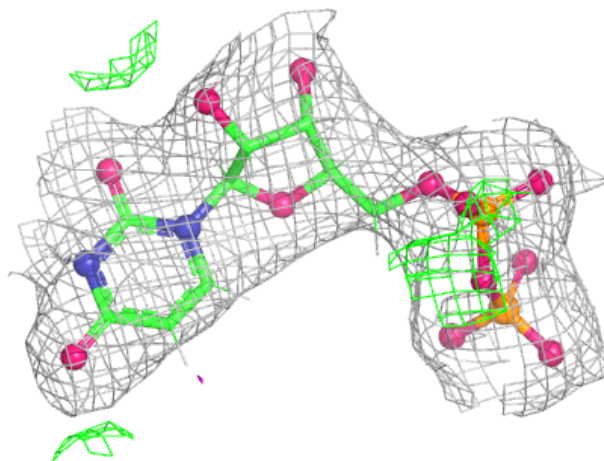
Electron density around UDP F 901:

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



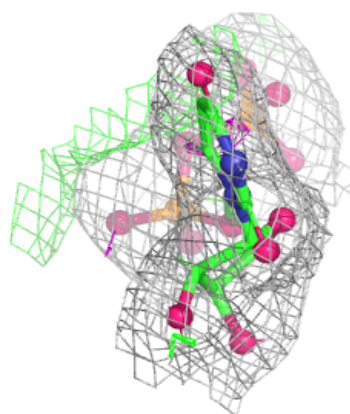
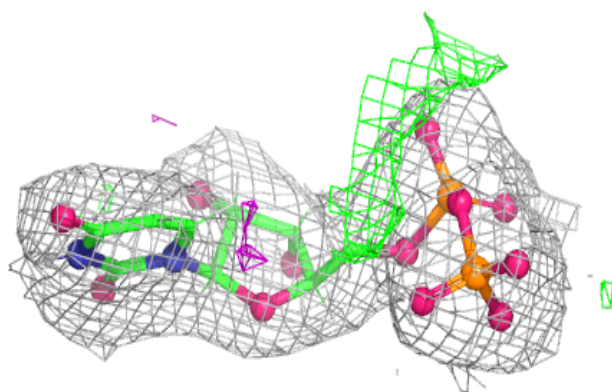
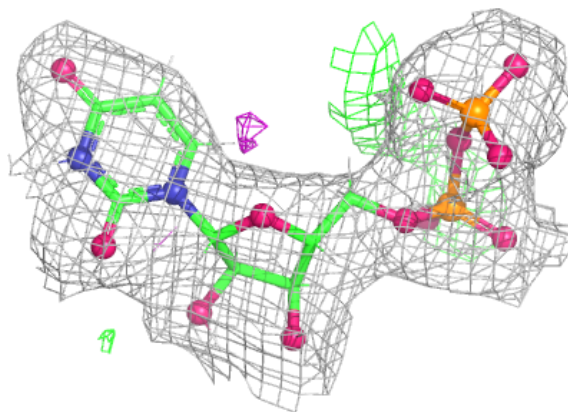
Electron density around UDP H 901:

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



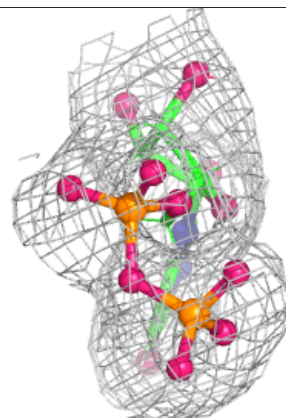
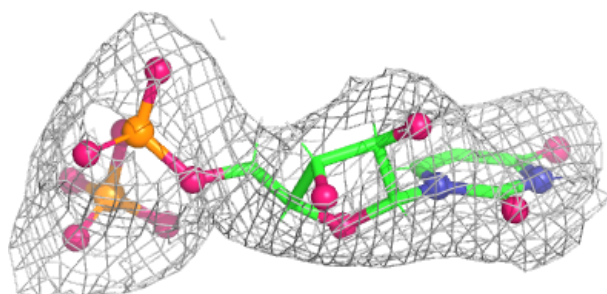
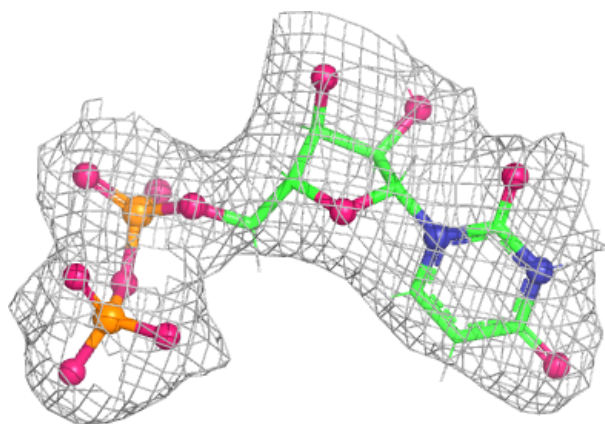
Electron density around UDP E 901:

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



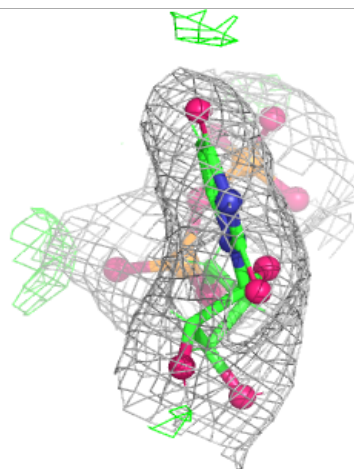
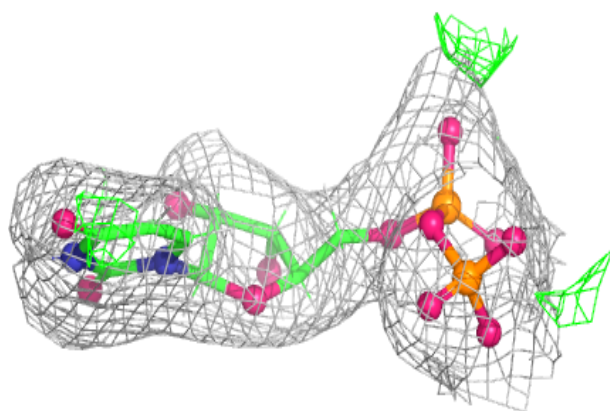
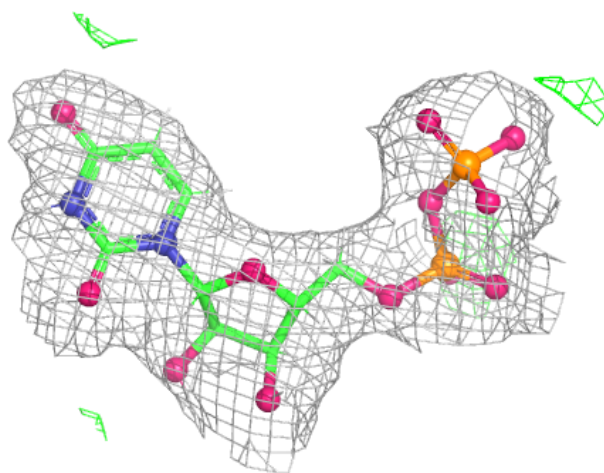
Electron density around UDP A 901:

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



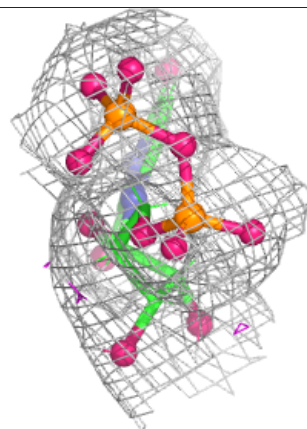
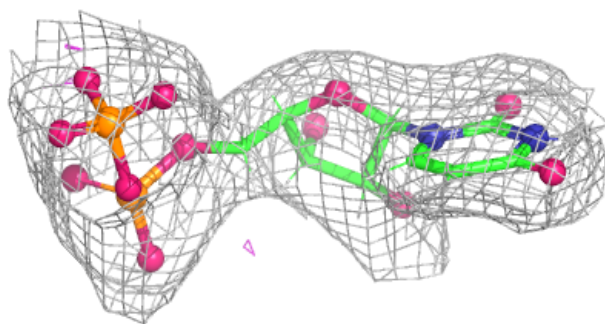
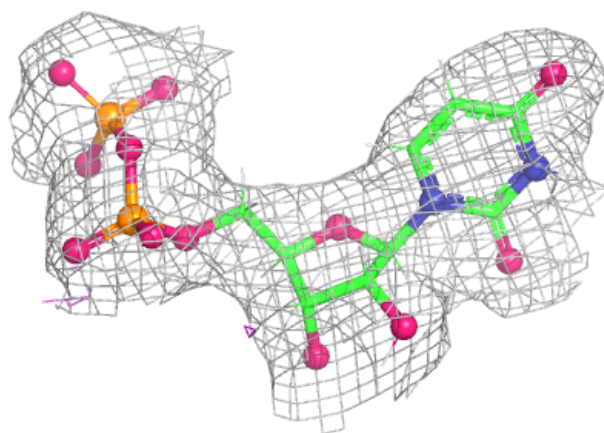
Electron density around UDP G 901:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.