



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:44 PM UTC

PDB ID : 9F3Y / pdb_00009f3y
Title : CutC choline lyase in complex with difluorocholine
Authors : Kalnins, G.
Deposited on : 2024-04-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

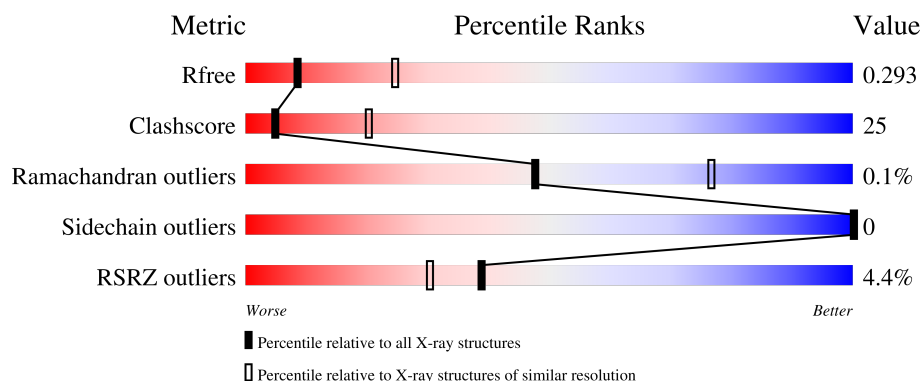
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



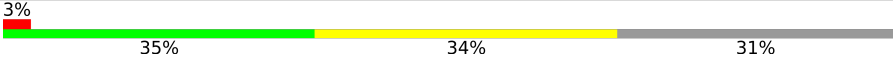
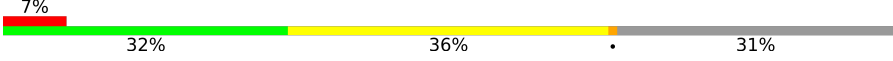
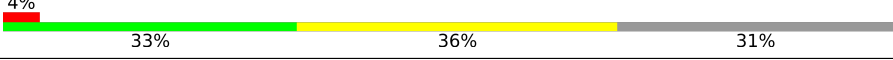
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1150	45% 24% 31%
1	B	1150	43% 25% 31%
1	C	1150	39% 30% 31%
1	D	1150	37% 31% 31%
1	E	1150	35% 33% 31%

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Mol	Chain	Length	Quality of chain
1	F	1150	 3% 35% 34% 31%
1	G	1150	 7% 32% 36% 31%
1	H	1150	 4% 33% 36% 31%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 50317 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Choline trimethylamine-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	B	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	C	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	D	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	E	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	F	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	G	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	H	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A486V7R5
A	-20	GLY	-	expression tag	UNP A0A486V7R5
A	-19	SER	-	expression tag	UNP A0A486V7R5
A	-18	SER	-	expression tag	UNP A0A486V7R5
A	-17	HIS	-	expression tag	UNP A0A486V7R5
A	-16	HIS	-	expression tag	UNP A0A486V7R5
A	-15	HIS	-	expression tag	UNP A0A486V7R5
A	-14	HIS	-	expression tag	UNP A0A486V7R5
A	-13	HIS	-	expression tag	UNP A0A486V7R5
A	-12	HIS	-	expression tag	UNP A0A486V7R5
A	-11	SER	-	expression tag	UNP A0A486V7R5
A	-10	GLN	-	expression tag	UNP A0A486V7R5
A	-9	ASP	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP A0A486V7R5
A	-7	GLU	-	expression tag	UNP A0A486V7R5
A	-6	ASN	-	expression tag	UNP A0A486V7R5
A	-5	LEU	-	expression tag	UNP A0A486V7R5
A	-4	TYR	-	expression tag	UNP A0A486V7R5
A	-3	PHE	-	expression tag	UNP A0A486V7R5
A	-2	GLN	-	expression tag	UNP A0A486V7R5
A	-1	GLY	-	expression tag	UNP A0A486V7R5
A	0	SER	-	expression tag	UNP A0A486V7R5
B	-21	MET	-	initiating methionine	UNP A0A486V7R5
B	-20	GLY	-	expression tag	UNP A0A486V7R5
B	-19	SER	-	expression tag	UNP A0A486V7R5
B	-18	SER	-	expression tag	UNP A0A486V7R5
B	-17	HIS	-	expression tag	UNP A0A486V7R5
B	-16	HIS	-	expression tag	UNP A0A486V7R5
B	-15	HIS	-	expression tag	UNP A0A486V7R5
B	-14	HIS	-	expression tag	UNP A0A486V7R5
B	-13	HIS	-	expression tag	UNP A0A486V7R5
B	-12	HIS	-	expression tag	UNP A0A486V7R5
B	-11	SER	-	expression tag	UNP A0A486V7R5
B	-10	GLN	-	expression tag	UNP A0A486V7R5
B	-9	ASP	-	expression tag	UNP A0A486V7R5
B	-8	HIS	-	expression tag	UNP A0A486V7R5
B	-7	GLU	-	expression tag	UNP A0A486V7R5
B	-6	ASN	-	expression tag	UNP A0A486V7R5
B	-5	LEU	-	expression tag	UNP A0A486V7R5
B	-4	TYR	-	expression tag	UNP A0A486V7R5
B	-3	PHE	-	expression tag	UNP A0A486V7R5
B	-2	GLN	-	expression tag	UNP A0A486V7R5
B	-1	GLY	-	expression tag	UNP A0A486V7R5
B	0	SER	-	expression tag	UNP A0A486V7R5
C	-21	MET	-	initiating methionine	UNP A0A486V7R5
C	-20	GLY	-	expression tag	UNP A0A486V7R5
C	-19	SER	-	expression tag	UNP A0A486V7R5
C	-18	SER	-	expression tag	UNP A0A486V7R5
C	-17	HIS	-	expression tag	UNP A0A486V7R5
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C	-15	HIS	-	expression tag	UNP A0A486V7R5
C	-14	HIS	-	expression tag	UNP A0A486V7R5
C	-13	HIS	-	expression tag	UNP A0A486V7R5
C	-12	HIS	-	expression tag	UNP A0A486V7R5
C	-11	SER	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLN	-	expression tag	UNP A0A486V7R5
C	-9	ASP	-	expression tag	UNP A0A486V7R5
C	-8	HIS	-	expression tag	UNP A0A486V7R5
C	-7	GLU	-	expression tag	UNP A0A486V7R5
C	-6	ASN	-	expression tag	UNP A0A486V7R5
C	-5	LEU	-	expression tag	UNP A0A486V7R5
C	-4	TYR	-	expression tag	UNP A0A486V7R5
C	-3	PHE	-	expression tag	UNP A0A486V7R5
C	-2	GLN	-	expression tag	UNP A0A486V7R5
C	-1	GLY	-	expression tag	UNP A0A486V7R5
C	0	SER	-	expression tag	UNP A0A486V7R5
D	-21	MET	-	initiating methionine	UNP A0A486V7R5
D	-20	GLY	-	expression tag	UNP A0A486V7R5
D	-19	SER	-	expression tag	UNP A0A486V7R5
D	-18	SER	-	expression tag	UNP A0A486V7R5
D	-17	HIS	-	expression tag	UNP A0A486V7R5
D	-16	HIS	-	expression tag	UNP A0A486V7R5
D	-15	HIS	-	expression tag	UNP A0A486V7R5
D	-14	HIS	-	expression tag	UNP A0A486V7R5
D	-13	HIS	-	expression tag	UNP A0A486V7R5
D	-12	HIS	-	expression tag	UNP A0A486V7R5
D	-11	SER	-	expression tag	UNP A0A486V7R5
D	-10	GLN	-	expression tag	UNP A0A486V7R5
D	-9	ASP	-	expression tag	UNP A0A486V7R5
D	-8	HIS	-	expression tag	UNP A0A486V7R5
D	-7	GLU	-	expression tag	UNP A0A486V7R5
D	-6	ASN	-	expression tag	UNP A0A486V7R5
D	-5	LEU	-	expression tag	UNP A0A486V7R5
D	-4	TYR	-	expression tag	UNP A0A486V7R5
D	-3	PHE	-	expression tag	UNP A0A486V7R5
D	-2	GLN	-	expression tag	UNP A0A486V7R5
D	-1	GLY	-	expression tag	UNP A0A486V7R5
D	0	SER	-	expression tag	UNP A0A486V7R5
E	-21	MET	-	initiating methionine	UNP A0A486V7R5
E	-20	GLY	-	expression tag	UNP A0A486V7R5
E	-19	SER	-	expression tag	UNP A0A486V7R5
E	-18	SER	-	expression tag	UNP A0A486V7R5
E	-17	HIS	-	expression tag	UNP A0A486V7R5
E	-16	HIS	-	expression tag	UNP A0A486V7R5
E	-15	HIS	-	expression tag	UNP A0A486V7R5
E	-14	HIS	-	expression tag	UNP A0A486V7R5
E	-13	HIS	-	expression tag	UNP A0A486V7R5

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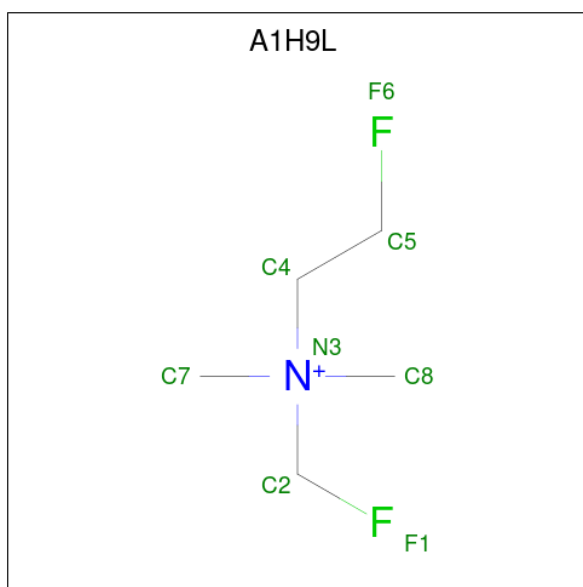
Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP A0A486V7R5
E	-11	SER	-	expression tag	UNP A0A486V7R5
E	-10	GLN	-	expression tag	UNP A0A486V7R5
E	-9	ASP	-	expression tag	UNP A0A486V7R5
E	-8	HIS	-	expression tag	UNP A0A486V7R5
E	-7	GLU	-	expression tag	UNP A0A486V7R5
E	-6	ASN	-	expression tag	UNP A0A486V7R5
E	-5	LEU	-	expression tag	UNP A0A486V7R5
E	-4	TYR	-	expression tag	UNP A0A486V7R5
E	-3	PHE	-	expression tag	UNP A0A486V7R5
E	-2	GLN	-	expression tag	UNP A0A486V7R5
E	-1	GLY	-	expression tag	UNP A0A486V7R5
E	0	SER	-	expression tag	UNP A0A486V7R5
F	-21	MET	-	initiating methionine	UNP A0A486V7R5
F	-20	GLY	-	expression tag	UNP A0A486V7R5
F	-19	SER	-	expression tag	UNP A0A486V7R5
F	-18	SER	-	expression tag	UNP A0A486V7R5
F	-17	HIS	-	expression tag	UNP A0A486V7R5
F	-16	HIS	-	expression tag	UNP A0A486V7R5
F	-15	HIS	-	expression tag	UNP A0A486V7R5
F	-14	HIS	-	expression tag	UNP A0A486V7R5
F	-13	HIS	-	expression tag	UNP A0A486V7R5
F	-12	HIS	-	expression tag	UNP A0A486V7R5
F	-11	SER	-	expression tag	UNP A0A486V7R5
F	-10	GLN	-	expression tag	UNP A0A486V7R5
F	-9	ASP	-	expression tag	UNP A0A486V7R5
F	-8	HIS	-	expression tag	UNP A0A486V7R5
F	-7	GLU	-	expression tag	UNP A0A486V7R5
F	-6	ASN	-	expression tag	UNP A0A486V7R5
F	-5	LEU	-	expression tag	UNP A0A486V7R5
F	-4	TYR	-	expression tag	UNP A0A486V7R5
F	-3	PHE	-	expression tag	UNP A0A486V7R5
F	-2	GLN	-	expression tag	UNP A0A486V7R5
F	-1	GLY	-	expression tag	UNP A0A486V7R5
F	0	SER	-	expression tag	UNP A0A486V7R5
G	-21	MET	-	initiating methionine	UNP A0A486V7R5
G	-20	GLY	-	expression tag	UNP A0A486V7R5
G	-19	SER	-	expression tag	UNP A0A486V7R5
G	-18	SER	-	expression tag	UNP A0A486V7R5
G	-17	HIS	-	expression tag	UNP A0A486V7R5
G	-16	HIS	-	expression tag	UNP A0A486V7R5
G	-15	HIS	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP A0A486V7R5
G	-13	HIS	-	expression tag	UNP A0A486V7R5
G	-12	HIS	-	expression tag	UNP A0A486V7R5
G	-11	SER	-	expression tag	UNP A0A486V7R5
G	-10	GLN	-	expression tag	UNP A0A486V7R5
G	-9	ASP	-	expression tag	UNP A0A486V7R5
G	-8	HIS	-	expression tag	UNP A0A486V7R5
G	-7	GLU	-	expression tag	UNP A0A486V7R5
G	-6	ASN	-	expression tag	UNP A0A486V7R5
G	-5	LEU	-	expression tag	UNP A0A486V7R5
G	-4	TYR	-	expression tag	UNP A0A486V7R5
G	-3	PHE	-	expression tag	UNP A0A486V7R5
G	-2	GLN	-	expression tag	UNP A0A486V7R5
G	-1	GLY	-	expression tag	UNP A0A486V7R5
G	0	SER	-	expression tag	UNP A0A486V7R5
H	-21	MET	-	initiating methionine	UNP A0A486V7R5
H	-20	GLY	-	expression tag	UNP A0A486V7R5
H	-19	SER	-	expression tag	UNP A0A486V7R5
H	-18	SER	-	expression tag	UNP A0A486V7R5
H	-17	HIS	-	expression tag	UNP A0A486V7R5
H	-16	HIS	-	expression tag	UNP A0A486V7R5
H	-15	HIS	-	expression tag	UNP A0A486V7R5
H	-14	HIS	-	expression tag	UNP A0A486V7R5
H	-13	HIS	-	expression tag	UNP A0A486V7R5
H	-12	HIS	-	expression tag	UNP A0A486V7R5
H	-11	SER	-	expression tag	UNP A0A486V7R5
H	-10	GLN	-	expression tag	UNP A0A486V7R5
H	-9	ASP	-	expression tag	UNP A0A486V7R5
H	-8	HIS	-	expression tag	UNP A0A486V7R5
H	-7	GLU	-	expression tag	UNP A0A486V7R5
H	-6	ASN	-	expression tag	UNP A0A486V7R5
H	-5	LEU	-	expression tag	UNP A0A486V7R5
H	-4	TYR	-	expression tag	UNP A0A486V7R5
H	-3	PHE	-	expression tag	UNP A0A486V7R5
H	-2	GLN	-	expression tag	UNP A0A486V7R5
H	-1	GLY	-	expression tag	UNP A0A486V7R5
H	0	SER	-	expression tag	UNP A0A486V7R5

- Molecule 2 is difluorocholine (CCD ID: A1H9L) (formula: $C_5H_{12}F_2N$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			8	5	2	1		
2	B	1	Total	C	F	N	0	0
			8	5	2	1		
2	C	1	Total	C	F	N	0	0
			8	5	2	1		
2	D	1	Total	C	F	N	0	0
			8	5	2	1		
2	E	1	Total	C	F	N	0	0
			8	5	2	1		
2	F	1	Total	C	F	N	0	0
			8	5	2	1		
2	G	1	Total	C	F	N	0	0
			8	5	2	1		
2	H	1	Total	C	F	N	0	0
			8	5	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	45	Total	O	0	0
			45	45		
3	C	40	Total	O	0	0
			40	40		
3	D	22	Total	O	0	0
			22	22		

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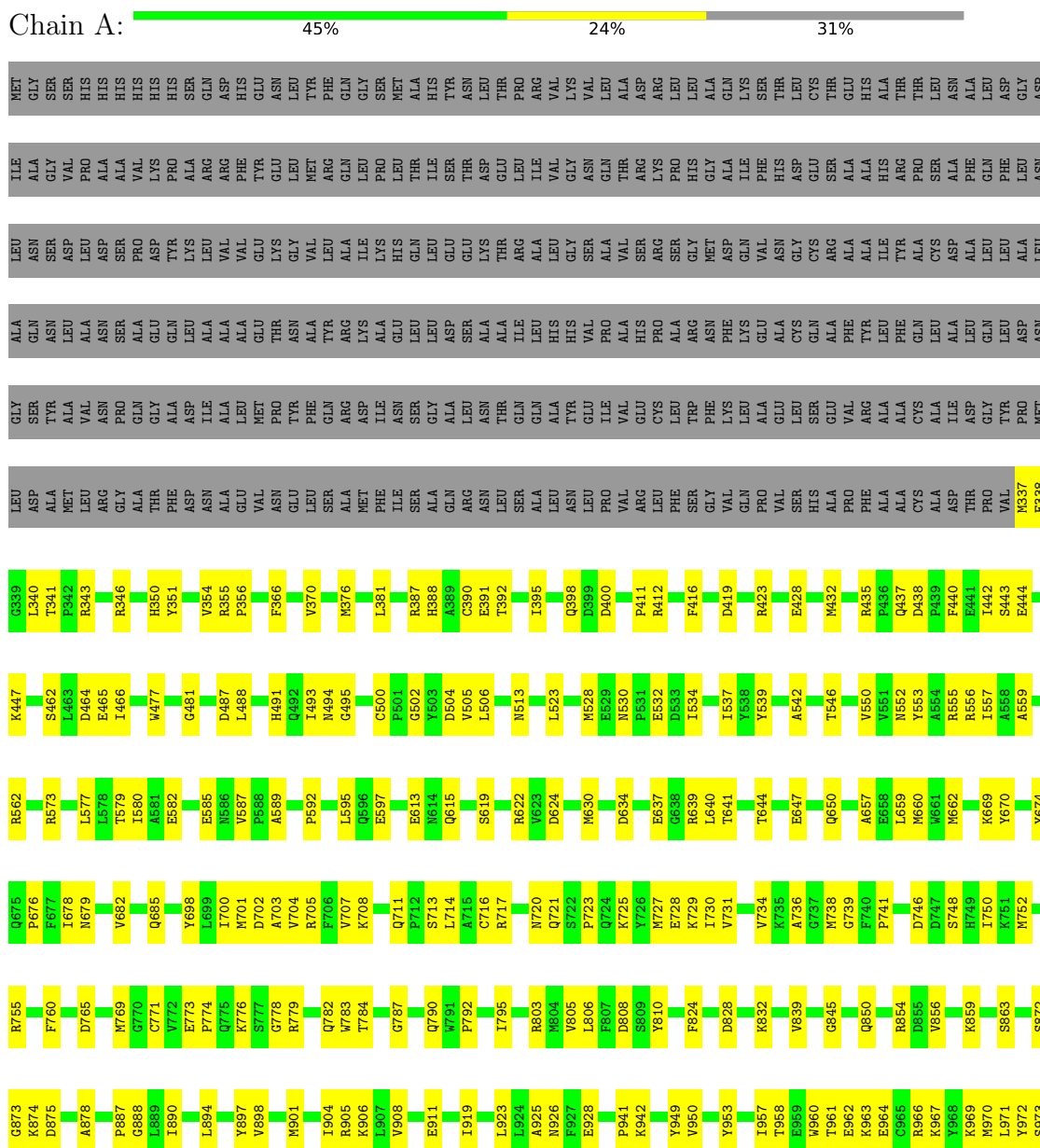
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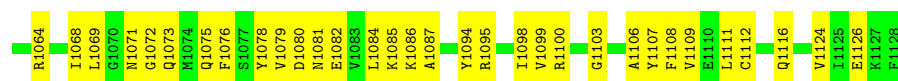
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	17	Total 17	O 17	0	0
3	F	17	Total 17	O 17	0	0
3	G	6	Total 6	O 6	0	0
3	H	7	Total 7	O 7	0	0

3 Residue-property plots

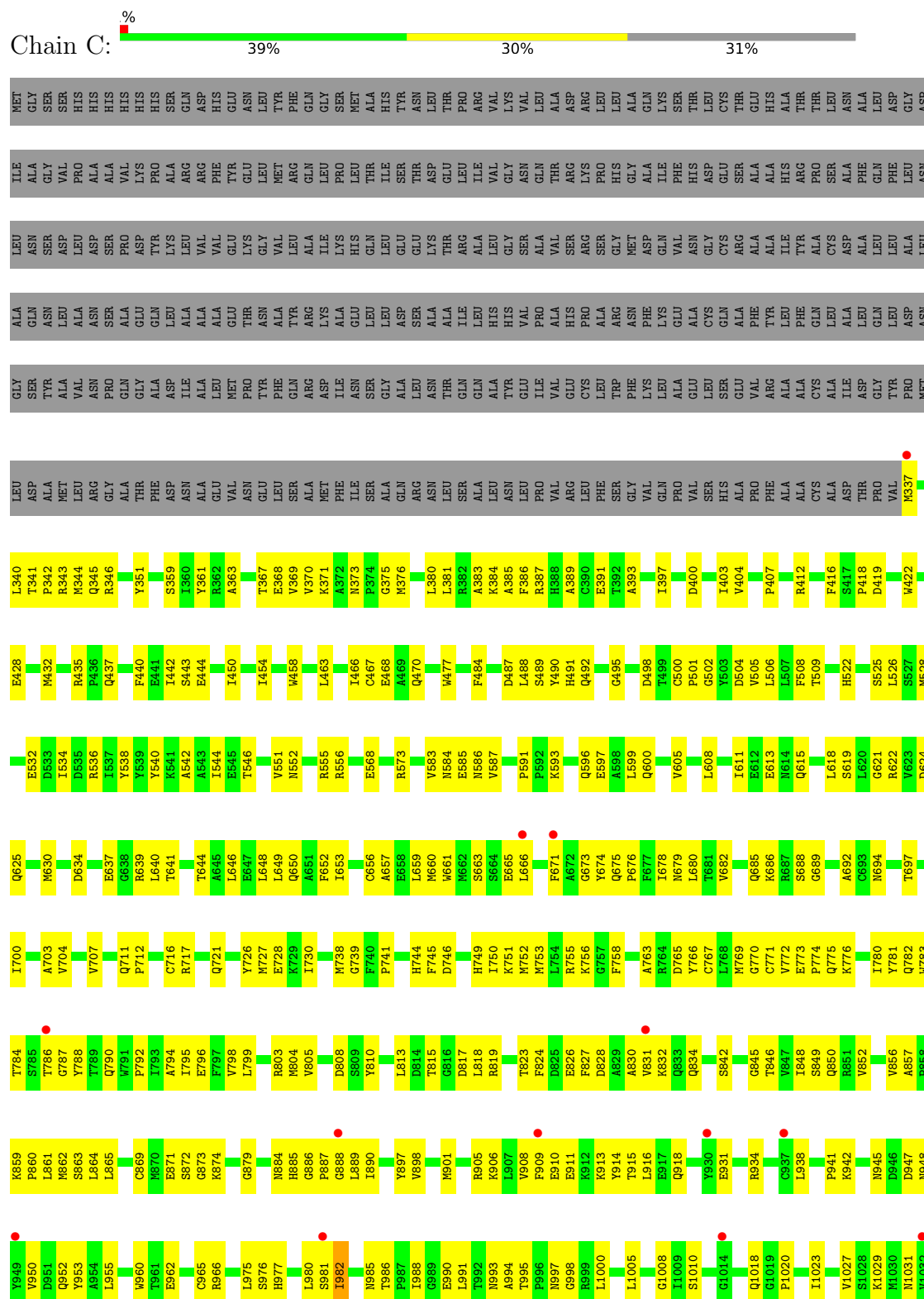
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

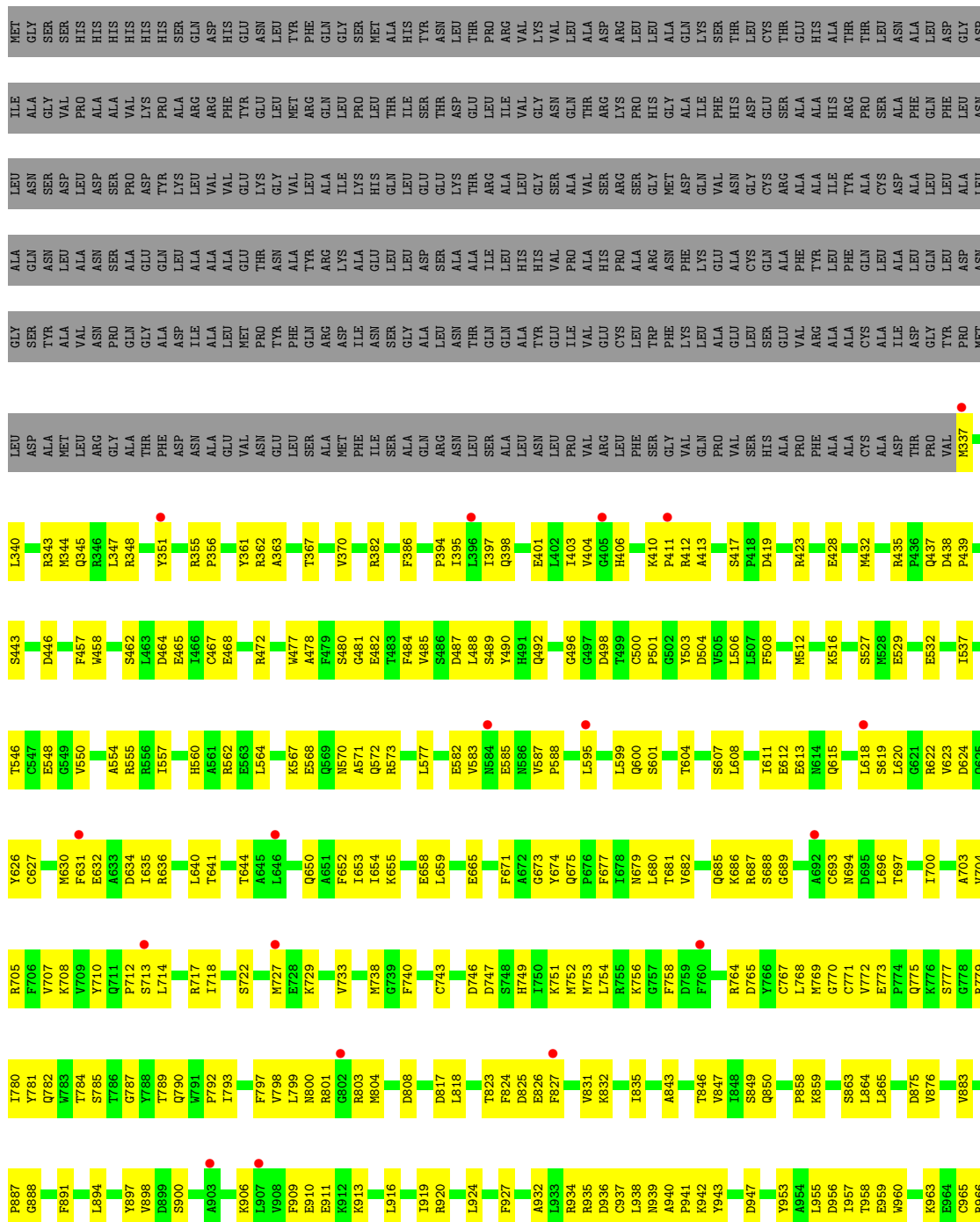




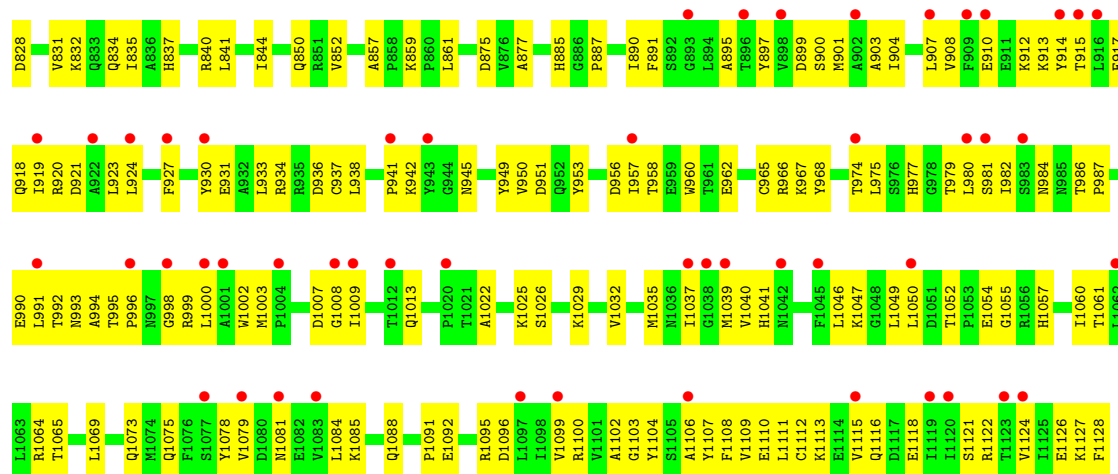
Molecule 1: Choline trimethylamine-lyase



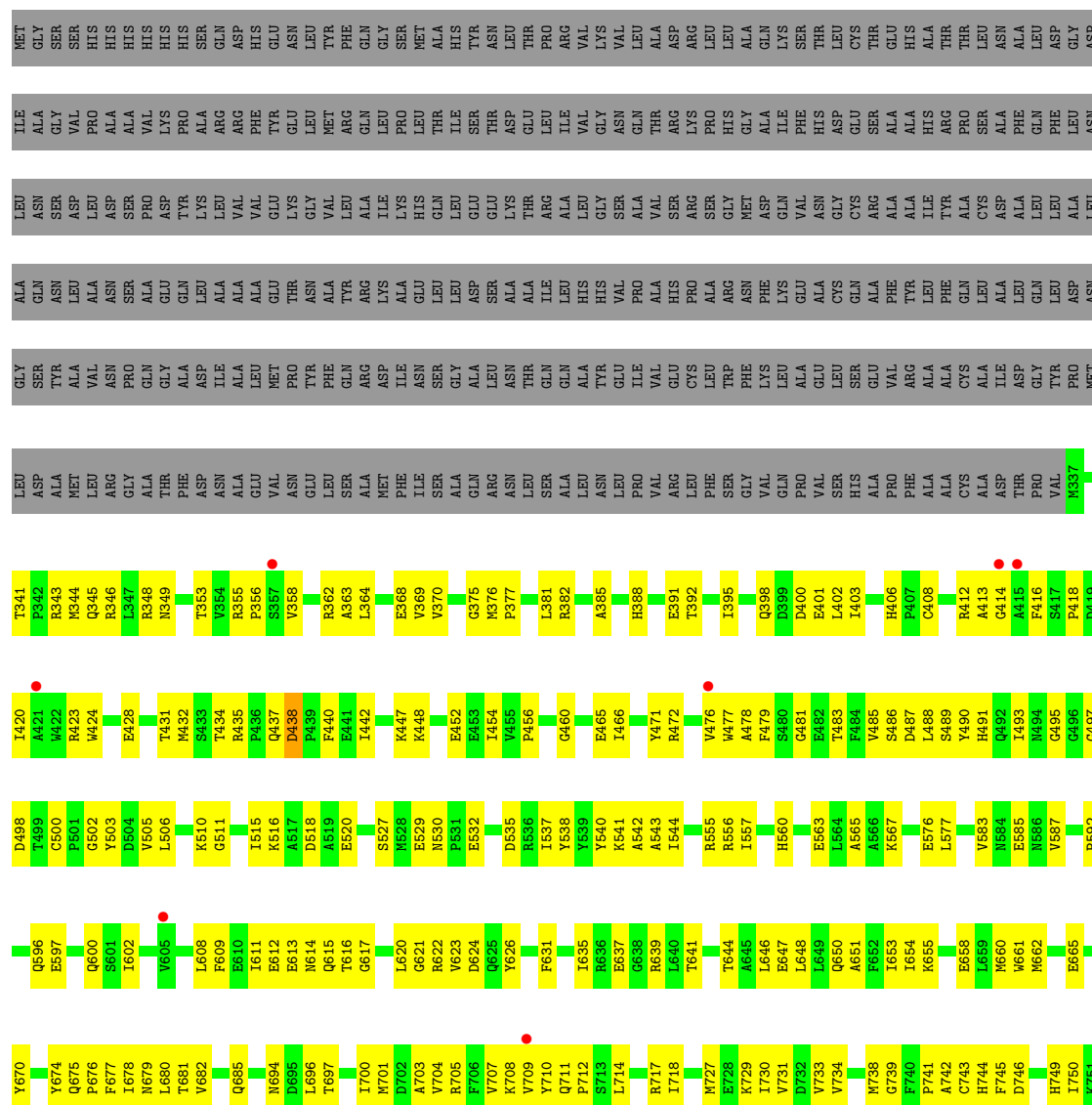
- Molecule 1: Choline trimethylamine-lyase

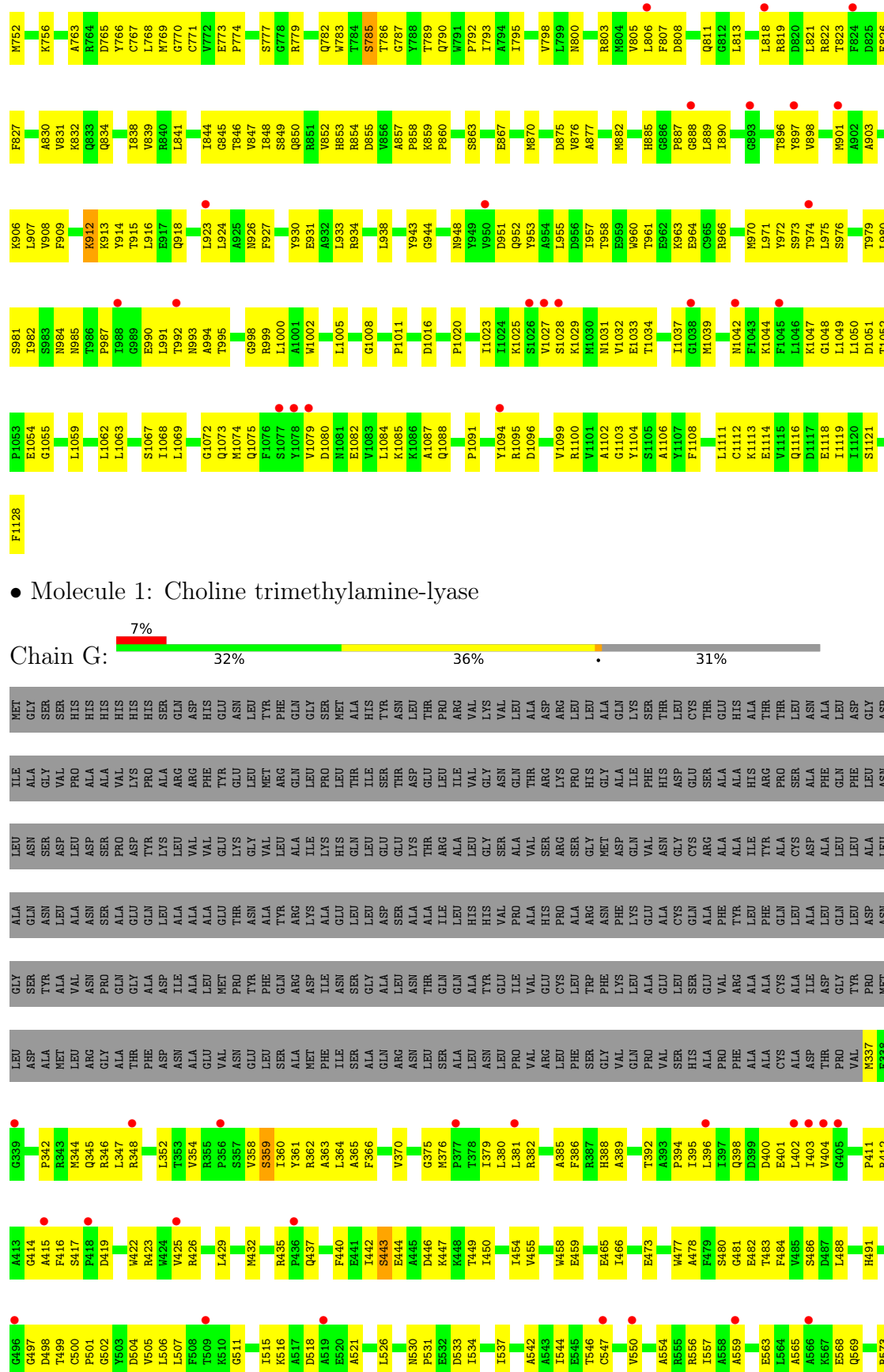


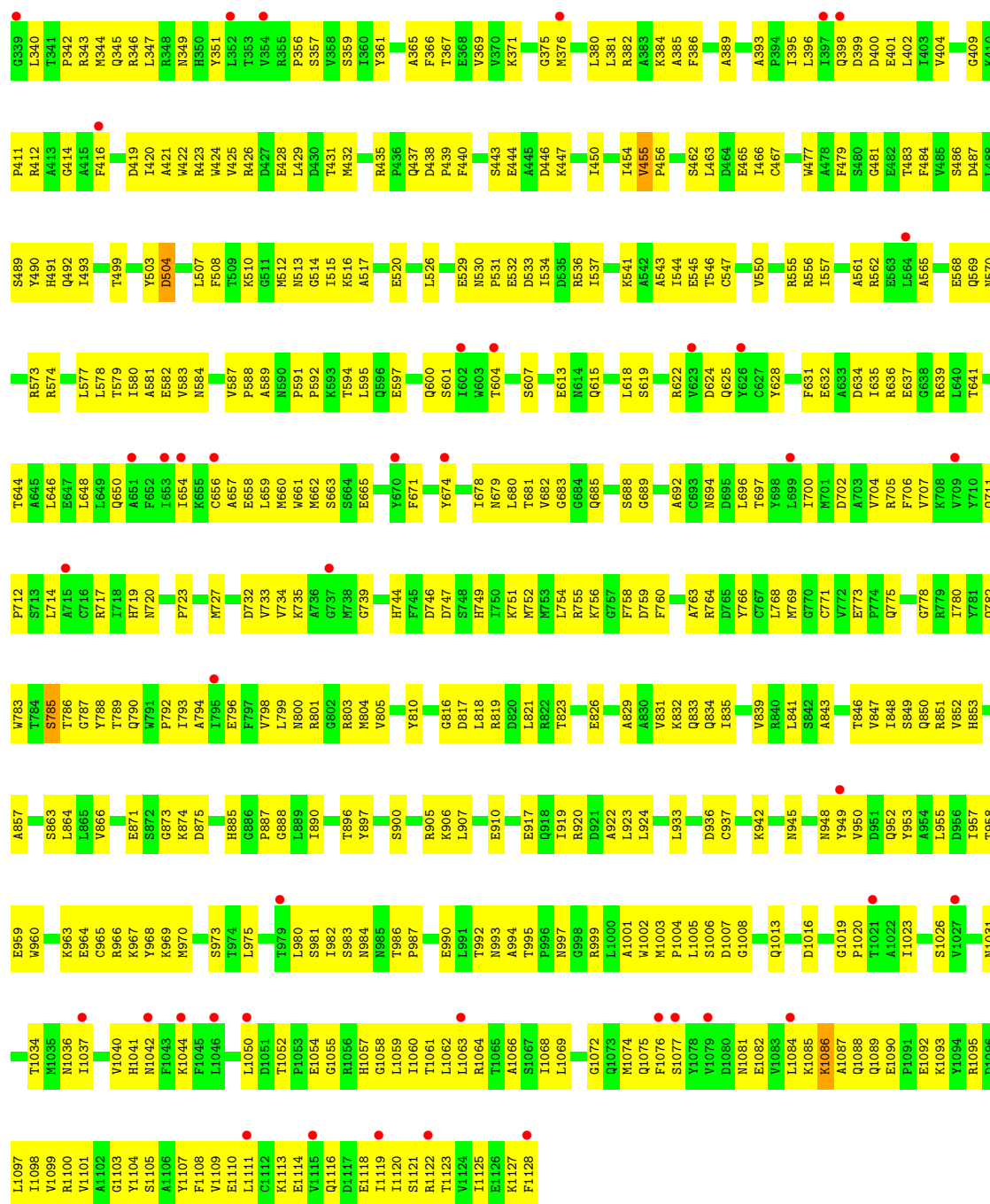




• Molecule 1: Choline trimethylamine-lyase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	88.37Å 117.57Å 212.53Å 77.65° 85.34° 70.01°	Depositor
Resolution (Å)	44.57 – 2.90 44.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.57-2.90) 95.9 (44.57-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.220 , 0.295 0.220 , 0.293	Depositor DCC
R_{free} test set	8188 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50317	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1H9L

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	0.54	0/6385	0.77	1/8640 (0.0%)
1	B	0.54	1/6385 (0.0%)	0.78	1/8640 (0.0%)
1	C	0.44	0/6385	0.73	2/8640 (0.0%)
1	D	0.43	0/6385	0.72	0/8640
1	E	0.43	0/6385	0.72	4/8640 (0.0%)
1	F	0.54	5/6385 (0.1%)	0.74	3/8640 (0.0%)
1	G	0.44	2/6385 (0.0%)	0.73	5/8640 (0.1%)
1	H	0.38	0/6385	0.70	1/8640 (0.0%)
All	All	0.47	8/51080 (0.0%)	0.73	17/69120 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	3
1	F	0	1
1	G	0	6
1	H	0	5
All	All	0	16

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	356	PRO	N-CD	-15.87	1.25	1.47
1	F	438	ASP	C-O	10.76	1.28	1.23
1	G	822	ARG	CZ-NH1	9.24	1.45	1.32
1	G	822	ARG	CD-NE	9.09	1.58	1.46
1	F	912	LYS	CB-CG	8.40	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	912	LYS	CD-CE	7.95	1.76	1.52
1	F	912	LYS	CA-CB	5.97	1.62	1.53
1	B	438	ASP	C-O	5.70	1.26	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	822	ARG	NE-CZ-NH2	-9.62	110.54	119.20
1	G	822	ARG	NH1-CZ-NH2	6.41	127.63	119.30
1	F	912	LYS	N-CA-C	-6.28	104.17	113.40
1	G	568	GLU	CA-C-N	6.23	128.63	120.28
1	G	568	GLU	C-N-CA	6.23	128.63	120.28
1	B	753	MET	CG-SD-CE	-5.97	87.77	100.90
1	C	856	VAL	CA-C-N	-5.95	116.83	122.37
1	C	856	VAL	C-N-CA	-5.95	116.83	122.37
1	E	589	ALA	CA-C-N	-5.64	115.84	123.96
1	E	589	ALA	C-N-CA	-5.64	115.84	123.96
1	E	437	GLN	CA-C-N	5.59	128.87	122.83
1	E	437	GLN	C-N-CA	5.59	128.87	122.83
1	A	1054	GLU	CA-CB-CG	-5.51	103.08	114.10
1	F	912	LYS	CB-CA-C	5.43	121.00	111.06
1	G	640	LEU	CA-CB-CG	5.41	135.24	116.30
1	H	455	VAL	CB-CA-C	-5.15	108.81	113.70
1	F	626	TYR	CA-CB-CG	5.05	122.99	113.90

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	981	SER	Peptide
1	E	353	THR	Peptide
1	E	377	PRO	Peptide
1	E	640	LEU	Peptide
1	F	785	SER	Peptide
1	G	359	SER	Peptide
1	G	443	SER	Peptide
1	G	641	THR	Peptide
1	G	663	SER	Peptide
1	G	780	ILE	Peptide
1	G	981	SER	Peptide
1	H	1086	LYS	Peptide
1	H	1093	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	H	431	THR	Peptide
1	H	504	ASP	Peptide
1	H	785	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6254	0	6171	217	3
1	B	6254	0	6171	216	2
1	C	6254	0	6171	315	0
1	D	6254	0	6171	326	3
1	E	6254	0	6171	332	1
1	F	6254	0	6171	349	2
1	G	6254	0	6171	413	1
1	H	6254	0	6171	376	0
2	A	8	0	0	0	0
2	B	8	0	0	1	0
2	C	8	0	0	1	0
2	D	8	0	0	1	0
2	E	8	0	0	1	0
2	F	8	0	0	0	0
2	G	8	0	0	1	0
2	H	8	0	0	1	0
3	A	67	0	0	4	0
3	B	45	0	0	3	0
3	C	40	0	0	6	0
3	D	22	0	0	2	0
3	E	17	0	0	5	0
3	F	17	0	0	1	0
3	G	6	0	0	1	0
3	H	7	0	0	1	0
All	All	50317	0	49368	2513	6

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 (2513) 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:F:912:LYS:CD	1:F:912:LYS:CE	1.76	1.63
1:F:912:LYS:CG	1:F:912:LYS:CB	1.77	1.61
1:H:568:GLU:OE1	1:H:570:ASN:N	1.72	1.20
1:A:957:ILE:HD12	1:A:958:THR:N	1.56	1.19
1:H:376:MET:HE3	1:H:380:LEU:HG	1.21	1.18
1:G:957:ILE:HD12	1:G:958:THR:N	1.58	1.17
1:A:739:GLY:HA3	1:A:1100:ARG:HG2	1.28	1.14
1:H:957:ILE:HD12	1:H:958:THR:H	1.17	1.07
1:G:380:LEU:HD23	1:G:380:LEU:O	1.60	1.01
1:G:595:LEU:HD12	1:G:631:PHE:HB2	1.40	1.00
1:H:376:MET:HE3	1:H:380:LEU:CG	1.95	0.96
1:H:1090:GLU:OE1	1:H:1090:GLU:O	1.83	0.96
1:G:635:ILE:CD1	1:G:641:THR:HA	1.95	0.96
1:H:376:MET:CE	1:H:380:LEU:HG	1.96	0.95
1:H:720:ASN:OD1	1:H:1064:ARG:NH2	2.00	0.94
1:G:1086:LYS:HE3	1:G:1094:TYR:OH	1.68	0.94
1:H:957:ILE:HD12	1:H:958:THR:N	1.85	0.92
1:G:380:LEU:HA	1:G:542:ALA:HB2	1.52	0.92
1:G:957:ILE:HD12	1:G:958:THR:H	1.28	0.92
1:C:432:MET:HG2	1:C:435:ARG:HH21	1.34	0.92
1:C:952:GLN:HA	1:C:1029:LYS:HZ3	1.34	0.91
1:H:437:GLN:NE2	1:H:1111:LEU:HA	1.85	0.91
1:G:606:GLU:OE1	1:G:678:ILE:CD1	2.19	0.91
1:G:1046:LEU:HD22	1:G:1126:GLU:HG2	1.51	0.91
1:G:596:GLN:HG3	1:G:648:LEU:HD11	1.52	0.90
1:F:818:LEU:CD2	1:F:916:LEU:HB2	2.02	0.90
1:C:952:GLN:HA	1:C:1029:LYS:NZ	1.86	0.90
1:H:1127:LYS:H	1:H:1127:LYS:HD2	1.35	0.90
1:H:437:GLN:OE1	1:H:438:ASP:N	2.04	0.90
1:F:1075:GLN:HE22	1:F:1103:GLY:HA2	1.37	0.89
1:H:536:ARG:HG2	1:H:873:GLY:HA3	1.55	0.89
1:H:1064:ARG:NH2	1:H:1068:ILE:HG13	1.88	0.88
1:A:337:MET:HB3	1:A:340:LEU:HD12	1.55	0.88
1:F:970:MET:HE3	1:F:975:LEU:HB2	1.52	0.88
1:F:818:LEU:HD21	1:F:916:LEU:HB2	1.54	0.87
1:A:957:ILE:HD12	1:A:958:THR:H	1.38	0.87
1:G:635:ILE:HD13	1:G:641:THR:HA	1.56	0.87
1:B:1075:GLN:HE22	1:B:1103:GLY:HA2	1.39	0.87
1:E:564:LEU:HA	1:E:567:LYS:HG2	1.56	0.87
1:E:583:VAL:HG23	1:E:597:GLU:HG2	1.58	0.86
1:E:486:SER:HB2	1:E:789:THR:HB	1.56	0.86
1:A:1075:GLN:HE22	1:A:1103:GLY:H	1.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:359:SER:HG	1:H:361:TYR:HD2	0.92	0.86
1:C:739:GLY:HA3	1:C:1100:ARG:HG2	1.57	0.85
1:G:1086:LYS:HE3	1:G:1094:TYR:CZ	2.11	0.85
1:D:437:GLN:NE2	1:D:1110:GLU:O	2.07	0.85
1:D:906:LYS:HZ2	1:D:911:GLU:HG3	1.41	0.85
1:E:1025:LYS:O	1:E:1029:LYS:NZ	2.09	0.85
1:H:624:ASP:HB3	1:H:682:VAL:HG12	1.59	0.85
1:G:379:ILE:HD12	1:G:858:PRO:HB2	1.56	0.85
1:F:1085:LYS:HD3	1:F:1088:GLN:HE21	1.43	0.84
1:H:1092:GLU:HA	1:H:1095:ARG:HG3	1.59	0.84
1:G:934:ARG:NH1	1:G:998:GLY:O	2.11	0.84
1:H:568:GLU:OE1	1:H:569:GLN:N	2.09	0.84
1:D:919:ILE:HD11	1:D:996:PRO:HB3	1.60	0.84
1:E:395:ILE:HD11	1:E:556:ARG:HG3	1.58	0.83
1:H:1064:ARG:HH22	1:H:1068:ILE:HG13	1.39	0.83
1:D:348:ARG:NH1	1:D:707:VAL:O	2.11	0.83
1:E:821:LEU:HD13	1:E:827:PHE:HA	1.60	0.83
1:F:963:LYS:NZ	1:G:761:GLU:OE2	2.12	0.83
1:C:758:PHE:HZ	1:C:780:ILE:HB	1.44	0.82
1:H:587:VAL:HB	1:H:601:SER:HB2	1.61	0.82
1:F:930:TYR:HB3	1:F:933:LEU:HB3	1.60	0.82
1:C:771:CYS:HB3	1:C:1103:GLY:HA3	1.62	0.82
1:D:798:VAL:HG21	1:D:831:VAL:HG12	1.62	0.82
1:E:512:MET:HE2	1:E:550:VAL:HG21	1.59	0.82
1:E:942:LYS:O	1:E:945:ASN:ND2	2.13	0.82
1:D:362:ARG:NH2	1:D:612:GLU:O	2.13	0.82
1:F:912:LYS:CE	1:F:912:LYS:CG	2.57	0.82
1:H:492:GLN:HG3	1:H:493:ILE:HG23	1.60	0.82
1:H:624:ASP:O	1:H:694:ASN:ND2	2.12	0.82
1:E:711:GLN:HG3	1:E:712:PRO:HA	1.62	0.81
1:G:650:GLN:HB2	1:G:707:VAL:HG21	1.60	0.81
1:H:970:MET:HE3	1:H:975:LEU:HB2	1.63	0.81
1:F:787:GLY:CA	1:F:889:LEU:HD11	2.10	0.81
1:H:395:ILE:HG23	1:H:557:ILE:HD13	1.60	0.81
1:D:428:GLU:OE2	1:D:435:ARG:NH1	2.12	0.81
1:F:1052:THR:HG23	1:F:1055:GLY:H	1.45	0.81
1:E:739:GLY:HA3	1:E:1100:ARG:HG2	1.62	0.80
1:F:857:ALA:O	1:F:859:LYS:NZ	2.12	0.80
1:E:806:LEU:HD22	1:E:991:LEU:HA	1.63	0.80
1:H:443:SER:OG	1:H:446:ASP:N	2.13	0.80
1:A:714:LEU:HD23	1:A:741:PRO:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:917:GLU:HB2	1:E:920:ARG:HH21	1.46	0.80
1:E:618:LEU:O	1:E:678:ILE:HD13	1.82	0.80
1:D:970:MET:HE3	1:D:975:LEU:HB2	1.64	0.80
1:E:724:GLN:HA	1:E:727:MET:HB2	1.64	0.80
1:G:587:VAL:HB	1:G:601:SER:HB2	1.63	0.80
1:E:727:MET:HG3	1:E:1064:ARG:HH11	1.47	0.79
1:D:936:ASP:HA	1:D:939:ASN:HB2	1.64	0.79
1:G:1003:MET:HE3	1:G:1004:PRO:HD2	1.63	0.79
1:A:771:CYS:HB3	1:A:1103:GLY:HA3	1.64	0.79
1:H:937:CYS:O	1:H:942:LYS:NZ	2.13	0.79
1:H:800:ASN:HB3	1:H:803:ARG:HG3	1.64	0.79
1:C:815:THR:HG23	1:C:834:GLN:HE21	1.48	0.79
1:D:898:VAL:HG13	1:D:953:TYR:HB2	1.62	0.79
1:E:598:ALA:HB2	1:E:630:MET:HE2	1.62	0.79
1:F:818:LEU:HD21	1:F:916:LEU:CB	2.13	0.79
1:C:432:MET:HE3	1:C:440:PHE:HB2	1.65	0.79
1:D:1095:ARG:HG3	1:D:1109:VAL:HG21	1.65	0.79
1:A:839:VAL:HG21	1:A:964:GLU:HG3	1.65	0.78
1:B:850:GLN:HB3	1:B:971:LEU:HD22	1.66	0.78
1:B:387:ARG:NH1	1:B:391:GLU:OE2	2.17	0.78
1:A:1054:GLU:HG3	1:E:912:LYS:HE2	1.64	0.78
1:G:402:LEU:HD11	1:G:596:GLN:HG2	1.64	0.78
1:B:1075:GLN:NE2	1:B:1100:ARG:HH21	1.82	0.78
1:B:753:MET:HE1	1:B:775:GLN:C	2.08	0.78
1:G:402:LEU:O	1:G:402:LEU:HD13	1.83	0.78
1:G:995:THR:HG23	1:G:999:ARG:HH21	1.47	0.78
1:H:1086:LYS:HG2	1:H:1089:GLN:HG2	1.64	0.78
1:A:850:GLN:HB3	1:A:971:LEU:HD22	1.66	0.77
1:B:435:ARG:NH2	1:B:438:ASP:O	2.17	0.77
1:D:641:THR:N	1:D:644:THR:OG1	2.17	0.77
1:E:429:LEU:HD22	1:E:447:LYS:HG2	1.66	0.77
1:F:813:LEU:O	1:F:834:GLN:NE2	2.17	0.77
1:F:938:LEU:HD21	1:F:998:GLY:HA3	1.66	0.77
1:G:444:GLU:HA	1:G:447:LYS:HB2	1.67	0.77
1:G:1021:THR:HG22	1:G:1062:LEU:HD13	1.65	0.77
1:B:428:GLU:OE2	1:B:435:ARG:HD2	1.84	0.77
1:C:769:MET:SD	1:C:770:GLY:N	2.57	0.76
1:E:742:ALA:HB2	1:E:1100:ARG:HH22	1.49	0.76
1:H:1118:GLU:HA	1:H:1121:SER:HB3	1.67	0.76
1:E:395:ILE:HG23	1:E:557:ILE:HD13	1.64	0.76
1:F:787:GLY:HA3	1:F:889:LEU:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:993:ASN:O	1:G:999:ARG:NH2	2.19	0.76
1:C:727:MET:HG3	1:C:1064:ARG:HH11	1.51	0.76
1:A:650:GLN:HB3	1:A:707:VAL:HG11	1.68	0.76
1:C:685:GLN:H	1:C:717:ARG:HH21	1.32	0.76
1:D:423:ARG:HH21	1:D:464:ASP:CG	1.94	0.76
1:E:771:CYS:HB3	1:E:1103:GLY:HA3	1.66	0.76
1:G:898:VAL:HG13	1:G:953:TYR:HB2	1.66	0.75
1:G:1086:LYS:HE3	1:G:1094:TYR:CE2	2.22	0.75
1:C:803:ARG:NH1	1:C:808:ASP:OD1	2.20	0.75
1:B:393:ALA:O	1:B:556:ARG:NH2	2.19	0.75
1:C:376:MET:HE1	1:C:384:LYS:HD2	1.69	0.75
1:F:739:GLY:HA3	1:F:1100:ARG:HB2	1.67	0.75
1:A:1100:ARG:NH2	1:A:1103:GLY:C	2.45	0.75
1:E:602:ILE:HG21	1:E:620:LEU:HD23	1.69	0.75
1:D:1003:MET:HG2	1:D:1004:PRO:HD2	1.66	0.75
1:F:943:TYR:OH	1:F:1027:VAL:HG12	1.87	0.74
1:G:354:VAL:HG11	1:G:411:PRO:HB2	1.69	0.74
1:G:633:ALA:HA	1:G:636:ARG:HG2	1.69	0.74
1:D:1033:GLU:H	1:D:1033:GLU:CD	1.93	0.74
1:C:1031:ASN:HD21	1:H:689:GLY:HA3	1.52	0.74
1:A:416:PHE:HA	1:A:662:MET:HE1	1.69	0.74
1:E:999:ARG:HH21	1:E:1003:MET:H	1.36	0.74
1:C:846:THR:O	1:C:849:SER:OG	2.05	0.74
1:F:914:TYR:HA	1:F:918:GLN:OE1	1.86	0.74
1:G:380:LEU:O	1:G:380:LEU:CD2	2.34	0.74
1:H:568:GLU:CD	1:H:569:GLN:H	1.96	0.74
1:H:775:GLN:HB3	1:H:780:ILE:HG21	1.68	0.74
1:C:962:GLU:HG2	1:C:977:HIS:CD2	2.23	0.74
1:G:635:ILE:HD12	1:G:641:THR:HA	1.70	0.74
1:G:613:GLU:OE2	1:G:859:LYS:NZ	2.19	0.73
1:H:561:ALA:HB3	1:H:581:ALA:HB2	1.68	0.73
1:E:653:ILE:HG23	1:E:712:PRO:HD2	1.70	0.73
1:H:782:GLN:O	3:H:1301:HOH:O	2.05	0.73
1:D:435:ARG:NH2	1:D:438:ASP:O	2.19	0.73
1:D:653:ILE:HG23	1:D:712:PRO:HD2	1.69	0.73
1:D:823:THR:HG22	1:D:825:ASP:H	1.52	0.73
1:G:1044:LYS:HE2	1:G:1122:ARG:HB2	1.70	0.73
1:A:579:THR:HA	1:A:582:GLU:HG2	1.69	0.73
1:B:423:ARG:NH2	1:B:468:GLU:OE1	2.22	0.73
1:E:643:ASP:HA	1:E:646:LEU:HB3	1.71	0.73
1:E:694:ASN:O	1:E:697:THR:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ASP:OD1	1:C:489:SER:HB3	1.89	0.73
1:D:554:ALA:HB2	1:D:588:PRO:HD2	1.71	0.73
1:E:775:GLN:HB3	1:E:780:ILE:HG21	1.70	0.73
1:D:562:ARG:HH21	1:D:582:GLU:HG2	1.52	0.72
1:G:641:THR:N	1:G:644:THR:OG1	2.22	0.72
1:H:444:GLU:HA	1:H:447:LYS:HE3	1.70	0.72
1:F:705:ARG:HA	1:F:738:MET:HE1	1.72	0.72
1:H:792:PRO:HG2	1:H:1005:LEU:HD13	1.71	0.72
1:D:1108:PHE:CZ	1:D:1116:GLN:HB2	2.25	0.72
1:G:416:PHE:HA	1:G:662:MET:HE1	1.69	0.72
1:G:615:GLN:HE21	1:G:618:LEU:HD21	1.55	0.72
1:A:720:ASN:OD1	1:A:1067:SER:OG	2.07	0.71
1:B:354:VAL:HG11	1:B:411:PRO:HB2	1.70	0.71
1:B:980:LEU:HD23	1:B:980:LEU:H	1.54	0.71
1:D:462:SER:OG	1:D:465:GLU:OE1	2.08	0.71
1:G:402:LEU:HD12	1:G:648:LEU:HD21	1.72	0.71
1:H:1099:VAL:HG11	1:H:1119:ILE:HG21	1.72	0.71
1:A:1108:PHE:CZ	1:A:1116:GLN:HB2	2.25	0.71
1:A:739:GLY:CA	1:A:1100:ARG:HG2	2.16	0.71
1:F:650:GLN:HB2	1:F:707:VAL:CG1	2.19	0.71
1:A:1016:ASP:HB2	1:A:1023:ILE:HD11	1.72	0.71
1:F:363:ALA:HB2	1:F:416:PHE:HB3	1.72	0.71
1:F:472:ARG:HE	1:F:477:TRP:CD1	2.09	0.71
1:C:993:ASN:OD1	1:C:994:ALA:N	2.23	0.71
1:G:1006:SER:HA	1:G:1013:GLN:HE22	1.55	0.70
1:C:952:GLN:CA	1:C:1029:LYS:NZ	2.54	0.70
1:D:727:MET:HG3	1:D:1064:ARG:HH11	1.55	0.70
1:E:750:ILE:HD13	1:E:764:ARG:HG2	1.74	0.70
1:C:432:MET:HE1	1:C:442:ILE:HB	1.73	0.70
1:E:715:ALA:HB1	1:E:768:LEU:HD23	1.74	0.70
1:F:1042:ASN:HD21	1:F:1102:ALA:HA	1.57	0.70
1:G:709:VAL:HG12	1:G:1107:TYR:OH	1.91	0.70
1:F:650:GLN:HB2	1:F:707:VAL:HG11	1.72	0.70
1:F:787:GLY:O	1:F:889:LEU:HD12	1.92	0.70
1:F:787:GLY:O	1:F:889:LEU:CD1	2.40	0.70
1:D:984:ASN:O	1:D:988:ILE:N	2.21	0.70
1:H:429:LEU:HD22	1:H:447:LYS:HB3	1.73	0.70
1:E:350:HIS:O	1:E:353:THR:OG1	2.07	0.70
1:G:606:GLU:OE1	1:G:678:ILE:HD13	1.90	0.70
1:G:1052:THR:HG21	1:G:1054:GLU:OE1	1.92	0.70
1:E:360:ILE:HG21	1:E:450:ILE:HD11	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:650:GLN:HB2	1:H:707:VAL:HG21	1.72	0.69
1:A:728:GLU:HG3	1:A:1056:ARG:HH21	1.57	0.69
1:C:848:ILE:O	1:C:852:VAL:HG23	1.92	0.69
1:D:570:ASN:OD1	1:D:571:ALA:N	2.25	0.69
1:G:813:LEU:HD11	1:G:837:HIS:HB2	1.74	0.69
1:H:516:LYS:O	1:H:520:GLU:HG3	1.92	0.69
1:H:999:ARG:NH1	1:H:1003:MET:O	2.25	0.69
1:H:1081:ASN:O	1:H:1085:LYS:HG2	1.92	0.69
1:B:999:ARG:NH1	1:B:1003:MET:O	2.24	0.69
1:D:355:ARG:NH1	1:H:1052:THR:OG1	2.24	0.69
1:E:711:GLN:NE2	3:E:1301:HOH:O	2.24	0.69
1:H:600:GLN:NE2	1:H:604:THR:OG1	2.25	0.69
1:A:354:VAL:HG11	1:A:411:PRO:HB2	1.74	0.69
1:C:738:MET:HG2	1:C:1098:ILE:HB	1.75	0.69
1:F:398:GLN:HB2	1:F:401:GLU:CD	2.17	0.69
1:H:568:GLU:CD	1:H:569:GLN:N	2.51	0.69
1:A:637:GLU:OE1	1:A:639:ARG:NH2	2.26	0.69
1:C:824:PHE:HD1	1:C:909:PHE:HD2	1.38	0.69
1:A:1054:GLU:CG	1:E:912:LYS:HE2	2.22	0.69
1:B:354:VAL:O	1:B:355:ARG:HD3	1.91	0.69
1:H:412:ARG:NH2	1:H:1110:GLU:OE2	2.24	0.69
1:C:532:GLU:OE1	1:C:532:GLU:N	2.25	0.69
1:F:785:SER:HA	1:F:888:GLY:O	1.93	0.69
1:G:337:MET:HB2	1:G:345:GLN:HE22	1.57	0.69
1:E:1095:ARG:HA	1:E:1109:VAL:HG21	1.75	0.68
1:F:341:THR:O	1:F:345:GLN:HG3	1.92	0.68
1:F:981:SER:OG	1:F:1008:GLY:N	2.25	0.68
1:H:702:ASP:OD1	1:H:705:ARG:NH2	2.24	0.68
1:C:753:MET:HE3	1:C:774:PRO:HB2	1.75	0.68
1:E:790:GLN:HB2	1:E:792:PRO:HD2	1.75	0.68
1:G:821:LEU:HB3	1:G:827:PHE:HB2	1.75	0.68
1:A:964:GLU:OE1	1:A:967:LYS:NZ	2.20	0.68
1:B:423:ARG:NH1	1:B:465:GLU:HG3	2.07	0.68
1:C:552:ASN:O	1:C:556:ARG:HG2	1.93	0.68
1:D:595:LEU:HD13	1:D:631:PHE:HB2	1.75	0.68
1:E:497:GLY:O	1:E:499:THR:OG1	2.11	0.68
1:G:641:THR:O	1:G:644:THR:OG1	2.09	0.68
1:C:879:GLY:O	1:C:884:ASN:ND2	2.23	0.68
1:H:949:TYR:HD1	1:H:949:TYR:O	1.76	0.68
1:C:1073:GLN:HE22	1:C:1075:GLN:NE2	1.92	0.68
1:F:502:GLY:HA3	1:F:505:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:986:THR:HG22	1:G:1004:PRO:HG3	1.74	0.68
1:D:398:GLN:NE2	1:D:401:GLU:OE2	2.27	0.68
1:E:522:HIS:HB3	1:E:540:TYR:CE2	2.28	0.68
1:E:857:ALA:O	1:E:859:LYS:NZ	2.23	0.68
1:F:848:ILE:O	1:F:852:VAL:HG23	1.94	0.68
1:A:776:LYS:HD2	1:A:779:ARG:HD2	1.75	0.68
1:B:432:MET:HA	1:B:435:ARG:HD3	1.75	0.68
1:E:912:LYS:HB2	1:E:912:LYS:NZ	2.09	0.68
1:F:995:THR:OG1	1:F:999:ARG:HB3	1.94	0.68
1:C:679:ASN:OD1	1:C:680:LEU:N	2.27	0.67
1:H:1019:GLY:CA	1:H:1127:LYS:HD3	2.23	0.67
1:D:708:LYS:HZ2	1:D:1098:ILE:HG13	1.59	0.67
1:D:367:THR:HG23	1:D:458:TRP:HE1	1.59	0.67
1:H:463:LEU:HD11	1:H:853:HIS:HA	1.76	0.67
1:H:1064:ARG:HH22	1:H:1068:ILE:CG1	2.07	0.67
1:G:806:LEU:HD23	1:G:991:LEU:HD23	1.76	0.67
1:H:948:ASN:O	1:H:952:GLN:HG3	1.94	0.67
1:D:467:CYS:HB3	1:D:492:GLN:HG3	1.74	0.67
1:E:770:GLY:HA3	2:E:1201:A1H9L:F1	1.85	0.67
1:F:730:ILE:O	1:F:734:VAL:HG23	1.92	0.67
1:G:1084:LEU:HB3	1:G:1120:ILE:HD11	1.76	0.67
1:H:398:GLN:NE2	1:H:401:GLU:OE2	2.28	0.67
1:H:489:SER:HA	1:H:492:GLN:HG2	1.77	0.67
1:H:919:ILE:HA	1:H:922:ALA:HB3	1.77	0.67
1:A:650:GLN:HB3	1:A:707:VAL:CG1	2.25	0.67
1:F:771:CYS:HB3	1:F:1103:GLY:HA3	1.76	0.67
1:H:734:VAL:HG12	1:H:1050:LEU:HD11	1.76	0.67
1:E:702:ASP:HA	1:E:705:ARG:HE	1.59	0.67
1:H:483:THR:HB	1:H:804:MET:HE1	1.75	0.67
1:H:541:LYS:HA	1:H:544:ILE:HD12	1.76	0.67
1:E:727:MET:HG3	1:E:1064:ARG:NH1	2.09	0.67
1:F:1048:GLY:HA2	1:F:1051:ASP:OD2	1.95	0.67
1:G:951:ASP:HB3	1:G:1029:LYS:HG3	1.77	0.67
1:C:872:SER:HB3	3:C:1338:HOH:O	1.94	0.66
1:D:1106:ALA:HB1	1:D:1111:LEU:HD11	1.76	0.66
1:G:854:ARG:HA	1:G:877:ALA:HB1	1.77	0.66
1:B:731:VAL:HG22	1:B:1059:LEU:HD23	1.77	0.66
1:C:419:ASP:HB3	1:C:458:TRP:CZ3	2.31	0.66
1:C:685:GLN:H	1:C:717:ARG:NH2	1.93	0.66
1:D:799:LEU:HA	1:D:818:LEU:HD21	1.77	0.66
1:D:1021:THR:HA	1:D:1024:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:527:SER:OG	1:F:529:GLU:HG2	1.94	0.66
1:F:787:GLY:C	1:F:889:LEU:HD11	2.20	0.66
1:E:678:ILE:CG2	1:E:712:PRO:HB3	2.24	0.66
1:F:344:MET:HE1	1:F:651:ALA:HB2	1.78	0.66
1:F:1114:GLU:OE1	1:F:1114:GLU:N	2.23	0.66
1:E:512:MET:CE	1:E:550:VAL:HG21	2.24	0.66
1:F:749:HIS:HA	1:F:752:MET:HG2	1.78	0.66
1:D:686:LYS:HD3	1:D:688:SER:H	1.60	0.66
1:A:957:ILE:HD12	1:A:957:ILE:C	2.20	0.66
1:G:396:LEU:CD1	1:G:398:GLN:HG2	2.26	0.66
1:G:1046:LEU:CD2	1:G:1126:GLU:HG2	2.26	0.66
1:C:500:CYS:SG	1:C:619:SER:HB2	2.36	0.66
1:E:993:ASN:ND2	1:E:994:ALA:H	1.94	0.66
1:G:364:LEU:HD22	1:G:454:ILE:HD11	1.78	0.66
1:C:727:MET:HE2	1:C:1064:ARG:HG3	1.78	0.66
1:C:608:LEU:O	1:C:611:ILE:N	2.29	0.65
1:C:790:GLN:HB2	1:C:792:PRO:HD2	1.77	0.65
1:F:483:THR:HG21	1:F:811:GLN:HG3	1.77	0.65
1:F:819:ARG:NH2	1:F:916:LEU:H	1.94	0.65
1:A:795:ILE:HG12	1:A:901:MET:HE1	1.76	0.65
1:C:703:ALA:O	1:C:707:VAL:HG12	1.96	0.65
1:D:803:ARG:NH1	1:D:808:ASP:OD1	2.29	0.65
1:G:400:ASP:H	1:G:573:ARG:HH12	1.45	0.65
1:G:569:GLN:H	1:G:569:GLN:CD	2.04	0.65
1:G:729:LYS:O	1:G:733:VAL:HG23	1.95	0.65
1:C:555:ARG:NH1	1:C:585:GLU:OE2	2.30	0.65
1:E:900:SER:O	1:E:904:ILE:HD12	1.95	0.65
1:F:442:ILE:HG23	1:F:447:LYS:HE3	1.79	0.65
1:F:1075:GLN:HE22	1:F:1103:GLY:CA	2.07	0.65
1:B:1021:THR:O	1:B:1025:LYS:HG2	1.96	0.65
1:C:1075:GLN:HE22	1:C:1103:GLY:HA2	1.62	0.65
1:E:803:ARG:HB2	1:E:810:TYR:CZ	2.30	0.65
1:F:742:ALA:HB2	1:F:1075:GLN:HE21	1.62	0.65
1:G:359:SER:HB3	1:G:415:ALA:HA	1.79	0.65
1:G:400:ASP:H	1:G:573:ARG:NH1	1.95	0.65
1:G:622:ARG:HA	1:G:681:THR:O	1.97	0.65
1:B:832:LYS:NZ	1:B:956:ASP:OD2	2.29	0.65
1:D:982:ILE:HG23	1:D:1104:TYR:CE1	2.32	0.65
1:D:966:ARG:HG2	1:D:975:LEU:O	1.97	0.65
1:C:656:CYS:HB2	1:C:712:PRO:HD3	1.77	0.65
1:E:1127:LYS:HG2	1:E:1128:PHE:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:VAL:HG21	1:A:714:LEU:HD22	1.79	0.65
1:F:822:ARG:HH11	1:F:823:THR:HG22	1.62	0.65
1:H:594:THR:HG23	1:H:597:GLU:H	1.62	0.65
1:E:697:THR:O	1:E:701:MET:HG3	1.97	0.64
1:F:756:LYS:HA	1:F:885:HIS:CD2	2.32	0.64
1:F:909:PHE:O	1:F:912:LYS:HE3	1.96	0.64
1:G:352:LEU:O	1:G:1095:ARG:NE	2.30	0.64
1:G:819:ARG:HD2	1:G:819:ARG:O	1.96	0.64
1:G:897:TYR:CE1	1:G:957:ILE:HG21	2.32	0.64
1:H:467:CYS:HB2	1:H:852:VAL:HG21	1.79	0.64
1:D:428:GLU:HB3	1:D:432:MET:HG3	1.79	0.64
1:F:376:MET:HG3	1:F:377:PRO:HD2	1.79	0.64
1:F:487:ASP:O	1:F:787:GLY:HA2	1.98	0.64
1:H:437:GLN:NE2	1:H:1110:GLU:O	2.25	0.64
1:H:923:LEU:HD12	1:H:994:ALA:C	2.23	0.64
1:A:343:ARG:HG3	1:A:400:ASP:HB3	1.79	0.64
1:A:435:ARG:NH2	1:A:438:ASP:O	2.27	0.64
1:B:897:TYR:CE2	1:B:901:MET:HE2	2.32	0.64
1:D:957:ILE:HD12	1:D:958:THR:H	1.62	0.64
1:G:366:PHE:O	1:G:370:VAL:HG23	1.97	0.64
1:H:1111:LEU:O	1:H:1116:GLN:NE2	2.29	0.64
1:A:530:ASN:HB3	1:A:532:GLU:OE2	1.97	0.64
1:C:584:ASN:OD1	1:C:600:GLN:NE2	2.25	0.64
1:C:637:GLU:OE1	1:C:639:ARG:NH1	2.29	0.64
1:C:728:GLU:HG2	1:C:1060:ILE:HD11	1.78	0.64
1:D:973:SER:OG	1:D:974:THR:N	2.31	0.64
1:E:739:GLY:HA3	1:E:1100:ARG:CG	2.28	0.64
1:F:800:ASN:O	1:F:803:ARG:HB2	1.96	0.64
1:C:756:LYS:NZ	1:C:782:GLN:OE1	2.28	0.64
1:G:625:GLN:OE1	1:G:692:ALA:HB1	1.98	0.64
1:E:790:GLN:HE22	1:E:992:THR:CG2	2.11	0.64
1:G:724:GLN:HA	1:G:727:MET:HB2	1.78	0.64
1:H:382:ARG:NH2	1:H:613:GLU:OE1	2.31	0.64
1:H:966:ARG:HD3	1:H:975:LEU:O	1.97	0.64
1:H:1013:GLN:HG2	1:H:1121:SER:OG	1.98	0.64
1:C:525:SER:O	1:C:525:SER:OG	2.16	0.64
1:D:770:GLY:HA3	2:D:1201:A1H9L:F1	1.87	0.64
1:F:1044:LYS:NZ	1:F:1119:ILE:O	2.30	0.64
1:G:635:ILE:HD13	1:G:641:THR:CA	2.26	0.64
1:E:348:ARG:HH21	1:E:352:LEU:HD11	1.63	0.64
1:G:635:ILE:HA	1:G:640:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:382:ARG:NH1	1:H:419:ASP:OD2	2.31	0.64
1:B:940:ALA:O	1:B:942:LYS:NZ	2.26	0.64
1:F:660:MET:HE1	1:F:674:TYR:HB3	1.79	0.64
1:G:635:ILE:CD1	1:G:641:THR:CA	2.75	0.64
1:F:897:TYR:CZ	1:F:901:MET:HE3	2.33	0.64
1:F:993:ASN:OD1	1:F:994:ALA:N	2.31	0.64
1:D:957:ILE:HD12	1:D:958:THR:N	2.13	0.63
1:E:503:TYR:HA	1:E:507:LEU:HB3	1.80	0.63
1:B:1095:ARG:HA	1:B:1109:VAL:HG21	1.80	0.63
1:D:673:GLY:O	1:D:675:GLN:NE2	2.26	0.63
1:F:486:SER:HB2	1:F:789:THR:HB	1.80	0.63
1:G:573:ARG:O	1:G:577:LEU:HG	1.98	0.63
1:G:803:ARG:NH1	1:G:808:ASP:OD1	2.31	0.63
1:G:905:ARG:NH1	1:G:910:GLU:OE2	2.31	0.63
1:G:980:LEU:HA	1:G:1040:VAL:HG12	1.80	0.63
1:H:531:PRO:HA	1:H:534:ILE:HD12	1.80	0.63
1:H:422:TRP:CE3	1:H:423:ARG:HA	2.33	0.63
1:B:748:SER:OG	1:B:1071:ASN:O	2.15	0.63
1:C:823:THR:OG1	1:C:826:GLU:N	2.19	0.63
1:F:424:TRP:O	1:F:428:GLU:HB2	1.98	0.63
1:H:437:GLN:HE21	1:H:1111:LEU:HA	1.62	0.63
1:F:701:MET:HE3	1:F:729:LYS:HG2	1.79	0.63
1:B:1016:ASP:HB2	1:B:1023:ILE:HD11	1.81	0.63
1:C:686:LYS:HB2	1:C:689:GLY:O	1.99	0.63
1:E:915:THR:HB	1:E:918:GLN:H	1.63	0.63
1:F:1073:GLN:HE22	1:F:1075:GLN:HG3	1.63	0.63
1:F:957:ILE:HD12	1:F:958:THR:N	2.13	0.63
1:E:467:CYS:HB3	1:E:492:GLN:HG3	1.81	0.63
1:E:532:GLU:CD	1:E:532:GLU:H	2.06	0.63
1:G:348:ARG:HH21	1:G:708:LYS:HB2	1.64	0.63
1:A:898:VAL:HG13	1:A:953:TYR:HB2	1.80	0.62
1:B:382:ARG:NH2	1:B:613:GLU:OE1	2.31	0.62
1:B:744:HIS:CE1	1:B:768:LEU:HG	2.33	0.62
1:B:779:ARG:HG2	1:B:882:MET:SD	2.38	0.62
1:G:504:ASP:OD1	1:G:505:VAL:N	2.32	0.62
1:G:666:LEU:HG	1:G:669:LYS:HZ1	1.63	0.62
1:A:897:TYR:CE1	1:A:901:MET:HE3	2.33	0.62
1:C:751:LYS:HE2	1:H:751:LYS:HG3	1.81	0.62
1:G:822:ARG:HG3	1:G:822:ARG:NH1	2.13	0.62
1:G:908:VAL:HG11	1:G:916:LEU:HG	1.80	0.62
1:H:424:TRP:O	1:H:428:GLU:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LYS:HE2	1:A:736:ALA:HB1	1.81	0.62
1:B:1073:GLN:HE22	1:B:1075:GLN:NE2	1.97	0.62
1:C:344:MET:HG3	1:C:650:GLN:NE2	2.13	0.62
1:C:795:ILE:HG12	1:C:901:MET:HE3	1.81	0.62
1:G:606:GLU:OE2	1:G:659:LEU:CD1	2.48	0.62
1:G:813:LEU:HD11	1:G:837:HIS:CB	2.30	0.62
1:H:917:GLU:O	1:H:920:ARG:HB3	1.99	0.62
1:D:439:PRO:O	1:D:674:TYR:OH	2.12	0.62
1:H:343:ARG:NH1	1:H:402:LEU:HD11	2.14	0.62
1:A:685:GLN:H	1:A:717:ARG:NH2	1.97	0.62
1:C:751:LYS:NZ	1:H:747:ASP:HA	2.15	0.62
1:G:498:ASP:OD1	1:G:784:THR:HG22	1.99	0.62
1:H:955:LEU:HD13	1:H:1031:ASN:H	1.64	0.62
1:B:831:VAL:HG21	1:B:901:MET:HE1	1.82	0.62
1:C:952:GLN:CA	1:C:1029:LYS:HZ2	2.12	0.62
1:F:1025:LYS:HA	1:F:1028:SER:HB3	1.81	0.62
1:H:510:LYS:HG3	1:H:514:GLY:HA3	1.80	0.62
1:H:526:LEU:HB3	1:H:533:ASP:HB3	1.82	0.62
1:C:621:GLY:HA2	1:C:767:CYS:HB2	1.80	0.62
1:E:727:MET:HE2	1:E:1064:ARG:HD2	1.82	0.62
1:G:437:GLN:OE1	1:G:1112:CYS:HB2	1.99	0.62
1:G:599:LEU:HD22	1:G:652:PHE:CG	2.35	0.62
1:A:999:ARG:NH1	1:A:1003:MET:O	2.33	0.62
1:D:340:LEU:HD12	1:D:345:GLN:HG2	1.81	0.62
1:E:499:THR:O	1:E:501:PRO:HD3	2.00	0.62
1:G:888:GLY:HA3	1:G:1037:ILE:HG13	1.82	0.62
1:F:966:ARG:HH11	1:F:974:THR:HG23	1.64	0.61
1:C:367:THR:O	1:C:371:LYS:HB2	2.00	0.61
1:C:596:GLN:HB2	1:C:648:LEU:HD11	1.80	0.61
1:E:795:ILE:HG12	1:E:901:MET:HE3	1.80	0.61
1:F:704:VAL:HG21	1:F:714:LEU:HD22	1.82	0.61
1:G:348:ARG:NE	1:G:707:VAL:O	2.31	0.61
1:H:890:ILE:HD11	1:H:1037:ILE:HD11	1.82	0.61
1:D:587:VAL:HB	1:D:601:SER:HB2	1.82	0.61
1:D:437:GLN:HG3	1:D:1112:CYS:H	1.66	0.61
1:D:564:LEU:HA	1:D:567:LYS:HG3	1.82	0.61
1:E:962:GLU:HB2	1:E:977:HIS:CD2	2.34	0.61
1:F:727:MET:HA	1:F:730:ILE:HD12	1.82	0.61
1:C:962:GLU:HG2	1:C:977:HIS:HD2	1.65	0.61
1:E:348:ARG:NH1	1:E:707:VAL:O	2.34	0.61
1:F:420:ILE:HD11	1:F:613:GLU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:981:SER:HB3	1:G:1008:GLY:H	1.64	0.61
1:H:344:MET:SD	1:H:650:GLN:HG3	2.40	0.61
1:F:858:PRO:O	1:F:860:PRO:HD3	1.99	0.61
1:A:1048:GLY:HA2	1:A:1051:ASP:OD2	2.01	0.60
1:B:685:GLN:NE2	1:B:746:ASP:OD2	2.33	0.60
1:E:927:PHE:HE2	1:E:1000:LEU:HA	1.66	0.60
1:F:346:ARG:NH1	1:F:400:ASP:OD1	2.33	0.60
1:G:767:CYS:SG	1:G:777:SER:HB3	2.41	0.60
1:H:744:HIS:HD2	1:H:749:HIS:HE1	1.48	0.60
1:H:1084:LEU:HA	1:H:1087:ALA:HB3	1.83	0.60
1:D:943:TYR:OH	1:D:1027:VAL:HG22	2.01	0.60
1:H:719:HIS:HB3	1:H:746:ASP:OD2	2.01	0.60
1:B:337:MET:HB3	1:B:340:LEU:HD12	1.83	0.60
1:B:477:TRP:O	1:B:481:GLY:N	2.35	0.60
1:H:600:GLN:NE2	1:H:604:THR:HG1	1.99	0.60
1:E:681:THR:HA	1:E:715:ALA:HB3	1.83	0.60
1:E:1000:LEU:HB2	1:E:1003:MET:SD	2.42	0.60
1:G:666:LEU:HG	1:G:669:LYS:NZ	2.16	0.60
1:D:782:GLN:NE2	1:D:1037:ILE:HD13	2.16	0.60
1:F:708:LYS:HA	1:F:738:MET:SD	2.41	0.60
1:F:839:VAL:HG11	1:F:964:GLU:O	2.02	0.60
1:G:896:THR:HG21	1:G:1005:LEU:HD22	1.82	0.60
1:B:1025:LYS:O	1:B:1028:SER:OG	2.15	0.60
1:G:412:ARG:NH2	1:G:1110:GLU:OE2	2.26	0.60
1:F:395:ILE:HG23	1:F:557:ILE:HD13	1.84	0.60
1:G:559:ALA:O	1:G:563:GLU:HG2	2.02	0.60
1:H:337:MET:HB2	1:H:345:GLN:HE21	1.67	0.60
1:H:957:ILE:CD1	1:H:958:THR:N	2.62	0.60
1:A:466:ILE:HD13	1:A:856:VAL:HG11	1.82	0.60
1:E:931:GLU:OE1	1:E:931:GLU:N	2.30	0.60
1:E:995:THR:HG21	1:E:999:ARG:HB3	1.84	0.60
1:F:602:ILE:HG21	1:F:620:LEU:HD22	1.82	0.60
1:F:1084:LEU:HD22	1:F:1108:PHE:CE2	2.37	0.60
1:B:579:THR:O	1:B:583:VAL:HG13	2.02	0.60
1:C:542:ALA:O	1:C:546:THR:HG22	2.02	0.60
1:D:846:THR:O	1:D:849:SER:OG	2.19	0.60
1:D:1084:LEU:HB2	1:D:1120:ILE:HD11	1.84	0.60
1:F:653:ILE:HG23	1:F:712:PRO:HD2	1.84	0.60
1:F:1085:LYS:HD3	1:F:1088:GLN:NE2	2.16	0.60
1:G:595:LEU:HD23	1:G:595:LEU:O	2.00	0.60
1:D:624:ASP:HB3	1:D:700:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:678:ILE:HG22	1:E:712:PRO:HB3	1.82	0.60
1:C:849:SER:OG	1:C:850:GLN:N	2.34	0.59
1:D:361:TYR:CD2	1:D:394:PRO:HG2	2.37	0.59
1:D:1021:THR:HG23	1:D:1024:ILE:HD11	1.84	0.59
1:H:717:ARG:NH1	1:H:766:TYR:O	2.35	0.59
1:A:432:MET:HA	1:A:435:ARG:HD3	1.84	0.59
1:B:395:ILE:HD11	1:B:556:ARG:HG2	1.84	0.59
1:E:827:PHE:HE2	1:E:901:MET:HE1	1.67	0.59
1:F:821:LEU:HD21	1:F:830:ALA:HB3	1.84	0.59
1:A:423:ARG:HH21	1:A:464:ASP:CG	2.11	0.59
1:B:435:ARG:NH2	1:B:438:ASP:HB2	2.17	0.59
1:D:1113:LYS:HD2	1:D:1113:LYS:H	1.67	0.59
1:E:483:THR:HB	1:E:804:MET:HE1	1.83	0.59
1:H:982:ILE:HG23	1:H:1104:TYR:CE1	2.38	0.59
1:H:382:ARG:NH2	1:H:857:ALA:HB1	2.17	0.59
1:A:419:ASP:N	1:A:419:ASP:OD1	2.36	0.59
1:B:799:LEU:HA	1:B:818:LEU:HD21	1.84	0.59
1:D:356:PRO:HG2	1:D:674:TYR:CZ	2.38	0.59
1:G:426:ARG:HG3	1:G:455:VAL:HG21	1.84	0.59
1:G:550:VAL:HG12	1:G:608:LEU:HD13	1.83	0.59
1:G:850:GLN:HB2	1:G:971:LEU:HD22	1.84	0.59
1:H:338:GLU:HG3	1:H:706:PHE:CD1	2.38	0.59
1:H:340:LEU:HD23	1:H:344:MET:HB3	1.84	0.59
1:H:515:ILE:HD12	1:H:864:LEU:HD22	1.83	0.59
1:B:973:SER:OG	1:B:974:THR:N	2.30	0.59
1:C:397:ILE:HG23	1:C:404:VAL:HG11	1.83	0.59
1:E:914:TYR:CZ	1:E:933:LEU:HB3	2.37	0.59
1:G:516:LYS:HG3	1:G:544:ILE:HA	1.84	0.59
1:G:982:ILE:H	1:G:982:ILE:HD12	1.67	0.59
1:H:1019:GLY:HA2	1:H:1127:LYS:HD3	1.83	0.59
1:A:897:TYR:CE2	1:A:957:ILE:HG21	2.37	0.59
1:C:487:ASP:O	1:C:787:GLY:HA2	2.01	0.59
1:C:739:GLY:HA3	1:C:1100:ARG:CG	2.32	0.59
1:D:640:LEU:HB3	1:D:644:THR:OG1	2.02	0.59
1:E:592:PRO:HG2	1:E:630:MET:HE3	1.83	0.59
1:G:587:VAL:HG11	1:G:592:PRO:HB3	1.84	0.59
1:G:793:ILE:HG13	1:G:796:GLU:HG3	1.84	0.59
1:H:398:GLN:HG3	1:H:401:GLU:CD	2.27	0.59
1:D:717:ARG:NH2	1:D:764:ARG:O	2.29	0.59
1:E:666:LEU:HA	1:E:669:LYS:HE3	1.83	0.59
1:G:914:TYR:CE2	1:G:933:LEU:HD13	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:450:ILE:HA	1:H:454:ILE:HB	1.84	0.59
1:A:985:ASN:HD21	1:A:1118:GLU:CD	2.11	0.59
1:B:890:ILE:HD12	1:B:980:LEU:HD21	1.84	0.59
1:F:912:LYS:CD	1:F:912:LYS:NZ	2.63	0.59
1:G:1042:ASN:ND2	1:G:1101:VAL:O	2.36	0.59
1:G:1107:TYR:HB2	1:G:1110:GLU:OE1	2.01	0.59
1:G:1108:PHE:CE1	1:G:1116:GLN:HG3	2.37	0.59
1:A:1041:HIS:NE2	1:A:1043:PHE:HE1	2.01	0.59
1:C:488:LEU:HD13	1:C:845:GLY:HA3	1.85	0.59
1:C:756:LYS:HA	1:C:885:HIS:CD2	2.38	0.59
1:D:634:ASP:HB3	1:D:640:LEU:HD12	1.85	0.59
1:D:897:TYR:CE2	1:D:957:ILE:HG21	2.37	0.59
1:D:1063:LEU:HD11	1:D:1076:PHE:CZ	2.37	0.59
1:E:361:TYR:CE2	1:E:394:PRO:HG3	2.37	0.59
1:G:361:TYR:CD2	1:G:394:PRO:HG3	2.38	0.59
1:G:362:ARG:NH1	1:G:417:SER:HA	2.17	0.59
1:G:443:SER:OG	1:G:446:ASP:N	2.32	0.59
1:G:1084:LEU:HD12	1:G:1097:LEU:HD21	1.85	0.59
1:D:1084:LEU:HA	1:D:1087:ALA:HB3	1.84	0.58
1:E:419:ASP:HB3	1:E:458:TRP:CH2	2.38	0.58
1:E:649:LEU:O	1:E:653:ILE:HG13	2.03	0.58
1:F:624:ASP:HB3	1:F:682:VAL:HG12	1.84	0.58
1:F:1108:PHE:CE1	1:F:1116:GLN:HB2	2.37	0.58
1:G:1061:THR:O	1:G:1065:THR:HG23	2.02	0.58
1:A:982:ILE:HA	3:A:1310:HOH:O	2.02	0.58
1:C:813:LEU:O	1:C:834:GLN:NE2	2.34	0.58
1:E:1113:LYS:HD3	1:E:1113:LYS:N	2.18	0.58
1:H:682:VAL:HG22	1:H:714:LEU:HD11	1.84	0.58
1:A:828:ASP:OD2	1:A:832:LYS:HE2	2.03	0.58
1:B:703:ALA:O	1:B:707:VAL:HG22	2.03	0.58
1:C:739:GLY:HA2	1:C:1076:PHE:O	2.03	0.58
1:D:615:GLN:HG3	1:D:618:LEU:HD21	1.84	0.58
1:D:1069:LEU:HA	1:E:721:GLN:NE2	2.19	0.58
1:E:1107:TYR:HB2	1:E:1110:GLU:OE1	2.03	0.58
1:F:583:VAL:HG22	1:F:597:GLU:HG3	1.84	0.58
1:D:694:ASN:OD1	1:D:697:THR:N	2.35	0.58
1:E:917:GLU:HA	1:E:920:ARG:HB3	1.84	0.58
1:H:356:PRO:HG2	1:H:674:TYR:CZ	2.38	0.58
1:B:753:MET:HE1	1:B:776:LYS:N	2.19	0.58
1:C:1020:PRO:HA	1:C:1023:ILE:HG12	1.85	0.58
1:D:362:ARG:NE	1:D:611:ILE:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1053:PRO:HA	1:D:1056:ARG:HB2	1.84	0.58
1:F:530:ASN:HB3	1:F:532:GLU:OE1	2.03	0.58
1:F:818:LEU:HD22	1:F:916:LEU:HB2	1.83	0.58
1:F:980:LEU:HD12	1:F:980:LEU:O	2.04	0.58
1:G:1086:LYS:CE	1:G:1094:TYR:CE2	2.86	0.58
1:E:356:PRO:HA	1:E:412:ARG:O	2.02	0.58
1:G:678:ILE:HG22	1:G:712:PRO:HB3	1.86	0.58
1:G:728:GLU:HG3	1:G:1056:ARG:HH21	1.69	0.58
1:A:941:PRO:HG2	1:A:949:TYR:CD2	2.38	0.58
1:C:805:VAL:HG21	1:C:993:ASN:CB	2.33	0.58
1:D:613:GLU:OE2	1:D:859:LYS:HD3	2.04	0.58
1:D:1127:LYS:HG2	1:D:1128:PHE:H	1.68	0.58
1:F:976:SER:HB3	1:F:1037:ILE:HD11	1.86	0.58
1:H:965:CYS:HB3	1:H:975:LEU:HG	1.84	0.58
1:D:700:ILE:O	1:D:704:VAL:HG23	2.04	0.58
1:D:1047:LYS:HD2	1:D:1079:VAL:HA	1.84	0.58
1:E:554:ALA:HB2	1:E:588:PRO:HD2	1.86	0.58
1:E:653:ILE:HG22	1:E:709:VAL:HG21	1.85	0.58
1:E:817:ASP:OD1	1:E:818:LEU:N	2.35	0.58
1:G:606:GLU:OE1	1:G:678:ILE:HD11	2.02	0.58
1:C:359:SER:HB2	1:C:361:TYR:HD2	1.69	0.58
1:C:730:ILE:HG23	1:C:741:PRO:CG	2.33	0.58
1:A:573:ARG:O	1:A:577:LEU:HG	2.04	0.58
1:B:769:MET:SD	1:B:770:GLY:N	2.77	0.58
1:C:522:HIS:HB3	1:C:540:TYR:CE2	2.39	0.58
1:C:1073:GLN:HE22	1:C:1075:GLN:HE21	1.50	0.58
1:F:927:PHE:CD2	1:F:934:ARG:HB2	2.39	0.58
1:G:676:PRO:HB2	1:G:678:ILE:HG12	1.85	0.58
1:H:1063:LEU:HD23	1:H:1074:MET:SD	2.44	0.58
1:B:801:ARG:HE	1:B:817:ASP:HA	1.70	0.57
1:D:356:PRO:HA	1:D:412:ARG:HB3	1.84	0.57
1:D:743:CYS:O	1:D:1073:GLN:HA	2.03	0.57
1:D:985:ASN:ND2	3:D:1302:HOH:O	2.37	0.57
1:E:596:GLN:HG3	1:E:648:LEU:HD21	1.86	0.57
1:F:745:PHE:O	1:F:749:HIS:ND1	2.37	0.57
1:F:476:VAL:HG12	1:F:841:LEU:HD22	1.86	0.57
1:F:908:VAL:HG11	1:F:916:LEU:HG	1.85	0.57
1:F:1079:VAL:HG21	1:F:1084:LEU:HD21	1.86	0.57
1:G:913:LYS:HD3	1:G:914:TYR:CE2	2.39	0.57
1:H:376:MET:HE3	1:H:380:LEU:CD2	2.35	0.57
1:H:759:ASP:OD1	1:H:760:PHE:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:981:SER:HB3	1:H:1008:GLY:H	1.69	0.57
1:C:665:GLU:HG2	1:C:666:LEU:HD22	1.84	0.57
1:D:832:LYS:HA	1:D:835:ILE:HD12	1.84	0.57
1:D:993:ASN:OD1	1:D:994:ALA:N	2.36	0.57
1:E:560:HIS:HA	1:E:563:GLU:HG2	1.85	0.57
1:E:930:TYR:HB3	1:E:933:LEU:CD2	2.34	0.57
1:H:356:PRO:HB3	1:H:660:MET:HE3	1.87	0.57
1:C:466:ILE:HA	1:G:375:GLY:HA3	1.86	0.57
1:F:483:THR:OG1	1:F:485:VAL:HG23	2.05	0.57
1:F:745:PHE:CD1	1:F:1067:SER:HB2	2.40	0.57
1:G:382:ARG:O	1:G:386:PHE:N	2.37	0.57
1:B:546:THR:O	1:B:550:VAL:HG23	2.03	0.57
1:C:827:PHE:HE2	1:C:901:MET:HE1	1.70	0.57
1:D:686:LYS:HE3	1:D:688:SER:HB3	1.85	0.57
1:E:1106:ALA:HB3	1:E:1111:LEU:HD21	1.87	0.57
1:F:1032:VAL:HB	1:F:1039:MET:HE1	1.87	0.57
1:C:905:ARG:NE	1:C:953:TYR:OH	2.38	0.57
1:D:435:ARG:HD2	1:D:665:GLU:HA	1.87	0.57
1:E:1118:GLU:HA	1:E:1121:SER:OG	2.04	0.57
1:E:612:GLU:OE2	1:E:861:LEU:N	2.37	0.57
1:E:1095:ARG:HG3	1:E:1096:ASP:H	1.69	0.57
1:F:654:ILE:O	1:F:658:GLU:HG3	2.03	0.57
1:H:367:THR:O	1:H:371:LYS:HB2	2.04	0.57
1:B:894:LEU:CD1	1:B:957:ILE:HD11	2.35	0.57
1:C:344:MET:HE2	1:C:650:GLN:HE21	1.69	0.57
1:D:887:PRO:HD2	1:D:970:MET:HG3	1.85	0.57
1:F:694:ASN:OD1	1:F:697:THR:N	2.35	0.57
1:F:952:GLN:HG3	1:F:953:TYR:CD1	2.39	0.57
1:F:1049:LEU:O	1:F:1055:GLY:HA3	2.05	0.57
1:G:516:LYS:HD3	1:G:547:CYS:HB2	1.87	0.57
1:G:594:THR:HG22	1:G:596:GLN:H	1.68	0.57
1:H:487:ASP:OD1	1:H:489:SER:OG	2.14	0.57
1:A:346:ARG:HD2	1:A:400:ASP:OD2	2.05	0.57
1:B:966:ARG:HH11	1:B:974:THR:CG2	2.17	0.57
1:C:660:MET:HE1	1:C:674:TYR:HB3	1.87	0.57
1:D:562:ARG:NH2	1:D:582:GLU:HG2	2.17	0.57
1:D:708:LYS:NZ	1:D:1098:ILE:HG13	2.20	0.57
1:E:915:THR:HG21	1:E:917:GLU:HG3	1.87	0.57
1:F:491:HIS:O	1:F:853:HIS:HE1	1.87	0.57
1:H:700:ILE:O	1:H:704:VAL:HG23	2.04	0.57
1:H:1057:HIS:O	1:H:1061:THR:OG1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:VAL:HG11	1:A:597:GLU:HB3	1.87	0.57
1:B:432:MET:HE3	1:B:440:PHE:HB2	1.87	0.57
1:D:620:LEU:HD12	1:D:680:LEU:HD12	1.86	0.57
1:E:813:LEU:HD11	1:E:837:HIS:HB2	1.87	0.57
1:E:1047:LYS:HE2	1:E:1079:VAL:HA	1.87	0.57
1:H:435:ARG:HD2	1:H:665:GLU:HG3	1.87	0.57
1:B:708:LYS:HA	1:B:738:MET:SD	2.44	0.56
1:B:917:GLU:HG3	3:B:1342:HOH:O	2.04	0.56
1:B:984:ASN:HA	1:B:987:PRO:HG2	1.86	0.56
1:C:745:PHE:CD1	1:C:1067:SER:HB3	2.40	0.56
1:C:952:GLN:CB	1:C:1029:LYS:NZ	2.68	0.56
1:F:641:THR:H	1:F:644:THR:HG1	1.50	0.56
1:G:423:ARG:HH11	1:G:465:GLU:HG2	1.69	0.56
1:G:839:VAL:HG11	1:G:964:GLU:HG3	1.88	0.56
1:C:842:SER:O	1:C:846:THR:OG1	2.23	0.56
1:D:564:LEU:HG	1:D:567:LYS:HE2	1.86	0.56
1:E:803:ARG:HB2	1:E:810:TYR:CE1	2.40	0.56
1:G:533:ASP:O	1:G:537:ILE:HG13	2.04	0.56
1:A:493:ILE:HG13	1:A:494:ASN:ND2	2.20	0.56
1:A:579:THR:HA	1:A:582:GLU:CG	2.35	0.56
1:A:731:VAL:HG12	1:A:1059:LEU:HD23	1.86	0.56
1:A:748:SER:O	1:A:752:MET:HG3	2.04	0.56
1:C:435:ARG:HD3	1:C:665:GLU:HA	1.88	0.56
1:D:685:GLN:NE2	1:D:746:ASP:OD2	2.23	0.56
1:D:703:ALA:O	1:D:707:VAL:HG22	2.06	0.56
1:D:900:SER:HB3	1:D:996:PRO:HB2	1.86	0.56
1:D:959:GLU:O	1:D:963:LYS:HG2	2.05	0.56
1:D:984:ASN:HA	1:D:987:PRO:HG2	1.86	0.56
1:E:957:ILE:HD12	1:E:958:THR:N	2.20	0.56
1:F:685:GLN:HG3	1:F:746:ASP:OD2	2.04	0.56
1:G:698:TYR:CD1	1:G:729:LYS:HG3	2.41	0.56
1:G:799:LEU:HD22	1:G:923:LEU:HD12	1.87	0.56
1:H:450:ILE:O	1:H:455:VAL:HG23	2.05	0.56
1:H:705:ARG:HB2	1:H:733:VAL:HG22	1.87	0.56
1:A:760:PHE:CZ	1:B:1033:GLU:HB3	2.40	0.56
1:B:1106:ALA:HB1	1:B:1111:LEU:HD11	1.86	0.56
1:D:927:PHE:CD1	1:D:934:ARG:HB2	2.40	0.56
1:D:995:THR:HG23	1:D:999:ARG:HH11	1.70	0.56
1:F:701:MET:HA	1:F:704:VAL:HG22	1.88	0.56
1:F:805:VAL:O	1:F:808:ASP:N	2.38	0.56
1:H:823:THR:HG1	1:H:826:GLU:H	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:LYS:HZ1	1:D:782:GLN:HE22	1.53	0.56
1:E:463:LEU:HG	1:E:852:VAL:HG12	1.87	0.56
1:E:938:LEU:HD11	1:E:998:GLY:HA3	1.88	0.56
1:E:1052:THR:CG2	1:E:1054:GLU:HB2	2.36	0.56
1:F:555:ARG:NH2	1:F:585:GLU:O	2.33	0.56
1:F:914:TYR:CE1	1:F:933:LEU:HD12	2.40	0.56
1:A:350:HIS:NE2	1:A:398:GLN:OE1	2.39	0.56
1:C:1075:GLN:NE2	1:C:1103:GLY:HA2	2.19	0.56
1:D:687:ARG:HD2	1:D:765:ASP:OD2	2.05	0.56
1:E:693:CYS:HA	1:E:697:THR:HG21	1.88	0.56
1:F:622:ARG:NH1	1:F:765:ASP:HA	2.21	0.56
1:F:938:LEU:CD2	1:F:998:GLY:HA3	2.36	0.56
1:G:429:LEU:HD23	1:G:442:ILE:HD11	1.88	0.56
1:G:635:ILE:HD13	1:G:640:LEU:C	2.30	0.56
1:A:388:HIS:CE1	1:A:392:THR:HG21	2.40	0.56
1:C:1100:ARG:HD3	1:C:1105:SER:OG	2.05	0.56
1:D:512:MET:HE3	1:D:550:VAL:HG11	1.87	0.56
1:E:758:PHE:CZ	1:E:780:ILE:HD12	2.41	0.56
1:E:1084:LEU:HD23	1:E:1108:PHE:CE1	2.41	0.56
1:F:452:GLU:O	1:F:456:PRO:HG2	2.06	0.56
1:F:646:LEU:O	1:F:650:GLN:HG2	2.05	0.56
1:F:733:VAL:HG13	1:F:741:PRO:HD3	1.88	0.56
1:F:822:ARG:NH1	1:F:823:THR:HG22	2.20	0.56
1:G:744:HIS:NE2	1:G:1073:GLN:HG3	2.21	0.56
1:G:1027:VAL:HG23	1:G:1071:ASN:ND2	2.20	0.56
1:H:526:LEU:HD21	1:H:536:ARG:HH21	1.69	0.56
1:H:969:LYS:O	1:H:970:MET:HE2	2.05	0.56
1:B:442:ILE:HG23	1:B:447:LYS:HE2	1.87	0.56
1:C:965:CYS:HA	1:C:975:LEU:HD23	1.88	0.56
1:H:450:ILE:HG13	1:H:454:ILE:HD12	1.87	0.56
1:D:355:ARG:NH1	1:H:1054:GLU:HB2	2.21	0.56
1:D:654:ILE:O	1:D:658:GLU:HG3	2.04	0.56
1:E:656:CYS:HB2	1:E:712:PRO:HD3	1.88	0.56
1:F:960:TRP:CH2	1:F:964:GLU:HG2	2.41	0.56
1:F:1047:LYS:HG3	1:F:1080:ASP:HB2	1.88	0.56
1:G:577:LEU:HD22	1:G:580:ILE:HD12	1.88	0.56
1:A:805:VAL:HG21	1:A:993:ASN:HD22	1.71	0.56
1:A:904:ILE:HD11	1:A:996:PRO:HG2	1.87	0.56
1:A:1039:MET:SD	1:A:1072:GLY:HA3	2.46	0.56
1:B:426:ARG:O	1:B:428:GLU:N	2.39	0.56
1:C:605:VAL:O	1:C:608:LEU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:SER:HB2	1:D:488:LEU:HD12	1.88	0.56
1:E:680:LEU:HD23	1:E:681:THR:N	2.21	0.56
1:H:573:ARG:O	1:H:577:LEU:HD23	2.06	0.56
1:H:1007:ASP:OD1	1:H:1007:ASP:N	2.37	0.56
1:H:1064:ARG:HH12	1:H:1068:ILE:HD11	1.71	0.56
1:A:428:GLU:O	1:A:432:MET:HG3	2.06	0.55
1:D:785:SER:HA	1:D:888:GLY:O	2.06	0.55
1:E:382:ARG:NH2	1:E:613:GLU:OE1	2.40	0.55
1:F:349:ASN:O	1:F:353:THR:HG23	2.05	0.55
1:H:546:THR:O	1:H:550:VAL:HG23	2.06	0.55
1:H:744:HIS:HD2	1:H:749:HIS:CE1	2.24	0.55
1:B:1047:LYS:HE3	1:B:1079:VAL:HA	1.87	0.55
1:E:487:ASP:O	1:E:787:GLY:HA2	2.06	0.55
1:E:900:SER:HB3	1:E:996:PRO:HB2	1.87	0.55
1:G:1045:PHE:HE1	1:G:1125:ILE:HD11	1.70	0.55
1:H:376:MET:HB3	1:H:381:LEU:HD22	1.88	0.55
1:A:1008:GLY:N	3:A:1308:HOH:O	2.37	0.55
1:B:450:ILE:HA	1:B:454:ILE:HD12	1.87	0.55
1:D:1080:ASP:O	1:D:1083:VAL:HG22	2.07	0.55
1:F:567:LYS:HG3	1:F:567:LYS:O	2.04	0.55
1:F:805:VAL:HG21	1:F:993:ASN:HD22	1.71	0.55
1:A:488:LEU:HD13	1:A:845:GLY:HA3	1.87	0.55
1:E:351:TYR:O	1:E:354:VAL:HG22	2.07	0.55
1:F:790:GLN:NE2	1:F:1005:LEU:HD11	2.22	0.55
1:F:821:LEU:HD12	1:F:826:GLU:HB3	1.89	0.55
1:F:844:ILE:HD11	1:H:529:GLU:HG2	1.87	0.55
1:G:554:ALA:O	1:G:557:ILE:HG22	2.07	0.55
1:B:705:ARG:NH1	1:B:732:ASP:HB3	2.22	0.55
1:B:964:GLU:HA	1:B:967:LYS:HE3	1.88	0.55
1:C:980:LEU:HA	1:C:1040:VAL:HG12	1.88	0.55
1:E:702:ASP:O	1:E:705:ARG:HG2	2.07	0.55
1:E:1032:VAL:HA	1:E:1035:MET:HE2	1.88	0.55
1:F:535:ASP:O	1:F:538:TYR:N	2.35	0.55
1:F:560:HIS:ND1	1:F:563:GLU:OE1	2.38	0.55
1:F:773:GLU:OE2	1:F:980:LEU:HD22	2.06	0.55
1:G:635:ILE:HD13	1:G:640:LEU:O	2.07	0.55
1:G:943:TYR:OH	1:G:1027:VAL:HG12	2.07	0.55
1:H:863:SER:OG	1:H:875:ASP:HB2	2.05	0.55
1:A:782:GLN:NE2	3:A:1303:HOH:O	2.32	0.55
1:B:536:ARG:HD3	1:B:872:SER:O	2.06	0.55
1:B:552:ASN:O	1:B:556:ARG:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ARG:HG2	1:C:873:GLY:HA3	1.88	0.55
1:C:656:CYS:CB	1:C:712:PRO:HD3	2.35	0.55
1:D:582:GLU:HA	1:D:585:GLU:HB3	1.88	0.55
1:D:752:MET:HE3	1:D:1036:ASN:HA	1.88	0.55
1:F:343:ARG:NH1	1:F:402:LEU:HD21	2.22	0.55
1:F:362:ARG:HG3	1:F:611:ILE:HA	1.89	0.55
1:G:761:GLU:O	1:G:765:ASP:HB2	2.05	0.55
1:A:713:SER:HB2	3:A:1356:HOH:O	2.06	0.55
1:C:432:MET:HG2	1:C:435:ARG:NH2	2.14	0.55
1:D:600:GLN:HE21	1:D:604:THR:CG2	2.20	0.55
1:D:916:LEU:HA	1:D:919:ILE:HG22	1.89	0.55
1:D:1046:LEU:HD13	1:D:1126:GLU:HG2	1.88	0.55
1:E:977:HIS:CE1	1:E:1035:MET:HG2	2.41	0.55
1:F:388:HIS:O	1:F:392:THR:HG23	2.06	0.55
1:G:1112:CYS:O	1:G:1116:GLN:HB2	2.07	0.55
1:H:416:PHE:CE1	1:H:425:VAL:HG11	2.42	0.55
1:H:437:GLN:NE2	1:H:1111:LEU:HD23	2.22	0.55
1:A:553:TYR:O	1:A:557:ILE:HG12	2.07	0.55
1:C:546:THR:HG23	1:C:864:LEU:HD11	1.88	0.55
1:C:765:ASP:HB3	1:C:776:LYS:HD3	1.88	0.55
1:D:634:ASP:CB	1:D:640:LEU:HD12	2.37	0.55
1:F:779:ARG:HD3	1:F:882:MET:SD	2.46	0.55
1:F:952:GLN:HG3	1:F:953:TYR:HD1	1.72	0.55
1:F:984:ASN:C	1:F:987:PRO:HD2	2.32	0.55
1:G:380:LEU:HA	1:G:542:ALA:CB	2.33	0.55
1:G:636:ARG:HG3	1:G:637:GLU:N	2.21	0.55
1:B:694:ASN:O	1:B:697:THR:HB	2.07	0.55
1:B:1084:LEU:HD22	1:B:1108:PHE:CE1	2.42	0.55
1:C:716:CYS:HB3	1:C:726:TYR:OH	2.07	0.55
1:G:937:CYS:O	1:G:942:LYS:NZ	2.35	0.55
1:G:1064:ARG:O	1:G:1068:ILE:HG13	2.06	0.55
1:H:359:SER:OG	1:H:361:TYR:HD2	1.74	0.55
1:H:919:ILE:HG22	1:H:933:LEU:HD11	1.89	0.55
1:A:698:TYR:CZ	1:A:725:LYS:HE2	2.41	0.55
1:B:428:GLU:O	1:B:432:MET:HG3	2.07	0.55
1:B:536:ARG:HG2	1:B:873:GLY:HA3	1.89	0.55
1:C:976:SER:HB3	1:C:1037:ILE:HD11	1.87	0.55
1:A:491:HIS:CE1	1:A:783:TRP:CG	2.95	0.54
1:D:995:THR:OG1	1:D:999:ARG:HB3	2.08	0.54
1:F:498:ASP:HA	1:F:769:MET:CE	2.37	0.54
1:H:574:ARG:C	1:H:578:LEU:HD12	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1084:LEU:HD21	1:C:1099:VAL:HG21	1.88	0.54
1:D:979:THR:O	1:D:1039:MET:HA	2.06	0.54
1:E:1057:HIS:O	1:E:1061:THR:HG23	2.07	0.54
1:F:1011:PRO:HG2	1:F:1023:ILE:HD13	1.89	0.54
1:H:755:ARG:HG2	1:H:1036:ASN:HD21	1.71	0.54
1:B:562:ARG:HG3	1:B:581:ALA:HB1	1.90	0.54
1:C:909:PHE:HZ	1:C:916:LEU:HD11	1.72	0.54
1:D:485:VAL:O	1:D:789:THR:OG1	2.17	0.54
1:D:713:SER:HA	1:D:740:PHE:CE2	2.43	0.54
1:F:500:CYS:SG	1:F:769:MET:HB2	2.48	0.54
1:G:359:SER:HB2	1:G:414:GLY:O	2.07	0.54
1:G:498:ASP:HA	1:G:769:MET:SD	2.47	0.54
1:A:619:SER:HB3	1:A:679:ASN:HB3	1.89	0.54
1:A:669:LYS:HE2	1:A:1112:CYS:SG	2.48	0.54
1:B:435:ARG:HH21	1:B:438:ASP:HB2	1.72	0.54
1:D:782:GLN:HE21	1:D:1037:ILE:HD13	1.73	0.54
1:E:899:ASP:OD1	1:E:942:LYS:HA	2.07	0.54
1:F:767:CYS:O	1:F:774:PRO:HA	2.08	0.54
1:G:735:LYS:NZ	1:G:1056:ARG:HH12	2.05	0.54
1:G:1075:GLN:HE22	1:G:1100:ARG:HH21	1.55	0.54
1:H:504:ASP:N	1:H:504:ASP:OD1	2.40	0.54
1:A:957:ILE:O	1:A:961:THR:N	2.33	0.54
1:C:962:GLU:HG3	1:C:1034:THR:O	2.08	0.54
1:E:510:LYS:NZ	1:E:518:ASP:OD2	2.25	0.54
1:F:846:THR:O	1:F:849:SER:OG	2.25	0.54
1:C:584:ASN:CG	1:C:600:GLN:HE22	2.14	0.54
1:D:940:ALA:O	1:D:942:LYS:NZ	2.33	0.54
1:F:912:LYS:CD	1:F:912:LYS:CB	2.77	0.54
1:H:574:ARG:HE	1:H:578:LEU:HD11	1.73	0.54
1:C:659:LEU:HD23	1:C:678:ILE:HD11	1.88	0.54
1:C:885:HIS:CE1	1:C:966:ARG:HH12	2.26	0.54
1:C:1027:VAL:HB	1:C:1071:ASN:HD21	1.73	0.54
1:E:728:GLU:O	1:E:731:VAL:HG22	2.07	0.54
1:G:964:GLU:OE1	1:G:967:LYS:NZ	2.28	0.54
1:G:1004:PRO:HB3	1:G:1118:GLU:HG3	1.88	0.54
1:H:443:SER:O	1:H:447:LYS:HG2	2.07	0.54
1:B:1084:LEU:HD21	1:B:1099:VAL:HG21	1.90	0.54
1:C:403:ILE:HD12	1:C:600:GLN:HB2	1.89	0.54
1:C:1075:GLN:HE22	1:C:1103:GLY:CA	2.20	0.54
1:E:796:GLU:OE1	1:E:805:VAL:HG23	2.08	0.54
1:G:402:LEU:HD13	1:G:402:LEU:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:499:THR:O	1:G:501:PRO:HD3	2.07	0.54
1:C:407:PRO:HB2	1:C:611:ILE:HD11	1.88	0.54
1:E:386:PHE:CE2	1:E:546:THR:HG23	2.42	0.54
1:E:915:THR:HG22	1:E:917:GLU:HG2	1.90	0.54
1:E:1100:ARG:HD2	1:E:1104:TYR:O	2.08	0.54
1:F:756:LYS:NZ	1:F:782:GLN:OE1	2.40	0.54
1:G:820:ASP:HA	1:G:822:ARG:HD3	1.88	0.54
1:G:1086:LYS:HZ2	1:G:1094:TYR:HE2	1.56	0.54
1:A:854:ARG:HG3	1:A:878:ALA:HA	1.89	0.54
1:A:1010:SER:HA	1:A:1041:HIS:CE1	2.43	0.54
1:B:1073:GLN:HE22	1:B:1075:GLN:HE21	1.56	0.54
1:E:917:GLU:HB2	1:E:920:ARG:NH2	2.19	0.54
1:H:489:SER:O	1:H:493:ILE:HG12	2.08	0.54
1:H:1001:ALA:HB1	1:H:1002:TRP:CE2	2.43	0.54
1:A:703:ALA:O	1:A:707:VAL:HG22	2.09	0.53
1:B:618:LEU:HD11	1:B:862:MET:HE1	1.89	0.53
1:C:888:GLY:HA2	1:C:976:SER:O	2.08	0.53
1:C:1062:LEU:HG	1:C:1074:MET:HE1	1.91	0.53
1:E:446:ASP:HA	1:E:449:THR:HG22	1.89	0.53
1:F:488:LEU:HD13	1:F:845:GLY:HA3	1.89	0.53
1:G:342:PRO:O	1:G:346:ARG:NH1	2.42	0.53
1:G:429:LEU:HD23	1:G:442:ILE:CD1	2.38	0.53
1:A:984:ASN:HA	1:A:987:PRO:HG2	1.90	0.53
1:B:337:MET:CB	1:B:340:LEU:HD12	2.39	0.53
1:C:653:ILE:HG23	1:C:712:PRO:HD2	1.90	0.53
1:D:337:MET:HB2	1:D:340:LEU:HG	1.89	0.53
1:G:660:MET:HE3	1:G:661:TRP:N	2.23	0.53
1:H:1019:GLY:HA3	1:H:1127:LYS:HD3	1.89	0.53
1:D:412:ARG:HH21	1:D:674:TYR:HB2	1.73	0.53
1:D:781:TYR:CD1	1:D:876:VAL:HB	2.43	0.53
1:D:1127:LYS:HG2	1:D:1128:PHE:N	2.23	0.53
1:E:358:VAL:HG21	1:E:432:MET:HE1	1.90	0.53
1:E:979:THR:HG21	1:E:1035:MET:SD	2.48	0.53
1:G:624:ASP:H	1:G:682:VAL:HG12	1.73	0.53
1:G:713:SER:HA	1:G:740:PHE:CZ	2.43	0.53
1:G:1111:LEU:HD23	1:G:1112:CYS:N	2.23	0.53
1:H:628:TYR:CE1	1:H:694:ASN:HB2	2.44	0.53
1:A:595:LEU:N	1:A:634:ASP:OD2	2.38	0.53
1:C:827:PHE:O	1:C:831:VAL:HG23	2.08	0.53
1:E:941:PRO:HG2	1:E:949:TYR:CD2	2.44	0.53
1:F:423:ARG:HH11	1:F:465:GLU:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1102:ALA:C	1:F:1104:TYR:H	2.15	0.53
1:H:537:ILE:O	1:H:541:LYS:HG2	2.09	0.53
1:H:579:THR:HA	1:H:582:GLU:HB3	1.89	0.53
1:A:803:ARG:HB2	1:A:810:TYR:CE1	2.43	0.53
1:B:555:ARG:HD2	1:B:555:ARG:N	2.22	0.53
1:D:920:ARG:O	1:D:924:LEU:HD13	2.09	0.53
1:C:817:ASP:OD2	1:C:819:ARG:NE	2.36	0.53
1:D:443:SER:HB2	1:D:446:ASP:H	1.73	0.53
1:D:583:VAL:O	1:D:587:VAL:HG22	2.08	0.53
1:D:906:LYS:NZ	1:D:911:GLU:HG3	2.20	0.53
1:G:792:PRO:HG2	1:G:1005:LEU:HD13	1.90	0.53
1:G:1024:ILE:HD13	1:G:1062:LEU:HD12	1.91	0.53
1:H:942:LYS:O	1:H:945:ASN:ND2	2.42	0.53
1:A:388:HIS:O	1:A:392:THR:HG23	2.09	0.53
1:A:495:GLY:HA3	1:A:615:GLN:HB3	1.90	0.53
1:C:1077:SER:HB2	1:C:1100:ARG:HB2	1.91	0.53
1:E:930:TYR:HB3	1:E:933:LEU:HD21	1.89	0.53
1:E:962:GLU:HB2	1:E:977:HIS:HD2	1.74	0.53
1:E:999:ARG:NH2	1:E:1003:MET:H	2.03	0.53
1:F:1052:THR:OG1	1:F:1054:GLU:OE1	2.27	0.53
1:G:480:SER:CB	1:G:488:LEU:HG	2.38	0.53
1:G:790:GLN:HB2	1:G:792:PRO:HD2	1.91	0.53
1:G:1080:ASP:O	1:G:1083:VAL:HG12	2.09	0.53
1:H:1058:GLY:O	1:H:1062:LEU:HB2	2.09	0.53
1:B:561:ALA:HB3	1:B:581:ALA:HB2	1.91	0.53
1:C:1029:LYS:O	1:C:1029:LYS:HD3	2.08	0.53
1:E:476:VAL:HG12	1:E:841:LEU:HD13	1.91	0.53
1:G:813:LEU:H	1:G:813:LEU:HD12	1.73	0.53
1:G:1010:SER:HG	1:G:1042:ASN:H	1.57	0.53
1:B:376:MET:HB3	1:B:381:LEU:HB2	1.91	0.53
1:B:428:GLU:OE2	1:B:665:GLU:HB2	2.09	0.53
1:C:466:ILE:HG23	1:G:375:GLY:HA2	1.91	0.53
1:D:468:GLU:OE2	1:D:472:ARG:NH1	2.42	0.53
1:E:450:ILE:HD12	1:E:454:ILE:HD12	1.91	0.53
1:E:758:PHE:HZ	1:E:780:ILE:HD12	1.73	0.53
1:E:828:ASP:OD2	1:E:832:LYS:NZ	2.42	0.53
1:F:616:THR:HB	1:F:661:TRP:CG	2.43	0.53
1:G:1049:LEU:O	1:G:1055:GLY:HA3	2.09	0.53
1:A:894:LEU:O	1:A:898:VAL:HG23	2.08	0.53
1:B:674:TYR:O	1:B:710:TYR:OH	2.21	0.53
1:B:797:PHE:HE1	1:B:804:MET:HB2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:780:ILE:HG12	1:C:781:TYR:N	2.24	0.53
1:D:846:THR:C	1:D:849:SER:HG	2.16	0.53
1:E:580:ILE:O	1:E:583:VAL:HG12	2.09	0.53
1:E:900:SER:O	1:E:903:ALA:N	2.42	0.53
1:F:491:HIS:HB2	1:F:786:THR:HG23	1.91	0.53
1:C:501:PRO:HB3	1:C:865:LEU:HB3	1.91	0.52
1:C:583:VAL:O	1:C:587:VAL:HG22	2.08	0.52
1:D:604:THR:O	1:D:607:SER:OG	2.27	0.52
1:E:395:ILE:CD1	1:E:556:ARG:HG3	2.37	0.52
1:F:679:ASN:HB2	1:F:770:GLY:O	2.09	0.52
1:G:984:ASN:O	1:G:988:ILE:HG13	2.09	0.52
1:H:735:LYS:HG3	1:H:1050:LEU:HD13	1.90	0.52
1:A:477:TRP:O	1:A:481:GLY:N	2.41	0.52
1:B:866:VAL:HG22	3:B:1333:HOH:O	2.08	0.52
1:D:686:LYS:HB3	1:D:689:GLY:O	2.08	0.52
1:F:414:GLY:HA3	1:F:662:MET:HG3	1.92	0.52
1:F:432:MET:SD	1:F:440:PHE:HB2	2.49	0.52
1:H:512:MET:HB2	1:H:589:ALA:HA	1.92	0.52
1:H:905:ARG:HD2	1:H:953:TYR:OH	2.08	0.52
1:B:803:ARG:HB2	1:B:810:TYR:CE1	2.45	0.52
1:C:952:GLN:HB3	1:C:1029:LYS:HZ2	1.73	0.52
1:D:595:LEU:CD1	1:D:631:PHE:HB2	2.40	0.52
1:E:831:VAL:O	1:E:834:GLN:N	2.42	0.52
1:E:979:THR:OG1	1:E:1039:MET:HA	2.09	0.52
1:E:1081:ASN:O	1:E:1085:LYS:HG3	2.09	0.52
1:F:739:GLY:CA	1:F:1100:ARG:HB2	2.37	0.52
1:G:1052:THR:HG22	1:G:1054:GLU:H	1.74	0.52
1:H:351:TYR:OH	1:H:657:ALA:O	2.18	0.52
1:E:587:VAL:HG12	1:E:590:ASN:O	2.10	0.52
1:E:938:LEU:CD1	1:E:998:GLY:HA3	2.39	0.52
1:G:717:ARG:NH1	1:G:764:ARG:O	2.35	0.52
1:G:788:TYR:OH	2:G:1201:A1H9L:F6	2.09	0.52
1:H:799:LEU:HA	1:H:818:LEU:HD11	1.90	0.52
1:C:646:LEU:O	1:C:650:GLN:HG3	2.10	0.52
1:C:751:LYS:HZ3	1:H:747:ASP:HA	1.74	0.52
1:D:934:ARG:O	1:D:938:LEU:HD12	2.10	0.52
1:F:511:GLY:O	1:F:515:ILE:HG13	2.09	0.52
1:F:745:PHE:HZ	1:F:1063:LEU:HD22	1.73	0.52
1:G:594:THR:HB	1:G:597:GLU:H	1.74	0.52
1:G:829:ALA:O	1:G:833:GLN:HG3	2.09	0.52
1:H:398:GLN:HG3	1:H:401:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1074:MET:HE2	1:H:1076:PHE:CZ	2.45	0.52
1:A:577:LEU:HA	1:A:580:ILE:HB	1.92	0.52
1:C:1045:PHE:HB3	1:C:1049:LEU:HD23	1.92	0.52
1:E:340:LEU:HD13	1:E:344:MET:HB3	1.92	0.52
1:E:950:VAL:HG13	1:E:951:ASP:OD2	2.09	0.52
1:E:966:ARG:HA	1:E:974:THR:HG22	1.91	0.52
1:F:608:LEU:O	1:F:611:ILE:N	2.39	0.52
1:F:621:GLY:O	1:F:623:VAL:N	2.43	0.52
1:H:790:GLN:HB2	1:H:792:PRO:HD2	1.91	0.52
1:B:376:MET:HE3	1:B:384:LYS:HE3	1.92	0.52
1:D:478:ALA:HA	1:D:482:GLU:HB2	1.90	0.52
1:D:573:ARG:O	1:D:577:LEU:HD12	2.09	0.52
1:D:995:THR:HG23	1:D:999:ARG:NH1	2.25	0.52
1:B:624:ASP:HB3	1:B:682:VAL:HG12	1.91	0.52
1:D:773:GLU:OE1	1:D:784:THR:HG21	2.10	0.52
1:E:398:GLN:HB2	1:E:401:GLU:CD	2.35	0.52
1:F:979:THR:O	1:F:1039:MET:HA	2.10	0.52
1:G:819:ARG:HD2	1:G:819:ARG:C	2.35	0.52
1:G:957:ILE:O	1:G:961:THR:N	2.35	0.52
1:A:850:GLN:NE2	1:A:887:PRO:HD3	2.25	0.52
1:B:650:GLN:HG2	1:B:707:VAL:HG13	1.91	0.52
1:F:375:GLY:HA3	1:H:466:ILE:HG12	1.92	0.52
1:F:703:ALA:O	1:F:707:VAL:HG22	2.10	0.52
1:F:955:LEU:HB2	1:F:1029:LYS:O	2.10	0.52
1:G:817:ASP:OD1	1:G:818:LEU:N	2.43	0.52
1:H:439:PRO:O	1:H:674:TYR:OH	2.25	0.52
1:A:462:SER:OG	1:A:465:GLU:OE1	2.25	0.52
1:A:963:LYS:HA	1:A:966:ARG:HB2	1.92	0.52
1:C:343:ARG:HD3	1:C:400:ASP:O	2.10	0.52
1:C:593:LYS:N	1:C:597:GLU:OE1	2.39	0.52
1:C:931:GLU:OE1	1:C:931:GLU:N	2.39	0.52
1:F:913:LYS:HE2	1:F:914:TYR:CZ	2.45	0.52
1:G:416:PHE:CE1	1:G:425:VAL:HG21	2.45	0.52
1:G:640:LEU:HD21	1:G:645:ALA:HB2	1.92	0.52
1:C:528:MET:SD	1:C:534:ILE:HG12	2.50	0.51
1:F:790:GLN:OE1	1:F:793:ILE:HB	2.10	0.51
1:G:504:ASP:HB3	1:G:626:TYR:CG	2.45	0.51
1:H:357:SER:N	1:H:412:ARG:O	2.36	0.51
1:B:364:LEU:HD21	1:B:449:THR:HG21	1.90	0.51
1:C:934:ARG:NH1	1:C:1000:LEU:HD21	2.26	0.51
1:D:640:LEU:HD22	1:D:644:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:718:ILE:HD11	1:G:743:CYS:HB3	1.91	0.51
1:G:1045:PHE:CE1	1:G:1125:ILE:HD11	2.44	0.51
1:A:444:GLU:OE2	1:C:342:PRO:HB3	2.11	0.51
1:B:995:THR:HG23	1:B:999:ARG:HH21	1.76	0.51
1:D:671:PHE:HD2	1:D:677:PHE:CE2	2.28	0.51
1:D:985:ASN:HD22	1:D:1007:ASP:HA	1.75	0.51
1:D:1042:ASN:OD1	1:D:1075:GLN:NE2	2.34	0.51
1:E:577:LEU:HA	1:E:580:ILE:HB	1.92	0.51
1:E:742:ALA:HB2	1:E:1100:ARG:NH2	2.22	0.51
1:E:908:VAL:O	1:E:912:LYS:HA	2.10	0.51
1:E:1065:THR:C	1:E:1069:LEU:HD12	2.35	0.51
1:G:396:LEU:HD11	1:G:398:GLN:HG2	1.92	0.51
1:G:813:LEU:HD11	1:G:837:HIS:CG	2.44	0.51
1:H:1127:LYS:HD2	1:H:1127:LYS:N	2.14	0.51
1:A:993:ASN:OD1	1:A:994:ALA:N	2.44	0.51
1:B:623:VAL:HG21	1:B:680:LEU:HD11	1.92	0.51
1:D:894:LEU:HD21	1:D:1030:MET:HE1	1.92	0.51
1:E:797:PHE:HE2	1:E:804:MET:HB2	1.74	0.51
1:E:1049:LEU:HD22	1:E:1126:GLU:O	2.11	0.51
1:G:347:LEU:CD1	1:G:400:ASP:HB2	2.40	0.51
1:G:798:VAL:HG21	1:G:831:VAL:HG22	1.92	0.51
1:A:390:CYS:HB3	1:A:553:TYR:HB2	1.92	0.51
1:A:790:GLN:HB2	1:A:792:PRO:HD2	1.92	0.51
1:B:540:TYR:O	1:B:544:ILE:HG13	2.10	0.51
1:B:1111:LEU:O	1:B:1116:GLN:NE2	2.43	0.51
1:C:470:GLN:NE2	1:G:375:GLY:O	2.32	0.51
1:C:657:ALA:HB2	1:C:711:GLN:O	2.10	0.51
1:D:411:PRO:HG3	1:D:658:GLU:OE1	2.10	0.51
1:E:753:MET:HE1	1:E:776:LYS:HB2	1.91	0.51
1:F:477:TRP:CZ3	1:F:481:GLY:HA3	2.46	0.51
1:F:622:ARG:HH11	1:F:765:ASP:HA	1.76	0.51
1:G:641:THR:H	1:G:644:THR:CG2	2.24	0.51
1:G:661:TRP:CZ2	1:G:663:SER:HB3	2.45	0.51
1:H:395:ILE:HD12	1:H:557:ILE:HG12	1.92	0.51
1:H:422:TRP:HZ3	1:H:426:ARG:HE	1.59	0.51
1:H:734:VAL:HG12	1:H:1050:LEU:CD1	2.41	0.51
1:D:411:PRO:HB3	1:D:658:GLU:HB3	1.93	0.51
1:E:980:LEU:HD12	1:E:982:ILE:HG13	1.93	0.51
1:G:863:SER:OG	1:G:875:ASP:HB2	2.10	0.51
1:H:607:SER:HA	1:H:659:LEU:CD1	2.41	0.51
1:A:437:GLN:OE1	1:A:1112:CYS:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:ASN:OD1	1:B:661:TRP:NE1	2.33	0.51
1:D:410:LYS:HB3	1:D:413:ALA:HB2	1.93	0.51
1:D:941:PRO:HB3	1:D:947:ASP:OD2	2.11	0.51
1:E:708:LYS:HA	1:E:738:MET:SD	2.50	0.51
1:F:631:PHE:CE1	1:F:635:ILE:HD11	2.45	0.51
1:F:744:HIS:CE1	1:F:768:LEU:HG	2.46	0.51
1:H:739:GLY:HA2	1:H:1076:PHE:O	2.11	0.51
1:H:1044:LYS:HB3	1:H:1123:THR:O	2.11	0.51
1:H:1095:ARG:HA	1:H:1109:VAL:CG2	2.41	0.51
1:B:516:LYS:O	1:B:520:GLU:HG2	2.10	0.51
1:D:823:THR:HG22	1:D:825:ASP:N	2.24	0.51
1:E:400:ASP:HA	1:E:573:ARG:NE	2.25	0.51
1:E:756:LYS:HA	1:E:885:HIS:CE1	2.45	0.51
1:E:840:ARG:O	1:E:844:ILE:HG13	2.10	0.51
1:F:943:TYR:OH	1:F:1027:VAL:CG1	2.58	0.51
1:G:923:LEU:HD11	1:G:996:PRO:HG3	1.93	0.51
1:G:957:ILE:CD1	1:G:958:THR:N	2.51	0.51
1:G:973:SER:OG	1:G:974:THR:N	2.43	0.51
1:G:1020:PRO:HA	1:G:1023:ILE:HD12	1.93	0.51
1:H:763:ALA:O	1:H:766:TYR:HB3	2.11	0.51
1:A:523:LEU:HD11	1:A:537:ILE:HG23	1.91	0.51
1:B:349:ASN:O	1:B:353:THR:HG23	2.10	0.51
1:B:553:TYR:CE1	1:B:557:ILE:HD11	2.45	0.51
1:G:395:ILE:HD11	1:G:556:ARG:NH1	2.25	0.51
1:B:897:TYR:CD1	1:B:897:TYR:C	2.89	0.51
1:C:676:PRO:HD2	1:C:711:GLN:HG3	1.93	0.51
1:D:779:ARG:O	1:D:883:VAL:HB	2.11	0.51
1:D:1113:LYS:H	1:D:1113:LYS:CD	2.24	0.51
1:E:793:ILE:HB	1:E:992:THR:HG22	1.92	0.51
1:F:343:ARG:HH12	1:F:576:GLU:CD	2.18	0.51
1:F:420:ILE:HD13	1:F:495:GLY:N	2.26	0.51
1:F:437:GLN:HE21	1:F:438:ASP:H	1.57	0.51
1:F:653:ILE:HG22	1:F:709:VAL:HG21	1.91	0.51
1:F:914:TYR:CZ	1:F:933:LEU:HD12	2.46	0.51
1:G:526:LEU:HB3	1:G:537:ILE:HD11	1.93	0.51
1:G:917:GLU:HA	1:G:920:ARG:HB2	1.93	0.51
1:H:530:ASN:HB3	1:H:532:GLU:OE1	2.11	0.51
1:B:487:ASP:O	1:B:787:GLY:HA2	2.11	0.50
1:E:797:PHE:O	1:E:802:GLY:N	2.36	0.50
1:F:1031:ASN:O	1:F:1034:THR:OG1	2.28	0.50
1:F:1091:PRO:O	1:F:1095:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1055:GLY:HA2	1:H:1128:PHE:HE2	1.75	0.50
1:A:1100:ARG:NH2	1:A:1103:GLY:CA	2.74	0.50
1:C:505:VAL:O	1:C:509:THR:OG1	2.29	0.50
1:D:623:VAL:HG21	1:D:680:LEU:HD11	1.94	0.50
1:D:823:THR:HB	1:D:826:GLU:HG3	1.94	0.50
1:G:450:ILE:HA	1:G:454:ILE:HB	1.93	0.50
1:G:965:CYS:HB3	1:G:975:LEU:HG	1.93	0.50
1:H:773:GLU:OE2	1:H:980:LEU:HD22	2.10	0.50
1:H:1004:PRO:HG2	1:H:1118:GLU:HB2	1.92	0.50
1:H:1020:PRO:HG3	1:H:1128:PHE:HA	1.92	0.50
1:C:508:PHE:O	1:C:591:PRO:HB3	2.11	0.50
1:C:593:LYS:O	1:C:593:LYS:HD2	2.11	0.50
1:C:938:LEU:HD21	1:C:998:GLY:HA3	1.92	0.50
1:D:356:PRO:HG3	1:D:412:ARG:HE	1.77	0.50
1:D:573:ARG:HG3	1:D:577:LEU:HD11	1.92	0.50
1:D:984:ASN:HB2	1:D:988:ILE:HG12	1.93	0.50
1:F:952:GLN:HE21	1:F:953:TYR:HE1	1.58	0.50
1:G:483:THR:HG21	1:G:811:GLN:HE21	1.77	0.50
1:G:905:ARG:HD2	1:G:953:TYR:OH	2.11	0.50
1:A:872:SER:HB2	1:A:874:LYS:NZ	2.27	0.50
1:B:771:CYS:HB3	1:B:1103:GLY:HA3	1.93	0.50
1:C:721:GLN:HG3	1:C:721:GLN:O	2.12	0.50
1:C:981:SER:OG	1:C:1008:GLY:N	2.36	0.50
1:C:1031:ASN:ND2	1:H:688:SER:O	2.45	0.50
1:D:1023:ILE:O	1:D:1027:VAL:HG23	2.11	0.50
1:E:941:PRO:O	1:E:942:LYS:HD2	2.11	0.50
1:F:1118:GLU:O	1:F:1121:SER:OG	2.21	0.50
1:G:480:SER:HB2	1:G:488:LEU:H	1.77	0.50
1:A:708:LYS:HA	1:A:738:MET:SD	2.52	0.50
1:A:1100:ARG:NH2	1:A:1104:TYR:N	2.59	0.50
1:B:832:LYS:HD2	1:B:960:TRP:CE2	2.46	0.50
1:D:686:LYS:HD3	1:D:688:SER:N	2.25	0.50
1:D:983:SER:O	1:D:987:PRO:HD2	2.12	0.50
1:F:631:PHE:CG	1:F:696:LEU:HD13	2.46	0.50
1:F:854:ARG:NH1	1:F:855:ASP:OD1	2.44	0.50
1:F:1075:GLN:NE2	1:F:1103:GLY:HA2	2.17	0.50
1:G:480:SER:HB3	1:G:488:LEU:HG	1.94	0.50
1:G:703:ALA:O	1:G:707:VAL:HG23	2.11	0.50
1:G:722:SER:O	1:G:1064:ARG:NH2	2.34	0.50
1:H:848:ILE:O	1:H:851:ARG:N	2.44	0.50
1:A:721:GLN:NE2	1:B:1069:LEU:HD23	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:HIS:CE1	1:B:783:TRP:CG	2.99	0.50
1:C:540:TYR:O	1:C:544:ILE:HG13	2.11	0.50
1:F:1039:MET:SD	1:F:1072:GLY:HA3	2.52	0.50
1:G:771:CYS:HB2	1:G:980:LEU:HD13	1.92	0.50
1:H:347:LEU:HD21	1:H:400:ASP:HB2	1.93	0.50
1:H:395:ILE:HG13	1:H:556:ARG:HG2	1.94	0.50
1:H:622:ARG:NH2	1:H:625:GLN:HG3	2.26	0.50
1:H:1066:ALA:HA	1:H:1069:LEU:HB2	1.93	0.50
1:A:622:ARG:NH1	1:A:765:ASP:HA	2.27	0.50
1:C:622:ARG:NH2	1:C:685:GLN:O	2.34	0.50
1:C:630:MET:SD	1:C:630:MET:N	2.76	0.50
1:D:382:ARG:HD3	1:D:858:PRO:HD2	1.92	0.50
1:E:701:MET:HE3	1:E:716:CYS:SG	2.52	0.50
1:G:542:ALA:O	1:G:546:THR:HG22	2.12	0.50
1:G:603:TRP:HB2	1:G:652:PHE:CE1	2.46	0.50
1:G:966:ARG:NH1	1:G:976:SER:HB2	2.27	0.50
1:H:657:ALA:HA	1:H:711:GLN:HB2	1.93	0.50
1:H:897:TYR:CE2	1:H:957:ILE:HG21	2.46	0.50
1:H:1064:ARG:NH1	1:H:1064:ARG:HG3	2.25	0.50
1:A:728:GLU:O	1:A:731:VAL:HG22	2.11	0.50
1:B:980:LEU:HA	1:B:1040:VAL:HG12	1.93	0.50
1:E:1124:VAL:HG13	1:E:1124:VAL:O	2.12	0.50
1:F:406:HIS:CE1	1:F:408:CYS:HB2	2.46	0.50
1:F:428:GLU:OE2	1:F:665:GLU:HB2	2.11	0.50
1:F:984:ASN:HA	1:F:987:PRO:HD2	1.94	0.50
1:H:850:GLN:NE2	1:H:887:PRO:HD3	2.27	0.50
1:A:736:ALA:HB3	1:A:738:MET:HE2	1.93	0.50
1:C:745:PHE:O	1:C:749:HIS:HB2	2.12	0.50
1:D:564:LEU:O	1:D:567:LYS:HE3	2.12	0.50
1:E:910:GLU:HA	1:E:910:GLU:OE2	2.10	0.50
1:E:1046:LEU:HB2	1:E:1126:GLU:HG2	1.94	0.50
1:E:1111:LEU:HB3	1:E:1115:VAL:HG11	1.93	0.50
1:F:403:ILE:HD12	1:F:600:GLN:HB2	1.94	0.50
1:F:479:PHE:HZ	1:F:838:ILE:HG12	1.76	0.50
1:F:973:SER:OG	1:F:974:THR:N	2.41	0.50
1:G:708:LYS:HA	1:G:738:MET:SD	2.52	0.50
1:H:775:GLN:HE21	1:H:780:ILE:CG2	2.23	0.50
1:H:986:THR:HB	1:H:987:PRO:HD3	1.94	0.50
1:B:488:LEU:HD13	1:B:845:GLY:HA3	1.93	0.49
1:C:491:HIS:HB2	1:C:786:THR:HG23	1.93	0.49
1:C:688:SER:O	1:H:955:LEU:HD21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1088:GLN:HG2	1:C:1116:GLN:OE1	2.12	0.49
1:E:962:GLU:OE1	1:E:977:HIS:N	2.40	0.49
1:F:362:ARG:HH21	1:F:613:GLU:HA	1.77	0.49
1:G:698:TYR:HE1	1:G:726:TYR:HA	1.76	0.49
1:G:762:ASP:OD1	1:G:779:ARG:NH1	2.45	0.49
1:H:793:ILE:HD12	1:H:992:THR:HG23	1.93	0.49
1:H:1118:GLU:O	1:H:1121:SER:OG	2.16	0.49
1:B:919:ILE:O	1:B:923:LEU:HG	2.12	0.49
1:C:815:THR:HG23	1:C:834:GLN:NE2	2.21	0.49
1:D:693:CYS:SG	3:D:1320:HOH:O	2.60	0.49
1:H:1095:ARG:HA	1:H:1109:VAL:HG22	1.92	0.49
1:B:739:GLY:HA2	1:B:1076:PHE:O	2.12	0.49
1:C:661:TRP:CH2	1:C:663:SER:HB2	2.47	0.49
1:C:782:GLN:NE2	1:C:1037:ILE:HD12	2.27	0.49
1:C:1073:GLN:NE2	1:C:1075:GLN:HE21	2.10	0.49
1:E:419:ASP:OD1	1:E:419:ASP:N	2.45	0.49
1:E:744:HIS:CD2	1:E:1073:GLN:HG2	2.47	0.49
1:F:742:ALA:CB	1:F:1075:GLN:HE21	2.23	0.49
1:H:734:VAL:CG1	1:H:1050:LEU:HD11	2.42	0.49
1:A:443:SER:O	1:A:447:LYS:HG3	2.12	0.49
1:E:595:LEU:O	1:E:599:LEU:HG	2.12	0.49
1:F:727:MET:O	1:F:731:VAL:HG23	2.13	0.49
1:F:1099:VAL:HG21	1:F:1108:PHE:CD2	2.47	0.49
1:G:733:VAL:HB	1:G:741:PRO:HD3	1.95	0.49
1:A:613:GLU:CD	1:A:859:LYS:HZ2	2.18	0.49
1:C:1039:MET:SD	1:C:1072:GLY:HA3	2.53	0.49
1:E:713:SER:HB2	3:E:1301:HOH:O	2.13	0.49
1:E:840:ARG:HG3	1:E:841:LEU:HD23	1.93	0.49
1:F:537:ILE:HG22	1:F:541:LYS:HD2	1.93	0.49
1:F:685:GLN:H	1:F:717:ARG:NH2	2.10	0.49
1:G:382:ARG:HG2	1:G:382:ARG:HH11	1.77	0.49
1:G:504:ASP:HB3	1:G:626:TYR:CD2	2.47	0.49
1:H:399:ASP:OD1	1:H:399:ASP:N	2.44	0.49
1:H:744:HIS:CD2	1:H:749:HIS:CE1	3.01	0.49
1:B:426:ARG:C	1:B:428:GLU:H	2.21	0.49
1:B:685:GLN:HG3	1:B:719:HIS:CD2	2.48	0.49
1:B:731:VAL:HG11	1:B:1056:ARG:HG2	1.93	0.49
1:B:851:ARG:O	1:B:854:ARG:HB3	2.13	0.49
1:C:795:ILE:CD1	1:C:901:MET:HE3	2.42	0.49
1:D:363:ALA:O	1:D:367:THR:OG1	2.23	0.49
1:D:775:GLN:HB3	1:D:780:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:ARG:HD3	1:F:465:GLU:HG3	1.95	0.49
1:F:694:ASN:OD1	1:F:696:LEU:N	2.46	0.49
1:G:381:LEU:O	1:G:385:ALA:N	2.40	0.49
1:G:742:ALA:HB2	1:G:1100:ARG:NH2	2.27	0.49
1:C:952:GLN:CB	1:C:1029:LYS:HZ2	2.24	0.49
1:C:1111:LEU:HB3	1:C:1115:VAL:HG23	1.93	0.49
1:D:437:GLN:CD	1:D:438:ASP:H	2.21	0.49
1:E:732:ASP:C	1:E:735:LYS:HB3	2.37	0.49
1:E:987:PRO:HA	1:E:990:GLU:OE1	2.13	0.49
1:F:792:PRO:HG2	1:F:896:THR:HB	1.93	0.49
1:G:478:ALA:O	1:G:483:THR:HG23	2.13	0.49
1:G:700:ILE:O	1:G:704:VAL:HG23	2.13	0.49
1:G:818:LEU:HD23	1:G:821:LEU:HD12	1.95	0.49
1:G:832:LYS:HB3	1:G:960:TRP:CZ2	2.47	0.49
1:H:420:ILE:HG13	1:H:421:ALA:N	2.28	0.49
1:C:568:GLU:HG2	1:C:573:ARG:HG3	1.95	0.49
1:C:952:GLN:HB3	1:C:1029:LYS:NZ	2.28	0.49
1:D:650:GLN:O	1:D:654:ILE:HD12	2.13	0.49
1:D:682:VAL:HG22	1:D:714:LEU:HD11	1.94	0.49
1:E:439:PRO:O	1:E:674:TYR:OH	2.26	0.49
1:E:915:THR:CG2	1:E:917:GLU:CG	2.90	0.49
1:E:999:ARG:HG2	1:E:1003:MET:HE2	1.95	0.49
1:F:821:LEU:HD21	1:F:830:ALA:CB	2.43	0.49
1:G:628:TYR:HB3	1:G:629:PRO:HD3	1.95	0.49
1:G:769:MET:HB2	1:G:775:GLN:HG3	1.95	0.49
1:G:905:ARG:HH11	1:G:949:TYR:HE1	1.61	0.49
1:G:1004:PRO:CB	1:G:1118:GLU:HG3	2.43	0.49
1:H:516:LYS:HB2	1:H:547:CYS:SG	2.52	0.49
1:H:796:GLU:HG3	1:H:800:ASN:HD22	1.78	0.49
1:D:571:ALA:HB1	1:D:572:GLN:NE2	2.28	0.49
1:D:573:ARG:HG3	1:D:577:LEU:CD1	2.41	0.49
1:D:677:PHE:O	1:D:770:GLY:HA2	2.12	0.49
1:D:679:ASN:ND2	1:D:770:GLY:O	2.34	0.49
1:E:815:THR:HG23	1:E:834:GLN:HE21	1.77	0.49
1:F:460:GLY:N	1:F:465:GLU:OE2	2.44	0.49
1:G:793:ILE:HA	1:G:796:GLU:HG3	1.95	0.49
1:G:1124:VAL:HG23	1:G:1124:VAL:O	2.13	0.49
1:H:694:ASN:OD1	1:H:697:THR:N	2.44	0.49
1:B:1087:ALA:HA	1:B:1094:TYR:CD2	2.48	0.49
1:C:368:GLU:O	1:C:371:LYS:HB3	2.13	0.49
1:C:885:HIS:ND1	1:C:886:GLY:N	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:993:ASN:O	1:C:995:THR:HG23	2.13	0.49
1:C:1095:ARG:HA	1:C:1109:VAL:HG21	1.95	0.49
1:D:622:ARG:HG3	1:D:767:CYS:HB3	1.95	0.49
1:G:906:LYS:O	1:G:911:GLU:HB2	2.13	0.49
1:G:907:LEU:HD21	1:G:936:ASP:HB3	1.94	0.49
1:G:1019:GLY:HA2	1:G:1127:LYS:HD2	1.95	0.49
1:G:1086:LYS:NZ	1:G:1094:TYR:HE2	2.11	0.49
1:C:488:LEU:CD1	1:C:845:GLY:HA3	2.43	0.48
1:C:934:ARG:CZ	1:C:1000:LEU:HD21	2.43	0.48
1:E:715:ALA:CB	1:E:768:LEU:HD23	2.42	0.48
1:F:460:GLY:H	1:F:465:GLU:CD	2.21	0.48
1:F:676:PRO:HG2	1:F:678:ILE:HG13	1.95	0.48
1:A:491:HIS:CE1	1:A:783:TRP:CD2	3.01	0.48
1:B:553:TYR:O	1:B:557:ILE:HG12	2.13	0.48
1:D:754:LEU:HA	1:D:754:LEU:HD23	1.60	0.48
1:D:758:PHE:HZ	1:D:780:ILE:HB	1.77	0.48
1:D:1027:VAL:HG21	1:D:1041:HIS:CE1	2.47	0.48
1:F:506:LEU:HD21	1:F:867:GLU:HG2	1.94	0.48
1:F:616:THR:OG1	1:F:617:GLY:N	2.45	0.48
1:G:440:PHE:CZ	1:G:660:MET:HE1	2.48	0.48
1:G:970:MET:HE3	1:G:975:LEU:HB2	1.94	0.48
1:H:508:PHE:O	1:H:591:PRO:HB3	2.13	0.48
1:H:622:ARG:NH1	1:H:683:GLY:O	2.45	0.48
1:H:634:ASP:HB3	1:H:639:ARG:HB2	1.95	0.48
1:A:698:TYR:CE2	1:A:725:LYS:HE2	2.48	0.48
1:A:773:GLU:OE2	1:A:980:LEU:HD22	2.14	0.48
1:B:437:GLN:HB2	1:B:1112:CYS:HB3	1.94	0.48
1:D:412:ARG:HH21	1:D:674:TYR:CB	2.26	0.48
1:D:789:THR:O	1:D:891:PHE:HA	2.13	0.48
1:E:341:THR:HG22	1:E:343:ARG:H	1.78	0.48
1:E:616:THR:OG1	1:E:677:PHE:HD2	1.97	0.48
1:F:624:ASP:HA	1:F:696:LEU:HD23	1.94	0.48
1:G:401:GLU:OE2	1:G:655:LYS:HE3	2.13	0.48
1:C:817:ASP:OD2	1:C:819:ARG:HB2	2.13	0.48
1:C:1080:ASP:HB3	1:C:1083:VAL:HG23	1.95	0.48
1:D:500:CYS:SG	1:D:619:SER:HB2	2.54	0.48
1:F:344:MET:HG2	1:F:650:GLN:OE1	2.13	0.48
1:F:377:PRO:HG2	1:F:538:TYR:CE1	2.49	0.48
1:F:1082:GLU:HA	1:F:1085:LYS:HB3	1.96	0.48
1:H:531:PRO:HA	1:H:534:ILE:CD1	2.43	0.48
1:H:1064:ARG:HG3	1:H:1064:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:VAL:HG21	1:A:964:GLU:CG	2.41	0.48
1:A:872:SER:HB2	1:A:874:LYS:HZ1	1.79	0.48
1:B:513:ASN:OD1	1:B:589:ALA:HB1	2.13	0.48
1:B:957:ILE:HD12	1:B:958:THR:N	2.28	0.48
1:B:966:ARG:HD3	1:B:975:LEU:O	2.12	0.48
1:C:351:TYR:CE1	1:C:412:ARG:HD3	2.47	0.48
1:C:889:LEU:O	1:C:977:HIS:HA	2.13	0.48
1:D:419:ASP:OD1	1:D:419:ASP:N	2.47	0.48
1:D:1118:GLU:HA	1:D:1121:SER:OG	2.14	0.48
1:E:347:LEU:O	1:E:351:TYR:N	2.45	0.48
1:F:476:VAL:CG1	1:F:841:LEU:HD22	2.43	0.48
1:H:648:LEU:HD23	1:H:648:LEU:HA	1.69	0.48
1:H:948:ASN:O	1:H:948:ASN:ND2	2.45	0.48
1:C:342:PRO:C	1:C:346:ARG:HH21	2.21	0.48
1:D:671:PHE:HD2	1:D:677:PHE:CZ	2.32	0.48
1:E:696:LEU:O	1:E:700:ILE:HG13	2.14	0.48
1:E:931:GLU:HA	1:E:934:ARG:HB3	1.95	0.48
1:E:934:ARG:O	1:E:937:CYS:HB2	2.13	0.48
1:F:944:GLY:HA3	1:F:1011:PRO:HG3	1.94	0.48
1:G:698:TYR:HB3	1:G:729:LYS:NZ	2.29	0.48
1:G:779:ARG:HG2	1:G:882:MET:SD	2.53	0.48
1:G:887:PRO:O	1:G:975:LEU:HD12	2.13	0.48
1:H:678:ILE:HG22	1:H:712:PRO:HB3	1.96	0.48
1:A:890:ILE:HD12	1:A:980:LEU:HG	1.95	0.48
1:A:980:LEU:HD12	1:A:980:LEU:O	2.14	0.48
1:B:773:GLU:OE2	1:B:980:LEU:HD13	2.14	0.48
1:C:613:GLU:HG2	1:C:615:GLN:NE2	2.29	0.48
1:E:520:GLU:HG2	1:E:544:ILE:HD11	1.96	0.48
1:E:631:PHE:O	1:E:635:ILE:HG12	2.14	0.48
1:E:672:ALA:O	1:E:1104:TYR:OH	2.24	0.48
1:F:821:LEU:HG	1:F:827:PHE:HA	1.94	0.48
1:G:783:TRP:HB2	1:G:887:PRO:HB3	1.96	0.48
1:G:1086:LYS:HE3	1:G:1094:TYR:HH	1.72	0.48
1:G:1096:ASP:HA	1:G:1107:TYR:HE2	1.78	0.48
1:H:386:PHE:CD2	1:H:546:THR:HG23	2.48	0.48
1:H:803:ARG:HB3	1:H:810:TYR:CE1	2.49	0.48
1:A:957:ILE:CD1	1:A:958:THR:N	2.51	0.48
1:B:502:GLY:HA3	1:B:505:VAL:HG12	1.94	0.48
1:B:687:ARG:HG3	1:B:765:ASP:HB2	1.96	0.48
1:C:796:GLU:OE2	1:C:805:VAL:HG22	2.14	0.48
1:C:824:PHE:CD1	1:C:909:PHE:HD2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:VAL:HG22	1:C:953:TYR:O	2.13	0.48
1:E:823:THR:HG22	1:E:826:GLU:HG3	1.95	0.48
1:F:369:VAL:HG11	1:F:385:ALA:HB2	1.95	0.48
1:F:382:ARG:NH2	1:F:613:GLU:OE1	2.45	0.48
1:H:788:TYR:HB3	1:H:984:ASN:HD22	1.79	0.48
1:H:949:TYR:O	1:H:949:TYR:CD1	2.64	0.48
1:A:366:PHE:O	1:A:370:VAL:HG23	2.14	0.48
1:C:599:LEU:HD22	1:C:652:PHE:CD2	2.48	0.48
1:D:640:LEU:CD2	1:D:644:THR:HB	2.44	0.48
1:D:650:GLN:HG2	1:D:707:VAL:HG13	1.96	0.48
1:E:472:ARG:CZ	1:E:477:TRP:CD1	2.97	0.48
1:G:713:SER:HA	1:G:740:PHE:CE1	2.48	0.48
1:H:783:TRP:HB2	1:H:887:PRO:HB3	1.95	0.48
1:H:910:GLU:OE1	1:H:949:TYR:OH	2.25	0.48
1:B:558:ALA:HB1	1:B:581:ALA:O	2.14	0.48
1:D:622:ARG:HH11	1:D:765:ASP:HA	1.79	0.48
1:D:824:PHE:HA	1:D:909:PHE:CD2	2.49	0.48
1:D:906:LYS:HA	1:D:910:GLU:HB2	1.95	0.48
1:D:1060:ILE:O	1:D:1064:ARG:HG2	2.14	0.48
1:E:678:ILE:HG21	1:E:712:PRO:HB3	1.93	0.48
1:E:924:LEU:O	1:E:924:LEU:HD23	2.14	0.48
1:F:510:LYS:NZ	1:F:518:ASP:OD2	2.29	0.48
1:G:906:LYS:HA	1:G:910:GLU:HB2	1.96	0.48
1:H:1042:ASN:ND2	1:H:1075:GLN:HE21	2.12	0.48
1:A:338:GLU:H	1:A:338:GLU:CD	2.22	0.47
1:A:700:ILE:O	1:A:704:VAL:HG22	2.13	0.47
1:B:948:ASN:O	1:B:952:GLN:HG2	2.14	0.47
1:C:468:GLU:HG3	1:C:477:TRP:CZ3	2.49	0.47
1:D:468:GLU:O	1:D:472:ARG:HG3	2.13	0.47
1:D:888:GLY:HA2	1:D:976:SER:O	2.13	0.47
1:D:984:ASN:N	1:D:984:ASN:OD1	2.47	0.47
1:E:572:GLN:O	1:E:576:GLU:HG3	2.14	0.47
1:F:783:TRP:HH2	1:F:853:HIS:ND1	2.11	0.47
1:G:806:LEU:HD22	1:G:991:LEU:HA	1.95	0.47
1:B:426:ARG:NE	1:B:427:ASP:OD1	2.47	0.47
1:C:375:GLY:HA3	1:G:466:ILE:HA	1.97	0.47
1:C:786:THR:OG1	1:C:846:THR:HG23	2.13	0.47
1:D:932:ALA:O	1:D:935:ARG:HB3	2.15	0.47
1:E:1052:THR:HG22	1:E:1054:GLU:H	1.79	0.47
1:F:391:GLU:O	1:F:556:ARG:NH1	2.47	0.47
1:G:507:LEU:HD21	1:G:605:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:735:LYS:HZ2	1:G:1056:ARG:HH12	1.61	0.47
1:G:946:ASP:OD1	1:G:1029:LYS:HE2	2.13	0.47
1:H:579:THR:O	1:H:583:VAL:HG22	2.14	0.47
1:H:587:VAL:HG11	1:H:592:PRO:HB3	1.96	0.47
1:B:623:VAL:HA	1:B:626:TYR:CE1	2.49	0.47
1:B:1064:ARG:O	1:B:1068:ILE:HD12	2.14	0.47
1:C:383:ALA:HB1	1:C:546:THR:HB	1.96	0.47
1:C:799:LEU:HA	1:C:818:LEU:HD21	1.96	0.47
1:G:669:LYS:HE2	1:G:987:PRO:HB3	1.95	0.47
1:G:694:ASN:N	1:G:697:THR:OG1	2.45	0.47
1:A:887:PRO:HD2	1:A:970:MET:HG3	1.96	0.47
1:A:941:PRO:HG2	1:A:949:TYR:HD2	1.78	0.47
1:C:344:MET:HE2	1:C:650:GLN:HB2	1.96	0.47
1:C:727:MET:HG3	1:C:1064:ARG:NH1	2.24	0.47
1:C:749:HIS:HA	1:C:752:MET:HG2	1.97	0.47
1:D:971:LEU:HB3	1:D:972:TYR:CD2	2.49	0.47
1:E:442:ILE:HG23	1:E:447:LYS:HE2	1.95	0.47
1:F:763:ALA:O	1:F:766:TYR:HD2	1.97	0.47
1:G:347:LEU:HD11	1:G:400:ASP:HB2	1.97	0.47
1:H:744:HIS:CE1	1:H:768:LEU:HG	2.50	0.47
1:H:984:ASN:HA	1:H:987:PRO:HD2	1.95	0.47
1:H:1098:ILE:HD11	1:H:1107:TYR:CZ	2.49	0.47
1:A:730:ILE:O	1:A:734:VAL:HG23	2.15	0.47
1:C:673:GLY:O	1:C:675:GLN:NE2	2.43	0.47
1:C:908:VAL:HG13	1:C:914:TYR:O	2.14	0.47
1:D:793:ILE:HD11	1:D:804:MET:HG3	1.97	0.47
1:D:849:SER:OG	1:D:850:GLN:N	2.47	0.47
1:E:442:ILE:HG13	1:E:447:LYS:HG3	1.96	0.47
1:F:650:GLN:HB2	1:F:707:VAL:HG13	1.96	0.47
1:F:746:ASP:HB3	1:F:750:ILE:CD1	2.44	0.47
1:G:806:LEU:CD2	1:G:991:LEU:HD23	2.43	0.47
1:G:966:ARG:HH11	1:G:974:THR:HG23	1.80	0.47
1:H:343:ARG:CG	1:H:400:ASP:HB3	2.45	0.47
1:H:796:GLU:HG3	1:H:800:ASN:ND2	2.29	0.47
1:A:674:TYR:HD2	1:A:1110:GLU:OE1	1.98	0.47
1:A:973:SER:OG	1:A:974:THR:N	2.44	0.47
1:A:1100:ARG:HH21	1:A:1103:GLY:CA	2.28	0.47
1:B:1020:PRO:HA	1:B:1023:ILE:HG12	1.96	0.47
1:B:1098:ILE:HG13	1:B:1107:TYR:CE1	2.49	0.47
1:C:341:THR:O	1:C:345:GLN:HG3	2.14	0.47
1:C:363:ALA:HB2	1:C:416:PHE:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ALA:HB2	1:C:860:PRO:CB	2.44	0.47
1:C:753:MET:HE2	1:C:756:LYS:HD2	1.96	0.47
1:C:788:TYR:CD1	1:C:890:ILE:HB	2.50	0.47
1:C:914:TYR:HA	1:C:918:GLN:OE1	2.14	0.47
1:D:347:LEU:O	1:D:351:TYR:N	2.42	0.47
1:G:531:PRO:HA	1:G:534:ILE:HD12	1.96	0.47
1:G:604:THR:O	1:G:608:LEU:HG	2.14	0.47
1:G:762:ASP:OD1	1:G:779:ARG:HD3	2.15	0.47
1:G:920:ARG:NH2	1:G:921:ASP:OD2	2.43	0.47
1:G:1008:GLY:HA3	1:G:1040:VAL:HG13	1.96	0.47
1:A:1020:PRO:HA	1:A:1023:ILE:HG13	1.96	0.47
1:C:765:ASP:HB3	1:C:776:LYS:CD	2.45	0.47
1:D:367:THR:HG23	1:D:458:TRP:NE1	2.28	0.47
1:D:406:HIS:NE2	1:D:410:LYS:O	2.47	0.47
1:D:527:SER:N	1:D:537:ILE:HD11	2.28	0.47
1:D:674:TYR:O	1:D:710:TYR:OH	2.29	0.47
1:D:1025:LYS:O	1:D:1028:SER:OG	2.18	0.47
1:E:750:ILE:O	1:E:754:LEU:HG	2.15	0.47
1:E:790:GLN:HE22	1:E:992:THR:HG23	1.79	0.47
1:F:655:LYS:NZ	3:F:1303:HOH:O	2.48	0.47
1:F:682:VAL:HB	1:F:697:THR:HG23	1.97	0.47
1:F:1050:LEU:HD21	1:F:1059:LEU:HB2	1.97	0.47
1:G:440:PHE:HE1	1:G:660:MET:HE2	1.80	0.47
1:G:505:VAL:HG13	1:G:506:LEU:HG	1.95	0.47
1:G:511:GLY:O	1:G:515:ILE:HG12	2.14	0.47
1:G:799:LEU:CD2	1:G:923:LEU:HD12	2.45	0.47
1:G:912:LYS:HA	1:G:912:LYS:HD2	1.68	0.47
1:G:916:LEU:HA	1:G:919:ILE:HG12	1.97	0.47
1:G:957:ILE:HD12	1:G:957:ILE:C	2.32	0.47
1:G:984:ASN:HB2	1:G:988:ILE:HG13	1.96	0.47
1:H:384:LYS:HE2	1:H:545:GLU:OE2	2.15	0.47
1:H:1082:GLU:HA	1:H:1085:LYS:HB2	1.95	0.47
1:A:412:ARG:HB3	1:A:660:MET:HE3	1.95	0.47
1:A:539:TYR:CD2	1:A:873:GLY:HA2	2.50	0.47
1:A:676:PRO:HG2	1:A:678:ILE:HG13	1.95	0.47
1:A:863:SER:OG	1:A:875:ASP:HB2	2.15	0.47
1:E:642:HIS:HA	1:E:699:LEU:HD11	1.96	0.47
1:E:700:ILE:O	1:E:704:VAL:HG23	2.15	0.47
1:G:550:VAL:HG12	1:G:608:LEU:CD1	2.45	0.47
1:G:678:ILE:CG2	1:G:712:PRO:HB3	2.44	0.47
1:G:710:TYR:HD2	1:G:1106:ALA:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:920:ARG:HE	1:G:921:ASP:CG	2.23	0.47
1:H:615:GLN:HG3	1:H:618:LEU:HD21	1.97	0.47
1:A:1097:LEU:O	1:A:1107:TYR:HA	2.14	0.47
1:B:565:ALA:O	1:B:574:ARG:HG3	2.15	0.47
1:C:758:PHE:CZ	1:C:780:ILE:HB	2.35	0.47
1:C:803:ARG:HB2	1:C:810:TYR:CE1	2.50	0.47
1:C:965:CYS:O	1:C:975:LEU:HB3	2.15	0.47
1:C:1068:ILE:HG23	1:H:1068:ILE:HG12	1.97	0.47
1:D:348:ARG:NH2	1:D:708:LYS:HD2	2.30	0.47
1:D:623:VAL:HG12	1:D:626:TYR:CZ	2.49	0.47
1:E:416:PHE:CE2	1:E:418:PRO:HG3	2.50	0.47
1:E:907:LEU:HD11	1:E:936:ASP:O	2.14	0.47
1:E:1013:GLN:HB3	1:E:1122:ARG:HA	1.96	0.47
1:F:472:ARG:NE	1:F:477:TRP:CD1	2.81	0.47
1:F:915:THR:OG1	1:F:918:GLN:HG2	2.15	0.47
1:G:614:ASN:ND2	1:G:662:MET:O	2.40	0.47
1:G:886:GLY:O	1:G:973:SER:HB3	2.15	0.47
1:G:1125:ILE:HA	1:G:1127:LYS:HE3	1.96	0.47
1:A:356:PRO:HA	1:A:412:ARG:HB2	1.97	0.47
1:A:774:PRO:HD2	1:A:1037:ILE:O	2.15	0.47
1:C:393:ALA:O	1:C:556:ARG:NH2	2.43	0.47
1:C:435:ARG:HH22	1:C:440:PHE:HD2	1.62	0.47
1:D:344:MET:HA	1:D:347:LEU:HD12	1.96	0.47
1:E:912:LYS:NZ	1:E:912:LYS:CB	2.78	0.47
1:F:613:GLU:O	1:F:615:GLN:HG2	2.15	0.47
1:G:388:HIS:CE1	1:G:392:THR:HG21	2.50	0.47
1:H:1075:GLN:HE22	1:H:1103:GLY:H	1.63	0.47
1:A:925:ALA:O	1:A:928:GLU:HB2	2.15	0.46
1:A:1016:ASP:HB2	1:A:1023:ILE:CD1	2.43	0.46
1:A:1042:ASN:OD1	1:A:1075:GLN:NE2	2.40	0.46
1:C:675:GLN:OE1	1:C:711:GLN:NE2	2.47	0.46
1:C:794:ALA:O	1:C:798:VAL:HG23	2.15	0.46
1:D:555:ARG:HA	1:D:555:ARG:HD3	1.66	0.46
1:F:518:ASP:HB2	1:F:870:MET:HE3	1.97	0.46
1:G:416:PHE:CZ	1:G:425:VAL:HG11	2.50	0.46
1:H:964:GLU:O	1:H:967:LYS:HB2	2.15	0.46
1:H:1020:PRO:HG3	1:H:1128:PHE:HD1	1.79	0.46
1:C:653:ILE:CD1	1:C:704:VAL:HG22	2.44	0.46
1:C:986:THR:O	1:C:990:GLU:HG3	2.16	0.46
1:D:504:ASP:OD1	1:D:504:ASP:N	2.46	0.46
1:D:599:LEU:HD13	1:D:652:PHE:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:832:LYS:HB3	1:D:960:TRP:CZ2	2.50	0.46
1:E:483:THR:OG1	1:E:485:VAL:HG23	2.14	0.46
1:F:486:SER:CB	1:F:789:THR:HB	2.45	0.46
1:G:621:GLY:HA2	1:G:767:CYS:HB3	1.97	0.46
1:G:791:TRP:CZ2	1:G:957:ILE:HD13	2.49	0.46
1:H:342:PRO:O	1:H:346:ARG:HG3	2.15	0.46
1:H:395:ILE:HG12	1:H:556:ARG:NH1	2.30	0.46
1:C:955:LEU:HB2	1:C:1029:LYS:O	2.15	0.46
1:D:771:CYS:HB2	1:D:772:VAL:HG22	1.97	0.46
1:E:674:TYR:O	1:E:710:TYR:OH	2.28	0.46
1:E:933:LEU:HD23	1:E:933:LEU:H	1.80	0.46
1:F:602:ILE:CG2	1:F:620:LEU:HD22	2.44	0.46
1:F:631:PHE:CD1	1:F:696:LEU:HD13	2.50	0.46
1:F:898:VAL:HG13	1:F:953:TYR:HB2	1.97	0.46
1:G:964:GLU:HA	1:G:967:LYS:HE3	1.96	0.46
1:G:1113:LYS:O	1:G:1116:GLN:HB3	2.15	0.46
1:H:986:THR:O	1:H:990:GLU:HG3	2.15	0.46
1:A:976:SER:HB3	1:A:1037:ILE:HD11	1.98	0.46
1:B:1081:ASN:HA	1:B:1084:LEU:HD12	1.98	0.46
1:C:653:ILE:HD13	1:C:704:VAL:HG22	1.96	0.46
1:C:730:ILE:HG23	1:C:741:PRO:HG3	1.97	0.46
1:C:962:GLU:O	1:C:966:ARG:HG2	2.15	0.46
1:D:395:ILE:HG23	1:D:557:ILE:HD13	1.96	0.46
1:D:790:GLN:NE2	1:D:992:THR:OG1	2.45	0.46
1:D:965:CYS:O	1:D:975:LEU:HB3	2.15	0.46
1:E:923:LEU:HA	1:E:994:ALA:HB3	1.98	0.46
1:F:991:LEU:O	1:F:1002:TRP:HZ3	1.98	0.46
1:G:364:LEU:HD21	1:G:449:THR:HG21	1.96	0.46
1:G:480:SER:HB2	1:G:486:SER:O	2.14	0.46
1:G:686:LYS:N	1:G:692:ALA:HB2	2.31	0.46
1:H:661:TRP:CH2	1:H:663:SER:HB3	2.50	0.46
1:H:768:LEU:HD13	1:H:768:LEU:HA	1.79	0.46
1:A:432:MET:CE	1:A:440:PHE:HB2	2.45	0.46
1:A:755:ARG:NH1	1:A:966:ARG:HH21	2.14	0.46
1:A:969:LYS:HD3	1:A:973:SER:O	2.16	0.46
1:A:1044:LYS:HB3	1:A:1123:THR:O	2.16	0.46
1:B:659:LEU:HD23	1:B:678:ILE:HD11	1.98	0.46
1:D:567:LYS:NZ	1:D:568:GLU:OE1	2.47	0.46
1:D:624:ASP:O	1:D:694:ASN:ND2	2.36	0.46
1:E:934:ARG:O	1:E:938:LEU:HD13	2.15	0.46
1:E:1060:ILE:O	1:E:1064:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:PRO:HG3	1:F:454:ILE:HG21	1.95	0.46
1:F:478:ALA:O	1:F:483:THR:HG23	2.15	0.46
1:F:805:VAL:HG21	1:F:993:ASN:ND2	2.29	0.46
1:G:606:GLU:OE2	1:G:659:LEU:HD12	2.16	0.46
1:G:768:LEU:HA	1:G:773:GLU:O	2.15	0.46
1:G:822:ARG:HG3	1:G:822:ARG:HH11	1.80	0.46
1:G:1104:TYR:C	1:G:1104:TYR:CD1	2.93	0.46
1:H:425:VAL:HA	1:H:428:GLU:HG3	1.96	0.46
1:H:1016:ASP:OD2	1:H:1023:ILE:HD11	2.16	0.46
1:A:702:ASP:HA	1:A:705:ARG:HG2	1.98	0.46
1:A:1097:LEU:HD12	1:A:1097:LEU:HA	1.69	0.46
1:B:898:VAL:HG13	1:B:953:TYR:HB2	1.96	0.46
1:B:951:ASP:CG	1:B:1026:SER:HB2	2.41	0.46
1:C:538:TYR:HE1	1:G:473:GLU:OE2	1.98	0.46
1:C:850:GLN:NE2	1:C:887:PRO:HD3	2.31	0.46
1:D:604:THR:O	1:D:608:LEU:HG	2.15	0.46
1:E:431:THR:HG22	1:E:434:THR:HB	1.97	0.46
1:E:1112:CYS:C	1:E:1113:LYS:HD3	2.40	0.46
1:F:596:GLN:HB2	1:F:648:LEU:HD11	1.96	0.46
1:G:365:ALA:HB1	1:G:389:ALA:HA	1.98	0.46
1:G:727:MET:O	1:G:731:VAL:HG23	2.15	0.46
1:A:942:LYS:C	1:A:950:VAL:HG11	2.41	0.46
1:B:897:TYR:CZ	1:B:957:ILE:HG21	2.50	0.46
1:C:428:GLU:OE2	1:C:665:GLU:HB2	2.16	0.46
1:C:646:LEU:HA	1:C:649:LEU:HD12	1.96	0.46
1:C:694:ASN:OD1	1:C:697:THR:N	2.48	0.46
1:C:859:LYS:O	1:C:863:SER:OG	2.25	0.46
1:D:817:ASP:OD1	1:D:818:LEU:N	2.49	0.46
1:E:472:ARG:NH2	1:E:477:TRP:NE1	2.63	0.46
1:E:680:LEU:O	1:E:715:ALA:N	2.47	0.46
1:E:1113:LYS:HA	1:E:1116:GLN:HG2	1.97	0.46
1:F:500:CYS:HB2	1:F:777:SER:CB	2.46	0.46
1:F:1062:LEU:HG	1:F:1074:MET:HE1	1.98	0.46
1:G:370:VAL:HG11	1:G:458:TRP:CH2	2.50	0.46
1:G:380:LEU:HD23	1:G:380:LEU:C	2.38	0.46
1:G:895:ALA:HB3	1:G:1006:SER:CB	2.45	0.46
1:H:366:PHE:CG	1:H:385:ALA:HB1	2.50	0.46
1:A:963:LYS:O	1:A:967:LYS:HG3	2.16	0.46
1:B:406:HIS:O	1:B:408:CYS:N	2.49	0.46
1:B:843:ALA:O	1:B:847:VAL:HG23	2.16	0.46
1:C:823:THR:HG1	1:C:826:GLU:H	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:ILE:O	1:G:363:ALA:N	2.49	0.46
1:G:664:SER:OG	1:G:665:GLU:N	2.49	0.46
1:G:908:VAL:HA	1:G:914:TYR:O	2.15	0.46
1:A:701:MET:HE3	1:A:716:CYS:SG	2.56	0.46
1:C:389:ALA:O	1:C:393:ALA:N	2.47	0.46
1:C:773:GLU:OE1	2:C:1201:A1H9L:F1	2.23	0.46
1:C:795:ILE:CG1	1:C:901:MET:HE3	2.45	0.46
1:C:871:GLU:OE1	1:C:871:GLU:N	2.42	0.46
1:C:1063:LEU:HD23	1:C:1074:MET:SD	2.56	0.46
1:D:987:PRO:HA	1:D:990:GLU:HG3	1.96	0.46
1:F:432:MET:HA	1:F:435:ARG:HD3	1.97	0.46
1:F:503:TYR:OH	1:F:609:PHE:HE2	1.99	0.46
1:F:889:LEU:HD12	1:F:889:LEU:HA	1.65	0.46
1:F:1087:ALA:HA	1:F:1094:TYR:CD2	2.51	0.46
1:G:625:GLN:CD	1:G:692:ALA:HB1	2.41	0.46
1:H:798:VAL:O	1:H:818:LEU:HD21	2.16	0.46
1:H:905:ARG:HD3	1:H:949:TYR:HE1	1.80	0.46
1:H:963:LYS:O	1:H:967:LYS:HG3	2.15	0.46
1:A:660:MET:SD	1:A:674:TYR:HB3	2.56	0.46
1:A:1001:ALA:C	1:A:1002:TRP:CG	2.92	0.46
1:D:988:ILE:HA	1:D:991:LEU:HD12	1.97	0.46
1:E:344:MET:HE1	1:E:651:ALA:HB2	1.98	0.46
1:E:749:HIS:HE1	3:E:1315:HOH:O	1.98	0.46
1:E:981:SER:OG	1:E:1008:GLY:N	2.49	0.46
1:H:555:ARG:HH11	1:H:555:ARG:HG3	1.81	0.46
1:A:442:ILE:HG23	1:A:447:LYS:HE2	1.98	0.45
1:A:592:PRO:HG2	1:A:630:MET:HE2	1.97	0.45
1:B:783:TRP:CH2	1:B:850:GLN:HA	2.51	0.45
1:C:675:GLN:CD	1:C:1104:TYR:CD2	2.94	0.45
1:D:1012:THR:HG22	1:D:1013:GLN:H	1.82	0.45
1:F:489:SER:O	1:F:493:ILE:HG12	2.16	0.45
1:F:497:GLY:HA3	1:F:616:THR:O	2.15	0.45
1:F:992:THR:HB	1:F:999:ARG:HH22	1.81	0.45
1:F:1063:LEU:HD23	1:F:1074:MET:SD	2.56	0.45
1:A:395:ILE:HD11	1:A:556:ARG:CZ	2.45	0.45
1:B:595:LEU:N	1:B:634:ASP:OD2	2.37	0.45
1:B:628:TYR:CD1	1:B:694:ASN:ND2	2.84	0.45
1:B:831:VAL:HG11	1:B:901:MET:CE	2.47	0.45
1:D:506:LEU:HD12	1:D:865:LEU:C	2.41	0.45
1:D:1012:THR:HG22	1:D:1013:GLN:N	2.31	0.45
1:D:1064:ARG:O	1:D:1068:ILE:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:ARG:NH1	1:E:464:ASP:OD2	2.50	0.45
1:E:446:ASP:O	1:E:450:ILE:HG12	2.16	0.45
1:E:553:TYR:HA	1:E:556:ARG:HG2	1.98	0.45
1:E:953:TYR:HA	1:E:956:ASP:CB	2.45	0.45
1:F:800:ASN:HD21	1:F:924:LEU:HD11	1.80	0.45
1:H:534:ILE:O	1:H:537:ILE:N	2.49	0.45
1:H:823:THR:OG1	1:H:826:GLU:N	2.37	0.45
1:C:386:PHE:CZ	1:C:861:LEU:HD22	2.51	0.45
1:C:506:LEU:HD13	1:C:864:LEU:O	2.15	0.45
1:C:624:ASP:HB3	1:C:682:VAL:HG12	1.97	0.45
1:C:874:LYS:HB2	1:C:874:LYS:HE2	1.64	0.45
1:D:516:LYS:NZ	1:D:548:GLU:OE2	2.40	0.45
1:E:912:LYS:HB2	1:E:912:LYS:HZ1	1.78	0.45
1:F:787:GLY:CA	1:F:889:LEU:CD1	2.91	0.45
1:F:1068:ILE:HG12	1:G:1068:ILE:HG23	1.99	0.45
1:H:583:VAL:HG23	1:H:584:ASN:OD1	2.17	0.45
1:H:801:ARG:HD2	1:H:816:GLY:O	2.16	0.45
1:A:824:PHE:CG	1:A:905:ARG:HD3	2.52	0.45
1:A:1062:LEU:HG	1:A:1074:MET:HE1	1.97	0.45
1:B:771:CYS:SG	2:B:1201:A1H9L:F1	2.65	0.45
1:C:370:VAL:HG22	1:C:381:LEU:HD21	1.99	0.45
1:C:502:GLY:N	1:C:865:LEU:O	2.46	0.45
1:C:756:LYS:HA	1:C:885:HIS:HD2	1.80	0.45
1:C:1010:SER:HA	1:C:1041:HIS:CE1	2.52	0.45
1:D:437:GLN:HB2	1:D:1112:CYS:HB2	1.98	0.45
1:D:738:MET:HG2	1:D:1098:ILE:HD12	1.98	0.45
1:E:957:ILE:HD12	1:E:958:THR:H	1.80	0.45
1:F:355:ARG:HD2	1:F:355:ARG:HA	1.68	0.45
1:F:617:GLY:HA2	1:F:677:PHE:HB2	1.98	0.45
1:G:364:LEU:HD21	1:G:449:THR:CG2	2.47	0.45
1:G:380:LEU:CD2	1:G:380:LEU:C	2.89	0.45
1:G:423:ARG:HH11	1:G:465:GLU:CG	2.29	0.45
1:H:487:ASP:O	1:H:787:GLY:HA2	2.17	0.45
1:H:896:THR:O	1:H:900:SER:OG	2.29	0.45
1:B:503:TYR:CE2	1:B:602:ILE:HG23	2.52	0.45
1:C:700:ILE:O	1:C:704:VAL:HG23	2.17	0.45
1:C:1027:VAL:HB	1:C:1071:ASN:ND2	2.32	0.45
1:C:1091:PRO:O	1:C:1109:VAL:HG11	2.16	0.45
1:D:986:THR:HB	1:D:987:PRO:CD	2.46	0.45
1:E:917:GLU:HG2	1:E:917:GLU:H	1.15	0.45
1:F:742:ALA:HB1	1:F:1073:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:890:ILE:CG2	1:F:980:LEU:H	2.29	0.45
1:G:483:THR:O	1:G:484:PHE:HB2	2.17	0.45
1:G:724:GLN:O	1:G:728:GLU:HB2	2.16	0.45
1:G:874:LYS:HB3	1:G:878:ALA:HB3	1.98	0.45
1:G:1084:LEU:HB3	1:G:1120:ILE:CD1	2.46	0.45
1:H:477:TRP:CH2	1:H:481:GLY:HA3	2.51	0.45
1:H:1020:PRO:HB2	1:H:1062:LEU:CD1	2.47	0.45
1:A:984:ASN:HB2	1:A:988:ILE:HG13	1.97	0.45
1:C:504:ASP:N	1:C:504:ASP:OD1	2.50	0.45
1:C:1111:LEU:O	1:C:1116:GLN:NE2	2.46	0.45
1:G:401:GLU:HB3	1:G:403:ILE:O	2.16	0.45
1:G:647:GLU:O	1:G:651:ALA:N	2.48	0.45
1:H:654:ILE:HD11	1:H:707:VAL:HG11	1.97	0.45
1:B:965:CYS:O	1:B:975:LEU:HB3	2.17	0.45
1:C:625:GLN:OE1	1:C:692:ALA:HB1	2.17	0.45
1:C:1084:LEU:HD23	1:C:1084:LEU:HA	1.81	0.45
1:D:1016:ASP:OD1	1:D:1016:ASP:N	2.46	0.45
1:D:1117:ASP:O	1:D:1120:ILE:N	2.49	0.45
1:F:348:ARG:NH1	1:F:1096:ASP:OD2	2.50	0.45
1:F:680:LEU:HD21	1:F:700:ILE:HG21	1.99	0.45
1:H:1055:GLY:HA2	1:H:1128:PHE:CE2	2.52	0.45
1:A:532:GLU:H	1:A:532:GLU:CD	2.25	0.45
1:A:729:LYS:HD3	1:A:729:LYS:HA	1.71	0.45
1:B:798:VAL:HG23	1:B:834:GLN:HG3	1.99	0.45
1:D:362:ARG:HH21	1:D:612:GLU:C	2.19	0.45
1:D:412:ARG:NH2	1:D:674:TYR:HB2	2.31	0.45
1:D:767:CYS:C	1:D:768:LEU:HD22	2.41	0.45
1:F:1084:LEU:HD22	1:F:1108:PHE:CD2	2.52	0.45
1:G:497:GLY:N	1:G:615:GLN:HB2	2.32	0.45
1:G:919:ILE:HG22	1:G:933:LEU:HD21	1.99	0.45
1:H:419:ASP:N	1:H:419:ASP:OD1	2.49	0.45
1:H:923:LEU:HA	1:H:923:LEU:HD13	1.73	0.45
1:H:1040:VAL:HG21	1:H:1103:GLY:N	2.32	0.45
1:A:832:LYS:HD3	1:A:960:TRP:CD2	2.52	0.45
1:B:529:GLU:O	1:B:529:GLU:HG2	2.16	0.45
1:B:699:LEU:HD23	1:B:699:LEU:HA	1.81	0.45
1:B:742:ALA:HA	1:B:1075:GLN:HG2	1.99	0.45
1:C:641:THR:N	1:C:644:THR:OG1	2.34	0.45
1:C:828:ASP:O	1:C:832:LYS:HG3	2.17	0.45
1:C:938:LEU:CD2	1:C:998:GLY:HA3	2.47	0.45
1:C:945:ASN:OD1	1:C:1018:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ARG:HA	1:D:351:TYR:HB3	1.99	0.45
1:D:599:LEU:HD22	1:D:652:PHE:CG	2.52	0.45
1:E:363:ALA:HB2	1:E:416:PHE:O	2.16	0.45
1:E:941:PRO:C	1:E:942:LYS:HD2	2.41	0.45
1:E:993:ASN:CG	1:E:994:ALA:H	2.25	0.45
1:F:901:MET:HB3	1:F:953:TYR:HD2	1.81	0.45
1:F:923:LEU:HB2	1:F:994:ALA:HB3	1.99	0.45
1:F:931:GLU:N	1:F:931:GLU:OE2	2.50	0.45
1:A:341:THR:HG21	1:A:647:GLU:HG3	1.99	0.45
1:A:624:ASP:HB3	1:A:682:VAL:HG12	1.99	0.45
1:C:369:VAL:HG21	1:C:385:ALA:HA	1.98	0.45
1:D:348:ARG:HH22	1:D:708:LYS:HD2	1.82	0.45
1:E:597:GLU:O	1:E:601:SER:HB2	2.16	0.45
1:F:370:VAL:HG13	1:F:381:LEU:HD21	1.98	0.45
1:F:479:PHE:HE2	1:F:838:ILE:HG23	1.82	0.45
1:G:376:MET:HE3	1:G:376:MET:HB2	1.78	0.45
1:G:698:TYR:HB3	1:G:729:LYS:HZ2	1.82	0.45
1:G:926:ASN:OD1	1:G:994:ALA:HB2	2.17	0.45
1:G:930:TYR:N	1:G:931:GLU:OE1	2.50	0.45
1:H:1113:LYS:NZ	1:H:1114:GLU:HG3	2.32	0.45
1:A:502:GLY:CA	1:A:778:GLY:HA3	2.47	0.44
1:A:727:MET:HA	1:A:730:ILE:HD12	1.98	0.44
1:A:906:LYS:HE3	1:A:911:GLU:OE2	2.16	0.44
1:A:984:ASN:HA	1:A:987:PRO:CG	2.46	0.44
1:B:411:PRO:HB3	1:B:658:GLU:HG2	2.00	0.44
1:C:815:THR:HG21	1:C:830:ALA:O	2.17	0.44
1:D:780:ILE:HD11	1:D:782:GLN:HB3	1.99	0.44
1:D:984:ASN:HB2	1:D:988:ILE:CG1	2.46	0.44
1:E:799:LEU:HA	1:E:818:LEU:HD21	1.99	0.44
1:F:516:LYS:O	1:F:520:GLU:HG2	2.18	0.44
1:G:850:GLN:CB	1:G:971:LEU:HD22	2.47	0.44
1:G:981:SER:O	1:G:982:ILE:C	2.59	0.44
1:H:411:PRO:HB3	1:H:658:GLU:HG2	1.97	0.44
1:H:587:VAL:HG11	1:H:597:GLU:HB3	1.99	0.44
1:A:1025:LYS:HD2	1:A:1025:LYS:HA	1.80	0.44
1:A:1041:HIS:CD2	1:A:1043:PHE:HE1	2.35	0.44
1:B:488:LEU:HD23	1:B:787:GLY:HA3	1.99	0.44
1:C:755:ARG:HG3	1:C:755:ARG:O	2.16	0.44
1:C:804:MET:HG2	3:C:1328:HOH:O	2.16	0.44
1:D:564:LEU:HA	1:D:567:LYS:CG	2.47	0.44
1:D:753:MET:HE3	1:D:753:MET:HB3	1.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:667:GLY:HA2	1:E:670:TYR:CD1	2.52	0.44
1:F:621:GLY:O	1:F:623:VAL:HG23	2.16	0.44
1:F:701:MET:HB3	1:F:714:LEU:HD21	2.00	0.44
1:F:752:MET:HE2	1:F:774:PRO:HG3	1.98	0.44
1:F:914:TYR:CD1	1:F:933:LEU:HD12	2.52	0.44
1:G:615:GLN:NE2	1:G:618:LEU:HD21	2.26	0.44
1:H:432:MET:HE3	1:H:440:PHE:HB2	1.98	0.44
1:A:919:ILE:O	1:A:923:LEU:HG	2.17	0.44
1:A:1043:PHE:HE2	1:A:1062:LEU:HD21	1.82	0.44
1:C:909:PHE:CZ	1:C:916:LEU:HD11	2.51	0.44
1:D:428:GLU:OE1	1:D:665:GLU:N	2.42	0.44
1:D:438:ASP:HA	1:D:674:TYR:CZ	2.52	0.44
1:D:1081:ASN:ND2	1:D:1120:ILE:O	2.49	0.44
1:E:1112:CYS:O	1:E:1115:VAL:HG12	2.16	0.44
1:F:358:VAL:HG23	1:F:440:PHE:HB3	1.98	0.44
1:G:480:SER:OG	1:G:481:GLY:N	2.50	0.44
1:G:717:ARG:HA	1:G:744:HIS:O	2.17	0.44
1:G:735:LYS:C	1:G:737:GLY:N	2.75	0.44
1:G:843:ALA:O	1:G:847:VAL:HG13	2.18	0.44
1:H:543:ALA:HB1	1:H:864:LEU:HD21	2.00	0.44
1:H:826:GLU:O	1:H:829:ALA:HB3	2.17	0.44
1:H:835:ILE:HG13	1:H:960:TRP:CZ3	2.52	0.44
1:H:843:ALA:O	1:H:847:VAL:HG23	2.17	0.44
1:A:622:ARG:HH11	1:A:765:ASP:HA	1.83	0.44
1:A:963:LYS:HZ3	1:A:963:LYS:HG3	1.70	0.44
1:B:653:ILE:HG21	1:B:707:VAL:HG21	2.00	0.44
1:B:775:GLN:HB3	1:B:780:ILE:HG21	1.98	0.44
1:B:1047:LYS:HE2	1:B:1078:TYR:O	2.18	0.44
1:C:911:GLU:OE2	1:C:913:LYS:HE2	2.18	0.44
1:D:620:LEU:HD13	1:D:652:PHE:HZ	1.82	0.44
1:D:622:ARG:NH1	1:D:717:ARG:HH12	2.14	0.44
1:E:732:ASP:O	1:E:735:LYS:HB3	2.17	0.44
1:E:875:ASP:OD1	1:E:877:ALA:N	2.47	0.44
1:F:1100:ARG:HH11	1:F:1104:TYR:C	2.24	0.44
1:G:500:CYS:O	1:G:778:GLY:N	2.46	0.44
1:G:576:GLU:HB3	1:G:577:LEU:HD23	1.99	0.44
1:H:574:ARG:O	1:H:578:LEU:HD12	2.16	0.44
1:H:727:MET:HE2	1:H:1060:ILE:HG23	1.98	0.44
1:B:370:VAL:HA	1:B:381:LEU:HD11	1.99	0.44
1:B:424:TRP:CE3	1:B:664:SER:HA	2.52	0.44
1:D:417:SER:HB2	1:D:419:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:840:ARG:HA	1:E:968:TYR:CE2	2.53	0.44
1:G:364:LEU:CD2	1:G:454:ILE:HD11	2.46	0.44
1:G:813:LEU:HD12	1:G:813:LEU:N	2.33	0.44
1:A:539:TYR:O	1:A:542:ALA:HB3	2.18	0.44
1:A:1118:GLU:OE2	1:A:1122:ARG:NE	2.39	0.44
1:B:362:ARG:NH1	1:B:417:SER:HA	2.32	0.44
1:D:348:ARG:NH2	1:D:1096:ASP:OD1	2.51	0.44
1:D:432:MET:O	1:D:439:PRO:HA	2.18	0.44
1:D:613:GLU:O	1:D:615:GLN:HG2	2.18	0.44
1:E:641:THR:O	1:E:643:ASP:N	2.51	0.44
1:E:980:LEU:HA	1:E:1040:VAL:HG12	1.98	0.44
1:G:423:ARG:NH1	1:G:465:GLU:HG2	2.33	0.44
1:H:340:LEU:HD23	1:H:344:MET:CB	2.48	0.44
1:H:1100:ARG:HA	1:H:1105:SER:HA	2.00	0.44
1:A:355:ARG:HD3	1:A:355:ARG:HA	1.63	0.44
1:A:432:MET:HE3	1:A:440:PHE:HB2	1.99	0.44
1:A:980:LEU:HA	1:A:1040:VAL:HG12	1.98	0.44
1:B:340:LEU:HD22	1:B:344:MET:CG	2.48	0.44
1:B:580:ILE:HA	1:B:583:VAL:HG22	2.00	0.44
1:B:862:MET:HB2	1:B:862:MET:HE2	1.73	0.44
1:B:864:LEU:C	1:B:865:LEU:HD23	2.43	0.44
1:C:988:ILE:HG22	1:C:1005:LEU:HD11	2.00	0.44
1:C:1075:GLN:HE22	1:C:1103:GLY:N	2.15	0.44
1:D:1106:ALA:CB	1:D:1111:LEU:HD11	2.46	0.44
1:E:681:THR:HG21	1:E:767:CYS:HA	1.99	0.44
1:E:982:ILE:O	1:E:1102:ALA:HB3	2.18	0.44
1:F:926:ASN:HD21	1:F:1000:LEU:HD22	1.82	0.44
1:G:724:GLN:NE2	1:G:1060:ILE:HD13	2.33	0.44
1:G:888:GLY:HA2	1:G:976:SER:O	2.17	0.44
1:H:398:GLN:HE21	1:H:401:GLU:CD	2.25	0.44
1:H:850:GLN:HE22	1:H:887:PRO:HD3	1.83	0.44
1:H:1097:LEU:HD12	1:H:1108:PHE:HB3	2.00	0.44
1:H:1121:SER:OG	1:H:1122:ARG:N	2.50	0.44
1:A:981:SER:OG	1:A:1008:GLY:N	2.50	0.44
1:A:985:ASN:OD1	1:A:986:THR:N	2.51	0.44
1:B:657:ALA:HA	1:B:711:GLN:HB2	1.99	0.44
1:B:739:GLY:HA3	1:B:1100:ARG:HB2	1.98	0.44
1:C:346:ARG:NH1	1:C:400:ASP:OD1	2.50	0.44
1:C:443:SER:OG	1:C:444:GLU:N	2.51	0.44
1:C:618:LEU:HD11	1:C:862:MET:HE1	2.00	0.44
1:C:750:ILE:O	1:C:753:MET:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:PHE:CE2	1:D:630:MET:HE1	2.52	0.44
1:D:624:ASP:OD1	1:D:682:VAL:HA	2.17	0.44
1:D:729:LYS:O	1:D:733:VAL:HG23	2.17	0.44
1:D:1095:ARG:CG	1:D:1109:VAL:HG21	2.44	0.44
1:E:726:TYR:HA	1:E:729:LYS:HB3	1.99	0.44
1:E:769:MET:HB3	1:E:769:MET:HE3	1.65	0.44
1:F:832:LYS:HD3	1:F:960:TRP:NE1	2.33	0.44
1:G:518:ASP:O	1:G:521:ALA:N	2.50	0.44
1:H:343:ARG:O	1:H:346:ARG:HB2	2.18	0.44
1:A:387:ARG:NE	1:A:391:GLU:OE2	2.50	0.44
1:A:984:ASN:HA	1:A:987:PRO:HD2	1.99	0.44
1:B:388:HIS:O	1:B:392:THR:HG23	2.18	0.44
1:B:432:MET:CE	1:B:440:PHE:HB2	2.46	0.44
1:B:572:GLN:O	1:B:576:GLU:HG3	2.17	0.44
1:B:908:VAL:O	1:B:912:LYS:HG2	2.17	0.44
1:D:746:ASP:O	1:D:749:HIS:N	2.49	0.44
1:E:698:TYR:CE1	1:E:726:TYR:HB2	2.53	0.44
1:E:1049:LEU:HD21	1:E:1128:PHE:CE2	2.53	0.44
1:F:631:PHE:O	1:F:635:ILE:HG13	2.17	0.44
1:F:907:LEU:HB3	1:F:914:TYR:HD2	1.82	0.44
1:H:491:HIS:CE1	1:H:783:TRP:CG	3.06	0.44
1:H:907:LEU:HD21	1:H:936:ASP:HB3	2.00	0.44
1:B:504:ASP:OD1	1:B:505:VAL:N	2.51	0.43
1:D:484:PHE:O	1:D:485:VAL:C	2.61	0.43
1:D:504:ASP:HB3	1:D:626:TYR:CD2	2.52	0.43
1:D:708:LYS:HE3	1:D:1096:ASP:O	2.17	0.43
1:D:1051:ASP:OD2	1:D:1078:TYR:OH	2.35	0.43
1:D:1113:LYS:O	1:D:1116:GLN:HG2	2.18	0.43
1:E:346:ARG:NH1	1:E:400:ASP:OD2	2.51	0.43
1:F:466:ILE:HA	1:H:375:GLY:HA3	2.00	0.43
1:F:1028:SER:HB2	1:F:1069:LEU:CD2	2.48	0.43
1:G:631:PHE:CE1	1:G:696:LEU:HB2	2.53	0.43
1:H:646:LEU:O	1:H:650:GLN:HG2	2.17	0.43
1:H:896:THR:HG22	1:H:997:ASN:HD21	1.83	0.43
1:H:1086:LYS:C	1:H:1088:GLN:N	2.75	0.43
1:A:487:ASP:O	1:A:787:GLY:HA2	2.17	0.43
1:A:957:ILE:C	1:A:957:ILE:CD1	2.89	0.43
1:C:824:PHE:HA	1:C:909:PHE:CD2	2.53	0.43
1:D:370:VAL:HG12	1:D:457:PHE:CZ	2.54	0.43
1:D:487:ASP:O	1:D:787:GLY:HA2	2.19	0.43
1:D:785:SER:OG	1:D:787:GLY:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1004:PRO:HB3	1:D:1118:GLU:HG3	2.01	0.43
1:E:425:VAL:O	1:E:429:LEU:HG	2.17	0.43
1:F:355:ARG:HD3	1:F:1095:ARG:HH12	1.82	0.43
1:F:957:ILE:O	1:F:961:THR:OG1	2.35	0.43
1:G:546:THR:HG23	1:G:864:LEU:HD11	2.00	0.43
1:G:565:ALA:O	1:G:574:ARG:HG3	2.18	0.43
1:G:600:GLN:HE21	1:G:604:THR:CG2	2.31	0.43
1:G:847:VAL:HA	1:G:850:GLN:OE1	2.18	0.43
1:G:1045:PHE:CZ	1:G:1059:LEU:HD13	2.53	0.43
1:H:479:PHE:CG	1:H:841:LEU:HD23	2.53	0.43
1:H:771:CYS:HB3	1:H:1103:GLY:HA3	1.99	0.43
1:H:906:LYS:HD2	1:H:949:TYR:CZ	2.53	0.43
1:A:641:THR:N	1:A:644:THR:OG1	2.41	0.43
1:B:340:LEU:HD22	1:B:344:MET:HG3	2.00	0.43
1:B:528:MET:HG3	1:B:534:ILE:HG12	1.99	0.43
1:C:526:LEU:HD21	1:C:536:ARG:HH21	1.83	0.43
1:C:648:LEU:HD23	1:C:648:LEU:HA	1.76	0.43
1:C:784:THR:HB	3:C:1302:HOH:O	2.19	0.43
1:E:818:LEU:N	1:E:818:LEU:HD12	2.33	0.43
1:E:1075:GLN:CD	1:E:1100:ARG:HH21	2.26	0.43
1:F:795:ILE:HA	1:F:798:VAL:HG12	1.98	0.43
1:F:821:LEU:HD12	1:F:821:LEU:HA	1.61	0.43
1:G:745:PHE:O	1:G:748:SER:OG	2.35	0.43
1:G:894:LEU:HD23	1:G:1009:ILE:HG22	2.00	0.43
1:G:955:LEU:HD23	1:G:959:GLU:HG3	1.99	0.43
1:G:1095:ARG:O	1:G:1107:TYR:HE2	2.01	0.43
1:H:632:GLU:OE2	1:H:636:ARG:HG3	2.19	0.43
1:A:806:LEU:HD22	1:A:990:GLU:O	2.19	0.43
1:A:1044:LYS:NZ	1:A:1119:ILE:O	2.51	0.43
1:B:477:TRP:CZ2	1:B:481:GLY:HA3	2.52	0.43
1:B:504:ASP:HB3	1:B:626:TYR:CG	2.53	0.43
1:B:512:MET:HB2	1:B:589:ALA:HA	2.01	0.43
1:B:783:TRP:O	1:B:784:THR:C	2.62	0.43
1:C:359:SER:HB2	1:C:361:TYR:CD2	2.50	0.43
1:D:546:THR:HB	1:D:864:LEU:HD11	2.00	0.43
1:D:650:GLN:O	1:D:653:ILE:N	2.52	0.43
1:D:769:MET:HE3	1:D:769:MET:HB3	1.74	0.43
1:E:384:LYS:HG2	1:E:545:GLU:OE1	2.18	0.43
1:E:1052:THR:HG22	1:E:1054:GLU:HB2	1.98	0.43
1:F:823:THR:OG1	1:F:826:GLU:N	2.46	0.43
1:F:943:TYR:O	1:F:1011:PRO:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:698:TYR:HD1	1:G:729:LYS:HG3	1.80	0.43
1:H:778:GLY:HA2	1:H:866:VAL:HG12	2.00	0.43
1:A:376:MET:HB3	1:A:381:LEU:HB2	2.00	0.43
1:A:1100:ARG:HH22	1:A:1103:GLY:C	2.26	0.43
1:C:941:PRO:HB2	1:C:950:VAL:HB	1.99	0.43
1:D:686:LYS:HD3	1:D:686:LYS:C	2.44	0.43
1:D:985:ASN:OD1	1:D:986:THR:N	2.51	0.43
1:E:730:ILE:O	1:E:734:VAL:HG23	2.18	0.43
1:E:915:THR:CG2	1:E:917:GLU:HG3	2.48	0.43
1:F:343:ARG:NH1	1:F:576:GLU:OE2	2.30	0.43
1:F:934:ARG:HH21	1:F:1000:LEU:HG	1.83	0.43
1:G:530:ASN:HB2	1:G:533:ASP:OD2	2.18	0.43
1:G:631:PHE:CD1	1:G:696:LEU:HB2	2.53	0.43
1:A:657:ALA:HA	1:A:711:GLN:HB2	2.00	0.43
1:E:1075:GLN:CG	1:E:1100:ARG:HH21	2.31	0.43
1:E:1084:LEU:HD21	1:E:1099:VAL:HG11	2.01	0.43
1:F:718:ILE:HD11	1:F:743:CYS:HB3	2.00	0.43
1:F:850:GLN:NE2	1:F:887:PRO:HD3	2.33	0.43
1:H:512:MET:HG2	1:H:588:PRO:HB2	2.00	0.43
1:H:1084:LEU:HB2	1:H:1120:ILE:HD11	1.99	0.43
1:B:1081:ASN:O	1:B:1085:LYS:HG2	2.18	0.43
1:C:435:ARG:HD2	1:C:437:GLN:O	2.19	0.43
1:C:746:ASP:O	1:C:750:ILE:N	2.34	0.43
1:C:966:ARG:HD3	1:C:975:LEU:O	2.18	0.43
1:C:985:ASN:OD1	1:C:985:ASN:N	2.47	0.43
1:D:685:GLN:HG3	1:D:746:ASP:OD2	2.18	0.43
1:D:843:ALA:HB1	1:D:970:MET:HE1	2.01	0.43
1:D:966:ARG:HA	1:D:974:THR:HG22	2.00	0.43
1:D:1045:PHE:CE2	1:D:1059:LEU:HD13	2.53	0.43
1:E:647:GLU:HA	1:E:650:GLN:NE2	2.33	0.43
1:E:803:ARG:HA	1:E:810:TYR:HA	1.99	0.43
1:F:343:ARG:NE	1:F:647:GLU:OE2	2.33	0.43
1:F:614:ASN:ND2	1:F:662:MET:HB2	2.33	0.43
1:F:863:SER:HA	1:F:876:VAL:HG13	2.01	0.43
1:F:948:ASN:HA	1:F:951:ASP:HB2	2.01	0.43
1:F:1112:CYS:O	1:F:1116:GLN:HG2	2.18	0.43
1:G:502:GLY:CA	1:G:778:GLY:HA3	2.49	0.43
1:G:594:THR:HG23	1:G:634:ASP:OD2	2.18	0.43
1:G:640:LEU:HG	1:G:644:THR:OG1	2.19	0.43
1:G:669:LYS:HE2	1:G:669:LYS:HB2	1.81	0.43
1:G:697:THR:H	1:G:697:THR:HG1	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:365:ALA:O	1:H:369:VAL:HG23	2.18	0.43
1:H:402:LEU:HA	1:H:580:ILE:HD11	1.99	0.43
1:H:562:ARG:O	1:H:565:ALA:HB3	2.18	0.43
1:H:631:PHE:CG	1:H:696:LEU:HD13	2.54	0.43
1:H:785:SER:HA	1:H:888:GLY:O	2.17	0.43
1:H:832:LYS:HA	1:H:835:ILE:HG12	2.00	0.43
1:A:1049:LEU:HD13	1:A:1126:GLU:O	2.18	0.43
1:B:990:GLU:HA	1:B:1002:TRP:O	2.19	0.43
1:C:857:ALA:O	1:C:859:LYS:NZ	2.47	0.43
1:E:599:LEU:HB3	1:E:652:PHE:CD1	2.53	0.43
1:E:850:GLN:NE2	1:E:887:PRO:HD3	2.33	0.43
1:F:428:GLU:CD	1:F:665:GLU:HB2	2.44	0.43
1:G:344:MET:HA	1:G:347:LEU:HD23	2.00	0.43
1:G:646:LEU:HB2	1:G:699:LEU:HD11	2.01	0.43
1:G:1074:MET:HE2	1:G:1076:PHE:HZ	1.84	0.43
1:H:656:CYS:HB2	1:H:712:PRO:HD3	2.00	0.43
1:H:775:GLN:HE21	1:H:780:ILE:HG21	1.83	0.43
1:H:803:ARG:HA	1:H:810:TYR:HA	2.00	0.43
1:H:885:HIS:HA	1:H:973:SER:HB3	2.01	0.43
1:B:423:ARG:HH11	1:B:465:GLU:HG3	1.82	0.43
1:B:489:SER:O	1:B:492:GLN:HB3	2.18	0.43
1:B:516:LYS:HB3	1:B:516:LYS:HE3	1.68	0.43
1:B:620:LEU:HD13	1:B:680:LEU:HD12	2.00	0.43
1:D:934:ARG:O	1:D:937:CYS:HB2	2.19	0.43
1:E:472:ARG:NH1	1:E:477:TRP:CD1	2.87	0.43
1:E:520:GLU:HG2	1:E:544:ILE:CD1	2.49	0.43
1:F:587:VAL:HG11	1:F:592:PRO:HB3	2.00	0.43
1:F:711:GLN:HE21	1:F:712:PRO:HA	1.84	0.43
1:F:985:ASN:N	1:F:985:ASN:OD1	2.51	0.43
1:G:477:TRP:NE1	1:G:482:GLU:OE1	2.49	0.43
1:G:587:VAL:HG21	1:G:597:GLU:O	2.18	0.43
1:G:999:ARG:HD2	1:G:1004:PRO:O	2.18	0.43
1:H:462:SER:OG	1:H:465:GLU:HG3	2.18	0.43
1:H:618:LEU:H	1:H:618:LEU:HD22	1.83	0.43
1:H:717:ARG:NH2	1:H:764:ARG:O	2.34	0.43
1:H:749:HIS:NE2	1:H:1072:GLY:O	2.46	0.43
1:H:993:ASN:OD1	1:H:994:ALA:N	2.44	0.43
1:C:551:VAL:O	1:C:555:ARG:HB2	2.19	0.43
1:C:649:LEU:O	1:C:652:PHE:HB3	2.19	0.43
1:C:783:TRP:HB2	1:C:887:PRO:HG3	2.01	0.43
1:C:1107:TYR:HB2	1:C:1110:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:ASP:HB3	1:D:626:TYR:CG	2.54	0.43
1:D:532:GLU:H	1:D:532:GLU:CD	2.27	0.43
1:E:914:TYR:CD1	1:E:933:LEU:HD13	2.53	0.43
1:E:966:ARG:NH1	1:E:974:THR:HB	2.33	0.43
1:F:505:VAL:O	1:F:506:LEU:HD23	2.19	0.43
1:F:675:GLN:HG3	1:F:1104:TYR:CD2	2.54	0.43
1:G:839:VAL:HG11	1:G:964:GLU:CG	2.49	0.43
1:G:1026:SER:O	1:G:1029:LYS:HG2	2.18	0.43
1:G:1112:CYS:SG	1:G:1113:LYS:N	2.91	0.43
1:H:486:SER:HB2	1:H:789:THR:HB	2.01	0.43
1:A:440:PHE:HE1	1:A:660:MET:SD	2.42	0.42
1:B:702:ASP:HA	1:B:705:ARG:HG3	2.01	0.42
1:D:423:ARG:NH2	1:D:464:ASP:OD2	2.47	0.42
1:E:437:GLN:OE1	1:E:437:GLN:HA	2.18	0.42
1:E:554:ALA:CB	1:E:588:PRO:HD2	2.49	0.42
1:E:850:GLN:HG2	3:E:1316:HOH:O	2.19	0.42
1:E:1095:ARG:HG3	1:E:1096:ASP:N	2.33	0.42
1:E:1108:PHE:CZ	1:E:1116:GLN:HB2	2.54	0.42
1:F:806:LEU:HD22	1:F:807:PHE:CE1	2.54	0.42
1:F:903:ALA:O	1:F:906:LYS:N	2.52	0.42
1:F:1016:ASP:CB	1:F:1023:ILE:HD11	2.49	0.42
1:G:621:GLY:O	1:G:623:VAL:N	2.52	0.42
1:G:710:TYR:CD2	1:G:1106:ALA:HA	2.54	0.42
1:H:345:GLN:O	1:H:349:ASN:HB2	2.19	0.42
1:H:414:GLY:HA3	1:H:662:MET:SD	2.58	0.42
1:H:839:VAL:HG12	1:H:968:TYR:CE2	2.54	0.42
1:A:351:TYR:CE1	1:A:412:ARG:HD3	2.54	0.42
1:A:660:MET:HE1	1:A:674:TYR:HB3	2.01	0.42
1:A:897:TYR:CE2	1:A:957:ILE:CG2	3.02	0.42
1:B:480:SER:OG	1:B:488:LEU:HB2	2.19	0.42
1:B:1039:MET:SD	1:B:1072:GLY:HA3	2.59	0.42
1:C:717:ARG:HD2	1:C:766:TYR:CE2	2.54	0.42
1:C:832:LYS:HB3	1:C:960:TRP:CZ2	2.54	0.42
1:C:947:ASP:O	1:C:950:VAL:HG12	2.19	0.42
1:D:953:TYR:O	1:D:957:ILE:HG13	2.20	0.42
1:D:1098:ILE:HG12	1:D:1107:TYR:CD1	2.55	0.42
1:E:463:LEU:HD23	1:E:467:CYS:HB2	2.01	0.42
1:E:686:LYS:NZ	1:E:691:ASP:O	2.39	0.42
1:E:841:LEU:HD22	1:E:844:ILE:HD12	2.00	0.42
1:E:953:TYR:HA	1:E:956:ASP:HB3	2.01	0.42
1:E:965:CYS:C	1:E:967:LYS:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:PRO:HG3	1:F:454:ILE:CG2	2.49	0.42
1:F:718:ILE:O	1:F:745:PHE:HA	2.20	0.42
1:F:1063:LEU:HD23	1:F:1063:LEU:HA	1.79	0.42
1:G:425:VAL:O	1:G:429:LEU:HG	2.19	0.42
1:G:429:LEU:O	1:G:447:LYS:HE3	2.19	0.42
1:H:366:PHE:HE1	1:H:389:ALA:HB2	1.83	0.42
1:H:376:MET:HB3	1:H:381:LEU:HB2	2.00	0.42
1:H:404:VAL:HG22	1:H:584:ASN:HD21	1.84	0.42
1:H:727:MET:HB3	1:H:1060:ILE:HD13	2.01	0.42
1:A:803:ARG:HD2	1:A:808:ASP:OD1	2.19	0.42
1:B:1044:LYS:HE3	1:B:1124:VAL:HG22	2.01	0.42
1:C:805:VAL:HG21	1:C:993:ASN:HB3	1.99	0.42
1:D:1098:ILE:HG22	1:D:1105:SER:HB3	2.01	0.42
1:E:1022:ALA:O	1:E:1026:SER:OG	2.27	0.42
1:F:637:GLU:OE1	1:F:639:ARG:NH2	2.43	0.42
1:G:419:ASP:OD1	1:G:419:ASP:N	2.52	0.42
1:H:435:ARG:CD	1:H:665:GLU:HG3	2.49	0.42
1:H:680:LEU:HD22	1:H:714:LEU:CD1	2.49	0.42
1:A:739:GLY:HA3	1:A:1100:ARG:CG	2.21	0.42
1:B:863:SER:OG	1:B:875:ASP:HB2	2.19	0.42
1:B:934:ARG:CZ	1:B:1000:LEU:HD21	2.48	0.42
1:C:784:THR:O	1:C:888:GLY:HA3	2.18	0.42
1:C:985:ASN:HB2	1:C:1005:LEU:O	2.20	0.42
1:D:635:ILE:HD13	1:D:640:LEU:O	2.20	0.42
1:D:696:LEU:O	1:D:700:ILE:HG13	2.18	0.42
1:D:751:LYS:HD2	1:D:1033:GLU:HG2	2.01	0.42
1:D:827:PHE:O	1:D:831:VAL:HG13	2.19	0.42
1:D:1084:LEU:HB2	1:D:1120:ILE:CD1	2.46	0.42
1:E:356:PRO:HB3	1:E:660:MET:HE3	2.02	0.42
1:E:564:LEU:HA	1:E:567:LYS:CG	2.38	0.42
1:E:908:VAL:HG13	1:E:914:TYR:O	2.20	0.42
1:F:466:ILE:HG23	1:H:375:GLY:HA2	2.01	0.42
1:F:771:CYS:HB3	1:F:1103:GLY:CA	2.46	0.42
1:F:854:ARG:HD3	1:F:972:TYR:OH	2.19	0.42
1:F:1106:ALA:HB3	1:F:1111:LEU:HD21	2.00	0.42
1:G:432:MET:HA	1:G:435:ARG:HB2	2.00	0.42
1:G:486:SER:HB2	1:G:789:THR:HB	2.01	0.42
1:G:846:THR:O	1:G:850:GLN:HG3	2.19	0.42
1:A:552:ASN:O	1:A:553:TYR:C	2.61	0.42
1:B:450:ILE:O	1:B:455:VAL:HG23	2.19	0.42
1:B:736:ALA:HB3	1:B:738:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:THR:HG21	1:B:980:LEU:HD11	2.01	0.42
1:B:923:LEU:HD13	1:B:994:ALA:O	2.19	0.42
1:C:337:MET:HG2	1:C:345:GLN:NE2	2.34	0.42
1:C:622:ARG:HH11	1:C:765:ASP:HA	1.85	0.42
1:C:716:CYS:SG	1:C:741:PRO:HB3	2.59	0.42
1:D:632:GLU:O	1:D:636:ARG:HG3	2.20	0.42
1:D:1046:LEU:O	1:D:1049:LEU:HB2	2.20	0.42
1:E:914:TYR:HD1	1:E:918:GLN:CD	2.27	0.42
1:F:448:LYS:HE2	1:F:452:GLU:CD	2.44	0.42
1:F:806:LEU:HB2	1:F:1002:TRP:CH2	2.55	0.42
1:F:908:VAL:HG21	1:F:916:LEU:HD23	2.01	0.42
1:G:616:THR:HB	1:G:661:TRP:CD1	2.54	0.42
1:G:691:ASP:OD2	1:G:723:PRO:HD3	2.18	0.42
1:H:790:GLN:CD	1:H:793:ILE:HB	2.44	0.42
1:A:685:GLN:HG3	1:A:746:ASP:OD2	2.19	0.42
1:B:959:GLU:HA	1:B:1034:THR:HG21	2.02	0.42
1:B:1080:ASP:OD2	1:B:1082:GLU:HB2	2.18	0.42
1:C:387:ARG:O	1:C:391:GLU:HG3	2.19	0.42
1:C:728:GLU:HG2	1:C:1060:ILE:CD1	2.47	0.42
1:C:750:ILE:HG23	1:C:763:ALA:HB1	2.01	0.42
1:C:751:LYS:HE2	1:H:751:LYS:CG	2.47	0.42
1:C:798:VAL:HG21	1:C:831:VAL:HG22	2.01	0.42
1:E:635:ILE:HD12	1:E:641:THR:HA	2.02	0.42
1:E:897:TYR:CE1	1:E:901:MET:HG3	2.54	0.42
1:E:917:GLU:HA	1:E:920:ARG:CB	2.48	0.42
1:E:1050:LEU:HD22	1:E:1055:GLY:O	2.19	0.42
1:F:413:ALA:C	1:F:660:MET:HB3	2.44	0.42
1:G:403:ILE:HG21	1:G:651:ALA:C	2.45	0.42
1:G:573:ARG:HA	1:G:576:GLU:HB2	2.01	0.42
1:G:691:ASP:OD1	1:G:692:ALA:N	2.53	0.42
1:H:631:PHE:CZ	1:H:635:ILE:HG13	2.55	0.42
1:H:723:PRO:O	1:H:727:MET:HG2	2.20	0.42
1:H:758:PHE:CE2	1:H:780:ILE:HD12	2.54	0.42
1:H:786:THR:HG21	1:H:846:THR:HA	2.02	0.42
1:H:803:ARG:NH1	1:H:805:VAL:HA	2.34	0.42
1:H:874:LYS:HD2	1:H:874:LYS:HA	1.68	0.42
1:H:1085:LYS:HD2	1:H:1085:LYS:HA	1.78	0.42
1:A:769:MET:HE1	1:A:784:THR:OG1	2.20	0.42
1:A:962:GLU:OE2	1:A:966:ARG:NH1	2.53	0.42
1:B:791:TRP:O	1:B:792:PRO:C	2.63	0.42
1:C:340:LEU:HD13	1:C:344:MET:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:PHE:HB2	1:C:991:LEU:CD1	2.49	0.42
1:C:593:LYS:NZ	3:C:1305:HOH:O	2.43	0.42
1:C:744:HIS:NE2	1:C:772:VAL:HG12	2.34	0.42
1:C:795:ILE:HG13	1:C:897:TYR:CE2	2.54	0.42
1:D:395:ILE:HG21	1:D:560:HIS:HB3	2.02	0.42
1:D:472:ARG:NH1	1:D:477:TRP:NE1	2.67	0.42
1:D:623:VAL:CG2	1:D:680:LEU:HD21	2.49	0.42
1:D:888:GLY:HA3	1:D:1037:ILE:HG13	2.02	0.42
1:D:1003:MET:HG2	1:D:1004:PRO:CD	2.43	0.42
1:E:508:PHE:O	1:E:591:PRO:HB3	2.19	0.42
1:F:805:VAL:O	1:F:806:LEU:C	2.63	0.42
1:G:1108:PHE:CD2	1:G:1111:LEU:HD13	2.55	0.42
1:H:520:GLU:HG2	1:H:544:ILE:CD1	2.50	0.42
1:H:769:MET:SD	2:H:1201:A1H9L:F1	2.67	0.42
1:H:920:ARG:O	1:H:924:LEU:HD12	2.20	0.42
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.69	0.42
1:B:625:GLN:NE2	1:B:692:ALA:HB1	2.34	0.42
1:B:993:ASN:O	1:B:999:ARG:NH2	2.52	0.42
1:C:948:ASN:OD1	1:C:1029:LYS:HE3	2.20	0.42
1:D:1027:VAL:HG21	1:D:1041:HIS:HE1	1.83	0.42
1:D:1099:VAL:HG23	1:D:1108:PHE:HB2	2.02	0.42
1:E:568:GLU:HG3	1:E:570:ASN:HB3	2.02	0.42
1:E:677:PHE:O	1:E:770:GLY:HA2	2.19	0.42
1:E:984:ASN:C	1:E:987:PRO:HD2	2.45	0.42
1:F:420:ILE:CD1	1:F:613:GLU:HB2	2.49	0.42
1:F:787:GLY:C	1:F:889:LEU:CD1	2.88	0.42
1:G:554:ALA:HB1	1:G:584:ASN:O	2.19	0.42
1:G:1031:ASN:O	1:G:1034:THR:HB	2.20	0.42
1:H:490:TYR:HE2	1:H:491:HIS:CE1	2.37	0.42
1:H:906:LYS:HA	1:H:910:GLU:HB2	2.02	0.42
1:H:1016:ASP:OD2	1:H:1123:THR:HG21	2.19	0.42
1:H:1041:HIS:O	1:H:1075:GLN:HG2	2.19	0.42
1:A:437:GLN:NE2	1:A:1110:GLU:O	2.48	0.42
1:A:888:GLY:HA3	1:A:1037:ILE:HG13	2.01	0.42
1:A:1046:LEU:HD13	1:A:1126:GLU:HG2	2.02	0.42
1:B:713:SER:HA	1:B:740:PHE:CE1	2.55	0.42
1:C:467:CYS:HB3	1:C:492:GLN:HG3	2.02	0.42
1:D:437:GLN:OE1	1:D:438:ASP:N	2.52	0.42
1:D:464:ASP:OD1	1:D:492:GLN:NE2	2.53	0.42
1:D:501:PRO:HB2	1:D:503:TYR:CE1	2.55	0.42
1:E:516:LYS:O	1:E:519:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:986:THR:OG1	1:E:987:PRO:HD3	2.19	0.42
1:F:385:ALA:O	1:F:388:HIS:N	2.53	0.42
1:F:822:ARG:HB3	1:F:826:GLU:OE2	2.20	0.42
1:F:1020:PRO:HG3	1:F:1128:PHE:HA	2.01	0.42
1:G:516:LYS:HB2	1:G:547:CYS:CB	2.50	0.42
1:H:455:VAL:HB	1:H:456:PRO:HD3	2.01	0.42
1:H:685:GLN:C	1:H:692:ALA:HB2	2.45	0.42
1:H:959:GLU:OE2	1:H:1034:THR:HG21	2.20	0.42
1:B:649:LEU:O	1:B:652:PHE:HB3	2.20	0.42
1:B:1003:MET:HE3	1:B:1003:MET:HB3	1.89	0.42
1:C:586:ASN:HB3	3:C:1323:HOH:O	2.20	0.42
1:C:634:ASP:OD1	1:C:639:ARG:NE	2.33	0.42
1:C:640:LEU:HD11	1:C:648:LEU:HD12	2.02	0.42
1:C:869:CYS:HB3	1:C:874:LYS:O	2.20	0.42
1:C:942:LYS:O	1:C:950:VAL:HG11	2.20	0.42
1:D:477:TRP:CH2	1:D:481:GLY:HA3	2.55	0.42
1:E:750:ILE:HG23	1:E:763:ALA:HB1	2.02	0.42
1:E:895:ALA:O	1:E:899:ASP:HB2	2.19	0.42
1:E:915:THR:HG21	1:E:917:GLU:CG	2.48	0.42
1:G:788:TYR:CE2	1:G:890:ILE:HG13	2.55	0.42
1:G:1028:SER:OG	1:G:1069:LEU:HD22	2.19	0.42
1:H:432:MET:HE2	1:H:432:MET:HB3	1.93	0.42
1:H:499:THR:O	1:H:618:LEU:HA	2.20	0.42
1:H:512:MET:SD	1:H:515:ILE:HD11	2.60	0.42
1:H:513:ASN:O	1:H:517:ALA:N	2.52	0.42
1:H:817:ASP:OD2	1:H:819:ARG:NH2	2.53	0.42
1:A:504:ASP:OD1	1:A:505:VAL:N	2.53	0.41
1:A:746:ASP:HB3	1:A:750:ILE:HD12	2.02	0.41
1:B:382:ARG:HH11	1:B:382:ARG:HG2	1.84	0.41
1:B:467:CYS:SG	1:B:471:TYR:CE1	3.13	0.41
1:B:823:THR:OG1	1:B:826:GLU:HG3	2.20	0.41
1:C:489:SER:O	1:C:490:TYR:C	2.63	0.41
1:D:622:ARG:HA	1:D:681:THR:O	2.20	0.41
1:D:775:GLN:HG2	1:D:780:ILE:HD13	2.01	0.41
1:E:919:ILE:O	1:E:923:LEU:HG	2.20	0.41
1:E:920:ARG:NH1	1:E:921:ASP:OD1	2.53	0.41
1:E:1091:PRO:HG2	1:E:1092:GLU:HG3	2.02	0.41
1:E:1106:ALA:CB	1:E:1111:LEU:HD21	2.49	0.41
1:F:362:ARG:NH2	1:F:613:GLU:HA	2.34	0.41
1:F:431:THR:O	1:F:434:THR:OG1	2.30	0.41
1:F:622:ARG:HA	1:F:681:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:656:CYS:HB2	1:G:712:PRO:HD3	2.02	0.41
1:H:503:TYR:HA	1:H:507:LEU:HB3	2.01	0.41
1:H:705:ARG:HD2	1:H:732:ASP:HB3	2.01	0.41
1:H:1101:VAL:HG11	1:H:1104:TYR:OH	2.20	0.41
1:A:528:MET:SD	1:A:534:ILE:HG23	2.60	0.41
1:B:1033:GLU:CD	1:B:1033:GLU:H	2.27	0.41
1:C:763:ALA:O	1:C:766:TYR:HD1	2.03	0.41
1:C:906:LYS:HA	1:C:910:GLU:HB2	2.02	0.41
1:D:386:PHE:CD2	1:D:546:THR:HG23	2.55	0.41
1:D:397:ILE:HG12	1:D:404:VAL:HB	2.02	0.41
1:E:502:GLY:HA3	1:E:778:GLY:HA3	2.02	0.41
1:E:674:TYR:HE1	1:E:1110:GLU:HG2	1.84	0.41
1:E:737:GLY:HA2	1:E:1078:TYR:O	2.20	0.41
1:E:813:LEU:HB2	1:E:834:GLN:HE22	1.85	0.41
1:E:981:SER:O	1:E:982:ILE:C	2.63	0.41
1:F:993:ASN:CG	1:F:994:ALA:N	2.78	0.41
1:G:394:PRO:C	1:G:395:ILE:HD13	2.45	0.41
1:G:422:TRP:HZ2	1:G:459:GLU:HG3	1.85	0.41
1:G:486:SER:CB	1:G:789:THR:HB	2.50	0.41
1:H:343:ARG:HG3	1:H:400:ASP:HB3	2.01	0.41
1:H:401:GLU:H	1:H:573:ARG:HH22	1.68	0.41
1:H:425:VAL:HA	1:H:428:GLU:CG	2.50	0.41
1:H:490:TYR:HD1	1:H:671:PHE:CZ	2.38	0.41
1:H:641:THR:N	1:H:644:THR:OG1	2.37	0.41
1:H:819:ARG:NE	1:H:917:GLU:OE2	2.53	0.41
1:H:885:HIS:HA	1:H:973:SER:CB	2.50	0.41
1:C:997:ASN:ND2	3:C:1308:HOH:O	2.53	0.41
1:C:1113:LYS:O	1:C:1116:GLN:HB2	2.20	0.41
1:D:641:THR:OG1	1:D:644:THR:N	2.36	0.41
1:D:1084:LEU:HD12	1:D:1084:LEU:H	1.85	0.41
1:D:1117:ASP:O	1:D:1120:ILE:HB	2.21	0.41
1:E:356:PRO:HG3	1:E:412:ARG:HB3	2.02	0.41
1:E:423:ARG:HH11	1:E:465:GLU:HG3	1.85	0.41
1:F:406:HIS:HE1	1:F:408:CYS:HB2	1.85	0.41
1:F:565:ALA:HB2	1:F:577:LEU:CB	2.50	0.41
1:F:987:PRO:O	1:F:990:GLU:HB3	2.20	0.41
1:F:987:PRO:O	1:F:991:LEU:HG	2.20	0.41
1:G:402:LEU:C	1:G:402:LEU:CD1	2.93	0.41
1:G:619:SER:HB3	1:G:679:ASN:O	2.20	0.41
1:G:1020:PRO:O	1:G:1023:ILE:HB	2.20	0.41
1:H:739:GLY:HA2	1:H:1077:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:771:CYS:HA	1:H:1103:GLY:O	2.20	0.41
1:H:873:GLY:O	1:H:874:LYS:HD2	2.21	0.41
1:B:479:PHE:CG	1:B:841:LEU:HD23	2.55	0.41
1:C:1018:GLN:OE1	1:C:1018:GLN:HA	2.20	0.41
1:D:490:TYR:OH	1:D:498:ASP:OD1	2.38	0.41
1:D:943:TYR:O	1:D:1011:PRO:HB3	2.21	0.41
1:E:445:ALA:HA	1:E:448:LYS:HD2	2.02	0.41
1:E:789:THR:HG23	1:E:891:PHE:CD1	2.55	0.41
1:E:791:TRP:HD1	1:E:835:ILE:HD13	1.85	0.41
1:E:806:LEU:HB2	1:E:1002:TRP:CZ3	2.55	0.41
1:E:832:LYS:HD3	1:E:960:TRP:CE2	2.55	0.41
1:E:890:ILE:HD11	1:E:1037:ILE:HG21	2.03	0.41
1:E:995:THR:CG2	1:E:999:ARG:HB3	2.49	0.41
1:F:364:LEU:HD23	1:F:364:LEU:O	2.20	0.41
1:F:957:ILE:HD12	1:F:957:ILE:C	2.45	0.41
1:G:646:LEU:HG	1:G:650:GLN:NE2	2.36	0.41
1:H:619:SER:OG	1:H:679:ASN:N	2.54	0.41
1:H:896:THR:HG23	1:H:1006:SER:OG	2.19	0.41
1:A:659:LEU:HD12	1:A:659:LEU:HA	1.76	0.41
1:C:538:TYR:HE1	1:G:473:GLU:CD	2.29	0.41
1:C:599:LEU:HD11	1:C:649:LEU:HD23	2.02	0.41
1:C:717:ARG:HD2	1:C:766:TYR:CZ	2.55	0.41
1:D:955:LEU:HD11	1:E:688:SER:O	2.19	0.41
1:E:749:HIS:O	1:E:752:MET:HG2	2.20	0.41
1:F:362:ARG:NH2	1:F:612:GLU:O	2.53	0.41
1:F:847:VAL:O	1:F:848:ILE:C	2.64	0.41
1:G:724:GLN:O	1:G:724:GLN:HG3	2.20	0.41
1:G:919:ILE:HG13	1:G:920:ARG:N	2.34	0.41
1:G:941:PRO:HG2	1:G:949:TYR:CD2	2.55	0.41
1:G:965:CYS:C	1:G:967:LYS:H	2.27	0.41
1:G:1009:ILE:HG13	1:G:1041:HIS:HD1	1.86	0.41
1:H:622:ARG:HA	1:H:681:THR:O	2.20	0.41
1:H:942:LYS:O	1:H:950:VAL:HG11	2.21	0.41
1:H:982:ILE:HG22	1:H:983:SER:N	2.35	0.41
1:H:1059:LEU:O	1:H:1062:LEU:HB3	2.21	0.41
1:H:1110:GLU:C	1:H:1111:LEU:HG	2.45	0.41
1:A:854:ARG:HD3	1:A:972:TYR:OH	2.21	0.41
1:B:617:GLY:HA2	1:B:677:PHE:O	2.19	0.41
1:B:1046:LEU:HB2	1:B:1126:GLU:HG2	2.03	0.41
1:C:463:LEU:HD23	1:C:463:LEU:O	2.21	0.41
1:C:751:LYS:HG2	1:H:751:LYS:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:965:CYS:CA	1:C:975:LEU:HD23	2.51	0.41
1:C:1073:GLN:HE22	1:C:1075:GLN:HG3	1.85	0.41
1:D:428:GLU:O	1:D:432:MET:HG3	2.20	0.41
1:D:655:LYS:HA	1:D:655:LYS:HD2	1.87	0.41
1:D:797:PHE:O	1:D:801:ARG:N	2.54	0.41
1:D:1045:PHE:CD2	1:D:1050:LEU:HD21	2.55	0.41
1:E:345:GLN:HA	1:E:348:ARG:HG2	2.02	0.41
1:E:567:LYS:HE2	1:E:567:LYS:N	2.35	0.41
1:E:1049:LEU:HG	1:E:1050:LEU:HD23	2.02	0.41
1:F:368:GLU:OE2	1:F:388:HIS:NE2	2.53	0.41
1:F:423:ARG:HH11	1:F:465:GLU:CG	2.32	0.41
1:F:827:PHE:O	1:F:831:VAL:HG23	2.20	0.41
1:F:854:ARG:HB3	1:F:877:ALA:O	2.21	0.41
1:G:337:MET:HB2	1:G:345:GLN:NE2	2.30	0.41
1:G:965:CYS:C	1:G:967:LYS:N	2.79	0.41
1:H:766:TYR:CD1	1:H:766:TYR:C	2.98	0.41
1:A:670:TYR:CD2	1:A:984:ASN:HB3	2.55	0.41
1:B:675:GLN:N	3:B:1308:HOH:O	2.41	0.41
1:C:380:LEU:HD12	1:C:542:ALA:HA	2.03	0.41
1:C:498:ASP:O	1:C:775:GLN:NE2	2.41	0.41
1:C:805:VAL:HG22	1:C:805:VAL:H	1.53	0.41
1:C:824:PHE:HD1	1:C:909:PHE:CD2	2.28	0.41
1:C:862:MET:HE2	1:C:862:MET:HB2	1.68	0.41
1:D:623:VAL:HG22	1:D:680:LEU:HD21	2.03	0.41
1:D:800:ASN:HB3	1:D:803:ARG:HB3	2.03	0.41
1:D:863:SER:OG	1:D:875:ASP:HB2	2.21	0.41
1:D:953:TYR:HA	1:D:956:ASP:HB3	2.02	0.41
1:E:447:LYS:O	1:E:451:ARG:HG3	2.20	0.41
1:E:576:GLU:O	1:E:580:ILE:N	2.46	0.41
1:F:466:ILE:HG23	1:H:375:GLY:CA	2.51	0.41
1:F:490:TYR:CD1	1:F:490:TYR:C	2.97	0.41
1:F:745:PHE:CZ	1:F:1063:LEU:HD22	2.54	0.41
1:F:953:TYR:HD1	1:F:953:TYR:N	2.18	0.41
1:G:718:ILE:HD12	1:G:745:PHE:HE1	1.85	0.41
1:H:754:LEU:HD23	1:H:758:PHE:O	2.20	0.41
1:A:555:ARG:NH1	1:A:585:GLU:O	2.53	0.41
1:A:723:PRO:O	1:A:727:MET:HG2	2.20	0.41
1:A:904:ILE:O	1:A:908:VAL:HB	2.21	0.41
1:C:418:PRO:HA	1:C:422:TRP:HB3	2.02	0.41
1:D:790:GLN:HB2	1:D:792:PRO:HD2	2.03	0.41
1:D:790:GLN:CD	1:D:793:ILE:HB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:913:LYS:HG2	1:E:914:TYR:CE2	2.56	0.41
1:E:1084:LEU:O	1:E:1088:GLN:HG3	2.21	0.41
1:F:412:ARG:NH2	1:F:710:TYR:OH	2.53	0.41
1:F:483:THR:HG21	1:F:811:GLN:CG	2.47	0.41
1:G:344:MET:HE1	1:G:651:ALA:HB2	2.01	0.41
1:G:435:ARG:NH1	1:G:664:SER:O	2.54	0.41
1:G:1074:MET:HE2	1:G:1076:PHE:CZ	2.56	0.41
1:H:424:TRP:HE3	1:H:428:GLU:OE2	2.03	0.41
1:H:594:THR:OG1	1:H:595:LEU:N	2.54	0.41
1:H:1023:ILE:O	1:H:1026:SER:HB2	2.20	0.41
1:A:500:CYS:SG	1:A:619:SER:HB2	2.61	0.41
1:A:513:ASN:OD1	1:A:589:ALA:HB1	2.20	0.41
1:A:970:MET:HE3	1:A:975:LEU:HB2	2.03	0.41
1:A:1046:LEU:HB2	1:A:1124:VAL:HG12	2.03	0.41
1:B:492:GLN:HG2	1:B:493:ILE:HG23	2.02	0.41
1:B:596:GLN:HB2	1:B:648:LEU:HD21	2.01	0.41
1:B:620:LEU:CD1	1:B:680:LEU:HD12	2.50	0.41
1:B:776:LYS:HD2	1:B:779:ARG:HD2	2.02	0.41
1:B:871:GLU:H	1:B:871:GLU:HG2	1.34	0.41
1:C:344:MET:HE2	1:C:650:GLN:CB	2.51	0.41
1:C:641:THR:H	1:C:644:THR:HG1	1.61	0.41
1:C:798:VAL:HG11	1:C:827:PHE:CE1	2.56	0.41
1:C:911:GLU:OE1	1:C:913:LYS:HB2	2.21	0.41
1:C:915:THR:OG1	1:C:918:GLN:N	2.51	0.41
1:D:343:ARG:HG3	1:D:344:MET:N	2.35	0.41
1:D:489:SER:HA	1:D:492:GLN:HB3	2.02	0.41
1:D:659:LEU:HD12	1:D:659:LEU:HA	1.85	0.41
1:D:718:ILE:CD1	1:D:743:CYS:HB3	2.51	0.41
1:D:747:ASP:O	1:D:751:LYS:HG3	2.21	0.41
1:D:955:LEU:HB2	1:D:1029:LYS:O	2.21	0.41
1:E:446:ASP:HA	1:E:449:THR:CG2	2.49	0.41
1:E:744:HIS:NE2	1:E:772:VAL:HG12	2.36	0.41
1:E:1052:THR:HB	1:E:1055:GLY:H	1.86	0.41
1:F:540:TYR:O	1:F:544:ILE:HD12	2.20	0.41
1:F:557:ILE:O	1:F:560:HIS:N	2.54	0.41
1:F:670:TYR:CD2	1:F:984:ASN:HB3	2.56	0.41
1:F:787:GLY:O	1:F:889:LEU:HD11	2.13	0.41
1:F:971:LEU:HD12	1:F:971:LEU:HA	1.66	0.41
1:F:1033:GLU:H	1:F:1033:GLU:CD	2.28	0.41
1:G:414:GLY:HA3	1:G:662:MET:SD	2.60	0.41
1:G:440:PHE:HZ	1:G:660:MET:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:755:ARG:HG2	3:G:1303:HOH:O	2.21	0.41
1:G:766:TYR:HE1	1:G:768:LEU:HD11	1.86	0.41
1:G:1024:ILE:HA	1:G:1027:VAL:HG22	2.03	0.41
1:H:340:LEU:HD12	1:H:706:PHE:HB3	2.02	0.41
1:H:396:LEU:HD22	1:H:409:GLY:O	2.21	0.41
1:H:659:LEU:HD22	1:H:678:ILE:HD11	2.02	0.41
1:H:680:LEU:CD2	1:H:682:VAL:HG13	2.51	0.41
1:H:794:ALA:HB2	1:H:835:ILE:HG23	2.03	0.41
1:H:818:LEU:HD23	1:H:821:LEU:HD12	2.01	0.41
1:H:923:LEU:HD12	1:H:994:ALA:O	2.20	0.41
1:H:965:CYS:O	1:H:967:LYS:N	2.54	0.41
1:A:983:SER:O	1:A:987:PRO:HD2	2.21	0.41
1:A:1100:ARG:HD2	1:A:1100:ARG:HA	1.68	0.41
1:B:576:GLU:O	1:B:580:ILE:HG13	2.20	0.41
1:B:620:LEU:HD12	1:B:680:LEU:HB2	2.03	0.41
1:C:450:ILE:HA	1:C:454:ILE:HB	2.02	0.41
1:D:582:GLU:HA	1:D:585:GLU:CB	2.50	0.41
1:D:1066:ALA:HA	1:D:1069:LEU:HB2	2.03	0.41
1:E:337:MET:O	1:E:345:GLN:NE2	2.54	0.41
1:E:494:ASN:ND2	1:E:661:TRP:HZ2	2.18	0.41
1:E:887:PRO:O	1:E:975:LEU:HD12	2.21	0.41
1:F:953:TYR:CD1	1:F:953:TYR:N	2.89	0.41
1:F:1113:LYS:HB3	1:F:1114:GLU:OE1	2.21	0.41
1:G:491:HIS:HB2	1:G:786:THR:HB	2.03	0.41
1:G:686:LYS:HG3	1:G:692:ALA:HA	2.03	0.41
1:G:740:PHE:CE1	1:G:1100:ARG:NH1	2.89	0.41
1:G:793:ILE:HD11	1:G:804:MET:HG3	2.03	0.41
1:G:795:ILE:HD13	1:G:901:MET:HG3	2.03	0.41
1:G:915:THR:OG1	1:G:918:GLN:HG3	2.21	0.41
1:H:923:LEU:HD11	1:H:995:THR:C	2.46	0.41
1:H:986:THR:HB	1:H:987:PRO:CD	2.51	0.41
1:H:1123:THR:HG22	1:H:1125:ILE:HD13	2.03	0.41
1:A:1042:ASN:C	1:A:1043:PHE:HD1	2.29	0.40
1:B:498:ASP:O	1:B:769:MET:HE2	2.21	0.40
1:B:701:MET:HE1	1:B:730:ILE:HG13	2.04	0.40
1:B:791:TRP:HB3	1:B:897:TYR:CD2	2.56	0.40
1:B:876:VAL:HG23	1:B:877:ALA:N	2.37	0.40
1:B:1086:LYS:HB2	1:B:1086:LYS:HE3	1.71	0.40
1:C:495:GLY:HA3	1:C:613:GLU:HG3	2.04	0.40
1:D:403:ILE:HG23	1:D:600:GLN:HA	2.03	0.40
1:D:504:ASP:CG	1:D:777:SER:HG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:CYS:HA	1:D:630:MET:CE	2.51	0.40
1:E:604:THR:O	1:E:607:SER:OG	2.38	0.40
1:E:1052:THR:HG21	1:E:1054:GLU:HB2	2.02	0.40
1:F:705:ARG:HA	1:F:738:MET:CE	2.47	0.40
1:F:783:TRP:HB2	1:F:887:PRO:HB3	2.03	0.40
1:G:607:SER:HA	1:G:659:LEU:HD11	2.02	0.40
1:G:671:PHE:HA	1:G:982:ILE:HG21	2.02	0.40
1:G:806:LEU:HD12	1:G:806:LEU:HA	1.86	0.40
1:G:955:LEU:CD2	1:G:959:GLU:HG3	2.51	0.40
1:G:982:ILE:HG23	1:G:1104:TYR:CE2	2.56	0.40
1:H:393:ALA:N	1:H:556:ARG:HH22	2.18	0.40
1:H:484:PHE:HD1	1:H:487:ASP:HB2	1.86	0.40
1:H:980:LEU:HD12	1:H:980:LEU:O	2.21	0.40
1:H:1042:ASN:HD21	1:H:1075:GLN:HE21	1.68	0.40
1:A:559:ALA:N	1:A:562:ARG:HH21	2.19	0.40
1:B:437:GLN:OE1	1:B:1112:CYS:N	2.47	0.40
1:B:438:ASP:HA	1:B:674:TYR:CZ	2.56	0.40
1:B:602:ILE:HG21	1:B:620:LEU:HD22	2.03	0.40
1:B:899:ASP:OD2	1:B:942:LYS:HD2	2.21	0.40
1:C:373:ASN:HB3	1:C:376:MET:HE3	2.03	0.40
1:C:671:PHE:HD1	1:C:982:ILE:HD13	1.86	0.40
1:C:744:HIS:CE1	1:C:772:VAL:HG12	2.56	0.40
1:C:824:PHE:HA	1:C:909:PHE:CE2	2.55	0.40
1:D:1035:MET:HE3	1:D:1035:MET:HB2	1.96	0.40
1:E:360:ILE:HD13	1:E:450:ILE:HD11	2.03	0.40
1:E:560:HIS:O	1:E:564:LEU:HG	2.22	0.40
1:E:749:HIS:CE1	3:E:1315:HOH:O	2.74	0.40
1:E:966:ARG:HG2	1:E:975:LEU:O	2.20	0.40
1:E:1009:ILE:HG13	1:E:1041:HIS:CD2	2.56	0.40
1:F:471:TYR:HE1	1:F:848:ILE:HB	1.87	0.40
1:F:542:ALA:O	1:F:543:ALA:C	2.64	0.40
1:F:909:PHE:CZ	1:F:916:LEU:HD11	2.56	0.40
1:F:1102:ALA:C	1:F:1104:TYR:N	2.79	0.40
1:H:752:MET:O	1:H:756:LYS:HG3	2.20	0.40
1:H:756:LYS:NZ	1:H:1036:ASN:O	2.49	0.40
1:H:942:LYS:C	1:H:950:VAL:HG11	2.46	0.40
1:A:736:ALA:CB	1:A:738:MET:HE2	2.51	0.40
1:A:792:PRO:HG2	1:A:1005:LEU:HD13	2.03	0.40
1:A:926:ASN:C	1:A:928:GLU:H	2.30	0.40
1:A:981:SER:O	1:A:982:ILE:C	2.64	0.40
1:D:705:ARG:HA	1:D:738:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:722:SER:O	1:D:1064:ARG:NH1	2.46	0.40
1:D:847:VAL:HA	1:D:850:GLN:HB2	2.03	0.40
1:E:397:ILE:HG23	1:E:404:VAL:CG1	2.52	0.40
1:E:444:GLU:HG3	1:E:447:LYS:HE3	2.02	0.40
1:E:759:ASP:OD1	1:E:760:PHE:N	2.50	0.40
1:E:1007:ASP:OD2	1:E:1122:ARG:NH1	2.53	0.40
1:F:500:CYS:HB2	1:F:777:SER:HB3	2.03	0.40
1:F:700:ILE:O	1:F:703:ALA:HB3	2.22	0.40
1:F:875:ASP:OD1	1:F:877:ALA:N	2.55	0.40
1:G:358:VAL:HG12	1:G:359:SER:O	2.21	0.40
1:G:382:ARG:HA	1:G:385:ALA:HB3	2.03	0.40
1:G:644:THR:H	1:G:644:THR:HG23	1.70	0.40
1:G:894:LEU:O	1:G:898:VAL:HG23	2.21	0.40
1:H:492:GLN:HG3	1:H:493:ILE:N	2.36	0.40
1:H:778:GLY:O	1:H:866:VAL:HA	2.22	0.40
1:H:849:SER:HA	1:H:852:VAL:HG22	2.03	0.40
1:H:871:GLU:H	1:H:871:GLU:CD	2.27	0.40
1:H:1119:ILE:HG12	1:H:1122:ARG:CZ	2.51	0.40
1:B:616:THR:OG1	1:B:617:GLY:N	2.55	0.40
1:B:944:GLY:HA3	1:B:1011:PRO:HG3	2.03	0.40
1:C:661:TRP:CZ3	1:C:663:SER:HB2	2.57	0.40
1:D:529:GLU:H	1:D:529:GLU:HG3	1.55	0.40
1:D:1027:VAL:HG13	1:D:1030:MET:HE3	2.03	0.40
1:D:1079:VAL:CG2	1:D:1084:LEU:HD11	2.51	0.40
1:F:944:GLY:HA3	1:F:1011:PRO:CG	2.51	0.40
1:G:916:LEU:O	1:G:920:ARG:HB2	2.22	0.40
1:G:966:ARG:CZ	1:G:976:SER:HB2	2.52	0.40
1:G:989:GLY:HA2	1:G:1005:LEU:HG	2.02	0.40
1:H:637:GLU:OE2	1:H:639:ARG:NH2	2.54	0.40
1:H:906:LYS:HZ3	1:H:949:TYR:HE2	1.69	0.40
1:A:506:LEU:HA	1:A:506:LEU:HD23	1.93	0.40
1:A:546:THR:O	1:A:550:VAL:HG23	2.22	0.40
1:B:622:ARG:NH2	1:B:685:GLN:O	2.48	0.40
1:B:627:CYS:HA	1:B:630:MET:SD	2.62	0.40
1:B:963:LYS:O	1:B:967:LYS:HG3	2.21	0.40
1:C:942:LYS:C	1:C:950:VAL:HG11	2.46	0.40
1:D:496:GLY:HA3	1:D:859:LYS:HE3	2.03	0.40
1:D:1098:ILE:HG12	1:D:1107:TYR:CE1	2.56	0.40
1:E:452:GLU:O	1:E:456:PRO:HG2	2.22	0.40
1:E:793:ILE:HD11	1:E:804:MET:HG3	2.04	0.40
1:E:1025:LYS:HD3	1:E:1029:LYS:HZ1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:650:GLN:HA	1:F:653:ILE:HD12	2.04	0.40
1:F:850:GLN:HE22	1:F:887:PRO:HD3	1.86	0.40
1:F:887:PRO:O	1:F:975:LEU:HD12	2.22	0.40
1:F:1108:PHE:HE1	1:F:1116:GLN:HE21	1.68	0.40
1:G:404:VAL:HG11	1:G:580:ILE:HG21	2.03	0.40
1:G:624:ASP:OD1	1:G:625:GLN:HG2	2.21	0.40
1:G:933:LEU:O	1:G:933:LEU:HD12	2.21	0.40
1:G:957:ILE:O	1:G:958:THR:C	2.63	0.40
1:G:993:ASN:OD1	1:G:994:ALA:N	2.53	0.40
1:H:829:ALA:O	1:H:833:GLN:HG3	2.21	0.40
1:H:831:VAL:O	1:H:834:GLN:HB2	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:GLU:OE2	1:D:913:LYS:NZ[1_655]	1.23	0.97
1:A:1054:GLU:OE2	1:D:913:LYS:CE[1_655]	1.93	0.27
1:F:822:ARG:O	1:G:819:ARG:NH2[1_455]	2.06	0.14
1:B:808:ASP:OD1	1:F:346:ARG:NH2[1_556]	2.17	0.03
1:A:1054:GLU:OE2	1:D:913:LYS:CD[1_655]	2.19	0.01
1:B:851:ARG:NH2	1:E:535:ASP:OD1[1_565]	2.19	0.01

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	790/1150 (69%)	727 (92%)	63 (8%)	0	100	100
1	B	790/1150 (69%)	726 (92%)	62 (8%)	2 (0%)	36	65
1	C	790/1150 (69%)	708 (90%)	81 (10%)	1 (0%)	48	77
1	D	790/1150 (69%)	701 (89%)	89 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	790/1150 (69%)	723 (92%)	67 (8%)	0	100	100
1	F	790/1150 (69%)	710 (90%)	79 (10%)	1 (0%)	48	77
1	G	790/1150 (69%)	711 (90%)	78 (10%)	1 (0%)	48	77
1	H	790/1150 (69%)	717 (91%)	73 (9%)	0	100	100
All	All	6320/9200 (69%)	5723 (91%)	592 (9%)	5 (0%)	48	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	982	ILE
1	B	427	ASP
1	C	982	ILE
1	G	982	ILE
1	F	982	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	668/955 (70%)	668 (100%)	0	100	100
1	B	668/955 (70%)	668 (100%)	0	100	100
1	C	668/955 (70%)	668 (100%)	0	100	100
1	D	668/955 (70%)	668 (100%)	0	100	100
1	E	668/955 (70%)	668 (100%)	0	100	100
1	F	668/955 (70%)	668 (100%)	0	100	100
1	G	668/955 (70%)	668 (100%)	0	100	100
1	H	668/955 (70%)	668 (100%)	0	100	100
All	All	5344/7640 (70%)	5344 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	GLN
1	A	721	GLN
1	A	811	GLN
1	A	853	HIS
1	B	350	HIS
1	B	513	ASN
1	B	530	ASN
1	B	719	HIS
1	B	744	HIS
1	B	1075	GLN
1	C	345	GLN
1	C	625	GLN
1	C	650	GLN
1	C	811	GLN
1	C	977	HIS
1	C	1031	ASN
1	C	1071	ASN
1	C	1075	GLN
1	D	513	ASN
1	D	572	GLN
1	D	650	GLN
1	D	749	HIS
1	D	811	GLN
1	D	1116	GLN
1	E	513	ASN
1	E	530	ASN
1	E	650	GLN
1	E	675	GLN
1	E	711	GLN
1	E	749	HIS
1	E	811	GLN
1	E	952	GLN
1	E	977	HIS
1	E	993	ASN
1	F	642	HIS
1	F	711	GLN
1	F	790	GLN
1	F	800	ASN
1	F	811	GLN
1	F	853	HIS
1	F	884	ASN
1	F	948	ASN

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Mol	Chain	Res	Type
1	F	952	GLN
1	F	1018	GLN
1	F	1042	ASN
1	F	1075	GLN
1	F	1088	GLN
1	F	1116	GLN
1	G	388	HIS
1	G	615	GLN
1	G	721	GLN
1	G	744	HIS
1	G	1013	GLN
1	G	1042	ASN
1	G	1089	GLN
1	H	345	GLN
1	H	373	ASN
1	H	406	HIS
1	H	596	GLN
1	H	614	ASN
1	H	724	GLN
1	H	744	HIS
1	H	884	ASN
1	H	1042	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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
2	A1H9L	D	1201	-	7,7,7	1.32	1 (14%)	7,9,9	1.06	0
2	A1H9L	F	1201	-	7,7,7	1.17	0	7,9,9	0.64	0
2	A1H9L	B	1201	-	7,7,7	1.30	1 (14%)	7,9,9	0.93	1 (14%)
2	A1H9L	A	1201	-	7,7,7	1.41	2 (28%)	7,9,9	0.89	0
2	A1H9L	E	1201	-	7,7,7	1.36	1 (14%)	7,9,9	0.82	0
2	A1H9L	G	1201	-	7,7,7	1.24	1 (14%)	7,9,9	0.90	0
2	A1H9L	H	1201	-	7,7,7	1.34	1 (14%)	7,9,9	0.77	0
2	A1H9L	C	1201	-	7,7,7	1.33	1 (14%)	7,9,9	0.84	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
2	A1H9L	D	1201	-	-	2/6/7/7	-
2	A1H9L	F	1201	-	-	5/6/7/7	-
2	A1H9L	B	1201	-	-	3/6/7/7	-
2	A1H9L	A	1201	-	-	0/6/7/7	-
2	A1H9L	E	1201	-	-	1/6/7/7	-
2	A1H9L	G	1201	-	-	3/6/7/7	-
2	A1H9L	H	1201	-	-	3/6/7/7	-
2	A1H9L	C	1201	-	-	3/6/7/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	A1H9L	C4-N3	-2.78	1.45	1.52
2	E	1201	A1H9L	C4-N3	-2.77	1.45	1.52
2	D	1201	A1H9L	C4-N3	-2.52	1.46	1.52
2	A	1201	A1H9L	C4-N3	-2.51	1.46	1.52
2	B	1201	A1H9L	C4-N3	-2.28	1.46	1.52
2	A	1201	A1H9L	C8-N3	-2.24	1.45	1.50
2	H	1201	A1H9L	C4-N3	-2.22	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1201	A1H9L	C4-N3	-2.15	1.47	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	A1H9L	C5-C4-N3	-2.12	105.45	119.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	A1H9L	N3-C4-C5-F6
2	C	1201	A1H9L	N3-C4-C5-F6
2	C	1201	A1H9L	F1-C2-N3-C7
2	C	1201	A1H9L	F1-C2-N3-C8
2	E	1201	A1H9L	N3-C4-C5-F6
2	F	1201	A1H9L	C5-C4-N3-C8
2	G	1201	A1H9L	N3-C4-C5-F6
2	G	1201	A1H9L	F1-C2-N3-C7
2	G	1201	A1H9L	F1-C2-N3-C8
2	H	1201	A1H9L	F1-C2-N3-C7
2	H	1201	A1H9L	F1-C2-N3-C8
2	D	1201	A1H9L	N3-C4-C5-F6
2	F	1201	A1H9L	N3-C4-C5-F6
2	H	1201	A1H9L	N3-C4-C5-F6
2	F	1201	A1H9L	C5-C4-N3-C2
2	F	1201	A1H9L	C5-C4-N3-C7
2	B	1201	A1H9L	F1-C2-N3-C7
2	B	1201	A1H9L	F1-C2-N3-C8
2	D	1201	A1H9L	F1-C2-N3-C8
2	F	1201	A1H9L	F1-C2-N3-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

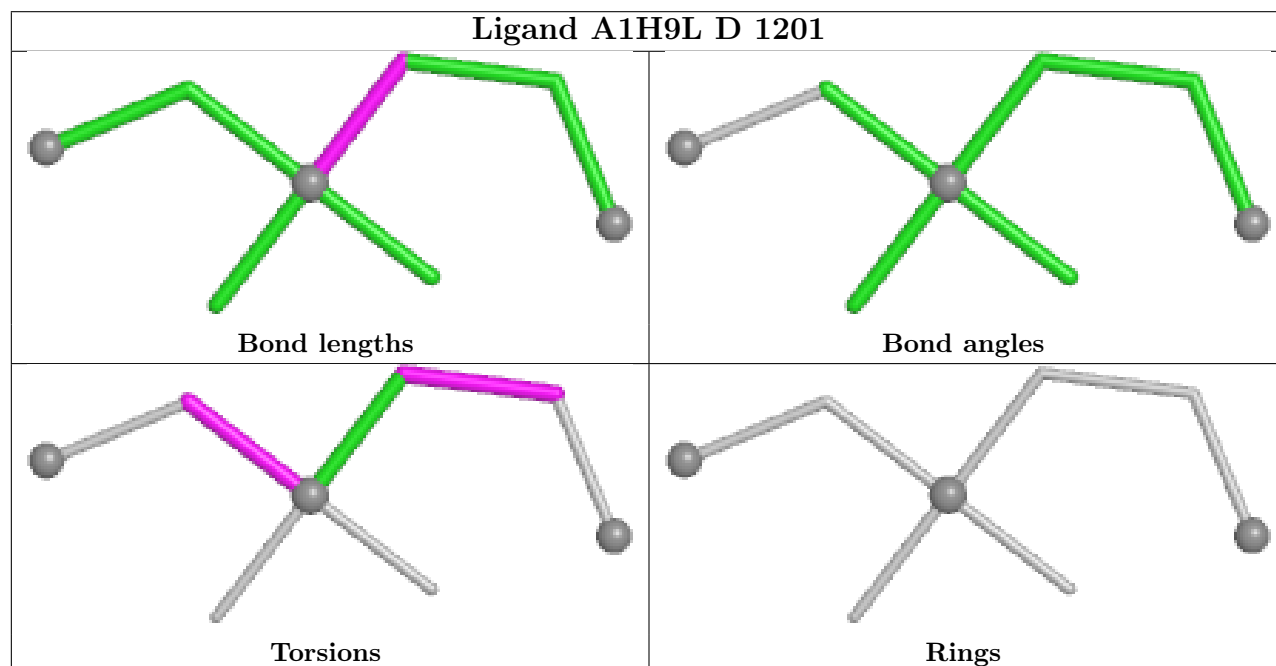
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1201	A1H9L	1	0
2	B	1201	A1H9L	1	0
2	E	1201	A1H9L	1	0
2	G	1201	A1H9L	1	0
2	H	1201	A1H9L	1	0

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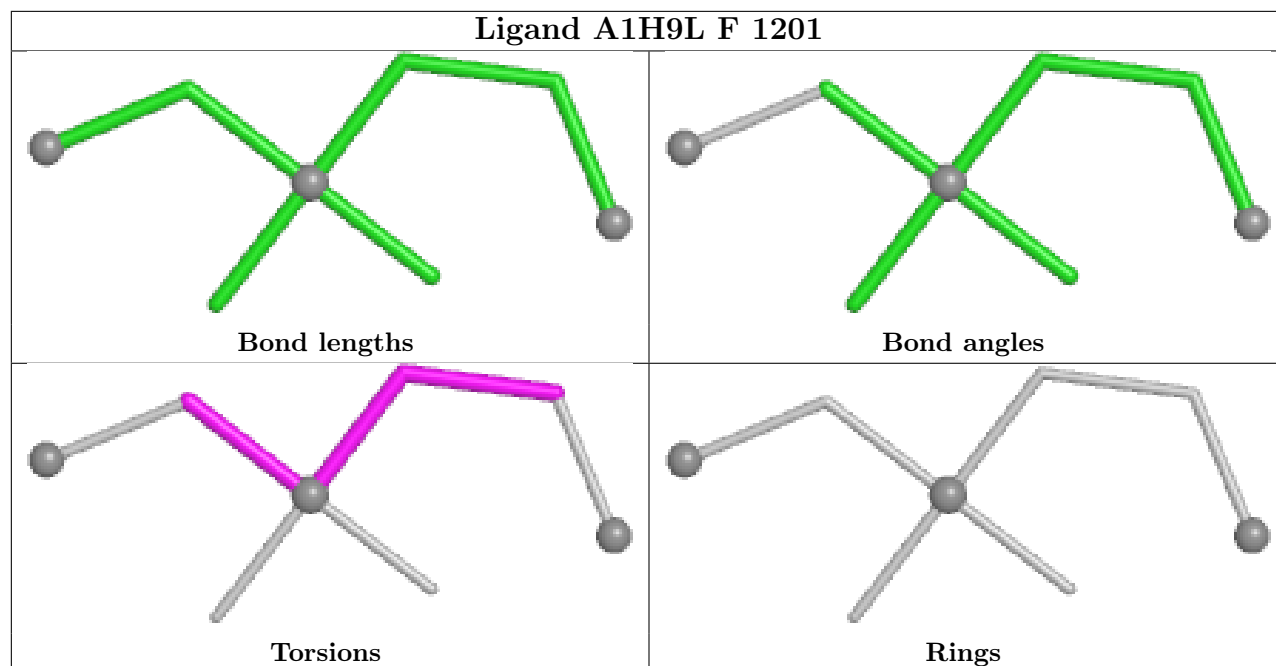
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1201	A1H9L	1	0

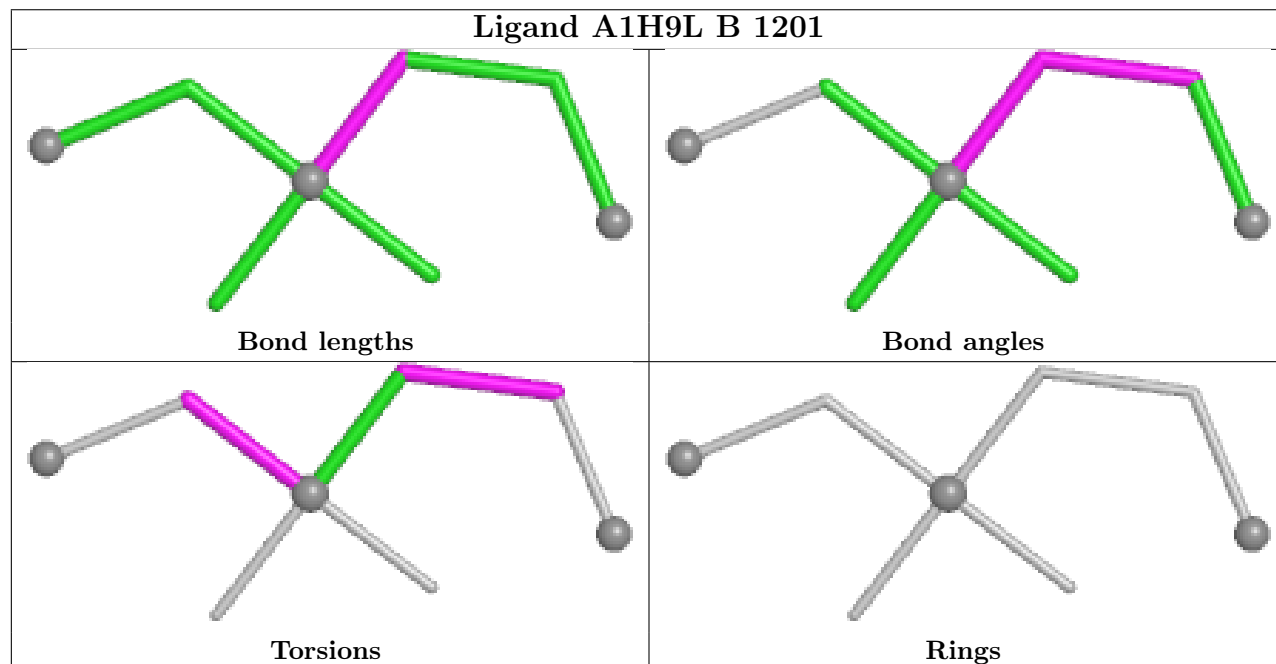
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



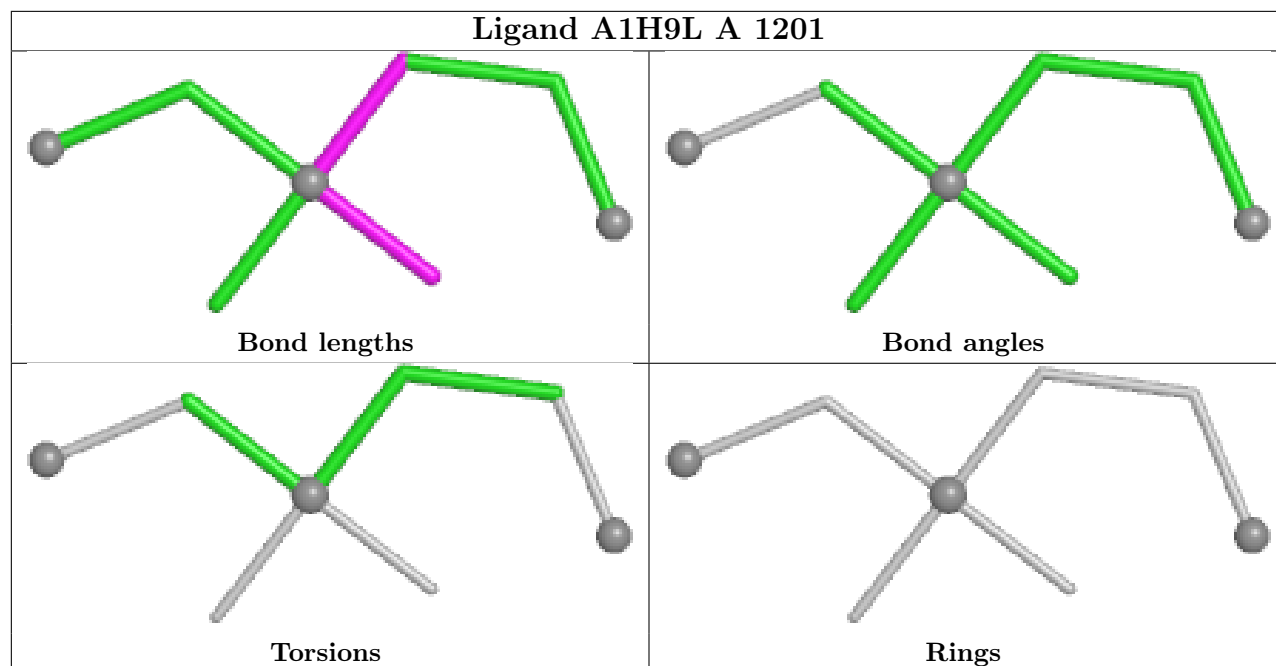
Ligand A1H9L F 1201



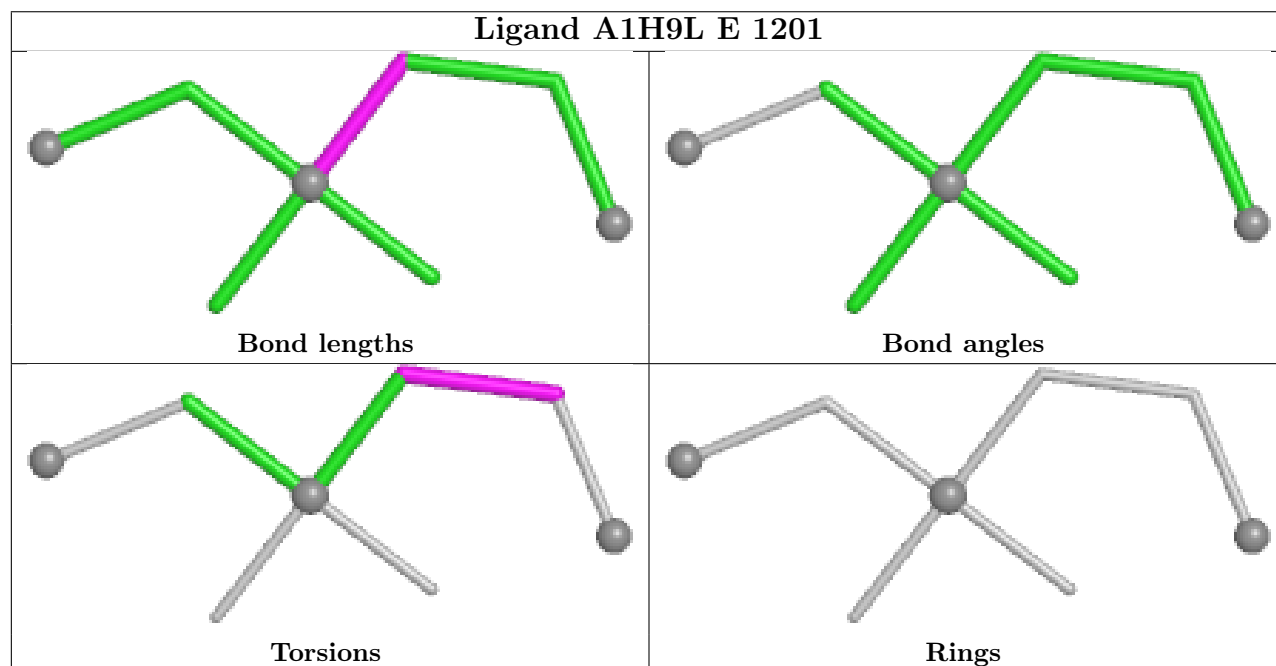
Ligand A1H9L B 1201



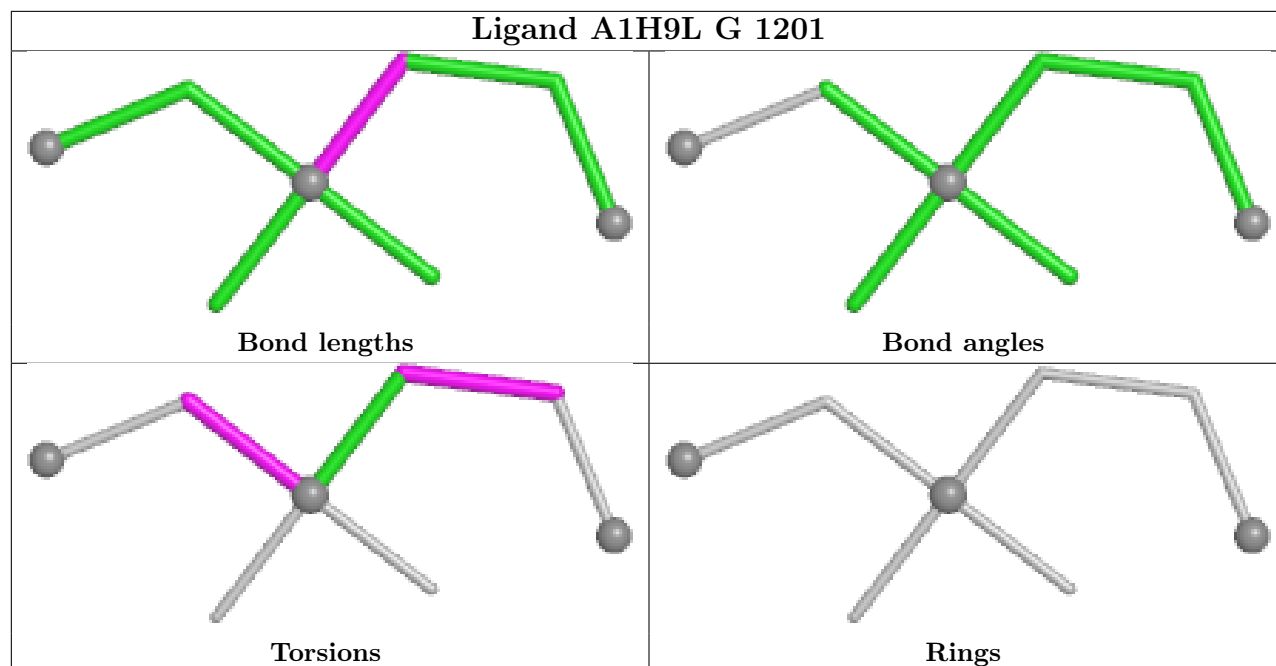
Ligand A1H9L A 1201



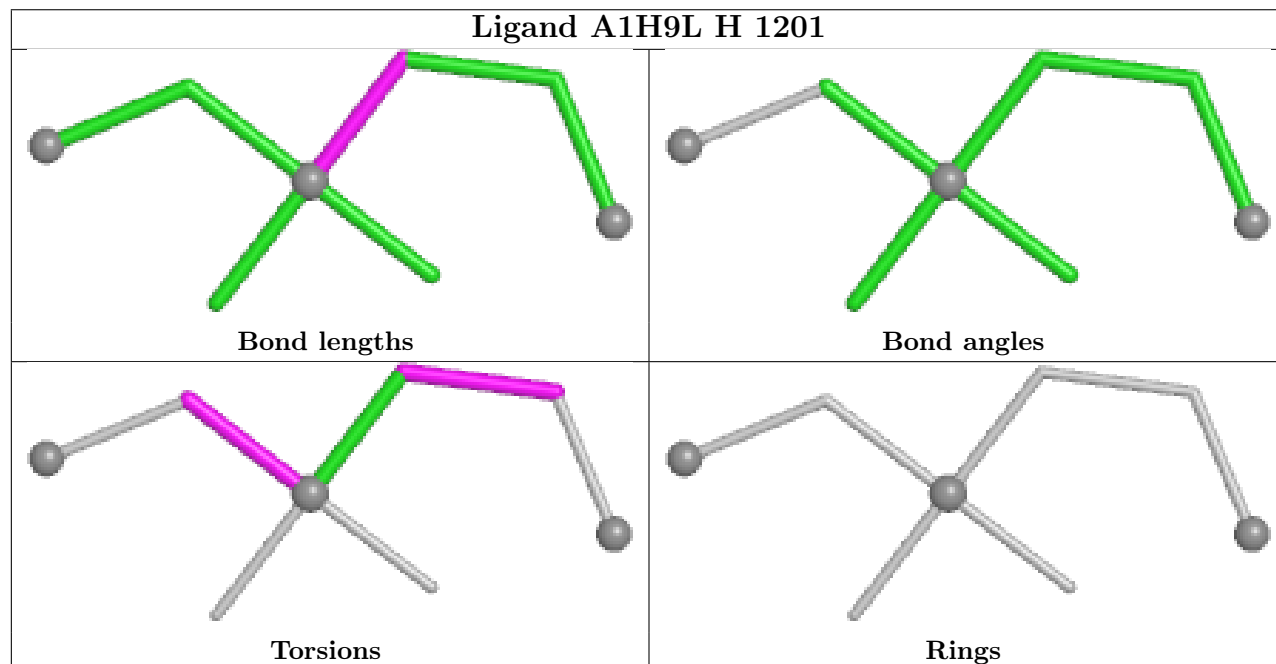
Ligand A1H9L E 1201

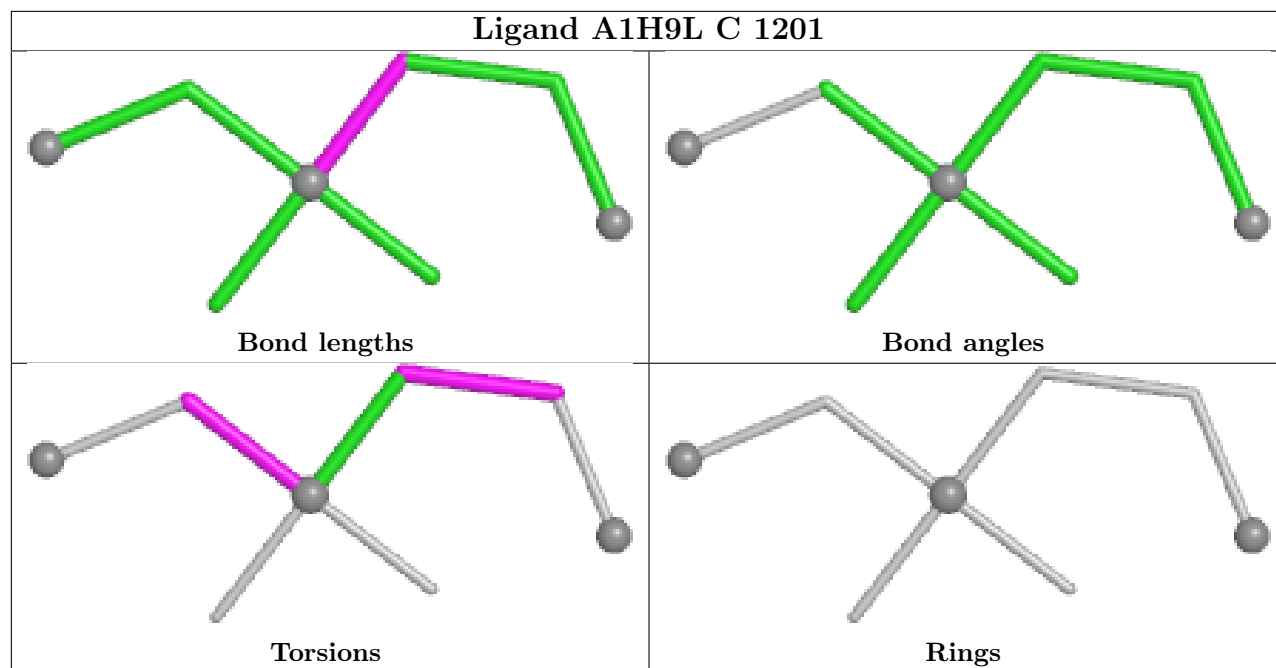


Ligand A1H9L G 1201



Ligand A1H9L H 1201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	792/1150 (68%)	-0.37	0	100	100	15, 28, 50, 86	0
1	B	792/1150 (68%)	-0.37	0	100	100	14, 29, 46, 67	0
1	C	792/1150 (68%)	0.29	17 (2%)	63	54	28, 51, 70, 112	0
1	D	792/1150 (68%)	0.55	34 (4%)	40	31	24, 59, 81, 102	0
1	E	792/1150 (68%)	0.76	73 (9%)	14	12	26, 65, 102, 121	0
1	F	792/1150 (68%)	0.46	29 (3%)	45	37	28, 54, 77, 95	0
1	G	792/1150 (68%)	0.86	83 (10%)	11	10	40, 72, 101, 113	0
1	H	792/1150 (68%)	0.73	44 (5%)	30	23	39, 71, 96, 121	0
All	All	6336/9200 (68%)	0.37	280 (4%)	39	30	14, 54, 90, 121	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	649	LEU	5.7
1	G	402	LEU	5.4
1	D	802	GLY	5.3
1	E	795	ILE	5.2
1	F	1038	GLY	4.7
1	E	1009	ILE	4.7
1	E	902	ALA	4.3
1	E	1115	VAL	4.1
1	H	651	ALA	4.0
1	C	337	MET	3.9
1	E	351	TYR	3.8
1	E	1038	GLY	3.8
1	F	1027	VAL	3.8
1	D	1099	VAL	3.8
1	G	405	GLY	3.7
1	H	1119	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	796	GLU	3.7
1	H	1063	LEU	3.6
1	E	919	ILE	3.6
1	F	897	TYR	3.6
1	E	916	LEU	3.6
1	G	1125	ILE	3.6
1	D	1062	LEU	3.5
1	H	709	VAL	3.5
1	E	898	VAL	3.4
1	F	476	VAL	3.4
1	G	1124	VAL	3.4
1	G	577	LEU	3.3
1	G	630	MET	3.3
1	G	550	VAL	3.3
1	G	1087	ALA	3.3
1	G	1106	ALA	3.3
1	E	983	SER	3.3
1	G	653	ILE	3.3
1	E	1045	PHE	3.2
1	D	1063	LEU	3.2
1	G	602	ILE	3.2
1	H	1042	ASN	3.2
1	G	1043	PHE	3.2
1	E	1008	GLY	3.2
1	F	1042	ASN	3.2
1	G	648	LEU	3.2
1	H	1115	VAL	3.1
1	G	581	ALA	3.1
1	E	981	SER	3.1
1	G	1108	PHE	3.1
1	G	1079	VAL	3.1
1	D	760	PHE	3.0
1	H	604	THR	3.0
1	E	671	PHE	3.0
1	E	930	TYR	3.0
1	E	1120	ILE	3.0
1	F	1077	SER	3.0
1	H	1077	SER	3.0
1	G	578	LEU	3.0
1	G	645	ALA	3.0
1	G	718	ILE	2.9
1	H	795	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	1094	TYR	2.9
1	C	1038	GLY	2.9
1	E	1004	PRO	2.9
1	E	1042	ASN	2.9
1	F	923	LEU	2.9
1	H	1079	VAL	2.8
1	H	1076	PHE	2.8
1	E	1050	LEU	2.8
1	H	653	ILE	2.8
1	H	397	ILE	2.8
1	D	903	ALA	2.8
1	G	1102	ALA	2.8
1	G	1097	LEU	2.8
1	G	547	CYS	2.8
1	D	1027	VAL	2.7
1	E	821	LEU	2.7
1	F	893	GLY	2.7
1	G	739	GLY	2.7
1	G	709	VAL	2.7
1	C	909	PHE	2.7
1	G	396	LEU	2.7
1	G	865	LEU	2.7
1	F	992	THR	2.7
1	G	348	ARG	2.7
1	E	1079	VAL	2.7
1	E	794	ALA	2.7
1	H	1084	LEU	2.7
1	E	747	ASP	2.7
1	G	1063	LEU	2.7
1	G	642	HIS	2.7
1	E	486	SER	2.7
1	H	626	TYR	2.6
1	E	818	LEU	2.6
1	F	1028	SER	2.6
1	D	1042	ASN	2.6
1	D	1050	LEU	2.6
1	G	1098	ILE	2.6
1	G	415	ALA	2.6
1	D	595	LEU	2.6
1	G	608	LEU	2.6
1	E	1037	ILE	2.6
1	H	623	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	994	ALA	2.6
1	H	339	GLY	2.6
1	E	1012	THR	2.6
1	H	1037	ILE	2.6
1	G	584	ASN	2.6
1	E	1119	ILE	2.5
1	G	1119	ILE	2.5
1	E	1123	THR	2.5
1	G	740	PHE	2.5
1	D	1011	PRO	2.5
1	H	376	MET	2.5
1	C	831	VAL	2.5
1	G	425	VAL	2.5
1	C	671	PHE	2.5
1	D	1076	PHE	2.5
1	E	927	PHE	2.5
1	E	1000	LEU	2.5
1	G	924	LEU	2.5
1	G	654	ILE	2.5
1	D	631	PHE	2.5
1	F	415	ALA	2.5
1	H	1021	THR	2.5
1	D	646	LEU	2.5
1	E	1039	MET	2.5
1	E	909	PHE	2.5
1	H	656	CYS	2.5
1	F	806	LEU	2.4
1	F	950	VAL	2.4
1	F	818	LEU	2.4
1	E	663	SER	2.4
1	E	1077	SER	2.4
1	D	692	ALA	2.4
1	C	1014	GLY	2.4
1	F	888	GLY	2.4
1	G	605	VAL	2.4
1	G	866	VAL	2.4
1	H	1027	VAL	2.4
1	G	559	ALA	2.4
1	G	603	TRP	2.4
1	E	670	TYR	2.4
1	D	727	MET	2.4
1	H	654	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	1020	PRO	2.4
1	E	907	LEU	2.4
1	E	1097	LEU	2.4
1	H	1046	LEU	2.4
1	G	403	ILE	2.4
1	E	339	GLY	2.3
1	G	879	GLY	2.3
1	H	1128	PHE	2.3
1	H	715	ALA	2.3
1	E	996	PRO	2.3
1	G	418	PRO	2.3
1	G	682	VAL	2.3
1	D	337	MET	2.3
1	C	981	SER	2.3
1	D	396	LEU	2.3
1	D	713	SER	2.3
1	E	943	TYR	2.3
1	E	974	THR	2.3
1	H	602	ILE	2.3
1	G	496	GLY	2.3
1	G	566	ALA	2.3
1	D	1003	MET	2.3
1	D	618	LEU	2.3
1	E	914	TYR	2.3
1	G	626	TYR	2.3
1	D	996	PRO	2.3
1	E	941	PRO	2.3
1	E	924	LEU	2.3
1	G	595	LEU	2.3
1	H	1044	LYS	2.3
1	F	974	THR	2.3
1	G	981	SER	2.3
1	G	741	PRO	2.3
1	G	638	GLY	2.3
1	G	706	PHE	2.2
1	G	633	ALA	2.2
1	E	714	LEU	2.2
1	H	564	LEU	2.2
1	E	915	THR	2.2
1	G	404	VAL	2.2
1	H	674	TYR	2.2
1	D	405	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	1015	ALA	2.2
1	E	340	LEU	2.2
1	E	402	LEU	2.2
1	G	1099	VAL	2.2
1	H	979	THR	2.2
1	F	357	SER	2.2
1	G	788	TYR	2.2
1	F	824	PHE	2.2
1	G	659	LEU	2.2
1	D	411	PRO	2.2
1	G	356	PRO	2.2
1	E	896	THR	2.2
1	C	888	GLY	2.2
1	C	1067	SER	2.2
1	E	893	GLY	2.2
1	E	922	ALA	2.2
1	E	1001	ALA	2.2
1	F	605	VAL	2.2
1	F	1079	VAL	2.2
1	H	737	GLY	2.2
1	F	1078	TYR	2.2
1	F	1094	TYR	2.2
1	G	1105	SER	2.2
1	F	421	ALA	2.2
1	E	1081	ASN	2.1
1	G	704	VAL	2.1
1	F	901	MET	2.1
1	G	509	THR	2.1
1	C	666	LEU	2.1
1	D	907	LEU	2.1
1	G	381	LEU	2.1
1	E	910	GLU	2.1
1	H	1122	ARG	2.1
1	D	584	ASN	2.1
1	E	799	LEU	2.1
1	H	699	LEU	2.1
1	D	351	TYR	2.1
1	G	519	ALA	2.1
1	C	937	CYS	2.1
1	E	743	CYS	2.1
1	F	1026	SER	2.1
1	C	1041	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1099	VAL	2.1
1	F	709	VAL	2.1
1	E	1062	LEU	2.1
1	G	868	GLY	2.1
1	G	1000	LEU	2.1
1	D	1128	PHE	2.1
1	E	789	THR	2.1
1	F	1045	PHE	2.1
1	H	416	PHE	2.1
1	C	1060	ILE	2.1
1	E	957	ILE	2.1
1	E	1106	ALA	2.1
1	G	1024	ILE	2.1
1	E	688	SER	2.1
1	H	398	GLN	2.1
1	H	337	MET	2.1
1	C	1032	VAL	2.1
1	G	436	PRO	2.1
1	E	991	LEU	2.1
1	H	352	LEU	2.1
1	D	827	PHE	2.1
1	E	998	GLY	2.1
1	F	414	GLY	2.1
1	C	786	THR	2.1
1	D	1096	ASP	2.1
1	E	791	TRP	2.1
1	F	988	ILE	2.1
1	H	338	GLU	2.1
1	C	949	TYR	2.1
1	G	1107	TYR	2.1
1	H	670	TYR	2.1
1	G	627	CYS	2.0
1	E	485	VAL	2.0
1	E	1124	VAL	2.0
1	H	1050	LEU	2.0
1	H	1111	LEU	2.0
1	G	631	PHE	2.0
1	G	689	GLY	2.0
1	D	982	ILE	2.0
1	G	730	ILE	2.0
1	C	930	TYR	2.0
1	D	1094	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	1127	LYS	2.0
1	H	949	TYR	2.0
1	E	1083	VAL	2.0
1	G	377	PRO	2.0
1	E	980	LEU	2.0
1	D	1108	PHE	2.0
1	G	339	GLY	2.0
1	G	652	PHE	2.0
1	E	815	THR	2.0
1	G	660	MET	2.0
1	G	1101	VAL	2.0
1	H	354	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

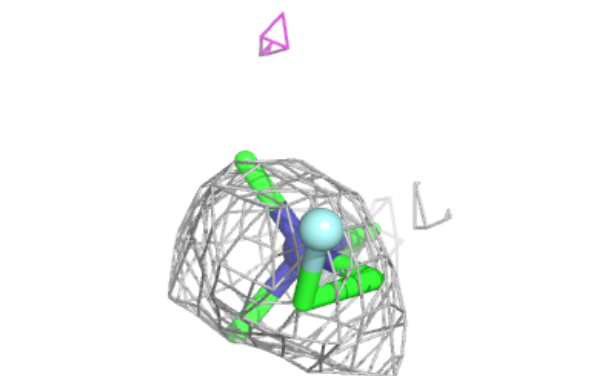
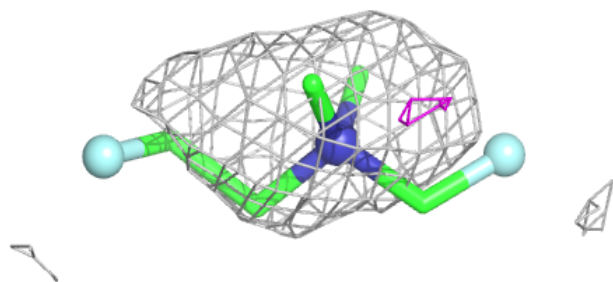
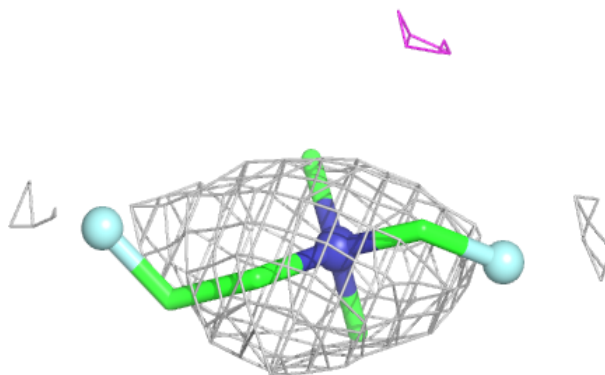
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1H9L	H	1201	8/8	0.85	0.24	70,75,81,86	0
2	A1H9L	G	1201	8/8	0.88	0.23	62,71,75,75	0
2	A1H9L	D	1201	8/8	0.88	0.18	48,54,58,64	0
2	A1H9L	C	1201	8/8	0.90	0.17	40,43,51,64	0
2	A1H9L	E	1201	8/8	0.92	0.12	48,55,57,58	0
2	A1H9L	F	1201	8/8	0.93	0.12	55,57,60,62	0
2	A1H9L	B	1201	8/8	0.94	0.11	20,23,27,30	0
2	A1H9L	A	1201	8/8	0.95	0.13	18,25,29,41	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.

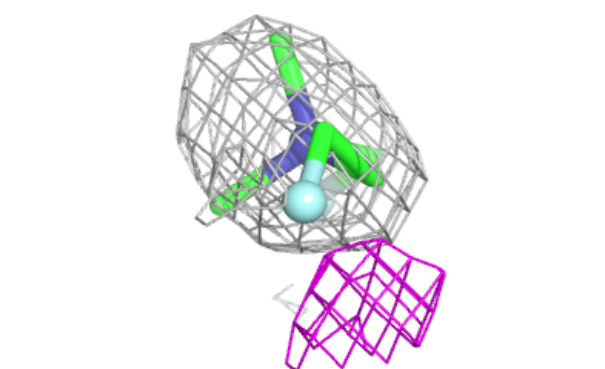
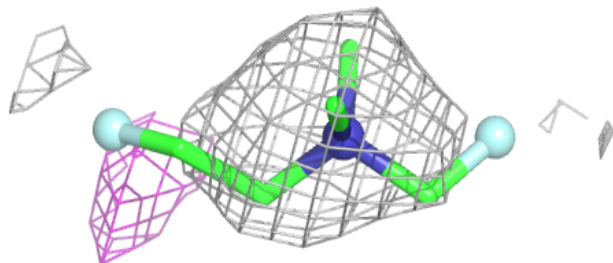
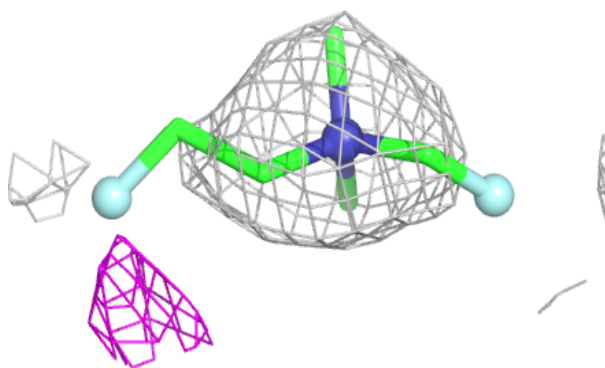
Electron density around A1H9L H 1201:

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



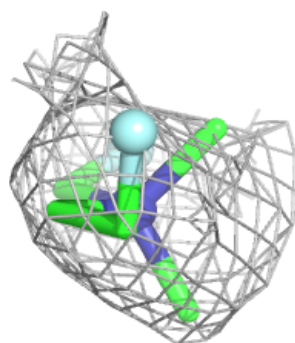
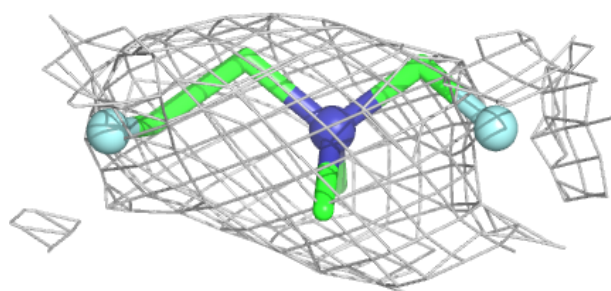
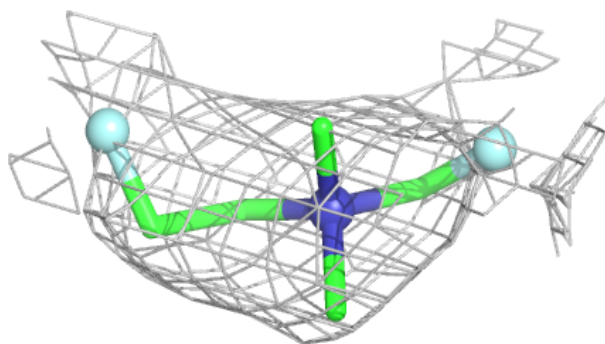
Electron density around A1H9L G 1201:

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

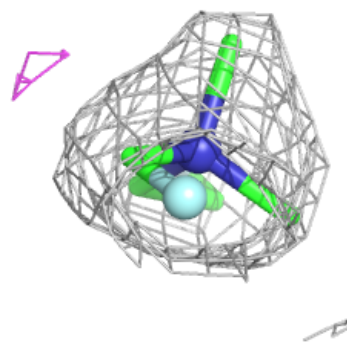
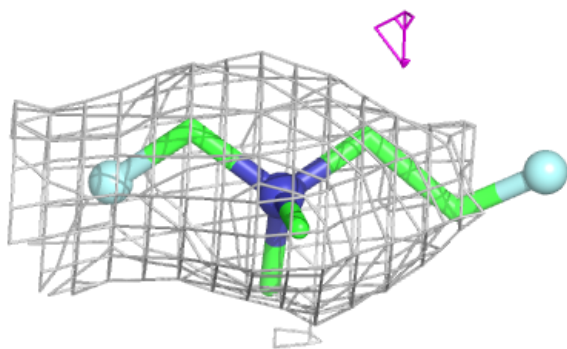
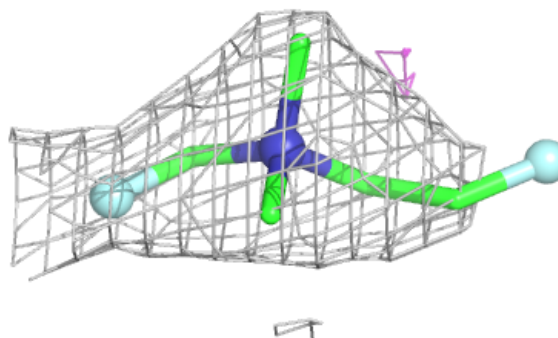


Electron density around A1H9L D 1201:

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

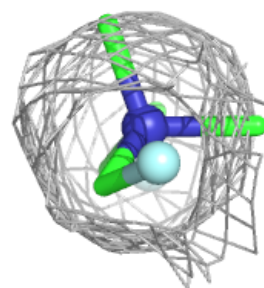
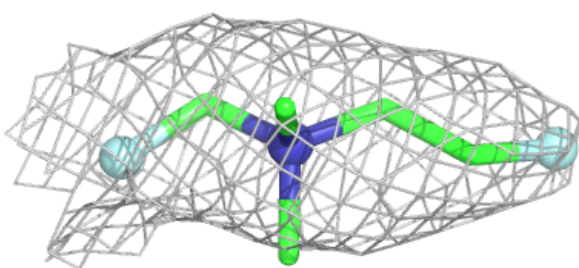
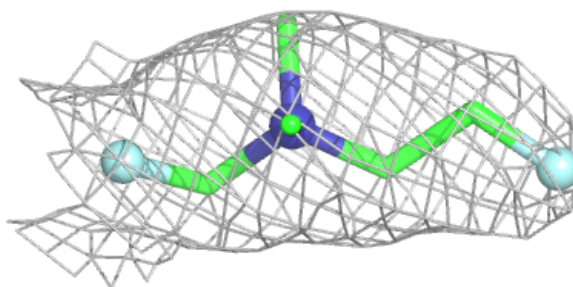
**Electron density around A1H9L C 1201:**

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

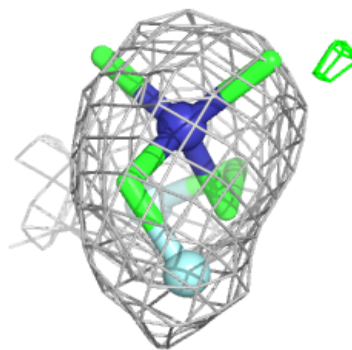
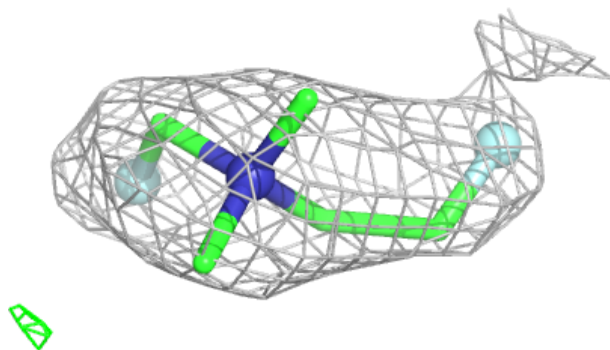
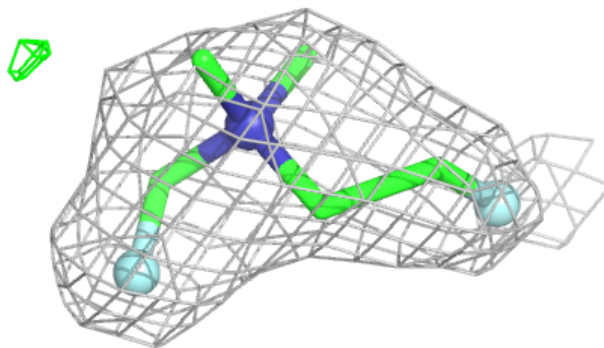


Electron density around A1H9L E 1201:

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

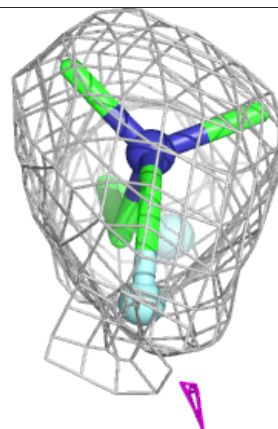
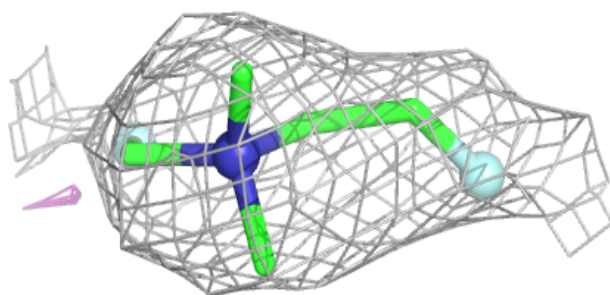
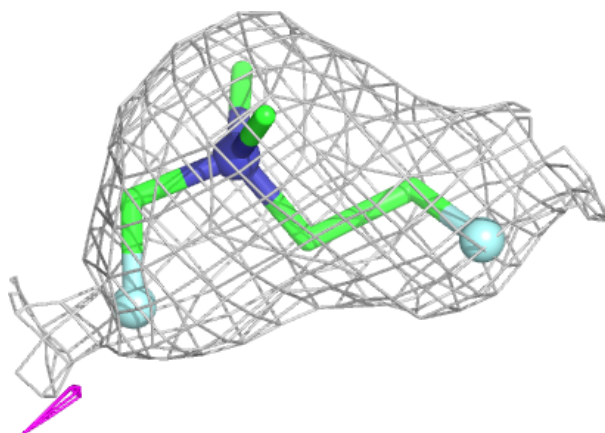
**Electron density around A1H9L F 1201:**

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



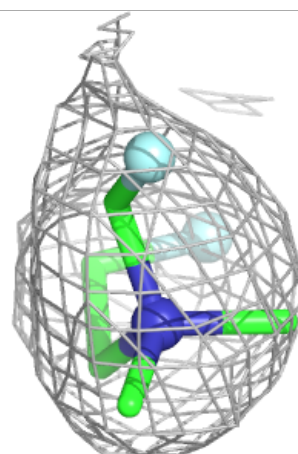
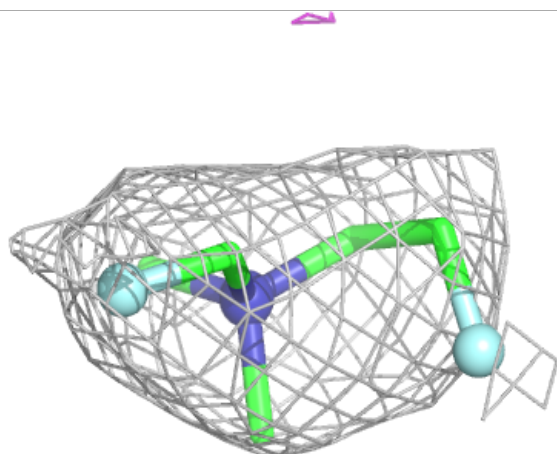
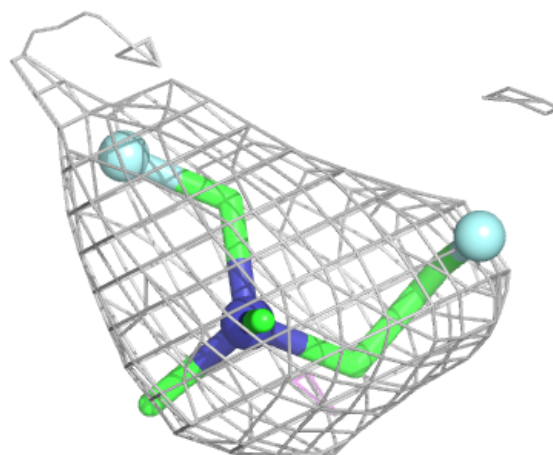
Electron density around A1H9L B 1201:

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



Electron density around A1H9L A 1201:

$2mF_o-DF_c$ (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.