Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2024 – 02:33 am BST

PDB ID	:	9F3W
Title	:	CutC choline lyase in complex with fluoromethylcholine
Authors	:	Kalnins, G.
Deposited on	:	2024-04-26
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

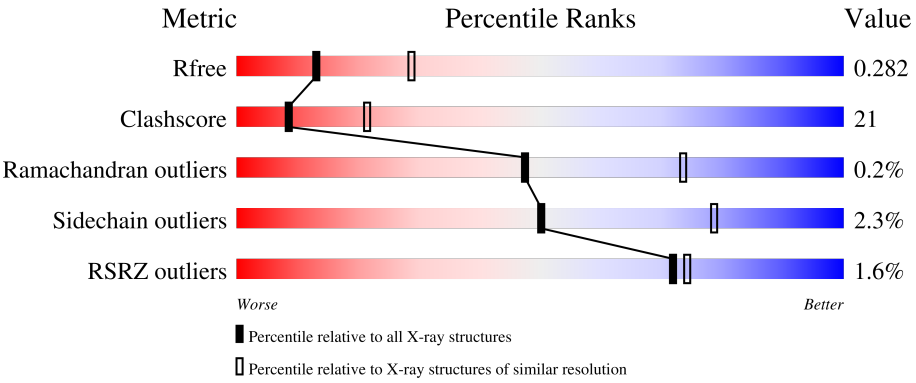
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	47% 22% 31%
1	B	1150	47% 21% · 31%
1	C	1150	45% 23% · 31%
1	D	1150	40% 28% · 31%
1	E	1150	% 41% 27% · 31%

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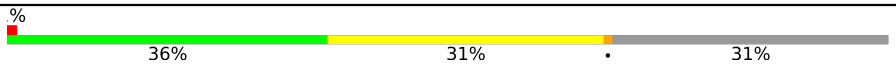
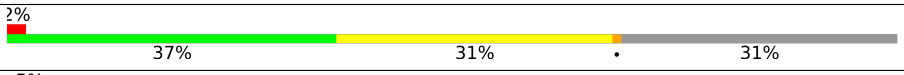
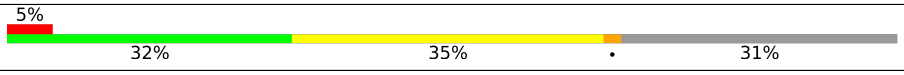
Mol	Chain	Length	Quality of chain
1	F	1150	
1	G	1150	
1	H	1150	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 50403 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
C	-16	HIS	-	expression tag	UNP A0A486V7R5
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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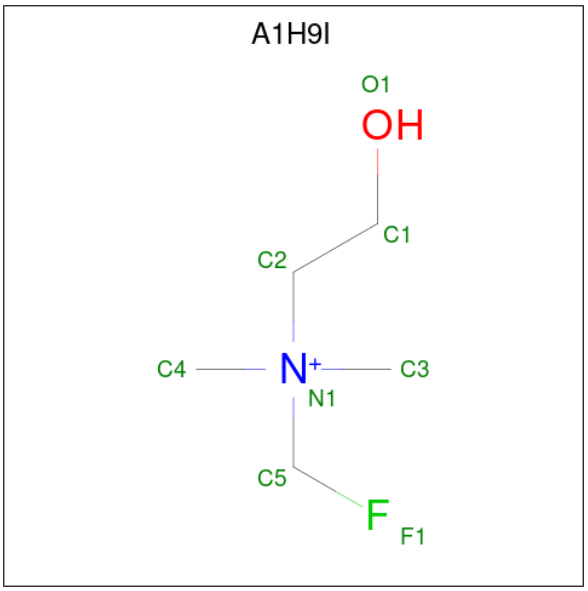
Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP A0A486V7R5
G	-13	HIS	-	expression tag	UNP A0A486V7R5
G	-12	HIS	-	expression tag	UNP A0A486V7R5
G	-11	SER	-	expression tag	UNP A0A486V7R5
G	-10	GLN	-	expression tag	UNP A0A486V7R5
G	-9	ASP	-	expression tag	UNP A0A486V7R5
G	-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 fluoromethylcholine (three-letter code: A1H9I) (formula: $C_5H_{13}FNO$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	60	Total O 60 60	0	0
3	C	62	Total O 62 62	0	0
3	D	26	Total O 26 26	0	0

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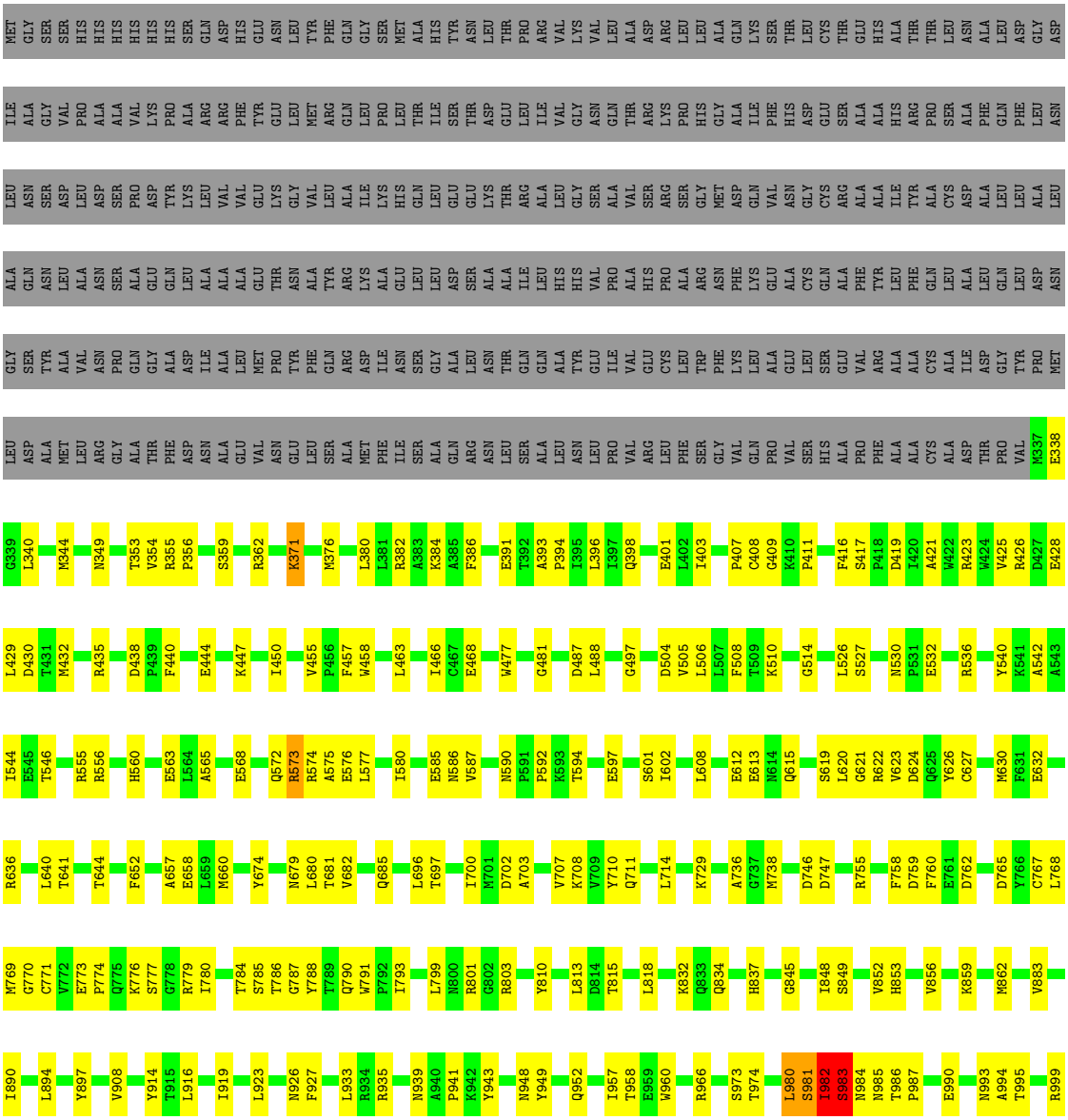
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	27	Total O 27 27	0	0
3	F	31	Total O 31 31	0	0
3	G	23	Total O 23 23	0	0
3	H	9	Total O 9 9	0	0

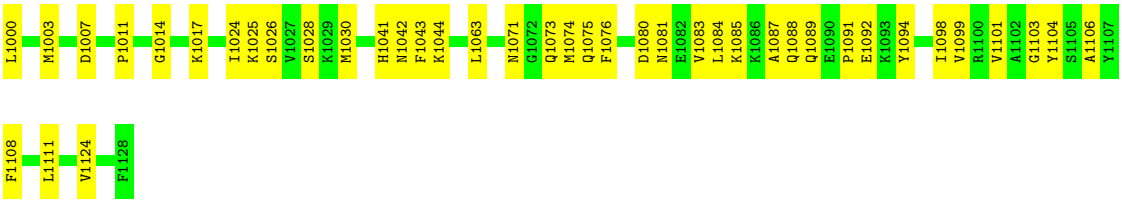
3 Residue-property plots (i)

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

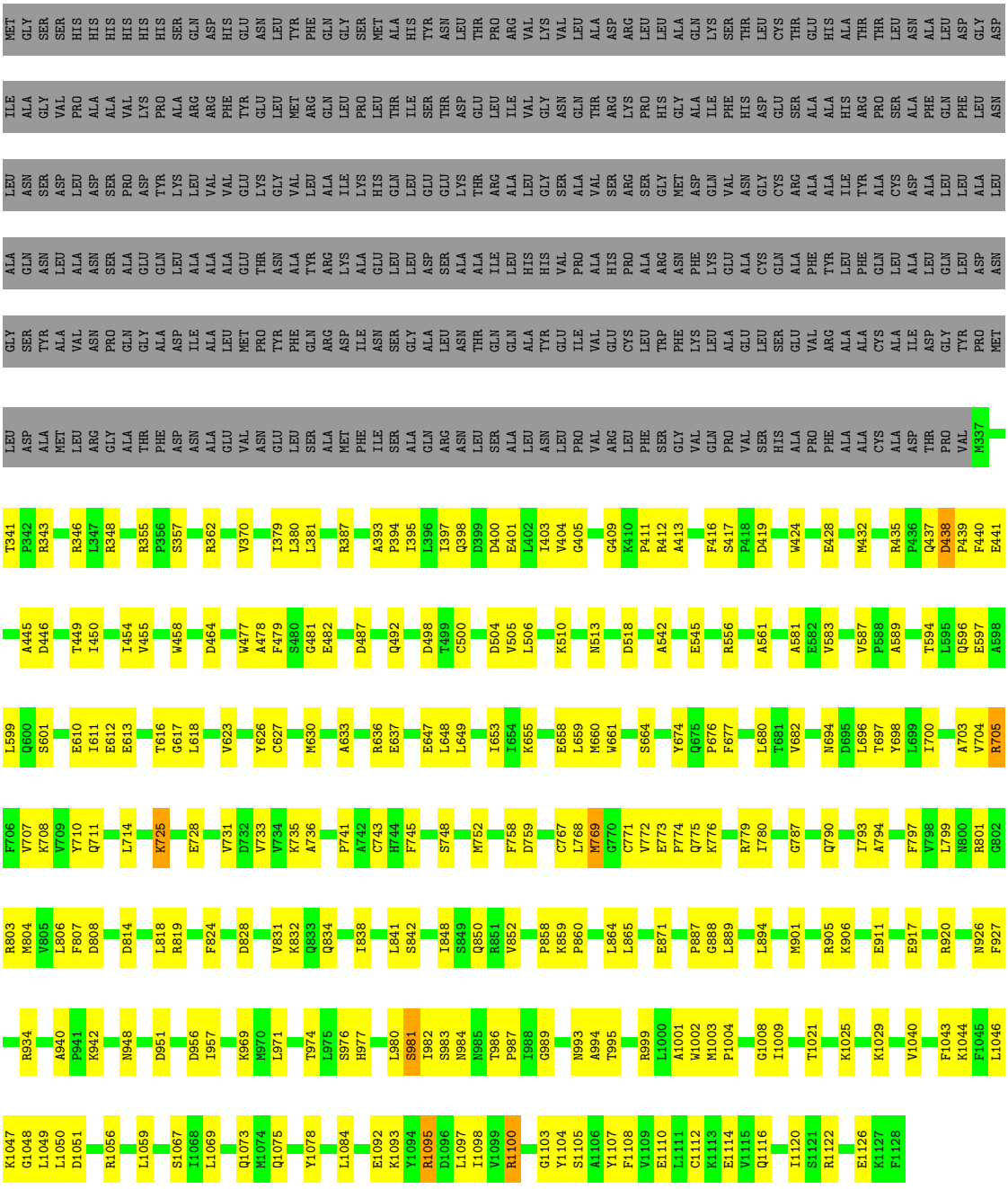
Chain A:





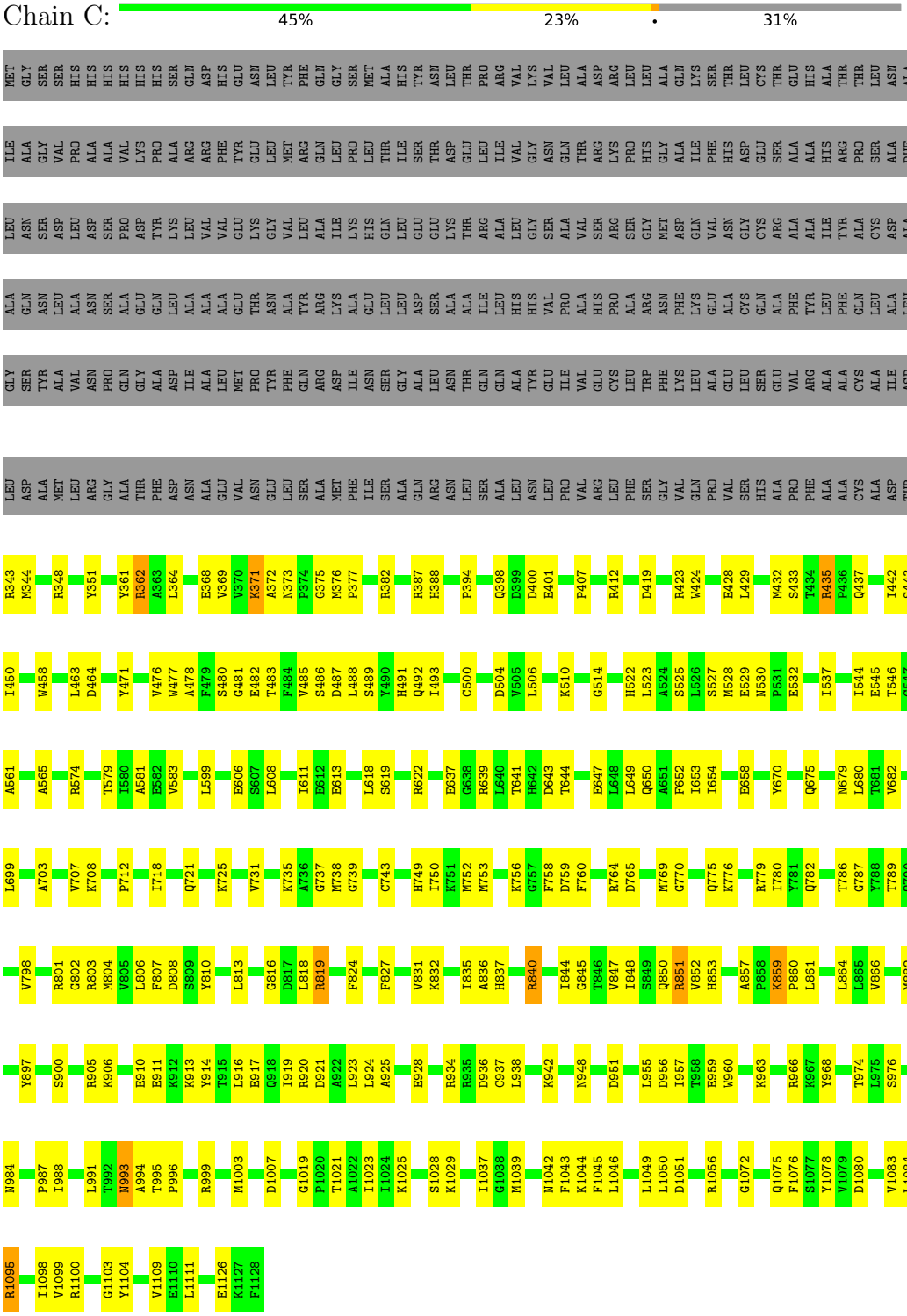
• Molecule 1: Choline trimethylamine-lyase

Chain B:



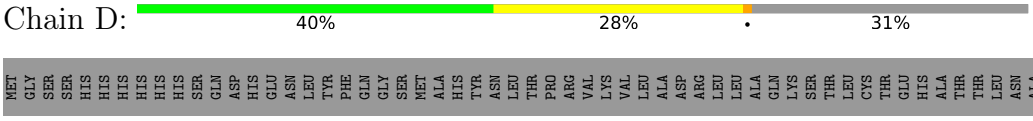
• Molecule 1: Choline trimethylamine-lyase

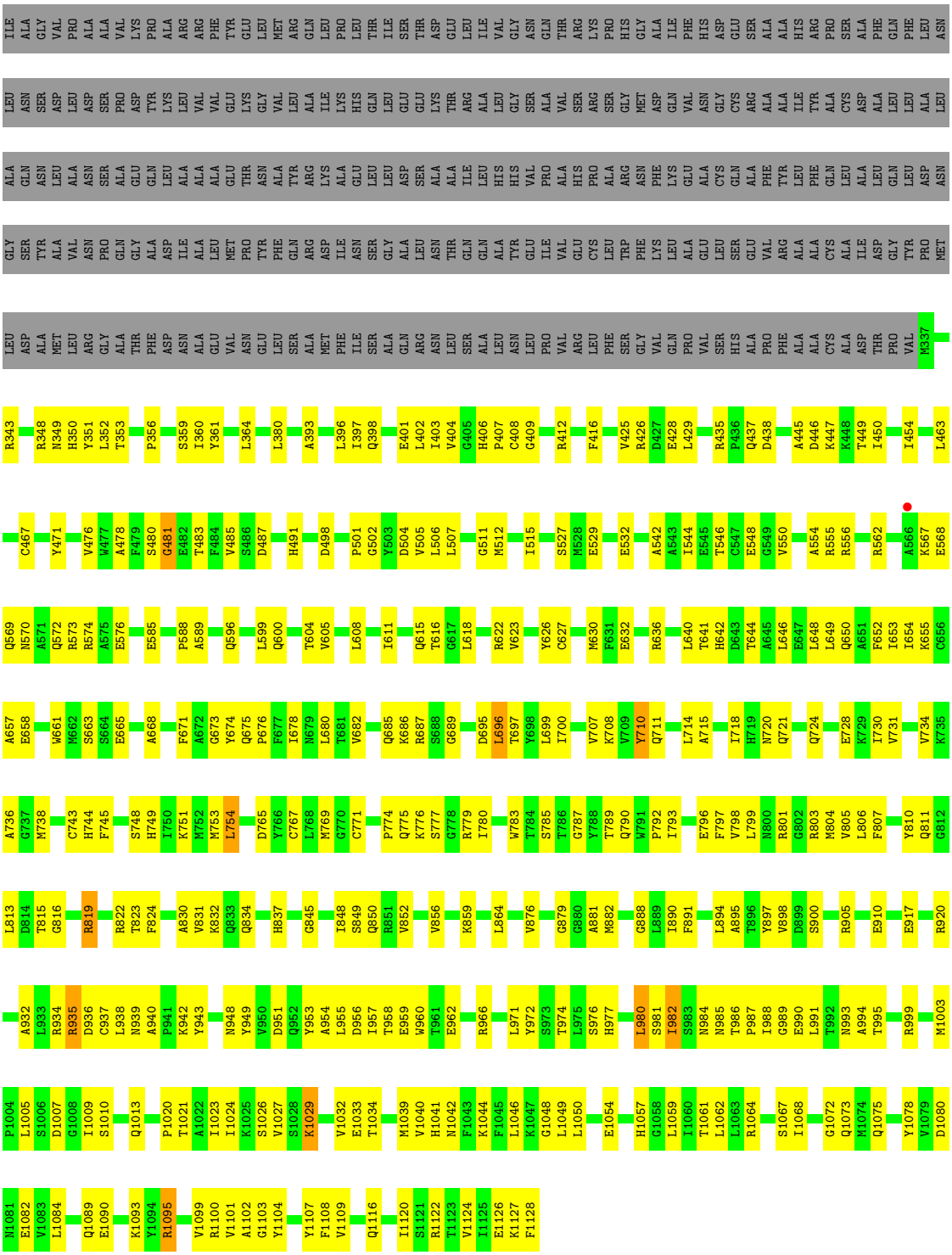
Chain C:



• Molecule 1: Choline trimethylamine-lyase

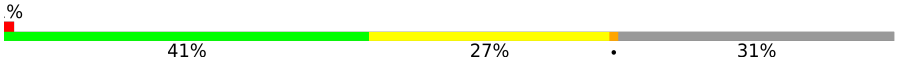
Chain D:

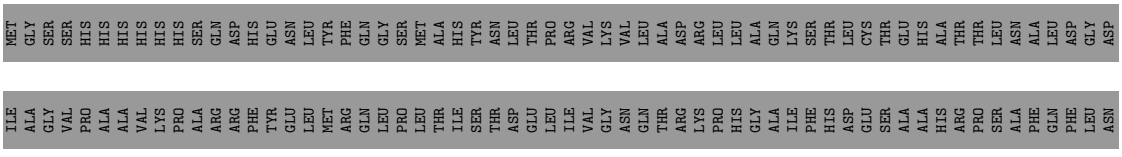


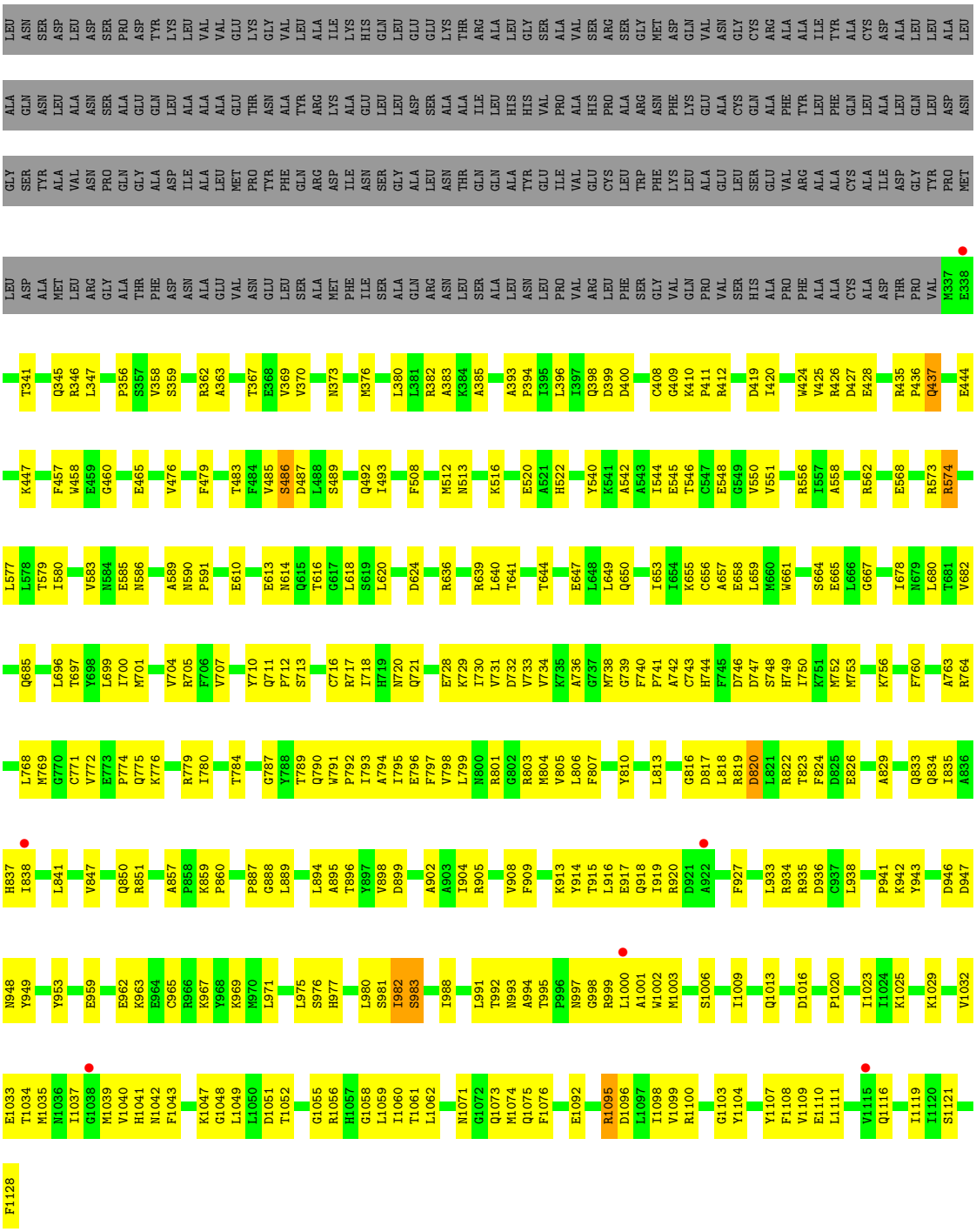


• Molecule 1: Choline trimethylamine-lyase

Chain E:

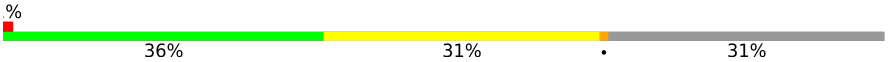


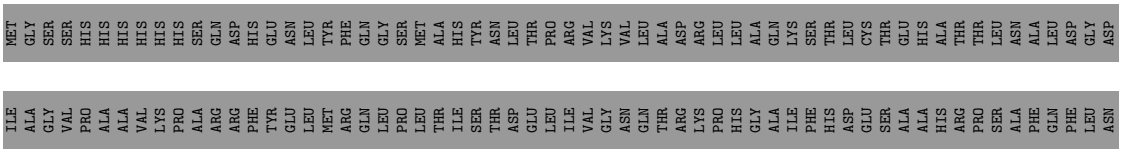


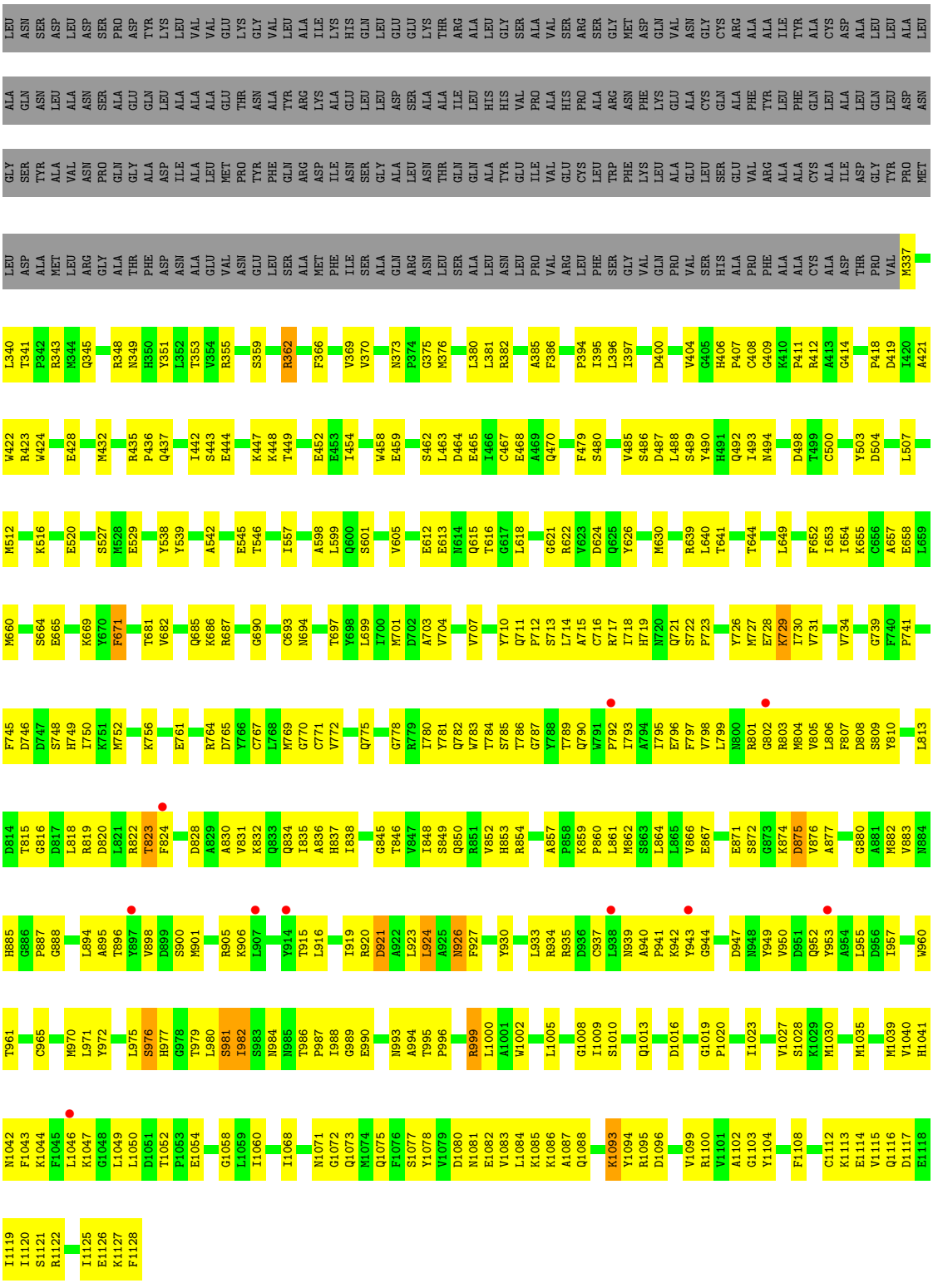


• Molecule 1: Choline trimethylamine-lyase

Chain F:

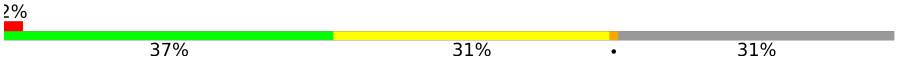


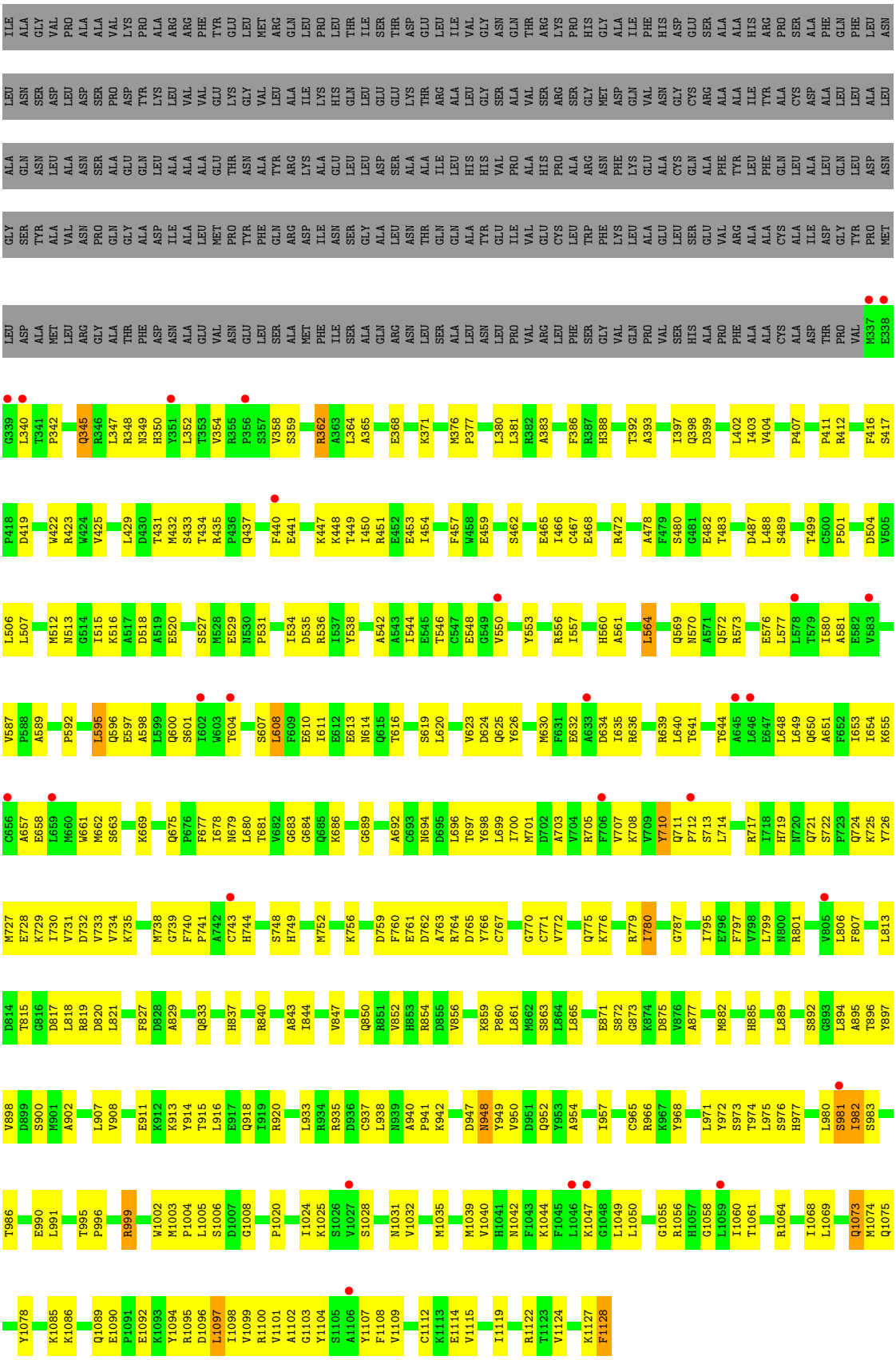




• Molecule 1: Choline trimethylamine-lyase

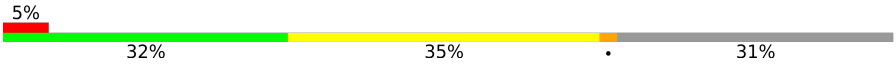
Chain G:

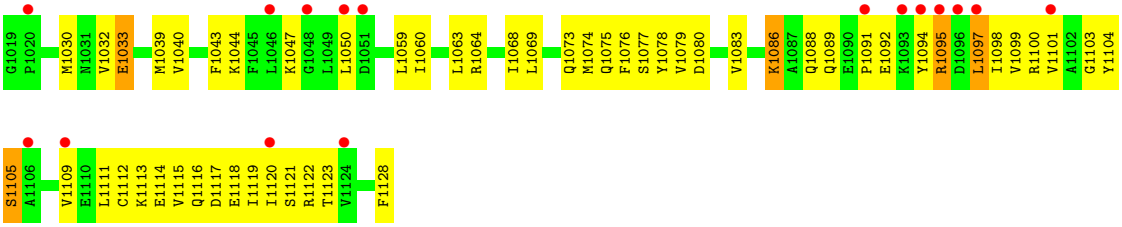




- Molecule 1: Choline trimethylamine-lyase

Chain H:




G1019
P1020
M1030
N1031
V1032
E1033
M1039
V1040
F1043
K1044
F1045
L1046
K1047
G1048
L1049
L1050
D1051
L1059
I1060
L1063
R1064
I1068
L1069
Q1073
M1074
Q1075
F1076
S1077
Y1078
V1079
D1080
V1083
K1086
A1087
Q1088
Q1089
E1090
P1091
E1092
K1093
Y1094
R1095
D1096
L1097
I1098
V1099
R1100
V1101
A1102
G1103
Y1104
S1105
A1106
V1109
E1110
L1111
C1112
K1113
E1114
V1115
Q1116
D1117
E1118
I1119
I1120
S1121
R1122
T1123
V1124
F1128

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	89.33Å 119.64Å 214.62Å 77.80° 85.16° 69.27°	Depositor
Resolution (Å)	83.54 – 2.70 90.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.7 (83.54-2.70) 85.8 (90.29-2.70)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.223 , 0.282 0.223 , 0.282	Depositor DCC
R_{free} test set	9642 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	50403	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1H9I

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	0.53	0/6385	0.70	0/8640
1	B	0.54	0/6385	0.69	2/8640 (0.0%)
1	C	0.49	1/6385 (0.0%)	0.65	0/8640
1	D	0.48	1/6385 (0.0%)	0.66	1/8640 (0.0%)
1	E	0.44	0/6385	0.64	1/8640 (0.0%)
1	F	0.50	1/6385 (0.0%)	0.69	4/8640 (0.0%)
1	G	0.45	0/6385	0.66	3/8640 (0.0%)
1	H	0.44	0/6385	0.68	3/8640 (0.0%)
All	All	0.49	3/51080 (0.0%)	0.67	14/69120 (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	A	0	3
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	3
1	H	0	6
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	500	CYS	CB-SG	-5.69	1.72	1.81
1	C	500	CYS	CB-SG	-5.47	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	467	CYS	CB-SG	-5.18	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	820	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	H	1097	LEU	CA-CB-CG	7.07	131.56	115.30
1	G	608	LEU	CA-CB-CG	6.87	131.10	115.30
1	D	696	LEU	CA-CB-CG	5.64	128.28	115.30
1	B	438	ASP	CB-CG-OD1	5.58	123.32	118.30
1	F	463	LEU	CA-CB-CG	5.53	128.01	115.30
1	F	823	THR	OG1-CB-CG2	-5.52	97.31	110.00
1	B	438	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	F	699	LEU	CA-CB-CG	5.25	127.38	115.30
1	G	564	LEU	CA-CB-CG	5.20	127.25	115.30
1	H	463	LEU	CA-CB-CG	5.11	127.05	115.30
1	G	1097	LEU	CA-CB-CG	5.08	126.99	115.30
1	F	924	LEU	CA-CB-CG	5.07	126.95	115.30
1	H	450	ILE	CG1-CB-CG2	-5.05	100.28	111.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLU	Peptide
1	A	981	SER	Mainchain
1	A	982	ILE	Mainchain
1	B	981	SER	Peptide
1	C	911	GLU	Peptide
1	C	981	SER	Peptide
1	D	981	SER	Peptide
1	E	981	SER	Peptide
1	F	981	SER	Peptide
1	G	595	LEU	Peptide
1	G	780	ILE	Peptide
1	G	981	SER	Peptide
1	H	1086	LYS	Peptide
1	H	344	MET	Peptide
1	H	443	SER	Peptide
1	H	489	SER	Peptide
1	H	636	ARG	Peptide
1	H	935	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6254	0	6171	171	0
1	B	6254	0	6171	183	0
1	C	6254	0	6171	203	1
1	D	6254	0	6171	241	0
1	E	6254	0	6171	249	0
1	F	6254	0	6171	336	0
1	G	6254	0	6171	296	0
1	H	6254	0	6171	390	0
2	A	8	0	0	0	0
2	B	8	0	0	1	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
2	E	8	0	0	0	0
2	F	8	0	0	2	0
2	G	8	0	0	0	0
2	H	8	0	0	0	0
3	A	69	0	0	7	0
3	B	60	0	0	0	0
3	C	62	0	0	4	0
3	D	26	0	0	0	0
3	E	27	0	0	4	0
3	F	31	0	0	6	0
3	G	23	0	0	2	0
3	H	9	0	0	1	0
All	All	50403	0	49368	2056	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (2056) 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:B:1100:ARG:HH12	1:B:1103:GLY:C	1.47	1.18
1:H:453:GLU:OE1	1:H:453:GLU:O	1.63	1.13
1:C:934:ARG:NH1	1:C:938:LEU:HD11	1.68	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1100:ARG:NH1	1:B:1104:TYR:N	2.03	1.07
1:C:934:ARG:HH11	1:C:938:LEU:HD11	1.11	1.07
1:G:348:ARG:HH21	1:G:708:LYS:HB2	1.17	1.05
1:F:850:GLN:NE2	1:F:887:PRO:HD3	1.74	1.02
1:H:343:ARG:HH12	1:H:573:ARG:NH1	1.57	1.02
1:C:1075:GLN:HE22	1:C:1103:GLY:H	1.07	0.99
1:F:479:PHE:HZ	1:F:838:ILE:HG22	1.28	0.98
1:H:400:ASP:HA	1:H:573:ARG:NH2	1.77	0.98
1:G:429:LEU:HD21	1:G:450:ILE:HD11	1.46	0.96
1:D:898:VAL:HG23	1:D:953:TYR:HB2	1.47	0.96
1:H:957:ILE:HD12	1:H:958:THR:N	1.81	0.96
1:F:798:VAL:HG21	1:F:831:VAL:HG12	1.48	0.95
1:D:696:LEU:HA	1:D:699:LEU:HB2	1.47	0.94
1:B:1100:ARG:NH1	1:B:1103:GLY:C	2.18	0.94
1:E:731:VAL:HG21	1:E:1060:ILE:HD11	1.50	0.93
1:F:1075:GLN:HE22	1:F:1103:GLY:HA2	1.30	0.92
1:G:623:VAL:HG22	1:G:680:LEU:HD21	1.51	0.92
1:D:1075:GLN:HE22	1:D:1103:GLY:H	1.16	0.92
1:G:604:THR:HA	1:G:607:SER:HB3	1.50	0.92
1:E:805:VAL:HG11	1:E:993:ASN:HB2	1.52	0.91
1:E:479:PHE:HZ	1:E:838:ILE:HG22	1.36	0.91
1:H:1063:LEU:HD21	1:H:1076:PHE:HZ	1.37	0.90
1:F:850:GLN:HE22	1:F:887:PRO:HD3	1.33	0.90
1:F:813:LEU:O	1:F:834:GLN:NE2	2.05	0.90
1:H:898:VAL:HG23	1:H:953:TYR:HB2	1.53	0.89
1:F:616:THR:HG23	2:F:1201:A1H9I:F1	1.63	0.89
1:E:739:GLY:HA3	1:E:1100:ARG:HB2	1.52	0.88
1:D:917:GLU:HA	1:D:920:ARG:HB3	1.54	0.88
1:E:917:GLU:HA	1:E:920:ARG:HD3	1.53	0.88
1:G:632:GLU:HG3	1:G:636:ARG:HH21	1.38	0.86
1:C:917:GLU:HG2	1:C:920:ARG:HH12	1.39	0.86
1:H:343:ARG:NH1	1:H:573:ARG:NH1	2.23	0.86
1:H:393:ALA:O	1:H:556:ARG:NH2	2.08	0.86
1:H:400:ASP:H	1:H:573:ARG:HH21	1.23	0.86
1:H:364:LEU:HD23	1:H:454:ILE:HD11	1.58	0.86
1:H:400:ASP:CA	1:H:573:ARG:NH2	2.39	0.86
1:A:1075:GLN:HE22	1:A:1103:GLY:H	1.22	0.85
1:H:401:GLU:HB3	1:H:404:VAL:HG11	1.58	0.85
1:H:467:CYS:HB2	1:H:852:VAL:HG21	1.58	0.85
1:C:483:THR:HB	1:C:804:MET:HE1	1.58	0.85
1:G:480:SER:HB2	1:G:488:LEU:HD12	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:GLN:HG3	1:D:648:LEU:HD21	1.59	0.84
1:E:857:ALA:O	1:E:859:LYS:NZ	2.09	0.84
1:G:771:CYS:HB3	1:G:1103:GLY:HA3	1.57	0.83
1:G:897:TYR:CE1	1:G:957:ILE:HG21	2.14	0.83
1:B:401:GLU:OE2	1:B:655:LYS:NZ	2.11	0.82
1:F:980:LEU:HD12	1:F:982:ILE:HG13	1.61	0.82
1:G:546:THR:HG21	1:G:860:PRO:HB2	1.60	0.81
1:C:653:ILE:HG23	1:C:712:PRO:HD2	1.60	0.81
1:F:480:SER:HB2	1:F:487:ASP:HA	1.63	0.81
1:F:872:SER:HB3	1:F:874:LYS:HG3	1.62	0.81
1:G:354:VAL:HG21	1:G:411:PRO:HB2	1.60	0.81
1:C:1093:LYS:HD3	1:C:1094:TYR:CD2	2.15	0.81
1:A:619:SER:HB3	1:A:679:ASN:HB3	1.63	0.80
1:G:561:ALA:HA	1:G:564:LEU:HD12	1.61	0.80
1:H:752:MET:CE	1:H:1033:GLU:HA	2.12	0.80
1:C:1075:GLN:NE2	1:C:1103:GLY:H	1.81	0.79
1:G:1095:ARG:HA	1:G:1109:VAL:HG21	1.64	0.79
1:F:1075:GLN:NE2	1:F:1103:GLY:HA2	1.98	0.79
1:D:483:THR:HB	1:D:804:MET:HE1	1.64	0.79
1:F:905:ARG:HD3	1:F:953:TYR:OH	1.83	0.79
1:D:995:THR:HG23	1:D:999:ARG:HH21	1.45	0.78
1:F:746:ASP:O	1:F:750:ILE:HG13	1.83	0.78
1:G:732:ASP:HA	1:G:735:LYS:HG2	1.65	0.78
1:C:1093:LYS:CD	1:C:1094:TYR:CE2	2.66	0.78
1:H:850:GLN:HG2	1:H:971:LEU:HD22	1.65	0.78
1:H:752:MET:HE1	1:H:1033:GLU:HA	1.64	0.78
1:C:344:MET:HE3	1:C:647:GLU:HG2	1.64	0.78
1:A:371:LYS:HD3	1:A:457:PHE:CE1	2.18	0.78
1:F:803:ARG:NH1	1:F:808:ASP:OD1	2.17	0.78
1:H:986:THR:HG23	1:H:1004:PRO:HG3	1.66	0.78
1:E:435:ARG:HD2	1:E:665:GLU:HA	1.66	0.77
1:C:1093:LYS:HD3	1:C:1094:TYR:CE2	2.19	0.77
1:B:1100:ARG:HH12	1:B:1104:TYR:N	1.68	0.77
1:G:403:ILE:HG23	1:G:600:GLN:HG3	1.66	0.77
1:C:443:SER:HB2	1:C:446:ASP:H	1.50	0.77
1:D:1075:GLN:HE21	1:D:1100:ARG:NE	1.81	0.77
1:E:486:SER:HB2	1:E:789:THR:HB	1.67	0.77
1:F:1073:GLN:HE22	1:F:1075:GLN:HG3	1.50	0.77
1:H:606:GLU:OE2	1:H:678:ILE:CD1	2.33	0.77
1:D:599:LEU:HD11	1:D:649:LEU:HD23	1.64	0.76
1:G:813:LEU:HD11	1:G:837:HIS:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:771:CYS:HB3	1:E:1103:GLY:HA3	1.68	0.76
1:F:624:ASP:HB2	1:F:697:THR:HG22	1.68	0.76
1:C:641:THR:HG22	1:C:643:ASP:H	1.50	0.76
1:G:570:ASN:HB3	1:G:573:ARG:HB3	1.68	0.76
1:H:605:VAL:HA	1:H:608:LEU:HB2	1.67	0.76
1:H:790:GLN:HB2	1:H:792:PRO:HD2	1.68	0.76
1:B:731:VAL:HG22	1:B:1059:LEU:HD23	1.66	0.76
1:H:437:GLN:HB2	1:H:1112:CYS:HB3	1.68	0.76
1:E:935:ARG:HA	1:E:938:LEU:HB2	1.68	0.75
1:A:982:ILE:HG22	1:A:983:SER:H	1.51	0.75
1:B:599:LEU:HD11	1:B:649:LEU:HD23	1.67	0.75
1:C:1075:GLN:HE22	1:C:1103:GLY:N	1.84	0.75
1:A:815:THR:HG23	1:A:834:GLN:HE21	1.52	0.75
1:E:411:PRO:HB3	1:E:658:GLU:HG2	1.67	0.75
1:B:379:ILE:HD13	1:B:858:PRO:HB2	1.68	0.74
1:H:900:SER:HB3	1:H:996:PRO:HD2	1.69	0.74
1:H:955:LEU:HD13	1:H:1030:MET:HA	1.69	0.74
1:B:1107:TYR:HB2	1:B:1110:GLU:HG3	1.69	0.74
1:F:653:ILE:HG23	1:F:712:PRO:HD2	1.70	0.74
1:D:1020:PRO:HB2	1:D:1062:LEU:HD21	1.69	0.74
1:F:806:LEU:HD12	1:F:807:PHE:CE1	2.22	0.74
1:H:772:VAL:HG11	1:H:1040:VAL:HB	1.70	0.74
1:G:634:ASP:HB3	1:G:640:LEU:HG	1.70	0.74
1:B:636:ARG:HH11	1:B:637:GLU:HG3	1.53	0.74
1:B:752:MET:HE3	1:B:774:PRO:HG2	1.69	0.74
1:F:382:ARG:NH2	1:F:613:GLU:OE1	2.20	0.74
1:A:391:GLU:O	1:A:556:ARG:NH1	2.21	0.73
1:F:449:THR:HA	1:F:452:GLU:HG2	1.70	0.73
1:E:999:ARG:NH1	1:E:1003:MET:O	2.22	0.73
1:G:772:VAL:HG11	1:G:1040:VAL:HG12	1.71	0.73
1:H:894:LEU:HD13	1:H:1009:ILE:HG22	1.69	0.73
1:B:980:LEU:HD12	1:B:980:LEU:O	1.88	0.73
1:F:981:SER:OG	1:F:1008:GLY:N	2.20	0.73
1:F:1044:LYS:NZ	1:F:1119:ILE:O	2.21	0.73
1:F:1082:GLU:HA	1:F:1085:LYS:HD2	1.70	0.73
1:A:555:ARG:NH1	1:A:585:GLU:O	2.22	0.73
1:F:359:SER:OG	1:F:414:GLY:O	2.07	0.73
1:F:771:CYS:HB3	1:F:1103:GLY:HA3	1.71	0.73
1:H:512:MET:CE	1:H:588:PRO:HG2	2.19	0.73
1:D:790:GLN:HB2	1:D:792:PRO:HD2	1.70	0.72
1:C:546:THR:HG21	1:C:860:PRO:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:653:ILE:HG23	1:G:712:PRO:HD2	1.70	0.72
1:G:1119:ILE:HA	1:G:1122:ARG:HD2	1.70	0.72
1:H:505:VAL:C	1:H:506:LEU:HD22	2.09	0.72
1:H:518:ASP:O	1:H:522:HIS:N	2.17	0.72
1:C:698:TYR:CZ	1:C:725:LYS:HD3	2.25	0.72
1:F:857:ALA:O	1:F:859:LYS:NZ	2.22	0.72
1:A:702:ASP:OD1	1:A:729:LYS:NZ	2.23	0.72
1:D:989:GLY:HA2	1:D:1005:LEU:HD13	1.70	0.72
1:H:596:GLN:HB3	1:H:648:LEU:HD21	1.72	0.72
1:D:988:ILE:HA	1:D:991:LEU:HD12	1.72	0.71
1:G:655:LYS:HA	1:G:658:GLU:HB3	1.72	0.71
1:G:684:GLY:HA3	1:G:717:ARG:HE	1.54	0.71
1:G:815:THR:HG22	1:G:833:GLN:HE21	1.55	0.71
1:D:744:HIS:CE1	1:D:1073:GLN:HG3	2.25	0.71
1:F:485:VAL:HG13	1:F:793:ILE:HD13	1.71	0.71
1:H:640:LEU:HD21	1:H:648:LEU:HD13	1.71	0.71
1:A:624:ASP:HA	1:A:696:LEU:HD23	1.73	0.71
1:D:476:VAL:O	1:D:480:SER:HB3	1.90	0.71
1:F:783:TRP:HH2	1:F:853:HIS:CD2	2.09	0.71
1:G:467:CYS:HB2	1:G:852:VAL:HG21	1.72	0.71
1:H:813:LEU:HD11	1:H:837:HIS:HB2	1.72	0.71
1:E:749:HIS:HE1	3:E:1316:HOH:O	1.74	0.71
1:A:423:ARG:NH2	1:A:468:GLU:OE1	2.23	0.71
1:G:1040:VAL:HA	1:G:1073:GLN:HE21	1.54	0.71
1:H:606:GLU:OE2	1:H:678:ILE:HD13	1.90	0.71
1:C:801:ARG:NE	1:C:816:GLY:O	2.23	0.70
1:D:428:GLU:OE1	1:D:435:ARG:NH1	2.23	0.70
1:E:713:SER:HB3	1:E:1100:ARG:HH12	1.56	0.70
1:H:907:LEU:HD13	1:H:914:TYR:HD2	1.56	0.70
1:B:831:VAL:HG21	1:B:901:MET:HE1	1.74	0.70
1:G:698:TYR:HD1	1:G:729:LYS:HD3	1.57	0.70
1:C:382:ARG:NH2	1:C:613:GLU:OE1	2.25	0.70
1:D:351:TYR:OH	1:D:710:TYR:HE1	1.74	0.70
1:G:759:ASP:OD1	1:G:760:PHE:N	2.22	0.70
1:E:479:PHE:CZ	1:E:838:ILE:HG22	2.24	0.70
1:G:641:THR:N	1:G:644:THR:OG1	2.25	0.70
1:C:463:LEU:HD11	1:C:853:HIS:CD2	2.26	0.69
1:D:393:ALA:O	1:D:556:ARG:NH2	2.25	0.69
1:H:570:ASN:HB3	1:H:573:ARG:HB3	1.74	0.69
1:F:850:GLN:NE2	1:F:887:PRO:CD	2.53	0.69
1:H:370:VAL:HG12	1:H:381:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:935:ARG:HG2	1:E:938:LEU:HD12	1.73	0.69
1:A:708:LYS:O	3:A:1301:HOH:O	2.11	0.69
1:A:815:THR:HG23	1:A:834:GLN:NE2	2.08	0.69
1:H:678:ILE:HG22	1:H:712:PRO:HB3	1.75	0.69
1:H:1092:GLU:HA	1:H:1095:ARG:HB2	1.75	0.69
1:H:1047:LYS:HE2	1:H:1079:VAL:HA	1.75	0.69
1:E:775:GLN:HB3	1:E:780:ILE:HG21	1.73	0.68
1:A:799:LEU:HA	1:A:818:LEU:HD21	1.75	0.68
1:B:771:CYS:HB3	1:B:1103:GLY:HA3	1.75	0.68
1:G:450:ILE:HG22	1:G:454:ILE:HD12	1.74	0.68
1:G:1040:VAL:HA	1:G:1073:GLN:NE2	2.07	0.68
1:H:1063:LEU:HD22	1:H:1074:MET:HE3	1.75	0.68
1:G:536:ARG:NH1	1:G:872:SER:O	2.26	0.68
1:A:435:ARG:NH2	1:A:438:ASP:O	2.25	0.68
1:F:993:ASN:OD1	1:F:994:ALA:N	2.27	0.68
1:G:437:GLN:NE2	1:G:1112:CYS:SG	2.67	0.68
1:H:980:LEU:HD23	1:H:980:LEU:H	1.58	0.68
1:C:753:MET:HA	1:C:756:LYS:HD2	1.75	0.68
1:C:966:ARG:HH11	1:C:974:THR:HG23	1.58	0.68
1:F:479:PHE:CZ	1:F:838:ILE:HG22	2.20	0.68
1:B:437:GLN:HE22	1:B:1112:CYS:H	1.41	0.68
1:C:492:GLN:HG2	1:C:493:ILE:HG23	1.75	0.68
1:A:1080:ASP:HB3	1:A:1083:VAL:HG23	1.76	0.67
1:F:424:TRP:CG	1:F:664:SER:OG	2.47	0.67
1:H:343:ARG:NH1	1:H:573:ARG:HH12	1.90	0.67
1:H:896:THR:O	1:H:900:SER:OG	2.12	0.67
1:H:999:ARG:NH1	1:H:1003:MET:O	2.28	0.67
1:F:848:ILE:O	1:F:852:VAL:HG23	1.94	0.67
1:B:435:ARG:HH21	1:B:438:ASP:HB2	1.58	0.67
1:G:1075:GLN:HE22	1:G:1103:GLY:HA2	1.59	0.67
1:H:362:ARG:HH21	1:H:417:SER:HA	1.58	0.67
1:H:400:ASP:N	1:H:573:ARG:HH21	1.92	0.67
1:B:403:ILE:O	1:B:655:LYS:HD2	1.93	0.67
1:H:390:CYS:HB3	1:H:553:TYR:HB2	1.76	0.67
1:H:957:ILE:HD12	1:H:958:THR:H	1.57	0.67
1:H:1086:LYS:HG2	1:H:1089:GLN:OE1	1.94	0.67
1:D:650:GLN:O	1:D:654:ILE:HG13	1.94	0.67
1:E:752:MET:HE2	1:E:1033:GLU:HA	1.76	0.67
1:H:1095:ARG:HG2	1:H:1095:ARG:HH11	1.60	0.67
1:E:913:LYS:HG3	1:E:914:TYR:CZ	2.29	0.66
1:E:933:LEU:O	1:E:936:ASP:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:613:GLU:O	1:F:615:GLN:HG2	1.96	0.66
1:D:1075:GLN:HE22	1:D:1103:GLY:N	1.90	0.66
1:F:835:ILE:O	1:F:838:ILE:HG12	1.95	0.66
1:H:510:LYS:HB3	1:H:514:GLY:HA3	1.76	0.66
1:E:696:LEU:O	1:E:700:ILE:HG12	1.96	0.66
1:D:627:CYS:HA	1:D:630:MET:HE2	1.77	0.66
1:H:945:ASN:HB3	1:H:1018:GLN:HG3	1.78	0.66
1:C:429:LEU:HD22	1:C:447:LYS:HB2	1.76	0.66
1:G:714:LEU:HD23	1:G:733:VAL:HG11	1.77	0.66
1:H:369:VAL:HG21	1:H:385:ALA:HA	1.77	0.66
1:G:364:LEU:HD12	1:G:365:ALA:N	2.11	0.66
1:E:934:ARG:CZ	1:E:1000:LEU:HD21	2.26	0.66
1:F:621:GLY:HA2	1:F:767:CYS:HB2	1.78	0.66
1:F:749:HIS:HA	1:F:752:MET:HG2	1.78	0.66
1:G:698:TYR:CD1	1:G:729:LYS:HD3	2.31	0.66
1:H:360:ILE:O	1:H:363:ALA:N	2.29	0.66
1:A:466:ILE:HD12	1:A:856:VAL:HG11	1.78	0.65
1:A:897:TYR:CE1	1:A:957:ILE:HG21	2.31	0.65
1:C:882:MET:HG2	1:C:883:VAL:HG23	1.77	0.65
1:D:640:LEU:HD21	1:D:648:LEU:HD12	1.78	0.65
1:B:1100:ARG:NH1	1:B:1103:GLY:CA	2.59	0.65
1:E:346:ARG:NH1	1:E:400:ASP:OD2	2.28	0.65
1:G:722:SER:OG	3:G:1301:HOH:O	2.13	0.65
1:D:897:TYR:CE2	1:D:957:ILE:HG21	2.31	0.65
1:G:598:ALA:HB2	1:G:630:MET:HE3	1.79	0.65
1:H:850:GLN:HE22	1:H:970:MET:HB3	1.61	0.65
1:A:773:GLU:OE2	1:A:980:LEU:HD13	1.97	0.65
1:C:1093:LYS:HD2	1:C:1094:TYR:CE2	2.30	0.65
1:B:362:ARG:NH2	1:B:417:SER:HB3	2.11	0.65
1:C:913:LYS:NZ	1:C:936:ASP:OD2	2.26	0.65
1:E:1040:VAL:HA	1:E:1073:GLN:HG2	1.79	0.65
1:G:342:PRO:HA	1:G:345:GLN:NE2	2.12	0.65
1:D:351:TYR:HH	1:D:710:TYR:HE1	1.40	0.65
1:D:632:GLU:O	1:D:636:ARG:HG2	1.97	0.65
1:H:771:CYS:HB3	1:H:1103:GLY:HA3	1.79	0.65
1:E:649:LEU:O	1:E:653:ILE:HG13	1.96	0.65
1:E:1020:PRO:HG3	1:E:1128:PHE:HA	1.79	0.65
1:H:733:VAL:HG13	1:H:741:PRO:HD3	1.79	0.65
1:A:428:GLU:HG2	1:A:432:MET:HG3	1.78	0.65
1:H:806:LEU:HD22	1:H:991:LEU:HA	1.79	0.65
1:C:488:LEU:HD23	1:C:787:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:981:SER:HG	1:F:1008:GLY:H	1.42	0.64
1:H:423:ARG:NH2	1:H:468:GLU:OE1	2.27	0.64
1:A:488:LEU:HD13	1:A:845:GLY:HA3	1.77	0.64
1:C:955:LEU:HD22	1:C:1029:LYS:HE3	1.79	0.64
1:G:623:VAL:HG12	1:G:626:TYR:CZ	2.32	0.64
1:H:443:SER:HB2	1:H:446:ASP:HB2	1.80	0.64
1:H:509:THR:HG23	1:H:510:LYS:HG3	1.78	0.64
1:H:678:ILE:CG2	1:H:712:PRO:HB3	2.28	0.64
1:A:641:THR:N	1:A:644:THR:OG1	2.28	0.64
1:C:1044:LYS:N	3:C:1302:HOH:O	2.29	0.64
1:E:742:ALA:HB2	1:E:1100:ARG:NH2	2.12	0.64
1:E:748:SER:OG	1:E:1071:ASN:O	2.14	0.64
1:H:854:ARG:HA	1:H:877:ALA:HB1	1.77	0.64
1:A:708:LYS:HE2	1:A:736:ALA:HB1	1.79	0.64
1:B:714:LEU:HD23	1:B:741:PRO:HB3	1.80	0.64
1:F:444:GLU:OE2	1:F:447:LYS:NZ	2.21	0.64
1:A:984:ASN:HA	1:A:987:PRO:HD2	1.78	0.64
1:B:395:ILE:HD11	1:B:556:ARG:CZ	2.26	0.64
1:C:637:GLU:OE1	1:C:639:ARG:NH1	2.29	0.64
1:D:962:GLU:HB2	1:D:977:HIS:CE1	2.32	0.64
1:E:730:ILE:O	1:E:734:VAL:HG23	1.97	0.64
1:H:650:GLN:HA	1:H:653:ILE:HG12	1.79	0.64
1:H:680:LEU:O	1:H:715:ALA:N	2.29	0.64
1:F:412:ARG:HB2	1:F:660:MET:HE2	1.80	0.64
1:F:905:ARG:HD3	1:F:953:TYR:HH	1.61	0.64
1:C:523:LEU:HD11	1:C:537:ILE:HG23	1.80	0.64
1:C:703:ALA:O	1:C:707:VAL:HG22	1.98	0.64
1:D:798:VAL:HG21	1:D:831:VAL:HG12	1.80	0.64
1:C:921:ASP:HA	1:C:924:LEU:HD12	1.81	0.63
1:D:696:LEU:O	1:D:700:ILE:HG13	1.98	0.63
1:H:360:ILE:HD11	1:H:446:ASP:HB3	1.79	0.63
1:H:512:MET:HE3	1:H:588:PRO:HG2	1.80	0.63
1:H:596:GLN:HG2	1:H:648:LEU:HD11	1.80	0.63
1:E:913:LYS:NZ	1:E:936:ASP:OD2	2.31	0.63
1:E:1107:TYR:HB2	1:E:1110:GLU:HG3	1.80	0.63
1:G:623:VAL:HG12	1:G:626:TYR:OH	1.97	0.63
1:H:821:LEU:HD22	1:H:827:PHE:HA	1.79	0.63
1:H:343:ARG:HD3	1:H:400:ASP:O	1.98	0.63
1:A:530:ASN:HB3	1:A:532:GLU:HG3	1.79	0.63
1:G:713:SER:HA	1:G:740:PHE:CE1	2.33	0.63
1:B:748:SER:O	1:B:752:MET:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1049:LEU:HD11	1:E:1128:PHE:HE2	1.64	0.63
1:F:875:ASP:OD1	1:F:877:ALA:N	2.31	0.63
1:G:999:ARG:HH12	1:G:1005:LEU:HD23	1.63	0.63
1:D:1073:GLN:NE2	1:D:1075:GLN:OE1	2.31	0.63
1:F:1052:THR:HG21	1:F:1054:GLU:HG2	1.81	0.63
1:A:776:LYS:NZ	1:A:777:SER:O	2.32	0.62
1:A:999:ARG:NH1	1:A:1003:MET:O	2.31	0.62
1:E:1060:ILE:H	1:E:1060:ILE:HD12	1.65	0.62
1:H:343:ARG:HG2	1:H:347:LEU:HG	1.80	0.62
1:F:701:MET:HE3	1:F:730:ILE:HG12	1.81	0.62
1:F:813:LEU:HD11	1:F:837:HIS:HB2	1.81	0.62
1:F:896:THR:HG21	1:F:1005:LEU:HD23	1.81	0.62
1:F:947:ASP:O	1:F:950:VAL:HG12	1.99	0.62
1:G:775:GLN:HB3	1:G:780:ILE:HG21	1.81	0.62
1:H:727:MET:HB3	1:H:1060:ILE:HD12	1.79	0.62
1:H:896:THR:HG23	1:H:1006:SER:OG	1.99	0.62
1:D:905:ARG:HD3	1:D:949:TYR:OH	1.99	0.62
1:F:1073:GLN:NE2	1:F:1075:GLN:HG3	2.15	0.62
1:D:1080:ASP:O	1:D:1084:LEU:HD23	2.00	0.62
1:E:1049:LEU:HD11	1:E:1128:PHE:CE2	2.34	0.62
1:G:980:LEU:HD12	1:G:982:ILE:HG13	1.80	0.62
1:H:822:ARG:N	1:H:826:GLU:OE1	2.27	0.62
1:H:919:ILE:O	1:H:923:LEU:HD12	1.99	0.62
1:D:682:VAL:HG13	1:D:697:THR:HG23	1.82	0.62
1:G:462:SER:OG	1:G:465:GLU:OE1	2.17	0.62
1:D:985:ASN:HD22	1:D:1007:ASP:HA	1.65	0.62
1:E:813:LEU:O	1:E:834:GLN:NE2	2.33	0.62
1:H:358:VAL:HG21	1:H:432:MET:HE1	1.81	0.62
1:B:424:TRP:CE3	1:B:664:SER:HA	2.34	0.62
1:B:995:THR:HG23	1:B:999:ARG:HH21	1.65	0.62
1:C:376:MET:HG3	1:C:377:PRO:HD2	1.81	0.62
1:C:999:ARG:NH1	1:C:1003:MET:O	2.33	0.62
1:G:623:VAL:HG21	1:G:680:LEU:HD11	1.82	0.62
1:G:908:VAL:HG11	1:G:914:TYR:HB2	1.82	0.62
1:E:705:ARG:HG2	1:E:736:ALA:HB2	1.81	0.62
1:F:694:ASN:H	1:F:697:THR:HG23	1.65	0.62
1:H:540:TYR:OH	1:H:870:MET:O	2.15	0.62
1:C:718:ILE:HD12	1:C:743:CYS:HB3	1.82	0.61
1:G:1032:VAL:HB	1:G:1039:MET:HE2	1.82	0.61
1:D:819:ARG:O	1:D:822:ARG:NH1	2.32	0.61
1:F:599:LEU:HD11	1:F:649:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1081:ASN:HA	1:F:1084:LEU:HD12	1.81	0.61
1:G:620:LEU:HD22	1:G:680:LEU:HD12	1.81	0.61
1:A:526:LEU:HD21	1:A:536:ARG:HH21	1.62	0.61
1:E:546:THR:HG21	1:E:860:PRO:HB2	1.83	0.61
1:F:362:ARG:NH2	1:F:612:GLU:O	2.29	0.61
1:F:739:GLY:HA3	1:F:1100:ARG:HB2	1.82	0.61
1:F:975:LEU:HD13	1:F:976:SER:N	2.15	0.61
1:G:607:SER:OG	1:G:608:LEU:N	2.32	0.61
1:H:954:ALA:O	1:H:958:THR:OG1	2.11	0.61
1:F:797:PHE:O	1:F:802:GLY:N	2.33	0.61
1:H:993:ASN:OD1	1:H:994:ALA:N	2.34	0.61
1:H:382:ARG:NH1	1:H:419:ASP:OD2	2.34	0.61
1:E:476:VAL:HG12	1:E:841:LEU:HG	1.83	0.61
1:F:815:THR:HG23	1:F:834:GLN:HE21	1.66	0.61
1:H:430:ASP:OD1	1:H:447:LYS:NZ	2.31	0.61
1:E:641:THR:H	1:E:644:THR:HG1	1.46	0.61
1:E:962:GLU:OE1	1:E:977:HIS:ND1	2.26	0.61
1:F:828:ASP:OD1	1:F:832:LYS:HE2	2.01	0.61
1:F:984:ASN:HB2	1:F:988:ILE:HG13	1.81	0.61
1:A:958:THR:HG21	1:A:1030:MET:CE	2.30	0.61
1:C:368:GLU:HA	1:C:371:LYS:HG2	1.81	0.61
1:E:753:MET:HE3	1:E:774:PRO:HB2	1.82	0.61
1:F:1052:THR:CG2	1:F:1054:GLU:HG2	2.30	0.61
1:C:432:MET:HA	1:C:435:ARG:HD2	1.83	0.61
1:D:1013:GLN:HB2	1:D:1122:ARG:HA	1.83	0.61
1:E:772:VAL:HG11	1:E:1040:VAL:HB	1.83	0.60
1:E:776:LYS:HD2	1:E:779:ARG:HD2	1.83	0.60
1:F:704:VAL:HG21	1:F:714:LEU:HD22	1.82	0.60
1:H:370:VAL:HG21	1:H:458:TRP:CZ2	2.35	0.60
1:H:650:GLN:HB3	1:H:707:VAL:HG21	1.83	0.60
1:H:960:TRP:O	1:H:963:LYS:HG3	2.01	0.60
1:E:647:GLU:HA	1:E:650:GLN:HE21	1.64	0.60
1:E:969:LYS:H	1:E:969:LYS:HE2	1.65	0.60
1:H:450:ILE:HD12	1:H:454:ILE:HB	1.82	0.60
1:H:576:GLU:O	1:H:579:THR:OG1	2.14	0.60
1:H:624:ASP:OD2	1:H:683:GLY:N	2.32	0.60
1:C:650:GLN:HB3	1:C:707:VAL:HG11	1.81	0.60
1:C:851:ARG:NH2	1:G:535:ASP:OD1	2.31	0.60
1:D:1032:VAL:HB	1:D:1039:MET:HE1	1.81	0.60
1:F:832:LYS:HD3	1:F:960:TRP:CE2	2.36	0.60
1:G:422:TRP:CZ2	1:G:459:GLU:HA	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:LYS:O	1:G:451:ARG:HG3	2.00	0.60
1:G:739:GLY:HA3	1:G:1100:ARG:HB2	1.83	0.60
1:H:416:PHE:CE2	1:H:450:ILE:HD13	2.36	0.60
1:D:416:PHE:CE1	1:D:425:VAL:HG11	2.37	0.60
1:D:1046:LEU:HD22	1:D:1126:GLU:HG2	1.83	0.60
1:F:805:VAL:HG21	1:F:993:ASN:HB2	1.82	0.60
1:H:422:TRP:NE1	1:H:458:TRP:O	2.35	0.60
1:H:641:THR:N	1:H:644:THR:OG1	2.34	0.60
1:H:1063:LEU:HD22	1:H:1074:MET:CE	2.32	0.60
1:C:478:ALA:HA	1:C:482:GLU:HB2	1.84	0.60
1:D:600:GLN:HE21	1:D:604:THR:HG23	1.65	0.60
1:H:486:SER:HA	1:H:789:THR:HB	1.84	0.60
1:A:354:VAL:HG11	1:A:411:PRO:HB2	1.82	0.60
1:E:487:ASP:O	1:E:787:GLY:HA2	2.01	0.60
1:F:685:GLN:H	1:F:717:ARG:NH2	2.00	0.60
1:G:698:TYR:CZ	1:G:725:LYS:HD3	2.37	0.60
1:G:908:VAL:HG12	1:G:914:TYR:H	1.67	0.60
1:H:404:VAL:HA	1:H:655:LYS:HE2	1.82	0.60
1:B:446:ASP:O	1:B:449:THR:OG1	2.19	0.60
1:C:489:SER:O	1:C:493:ILE:HG12	2.01	0.60
1:C:798:VAL:HG21	1:C:831:VAL:HG22	1.83	0.60
1:D:1021:THR:HA	1:D:1024:ILE:HG12	1.83	0.60
1:D:1044:LYS:NZ	1:D:1120:ILE:O	2.35	0.60
1:E:562:ARG:HH22	1:E:585:GLU:HG3	1.65	0.60
1:G:743:CYS:HB2	1:G:1074:MET:O	2.02	0.60
1:H:1013:GLN:NE2	1:H:1118:GLU:OE2	2.35	0.60
1:E:610:GLU:HG3	1:E:659:LEU:HD11	1.82	0.60
1:E:917:GLU:HA	1:E:920:ARG:CD	2.27	0.60
1:G:416:PHE:HE1	1:G:425:VAL:HG21	1.66	0.60
1:G:466:ILE:HD13	1:G:856:VAL:HG21	1.83	0.60
1:H:488:LEU:HD23	1:H:787:GLY:HA3	1.83	0.60
1:B:993:ASN:O	1:B:999:ARG:NH2	2.35	0.60
1:F:465:GLU:O	1:F:468:GLU:HB3	2.02	0.60
1:A:572:GLN:O	1:A:575:ALA:N	2.35	0.60
1:D:570:ASN:OD1	1:D:572:GLN:N	2.35	0.60
1:G:340:LEU:HB3	1:G:345:GLN:OE1	2.01	0.60
1:H:777:SER:O	1:H:779:ARG:N	2.34	0.60
1:H:980:LEU:HD12	1:H:982:ILE:HD11	1.83	0.60
1:A:623:VAL:HG23	1:A:627:CYS:SG	2.41	0.59
1:C:848:ILE:O	1:C:852:VAL:HG12	2.02	0.59
1:F:726:TYR:O	1:F:730:ILE:HG13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1112:CYS:HB3	1:F:1115:VAL:H	1.66	0.59
1:G:623:VAL:CG2	1:G:680:LEU:HD21	2.27	0.59
1:H:849:SER:HA	1:H:852:VAL:HG22	1.84	0.59
1:C:835:ILE:HD13	1:C:957:ILE:HD11	1.82	0.59
1:D:599:LEU:HD22	1:D:652:PHE:CG	2.37	0.59
1:F:694:ASN:H	1:F:697:THR:CG2	2.14	0.59
1:H:624:ASP:HB3	1:H:682:VAL:HG23	1.84	0.59
1:H:845:GLY:HA2	1:H:848:ILE:HD12	1.84	0.59
1:A:432:MET:HE3	1:A:440:PHE:HB2	1.84	0.59
1:B:850:GLN:NE2	1:B:887:PRO:HD3	2.17	0.59
1:D:650:GLN:OE1	1:D:707:VAL:HG13	2.02	0.59
1:G:347:LEU:HB3	1:G:654:ILE:HD13	1.82	0.59
1:H:594:THR:OG1	1:H:595:LEU:N	2.35	0.59
1:H:852:VAL:O	1:H:856:VAL:HG12	2.01	0.59
1:F:955:LEU:HD13	1:F:1030:MET:HA	1.82	0.59
1:C:488:LEU:HD13	1:C:845:GLY:HA3	1.85	0.59
1:H:1091:PRO:HG2	1:H:1092:GLU:OE1	2.02	0.59
1:G:1064:ARG:O	1:G:1068:ILE:HD12	2.02	0.59
1:H:341:THR:HG22	1:H:343:ARG:H	1.67	0.59
1:H:344:MET:HE3	1:H:650:GLN:HB2	1.85	0.59
1:A:790:GLN:NE2	1:A:793:ILE:HB	2.16	0.59
1:B:698:TYR:CZ	1:B:725:LYS:HD3	2.38	0.59
1:D:797:PHE:HE1	1:D:804:MET:HB2	1.68	0.59
1:D:999:ARG:NH1	1:D:1003:MET:O	2.35	0.59
1:E:805:VAL:HG11	1:E:993:ASN:CB	2.31	0.59
1:F:730:ILE:O	1:F:734:VAL:HG23	2.03	0.59
1:H:981:SER:OG	1:H:985:ASN:HB3	2.03	0.59
1:H:1044:LYS:HB3	1:H:1123:THR:O	2.02	0.59
1:A:505:VAL:HG13	1:A:506:LEU:HG	1.85	0.59
1:F:369:VAL:O	1:F:373:ASN:ND2	2.36	0.59
1:F:935:ARG:O	1:F:939:ASN:ND2	2.35	0.59
1:H:443:SER:HB2	1:H:446:ASP:H	1.66	0.59
1:C:934:ARG:HH11	1:C:938:LEU:CD1	2.01	0.59
1:E:742:ALA:HB2	1:E:1100:ARG:HH21	1.68	0.59
1:F:351:TYR:OH	1:F:412:ARG:NH1	2.35	0.59
1:F:1027:VAL:HG23	1:F:1071:ASN:ND2	2.18	0.59
1:G:350:HIS:NE2	1:G:398:GLN:OE1	2.32	0.59
1:H:705:ARG:HB3	1:H:733:VAL:HG23	1.85	0.59
1:D:1075:GLN:NE2	1:D:1103:GLY:H	1.96	0.59
1:G:419:ASP:OD1	1:G:419:ASP:N	2.36	0.59
1:H:790:GLN:NE2	1:H:793:ILE:HB	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ALA:O	1:E:367:THR:OG1	2.18	0.58
1:F:862:MET:O	1:F:866:VAL:HG23	2.03	0.58
1:A:771:CYS:HB3	1:A:1103:GLY:HA3	1.86	0.58
1:A:786:THR:N	3:A:1302:HOH:O	2.31	0.58
1:B:871:GLU:OE1	1:B:871:GLU:N	2.35	0.58
1:C:750:ILE:HD11	1:C:764:ARG:HG2	1.85	0.58
1:C:759:ASP:OD1	1:C:760:PHE:N	2.36	0.58
1:F:435:ARG:HG3	1:F:665:GLU:HG2	1.84	0.58
1:H:423:ARG:HH11	1:H:465:GLU:HG2	1.68	0.58
1:H:935:ARG:HA	1:H:938:LEU:H	1.68	0.58
1:A:504:ASP:HB3	1:A:626:TYR:CD2	2.37	0.58
1:A:803:ARG:HB2	1:A:810:TYR:CE1	2.38	0.58
1:F:806:LEU:HD12	1:F:807:PHE:CD1	2.38	0.58
1:G:898:VAL:HG11	1:G:954:ALA:HB2	1.85	0.58
1:G:1047:LYS:HA	1:G:1078:TYR:CE1	2.38	0.58
1:H:527:SER:O	1:H:537:ILE:HD11	2.03	0.58
1:B:432:MET:HG2	1:B:440:PHE:HB2	1.85	0.58
1:E:420:ILE:HD11	1:E:614:ASN:HB3	1.85	0.58
1:H:792:PRO:HG3	1:H:896:THR:OG1	2.03	0.58
1:H:896:THR:HG23	1:H:1006:SER:H	1.69	0.58
1:C:934:ARG:NH1	1:C:938:LEU:CD1	2.57	0.58
1:F:799:LEU:HA	1:F:818:LEU:HD21	1.85	0.58
1:F:1125:ILE:H	1:F:1125:ILE:HD12	1.66	0.58
1:H:599:LEU:HD23	1:H:652:PHE:HB3	1.86	0.58
1:F:486:SER:HB2	1:F:789:THR:HB	1.85	0.58
1:G:364:LEU:HD12	1:G:365:ALA:H	1.68	0.58
1:G:703:ALA:O	1:G:707:VAL:HG22	2.04	0.58
1:C:801:ARG:HE	1:C:816:GLY:C	2.06	0.58
1:F:516:LYS:O	1:F:520:GLU:HG2	2.03	0.58
1:F:806:LEU:HD12	1:F:807:PHE:CZ	2.39	0.58
1:H:345:GLN:O	1:H:349:ASN:N	2.31	0.58
1:H:614:ASN:ND2	1:H:662:MET:HB2	2.19	0.58
1:B:752:MET:CE	1:B:774:PRO:HG2	2.33	0.58
1:C:504:ASP:N	1:C:504:ASP:OD1	2.35	0.58
1:E:356:PRO:HG3	1:E:412:ARG:HH11	1.67	0.58
1:E:1042:ASN:OD1	1:E:1075:GLN:NE2	2.37	0.58
1:F:1000:LEU:H	1:F:1000:LEU:HD12	1.69	0.58
1:C:362:ARG:HH21	1:C:613:GLU:HA	1.69	0.58
1:C:1021:THR:O	1:C:1025:LYS:HG3	2.03	0.58
1:E:558:ALA:CB	1:E:585:GLU:HG2	2.34	0.58
1:E:738:MET:HG2	1:E:1098:ILE:HB	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1108:PHE:CZ	1:F:1116:GLN:HG2	2.38	0.57
1:G:411:PRO:HB3	1:G:658:GLU:HG3	1.86	0.57
1:G:512:MET:HE3	1:G:550:VAL:HG11	1.85	0.57
1:H:687:ARG:NH1	1:H:765:ASP:OD2	2.36	0.57
1:E:653:ILE:HG23	1:E:712:PRO:HD2	1.85	0.57
1:G:986:THR:HG21	1:G:1115:VAL:HA	1.86	0.57
1:D:1095:ARG:HA	1:D:1109:VAL:HG21	1.87	0.57
1:E:1111:LEU:O	1:E:1116:GLN:NE2	2.37	0.57
1:F:796:GLU:OE1	3:F:1302:HOH:O	2.17	0.57
1:H:512:MET:SD	1:H:550:VAL:HG21	2.44	0.57
1:A:497:GLY:N	1:A:615:GLN:OE1	2.34	0.57
1:D:403:ILE:HD13	1:D:652:PHE:HB2	1.85	0.57
1:E:682:VAL:HG13	1:E:697:THR:HG23	1.86	0.57
1:H:435:ARG:NH2	1:H:438:ASP:O	2.28	0.57
1:H:437:GLN:HG3	1:H:438:ASP:N	2.19	0.57
1:C:483:THR:HB	1:C:804:MET:CE	2.32	0.57
1:C:527:SER:OG	1:C:529:GLU:HG2	2.04	0.57
1:D:653:ILE:HG21	1:D:707:VAL:HG21	1.87	0.57
1:E:489:SER:HA	1:E:492:GLN:HB3	1.86	0.57
1:G:371:LYS:HG3	1:G:457:PHE:CE1	2.40	0.57
1:G:407:PRO:HG3	1:G:608:LEU:HD12	1.87	0.57
1:H:370:VAL:HG23	1:H:371:LYS:H	1.69	0.57
1:A:980:LEU:HD23	1:A:980:LEU:H	1.69	0.57
1:B:487:ASP:O	1:B:787:GLY:HA2	2.04	0.57
1:C:776:LYS:HD2	1:C:779:ARG:HD2	1.86	0.57
1:E:1095:ARG:HA	1:E:1109:VAL:HG21	1.86	0.57
1:G:348:ARG:NH2	1:G:708:LYS:HB2	2.02	0.57
1:H:437:GLN:HE22	1:H:1111:LEU:HA	1.70	0.57
1:A:815:THR:CG2	1:A:834:GLN:HE21	2.17	0.57
1:F:546:THR:OG1	1:F:864:LEU:HD11	2.04	0.57
1:H:358:VAL:HB	1:H:442:ILE:HG22	1.86	0.57
1:A:986:THR:HB	1:A:987:PRO:HD3	1.86	0.57
1:C:1095:ARG:HA	1:C:1109:VAL:HG21	1.87	0.57
1:D:396:LEU:HD23	1:D:406:HIS:HB3	1.87	0.57
1:D:554:ALA:HB2	1:D:588:PRO:HD2	1.87	0.57
1:D:790:GLN:NE2	1:D:793:ILE:HB	2.19	0.57
1:D:1033:GLU:HB2	1:E:760:PHE:CZ	2.40	0.57
1:G:895:ALA:HA	1:G:898:VAL:HG22	1.85	0.57
1:G:1099:VAL:HG21	1:G:1108:PHE:CD1	2.40	0.57
1:H:599:LEU:HD23	1:H:652:PHE:CB	2.35	0.57
1:F:382:ARG:NH1	1:F:419:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:900:SER:HB3	1:F:996:PRO:HD2	1.85	0.57
1:F:986:THR:O	1:F:990:GLU:HG3	2.04	0.57
1:G:1042:ASN:ND2	1:G:1101:VAL:O	2.38	0.57
1:C:775:GLN:HB3	1:C:780:ILE:HG21	1.85	0.57
1:G:980:LEU:HD12	1:G:982:ILE:CG1	2.34	0.57
1:H:739:GLY:HA3	1:H:1100:ARG:HG2	1.86	0.57
1:A:1014:GLY:O	1:A:1017:LYS:HE2	2.05	0.56
1:C:948:ASN:HA	1:C:951:ASP:HB2	1.86	0.56
1:E:437:GLN:HA	1:E:437:GLN:HE21	1.70	0.56
1:E:650:GLN:HB2	1:E:707:VAL:HG11	1.87	0.56
1:E:803:ARG:HA	1:E:810:TYR:HA	1.87	0.56
1:B:1048:GLY:HA2	1:B:1051:ASP:OD2	2.05	0.56
1:C:1084:LEU:HD21	1:C:1099:VAL:HG21	1.86	0.56
1:F:818:LEU:H	1:F:818:LEU:HD12	1.69	0.56
1:F:906:LYS:HB2	1:F:949:TYR:OH	2.05	0.56
1:F:1044:LYS:HA	1:F:1077:SER:HB2	1.88	0.56
1:G:632:GLU:HG3	1:G:636:ARG:NH2	2.14	0.56
1:G:799:LEU:HB3	1:G:920:ARG:HG2	1.87	0.56
1:B:405:GLY:O	1:B:655:LYS:HE2	2.06	0.56
1:D:751:LYS:HA	1:D:754:LEU:HD12	1.86	0.56
1:G:708:LYS:HE2	1:G:738:MET:SD	2.45	0.56
1:G:722:SER:O	1:G:1064:ARG:NH2	2.38	0.56
1:H:479:PHE:CG	1:H:841:LEU:HD23	2.40	0.56
1:D:445:ALA:O	1:D:449:THR:HG23	2.05	0.56
1:F:927:PHE:CD1	1:F:934:ARG:HB2	2.40	0.56
1:G:717:ARG:HD2	1:G:766:TYR:CE1	2.41	0.56
1:H:522:HIS:O	1:H:525:SER:HB3	2.05	0.56
1:E:382:ARG:NH2	1:E:613:GLU:OE1	2.37	0.56
1:G:1025:LYS:O	1:G:1028:SER:OG	2.23	0.56
1:H:813:LEU:HD11	1:H:837:HIS:CB	2.36	0.56
1:H:828:ASP:CG	1:H:832:LYS:HZ3	2.09	0.56
1:C:851:ARG:HH22	1:G:535:ASP:CG	2.08	0.56
1:D:993:ASN:OD1	1:D:994:ALA:N	2.38	0.56
1:F:487:ASP:O	1:F:787:GLY:HA2	2.06	0.56
1:G:1127:LYS:O	1:G:1128:PHE:HD1	1.89	0.56
1:C:844:ILE:O	1:C:848:ILE:HG13	2.06	0.56
1:D:1080:ASP:OD1	1:D:1082:GLU:N	2.39	0.56
1:F:1049:LEU:HD11	1:F:1126:GLU:HA	1.87	0.56
1:G:829:ALA:O	1:G:833:GLN:HG2	2.05	0.56
1:H:400:ASP:N	1:H:573:ARG:NH2	2.52	0.56
1:C:1093:LYS:NZ	1:C:1094:TYR:CZ	2.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:948:ASN:O	1:G:948:ASN:ND2	2.34	0.56
1:H:799:LEU:HA	1:H:818:LEU:HD11	1.88	0.56
1:B:981:SER:HB3	1:B:1008:GLY:H	1.71	0.56
1:B:1046:LEU:HD22	1:B:1126:GLU:HG2	1.88	0.56
1:B:1084:LEU:HD23	1:B:1097:LEU:HD21	1.88	0.55
1:D:512:MET:SD	1:D:550:VAL:HG11	2.46	0.55
1:F:395:ILE:HD12	1:F:557:ILE:HD13	1.87	0.55
1:G:487:ASP:OD1	1:G:489:SER:HB3	2.06	0.55
1:G:608:LEU:HA	1:G:611:ILE:HG12	1.88	0.55
1:A:759:ASP:OD1	1:A:760:PHE:N	2.34	0.55
1:B:926:ASN:ND2	1:B:1001:ALA:HB3	2.21	0.55
1:C:348:ARG:HH21	1:C:708:LYS:HB2	1.71	0.55
1:D:905:ARG:O	1:D:910:GLU:HG3	2.07	0.55
1:D:986:THR:HB	1:D:987:PRO:HD3	1.88	0.55
1:D:1040:VAL:HA	1:D:1073:GLN:OE1	2.05	0.55
1:E:732:ASP:OD1	1:E:1056:ARG:NH2	2.34	0.55
1:H:713:SER:HA	1:H:740:PHE:CE1	2.41	0.55
1:A:682:VAL:HG21	1:A:700:ILE:HG21	1.89	0.55
1:C:423:ARG:HD3	1:C:464:ASP:OD2	2.07	0.55
1:C:480:SER:HB2	1:C:486:SER:O	2.06	0.55
1:F:748:SER:OG	1:F:1071:ASN:O	2.16	0.55
1:G:416:PHE:CE1	1:G:425:VAL:HG21	2.40	0.55
1:H:995:THR:OG1	1:H:997:ASN:OD1	2.24	0.55
1:F:887:PRO:HD2	1:F:970:MET:HE2	1.88	0.55
1:F:1127:LYS:HZ3	1:F:1128:PHE:HB2	1.72	0.55
1:G:677:PHE:HB3	1:G:770:GLY:HA2	1.88	0.55
1:H:423:ARG:HG3	3:H:1306:HOH:O	2.06	0.55
1:H:437:GLN:NE2	1:H:672:ALA:HB1	2.22	0.55
1:H:1088:GLN:HG2	1:H:1116:GLN:OE1	2.07	0.55
1:A:813:LEU:HD11	1:A:837:HIS:HB2	1.88	0.55
1:D:987:PRO:HA	1:D:990:GLU:HG3	1.88	0.55
1:G:694:ASN:N	1:G:697:THR:OG1	2.37	0.55
1:G:981:SER:HB3	1:G:1008:GLY:H	1.71	0.55
1:H:423:ARG:HH11	1:H:465:GLU:CG	2.19	0.55
1:H:1118:GLU:HA	1:H:1121:SER:OG	2.06	0.55
1:D:546:THR:HB	1:D:864:LEU:HD11	1.89	0.55
1:F:454:ILE:O	1:F:458:TRP:HD1	1.90	0.55
1:H:938:LEU:HG	1:H:998:GLY:HA3	1.87	0.55
1:H:1075:GLN:OE1	1:H:1100:ARG:NH2	2.36	0.55
1:C:850:GLN:NE2	3:C:1306:HOH:O	2.39	0.55
1:D:730:ILE:O	1:D:734:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:624:ASP:O	1:G:694:ASN:ND2	2.39	0.55
1:B:583:VAL:HG13	1:B:597:GLU:HG2	1.87	0.55
1:C:832:LYS:NZ	1:C:956:ASP:OD2	2.37	0.55
1:G:719:HIS:CD2	1:G:721:GLN:H	2.25	0.55
1:G:937:CYS:O	1:G:942:LYS:NZ	2.30	0.55
1:B:380:LEU:HA	1:B:542:ALA:HB2	1.87	0.55
1:C:485:VAL:O	1:C:789:THR:OG1	2.16	0.55
1:D:745:PHE:CD1	1:D:1067:SER:HB2	2.41	0.55
1:F:783:TRP:CH2	1:F:853:HIS:CD2	2.93	0.55
1:F:418:PRO:HA	1:F:421:ALA:O	2.07	0.54
1:F:641:THR:H	1:F:644:THR:HG1	1.54	0.54
1:H:500:CYS:SG	1:H:619:SER:HB2	2.46	0.54
1:H:828:ASP:OD1	1:H:832:LYS:NZ	2.39	0.54
1:B:999:ARG:NH1	1:B:1003:MET:O	2.40	0.54
1:C:487:ASP:O	1:C:787:GLY:HA2	2.06	0.54
1:F:926:ASN:HD21	1:F:1000:LEU:HD23	1.71	0.54
1:G:449:THR:O	1:G:453:GLU:HB2	2.08	0.54
1:H:653:ILE:HD11	1:H:707:VAL:HG21	1.88	0.54
1:B:500:CYS:SG	1:B:769:MET:HB2	2.47	0.54
1:C:344:MET:HE3	1:C:647:GLU:CG	2.33	0.54
1:C:749:HIS:HA	1:C:752:MET:HG2	1.89	0.54
1:G:1086:LYS:HE2	1:G:1094:TYR:OH	2.07	0.54
1:H:422:TRP:CE3	1:H:423:ARG:HA	2.42	0.54
1:H:641:THR:HG22	1:H:642:HIS:N	2.23	0.54
1:B:772:VAL:HG22	1:B:773:GLU:OE2	2.07	0.54
1:C:682:VAL:HG13	1:C:697:THR:HG23	1.90	0.54
1:D:655:LYS:NZ	1:D:658:GLU:OE2	2.30	0.54
1:D:980:LEU:HA	1:D:1040:VAL:HG12	1.89	0.54
1:E:369:VAL:HG21	1:E:385:ALA:HA	1.90	0.54
1:C:850:GLN:HE22	1:C:887:PRO:HD3	1.72	0.54
1:E:750:ILE:HD13	1:E:764:ARG:HG2	1.90	0.54
1:E:804:MET:HE1	1:E:807:PHE:HD2	1.71	0.54
1:G:1020:PRO:HD3	1:G:1127:LYS:HB2	1.88	0.54
1:F:622:ARG:HH11	1:F:765:ASP:HA	1.73	0.54
1:F:801:ARG:NE	1:F:816:GLY:O	2.39	0.54
1:F:849:SER:OG	1:F:850:GLN:N	2.41	0.54
1:F:898:VAL:HG13	1:F:953:TYR:HB2	1.90	0.54
1:G:354:VAL:HG11	1:G:411:PRO:O	2.08	0.54
1:B:1009:ILE:HG12	1:B:1040:VAL:O	2.08	0.54
1:C:599:LEU:HD22	1:C:652:PHE:CG	2.43	0.54
1:D:932:ALA:O	1:D:935:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:396:LEU:HD13	1:E:409:GLY:O	2.08	0.54
1:F:746:ASP:HB3	1:F:750:ILE:HD11	1.89	0.54
1:G:749:HIS:HA	1:G:752:MET:HG3	1.89	0.54
1:H:694:ASN:OD1	1:H:694:ASN:N	2.39	0.54
1:C:850:GLN:NE2	1:C:887:PRO:HD3	2.23	0.54
1:E:1041:HIS:H	1:E:1073:GLN:HG3	1.73	0.54
1:F:872:SER:HB3	1:F:874:LYS:H	1.73	0.54
1:F:979:THR:HG21	1:F:1035:MET:SD	2.48	0.54
1:H:818:LEU:HD23	1:H:821:LEU:HD12	1.90	0.54
1:H:981:SER:HB3	1:H:1008:GLY:H	1.73	0.54
1:B:1075:GLN:OE1	1:B:1100:ARG:HD3	2.08	0.54
1:D:600:GLN:NE2	1:D:604:THR:HG23	2.23	0.54
1:E:899:ASP:HB3	1:E:942:LYS:HG2	1.90	0.54
1:F:798:VAL:HG23	1:F:834:GLN:HG3	1.89	0.54
1:G:739:GLY:CA	1:G:1100:ARG:HB2	2.38	0.54
1:H:400:ASP:H	1:H:573:ARG:NH2	1.99	0.54
1:A:1075:GLN:NE2	1:A:1103:GLY:H	1.99	0.54
1:B:728:GLU:HG3	1:B:1056:ARG:HH21	1.72	0.54
1:C:561:ALA:HB3	1:C:581:ALA:HB2	1.89	0.54
1:D:478:ALA:HB1	1:D:811:GLN:HE22	1.72	0.54
1:E:574:ARG:HA	1:E:577:LEU:HD12	1.90	0.54
1:F:1080:ASP:HB3	1:F:1083:VAL:HG23	1.90	0.54
1:F:423:ARG:HG3	3:F:1319:HOH:O	2.08	0.53
1:F:990:GLU:HG2	1:F:1002:TRP:O	2.08	0.53
1:F:1020:PRO:HG3	1:F:1128:PHE:HD1	1.73	0.53
1:H:443:SER:CB	1:H:446:ASP:H	2.20	0.53
1:D:803:ARG:HA	1:D:810:TYR:HA	1.91	0.53
1:E:382:ARG:NH1	3:E:1303:HOH:O	2.41	0.53
1:F:442:ILE:HG23	1:F:447:LYS:HE3	1.89	0.53
1:F:1127:LYS:HD2	1:F:1128:PHE:H	1.73	0.53
1:G:504:ASP:HB3	1:G:626:TYR:CD2	2.43	0.53
1:G:573:ARG:HE	1:G:577:LEU:HD11	1.72	0.53
1:H:771:CYS:SG	1:H:982:ILE:HG12	2.47	0.53
1:C:993:ASN:ND2	1:C:994:ALA:H	2.07	0.53
1:D:934:ARG:NH1	1:D:938:LEU:HD21	2.23	0.53
1:F:394:PRO:HD2	1:F:407:PRO:O	2.07	0.53
1:E:516:LYS:NZ	1:E:548:GLU:OE2	2.29	0.53
1:E:705:ARG:HG3	1:E:733:VAL:HA	1.91	0.53
1:F:769:MET:SD	1:F:770:GLY:N	2.81	0.53
1:C:437:GLN:HE22	1:C:1111:LEU:HA	1.74	0.53
1:E:664:SER:OG	1:E:667:GLY:N	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:794:ALA:O	1:E:797:PHE:HB2	2.08	0.53
1:E:934:ARG:O	1:E:938:LEU:HG	2.08	0.53
1:E:980:LEU:HA	1:E:1040:VAL:HG12	1.89	0.53
1:F:756:LYS:NZ	1:F:782:GLN:HE22	2.07	0.53
1:F:1112:CYS:HB2	1:F:1115:VAL:HG23	1.90	0.53
1:G:404:VAL:O	1:G:600:GLN:NE2	2.41	0.53
1:G:483:THR:HG22	1:G:807:PHE:CD2	2.43	0.53
1:F:882:MET:HG2	1:F:883:VAL:HG23	1.91	0.53
1:G:536:ARG:HG2	1:G:873:GLY:HA3	1.89	0.53
1:H:405:GLY:H	1:H:655:LYS:HZ1	1.57	0.53
1:A:758:PHE:HE2	1:A:780:ILE:HD12	1.74	0.53
1:B:412:ARG:HH12	1:B:1095:ARG:HH22	1.55	0.53
1:D:632:GLU:HG2	1:D:636:ARG:HE	1.74	0.53
1:D:676:PRO:HB2	1:D:678:ILE:HG13	1.89	0.53
1:E:620:LEU:HD12	1:E:680:LEU:HD12	1.91	0.53
1:F:806:LEU:O	1:F:806:LEU:HD13	2.08	0.53
1:G:756:LYS:HG2	1:G:885:HIS:CE1	2.42	0.53
1:H:495:GLY:HA3	1:H:613:GLU:HG3	1.90	0.53
1:H:618:LEU:H	1:H:618:LEU:HD22	1.72	0.53
1:H:761:GLU:O	1:H:765:ASP:HB2	2.09	0.53
1:C:760:PHE:HB3	1:C:764:ARG:HH12	1.74	0.53
1:E:738:MET:HB3	1:E:1098:ILE:HG22	1.90	0.53
1:E:749:HIS:HA	1:E:752:MET:CG	2.39	0.53
1:F:989:GLY:CA	1:F:1005:LEU:HD11	2.39	0.53
1:B:437:GLN:NE2	1:B:1112:CYS:H	2.06	0.53
1:C:721:GLN:NE2	1:H:1069:LEU:HA	2.24	0.53
1:C:756:LYS:NZ	1:C:782:GLN:OE1	2.42	0.53
1:E:435:ARG:HG3	1:E:436:PRO:HD2	1.89	0.53
1:G:364:LEU:O	1:G:368:GLU:HG3	2.08	0.53
1:G:797:PHE:O	1:G:801:ARG:N	2.41	0.53
1:A:958:THR:HG21	1:A:1030:MET:HE3	1.89	0.53
1:A:1075:GLN:HE22	1:A:1103:GLY:N	2.00	0.53
1:C:622:ARG:HH11	1:C:765:ASP:HA	1.73	0.53
1:E:793:ILE:HD13	1:E:992:THR:HG23	1.91	0.53
1:F:437:GLN:HE22	1:F:1112:CYS:N	2.06	0.53
1:G:404:VAL:H	1:G:600:GLN:NE2	2.07	0.53
1:G:765:ASP:HB3	1:G:776:LYS:HD3	1.91	0.53
1:H:370:VAL:HG21	1:H:458:TRP:CH2	2.43	0.53
1:H:503:TYR:OH	1:H:606:GLU:OE1	2.26	0.53
1:A:758:PHE:HZ	1:A:780:ILE:HB	1.73	0.52
1:B:428:GLU:OE1	1:B:435:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:GLN:HB3	1:B:971:LEU:HD22	1.89	0.52
1:C:847:VAL:O	1:C:851:ARG:HB2	2.09	0.52
1:D:562:ARG:NH2	1:D:585:GLU:HG3	2.24	0.52
1:F:369:VAL:HG11	1:F:385:ALA:CB	2.38	0.52
1:F:693:CYS:HA	1:F:697:THR:HG21	1.90	0.52
1:F:1027:VAL:HG23	1:F:1071:ASN:HD21	1.74	0.52
1:G:1058:GLY:C	1:G:1128:PHE:CE2	2.82	0.52
1:G:1085:LYS:O	1:G:1089:GLN:NE2	2.42	0.52
1:H:352:LEU:HG	1:H:1095:ARG:HE	1.74	0.52
1:H:512:MET:HE1	1:H:550:VAL:HB	1.90	0.52
1:E:915:THR:O	1:E:919:ILE:HD12	2.08	0.52
1:H:586:ASN:O	1:H:590:ASN:HB2	2.09	0.52
1:B:348:ARG:HH21	1:B:708:LYS:HB2	1.74	0.52
1:B:513:ASN:OD1	1:B:589:ALA:HB1	2.09	0.52
1:C:737:GLY:HA2	1:C:1078:TYR:HB3	1.91	0.52
1:D:505:VAL:HG23	1:D:506:LEU:HG	1.91	0.52
1:F:982:ILE:O	1:F:1102:ALA:HB3	2.09	0.52
1:G:701:MET:HG2	1:G:714:LEU:HD21	1.90	0.52
1:H:740:PHE:CZ	1:H:1105:SER:HB2	2.44	0.52
1:H:908:VAL:HG23	1:H:914:TYR:O	2.10	0.52
1:A:973:SER:OG	1:A:974:THR:N	2.40	0.52
1:C:917:GLU:HG2	1:C:920:ARG:NH1	2.18	0.52
1:D:686:LYS:HB2	1:D:689:GLY:O	2.09	0.52
1:D:845:GLY:HA2	1:D:848:ILE:HD12	1.91	0.52
1:D:852:VAL:O	1:D:856:VAL:HG22	2.08	0.52
1:D:959:GLU:HA	1:D:1034:THR:HG21	1.91	0.52
1:D:1075:GLN:HE21	1:D:1100:ARG:HE	1.52	0.52
1:E:697:THR:O	1:E:701:MET:HG3	2.09	0.52
1:E:1095:ARG:HG3	1:E:1096:ASP:N	2.24	0.52
1:G:678:ILE:HG22	1:G:712:PRO:HB3	1.92	0.52
1:G:965:CYS:HB3	1:G:975:LEU:HG	1.91	0.52
1:G:1044:LYS:HE3	1:G:1124:VAL:HG13	1.91	0.52
1:H:496:GLY:N	1:H:613:GLU:OE2	2.41	0.52
1:B:948:ASN:HA	1:B:951:ASP:HB2	1.92	0.52
1:C:735:LYS:HE3	1:C:1051:ASP:OD1	2.09	0.52
1:D:803:ARG:HB2	1:D:810:TYR:CE2	2.44	0.52
1:F:618:LEU:HD22	1:F:618:LEU:H	1.74	0.52
1:G:940:ALA:O	1:G:942:LYS:NZ	2.42	0.52
1:A:602:ILE:HD11	1:A:626:TYR:HE1	1.74	0.52
1:F:792:PRO:HG2	1:F:1005:LEU:CD2	2.39	0.52
1:G:402:LEU:HD21	1:G:596:GLN:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:915:THR:OG1	1:G:918:GLN:HB2	2.10	0.52
1:H:739:GLY:HA2	1:H:1077:SER:HA	1.90	0.52
1:H:1091:PRO:O	1:H:1109:VAL:HG11	2.09	0.52
1:E:801:ARG:NH2	1:E:816:GLY:HA2	2.24	0.52
1:E:1052:THR:OG1	1:E:1055:GLY:N	2.38	0.52
1:G:683:GLY:HA3	1:G:726:TYR:OH	2.10	0.52
1:H:731:VAL:HG22	1:H:1059:LEU:HD22	1.91	0.52
1:A:380:LEU:HA	1:A:542:ALA:HB2	1.92	0.52
1:A:394:PRO:HB2	1:A:409:GLY:HA2	1.92	0.52
1:A:504:ASP:HB3	1:A:626:TYR:CG	2.45	0.52
1:D:350:HIS:O	1:D:353:THR:OG1	2.21	0.52
1:D:356:PRO:HG2	1:D:674:TYR:CZ	2.45	0.52
1:E:752:MET:O	1:E:756:LYS:HG3	2.10	0.52
1:G:423:ARG:NH1	1:G:465:GLU:HG3	2.25	0.52
1:G:516:LYS:HE3	1:G:544:ILE:HG23	1.92	0.52
1:H:904:ILE:O	1:H:908:VAL:HG12	2.09	0.52
1:B:341:THR:HG21	1:B:647:GLU:HG3	1.91	0.52
1:C:486:SER:HA	1:C:789:THR:HB	1.92	0.52
1:D:796:GLU:OE1	1:D:805:VAL:HG23	2.09	0.52
1:D:1010:SER:HA	1:D:1041:HIS:CE1	2.45	0.52
1:F:952:GLN:HG3	1:F:953:TYR:CD1	2.45	0.52
1:F:971:LEU:HD23	1:F:972:TYR:CZ	2.45	0.52
1:G:412:ARG:HH11	1:G:412:ARG:HG3	1.73	0.52
1:G:432:MET:HB3	1:G:440:PHE:H	1.73	0.52
1:G:710:TYR:HB3	1:G:1107:TYR:CE1	2.45	0.52
1:G:762:ASP:OD1	1:G:779:ARG:NH1	2.43	0.52
1:H:904:ILE:HG23	1:H:908:VAL:CG1	2.39	0.52
1:A:682:VAL:HG13	1:A:697:THR:HG23	1.92	0.52
1:B:500:CYS:HG	1:B:767:CYS:HG	1.58	0.52
1:D:485:VAL:O	1:D:789:THR:OG1	2.26	0.52
1:D:1090:GLU:OE2	1:D:1093:LYS:NZ	2.43	0.52
1:E:624:ASP:HA	1:E:696:LEU:HD23	1.92	0.52
1:H:1101:VAL:HB	1:H:1104:TYR:CZ	2.44	0.52
1:E:356:PRO:HG3	1:E:412:ARG:NH1	2.25	0.51
1:E:380:LEU:HA	1:E:542:ALA:HB2	1.92	0.51
1:E:927:PHE:CD1	1:E:934:ARG:HB2	2.44	0.51
1:G:362:ARG:HG3	1:G:611:ILE:HA	1.91	0.51
1:G:604:THR:CA	1:G:607:SER:HB3	2.34	0.51
1:G:697:THR:HG22	1:G:701:MET:HE1	1.92	0.51
1:H:727:MET:HG3	1:H:1064:ARG:NH2	2.24	0.51
1:H:771:CYS:HB2	1:H:772:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1100:ARG:HH11	1:B:1104:TYR:N	2.04	0.51
1:D:948:ASN:HA	1:D:951:ASP:HB2	1.92	0.51
1:G:587:VAL:HB	1:G:601:SER:HB2	1.92	0.51
1:G:908:VAL:HB	1:G:914:TYR:O	2.09	0.51
1:H:347:LEU:HD21	1:H:400:ASP:C	2.31	0.51
1:H:453:GLU:O	1:H:453:GLU:CD	2.43	0.51
1:H:785:SER:OG	1:H:787:GLY:O	2.26	0.51
1:C:530:ASN:HB3	1:C:532:GLU:OE1	2.11	0.51
1:C:906:LYS:HA	1:C:910:GLU:HB2	1.92	0.51
1:F:599:LEU:HD22	1:F:652:PHE:CG	2.46	0.51
1:F:785:SER:HA	1:F:888:GLY:O	2.10	0.51
1:F:980:LEU:HD12	1:F:982:ILE:CG1	2.38	0.51
1:H:457:PHE:O	1:H:461:ARG:NE	2.33	0.51
1:A:703:ALA:O	1:A:707:VAL:HG22	2.11	0.51
1:B:832:LYS:NZ	1:B:956:ASP:OD1	2.43	0.51
1:B:1116:GLN:O	1:B:1120:ILE:HG13	2.11	0.51
1:D:776:LYS:HD2	1:D:779:ARG:HD2	1.92	0.51
1:E:685:GLN:NE2	1:E:746:ASP:OD2	2.43	0.51
1:F:624:ASP:HB3	1:F:682:VAL:HG22	1.92	0.51
1:G:402:LEU:HD22	1:G:648:LEU:HD21	1.92	0.51
1:G:1020:PRO:HG3	1:G:1128:PHE:HA	1.92	0.51
1:C:419:ASP:HB3	1:C:458:TRP:CH2	2.45	0.51
1:D:348:ARG:O	1:D:352:LEU:HD12	2.11	0.51
1:D:673:GLY:O	1:D:675:GLN:NE2	2.31	0.51
1:E:1016:ASP:OD2	1:E:1023:ILE:HD11	2.10	0.51
1:A:927:PHE:HD2	1:A:1000:LEU:HD23	1.76	0.51
1:C:344:MET:CE	1:C:647:GLU:CG	2.89	0.51
1:C:1045:PHE:HB3	1:C:1049:LEU:HD23	1.92	0.51
1:E:419:ASP:HB3	1:E:458:TRP:CH2	2.46	0.51
1:B:680:LEU:HD21	1:B:700:ILE:HG21	1.93	0.51
1:D:775:GLN:HB3	1:D:780:ILE:HG21	1.92	0.51
1:F:343:ARG:HG3	1:F:400:ASP:HB3	1.92	0.51
1:G:694:ASN:O	1:G:697:THR:HB	2.11	0.51
1:H:775:GLN:HB3	1:H:780:ILE:HD13	1.92	0.51
1:H:1086:LYS:HB3	1:H:1089:GLN:OE1	2.10	0.51
1:E:824:PHE:CZ	1:E:953:TYR:HE2	2.29	0.51
1:F:756:LYS:HZ3	1:F:782:GLN:HE22	1.59	0.51
1:H:641:THR:HB	1:H:644:THR:H	1.76	0.51
1:H:677:PHE:HE1	1:H:1104:TYR:CD1	2.29	0.51
1:A:340:LEU:HB3	1:A:344:MET:HB3	1.93	0.51
1:E:793:ILE:HG13	1:E:797:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:613:GLU:OE2	1:G:859:LYS:NZ	2.38	0.51
1:G:935:ARG:HA	1:G:938:LEU:HB2	1.92	0.51
1:H:573:ARG:NH1	1:H:576:GLU:OE1	2.43	0.51
1:A:981:SER:O	1:A:982:ILE:O	2.28	0.51
1:B:617:GLY:HA2	1:B:677:PHE:O	2.10	0.51
1:C:984:ASN:O	1:C:988:ILE:HB	2.11	0.51
1:D:714:LEU:HD12	1:D:715:ALA:N	2.26	0.51
1:E:542:ALA:O	1:E:546:THR:HG23	2.10	0.51
1:H:366:PHE:O	1:H:370:VAL:HG22	2.10	0.51
1:A:818:LEU:HD13	1:A:916:LEU:HB3	1.93	0.50
1:B:362:ARG:HD2	1:B:611:ILE:O	2.11	0.50
1:D:480:SER:OG	1:D:481:GLY:N	2.44	0.50
1:E:420:ILE:HD12	1:E:493:ILE:O	2.11	0.50
1:E:731:VAL:CG2	1:E:1060:ILE:HD11	2.31	0.50
1:E:993:ASN:OD1	1:E:994:ALA:N	2.33	0.50
1:F:1075:GLN:HE22	1:F:1103:GLY:CA	2.14	0.50
1:F:1114:GLU:H	1:F:1114:GLU:CD	2.10	0.50
1:G:362:ARG:NH1	1:G:417:SER:HA	2.26	0.50
1:G:504:ASP:HB3	1:G:626:TYR:CG	2.46	0.50
1:G:911:GLU:HG2	1:G:913:LYS:HB2	1.94	0.50
1:H:504:ASP:OD1	1:H:777:SER:HB2	2.10	0.50
1:D:682:VAL:HB	1:D:714:LEU:HD11	1.93	0.50
1:E:396:LEU:HD21	1:E:398:GLN:HG2	1.92	0.50
1:E:522:HIS:HB3	1:E:540:TYR:CE2	2.47	0.50
1:E:685:GLN:H	1:E:717:ARG:NH2	2.10	0.50
1:G:468:GLU:O	1:G:472:ARG:HG3	2.10	0.50
1:G:743:CYS:O	1:G:1073:GLN:HA	2.11	0.50
1:H:447:LYS:HB2	1:H:448:LYS:HE3	1.94	0.50
1:E:902:ALA:HB1	1:E:949:TYR:CE2	2.47	0.50
1:E:997:ASN:OD1	1:E:998:GLY:N	2.44	0.50
1:G:948:ASN:HD21	1:G:952:GLN:HB3	1.75	0.50
1:H:576:GLU:HB2	1:H:577:LEU:HD12	1.92	0.50
1:B:343:ARG:HD3	1:B:400:ASP:O	2.11	0.50
1:B:986:THR:HG21	1:B:1114:GLU:HB3	1.92	0.50
1:B:1075:GLN:HE22	1:B:1103:GLY:HA2	1.76	0.50
1:E:796:GLU:OE2	1:E:805:VAL:N	2.39	0.50
1:E:909:PHE:HZ	1:E:916:LEU:HD11	1.77	0.50
1:F:722:SER:HB3	1:F:726:TYR:HD2	1.77	0.50
1:A:419:ASP:OD1	1:A:419:ASP:N	2.44	0.50
1:B:428:GLU:O	1:B:432:MET:HB2	2.12	0.50
1:D:437:GLN:HG3	1:D:668:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:LEU:HD22	1:F:409:GLY:O	2.12	0.50
1:F:1039:MET:SD	1:F:1072:GLY:HA3	2.52	0.50
1:H:1075:GLN:HE22	1:H:1103:GLY:H	1.58	0.50
1:A:1063:LEU:HD21	1:A:1076:PHE:HE2	1.77	0.50
1:B:370:VAL:HG22	1:B:381:LEU:HD21	1.94	0.50
1:D:1020:PRO:HA	1:D:1023:ILE:HD12	1.92	0.50
1:G:897:TYR:HE1	1:G:957:ILE:HG21	1.74	0.50
1:H:735:LYS:HA	1:H:1078:TYR:CD2	2.47	0.50
1:H:935:ARG:O	1:H:939:ASN:HB2	2.12	0.50
1:A:738:MET:HG3	1:A:1098:ILE:HB	1.94	0.50
1:B:660:MET:SD	1:B:674:TYR:HB3	2.51	0.50
1:E:1059:LEU:O	1:E:1062:LEU:N	2.44	0.50
1:E:1116:GLN:HA	1:E:1119:ILE:HD12	1.94	0.50
1:F:348:ARG:NH2	1:F:1096:ASP:OD1	2.44	0.50
1:G:450:ILE:HA	1:G:454:ILE:HB	1.94	0.50
1:G:728:GLU:HA	1:G:731:VAL:HG23	1.93	0.50
1:G:850:GLN:HB3	1:G:971:LEU:HD22	1.92	0.50
1:H:504:ASP:OD1	1:H:505:VAL:HG23	2.12	0.50
1:B:682:VAL:HG13	1:B:697:THR:HG23	1.93	0.50
1:C:443:SER:HB2	1:C:446:ASP:HB2	1.93	0.50
1:E:513:ASN:OD1	1:E:551:VAL:HG21	2.12	0.50
1:E:784:THR:HB	3:E:1309:HOH:O	2.12	0.50
1:F:797:PHE:HE1	1:F:804:MET:HA	1.77	0.50
1:G:560:HIS:O	1:G:564:LEU:HG	2.11	0.50
1:G:821:LEU:HD13	1:G:827:PHE:HD2	1.76	0.50
1:H:628:TYR:OH	1:H:632:GLU:HG3	2.12	0.50
1:H:655:LYS:HA	1:H:658:GLU:HG3	1.94	0.50
1:H:752:MET:HE2	1:H:1033:GLU:HA	1.91	0.50
1:B:705:ARG:HG3	1:B:733:VAL:HA	1.94	0.50
1:D:527:SER:OG	1:D:529:GLU:OE1	2.30	0.50
1:E:818:LEU:C	1:E:820:ASP:H	2.15	0.50
1:F:927:PHE:CD2	1:F:934:ARG:HD3	2.47	0.50
1:F:989:GLY:CA	1:F:1005:LEU:CD1	2.90	0.50
1:G:686:LYS:N	1:G:692:ALA:HB2	2.26	0.50
1:G:772:VAL:CG1	1:G:1040:VAL:HG12	2.39	0.50
1:G:854:ARG:HA	1:G:877:ALA:HB1	1.93	0.50
1:H:506:LEU:HD22	1:H:506:LEU:N	2.26	0.50
1:B:850:GLN:HE22	1:B:887:PRO:HD3	1.77	0.49
1:C:682:VAL:CG1	1:C:697:THR:HG23	2.42	0.49
1:C:813:LEU:HD13	1:C:837:HIS:CG	2.47	0.49
1:D:980:LEU:HD23	1:D:980:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:GLU:HG2	1:E:544:ILE:HD11	1.94	0.49
1:E:959:GLU:HA	1:E:1034:THR:HG21	1.93	0.49
1:G:403:ILE:HD12	1:G:600:GLN:HB2	1.94	0.49
1:G:915:THR:H	1:G:918:GLN:HB2	1.76	0.49
1:H:340:LEU:HD11	1:H:706:PHE:HB3	1.94	0.49
1:A:1042:ASN:ND2	1:A:1101:VAL:O	2.45	0.49
1:C:803:ARG:HD2	1:C:808:ASP:OD1	2.12	0.49
1:F:542:ALA:O	1:F:545:GLU:N	2.45	0.49
1:F:622:ARG:NH1	1:F:765:ASP:HA	2.28	0.49
1:G:516:LYS:HE2	1:G:520:GLU:OE2	2.12	0.49
1:A:612:GLU:OE2	1:A:862:MET:N	2.43	0.49
1:C:897:TYR:CZ	1:C:957:ILE:HD12	2.47	0.49
1:D:966:ARG:HH11	1:D:974:THR:HG23	1.78	0.49
1:F:989:GLY:O	1:F:999:ARG:NH2	2.46	0.49
1:F:1087:ALA:HA	1:F:1094:TYR:CD2	2.47	0.49
1:H:660:MET:HE1	1:H:674:TYR:HB3	1.95	0.49
1:H:694:ASN:ND2	1:H:696:LEU:HB3	2.27	0.49
1:H:1112:CYS:O	1:H:1116:GLN:HG2	2.12	0.49
1:C:362:ARG:NH2	1:C:613:GLU:HA	2.27	0.49
1:C:731:VAL:HG11	1:C:1056:ARG:HG2	1.94	0.49
1:D:507:LEU:HD12	1:D:507:LEU:O	2.12	0.49
1:E:358:VAL:HG23	1:E:358:VAL:O	2.13	0.49
1:E:720:ASN:HB2	1:E:721:GLN:OE1	2.12	0.49
1:F:798:VAL:CG2	1:F:831:VAL:HG12	2.31	0.49
1:F:1019:GLY:O	1:F:1023:ILE:HG13	2.12	0.49
1:G:504:ASP:OD1	1:G:504:ASP:N	2.45	0.49
1:H:420:ILE:O	1:H:463:LEU:HB3	2.12	0.49
1:H:609:PHE:CD1	1:H:861:LEU:HD23	2.47	0.49
1:H:986:THR:CB	1:H:1115:VAL:HG12	2.43	0.49
1:A:428:GLU:OE1	1:A:435:ARG:NH1	2.28	0.49
1:F:1041:HIS:CE1	1:F:1043:PHE:HE1	2.31	0.49
1:G:380:LEU:HA	1:G:542:ALA:HB2	1.93	0.49
1:G:587:VAL:HG11	1:G:592:PRO:HB3	1.93	0.49
1:G:896:THR:O	1:G:900:SER:OG	2.17	0.49
1:H:708:LYS:HG2	1:H:1098:ILE:HD12	1.93	0.49
1:H:744:HIS:HB3	1:H:749:HIS:CE1	2.47	0.49
1:A:995:THR:OG1	1:A:999:ARG:HB3	2.13	0.49
1:B:387:ARG:HD3	1:B:545:GLU:OE2	2.12	0.49
1:B:682:VAL:CG1	1:B:697:THR:HG23	2.42	0.49
1:C:827:PHE:O	1:C:831:VAL:HG23	2.12	0.49
1:D:850:GLN:HB3	1:D:971:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:ASP:OD1	1:E:419:ASP:N	2.38	0.49
1:F:376:MET:HB3	1:F:381:LEU:HD13	1.95	0.49
1:F:815:THR:HG23	1:F:834:GLN:NE2	2.28	0.49
1:F:975:LEU:HD13	1:F:976:SER:H	1.77	0.49
1:G:730:ILE:O	1:G:734:VAL:HG23	2.12	0.49
1:G:966:ARG:NH1	1:G:976:SER:HB2	2.27	0.49
1:B:708:LYS:HE2	1:B:736:ALA:HB1	1.94	0.49
1:C:477:TRP:O	1:C:481:GLY:N	2.46	0.49
1:D:407:PRO:HB2	1:D:611:ILE:HD11	1.94	0.49
1:D:615:GLN:HG3	1:D:618:LEU:HD21	1.95	0.49
1:D:687:ARG:HG3	1:D:765:ASP:HB2	1.94	0.49
1:D:823:THR:HG22	1:D:824:PHE:H	1.78	0.49
1:D:905:ARG:HD3	1:D:949:TYR:CZ	2.48	0.49
1:E:410:LYS:HG3	1:E:411:PRO:HD2	1.95	0.49
1:E:776:LYS:C	1:E:776:LYS:HD3	2.32	0.49
1:F:527:SER:OG	1:F:529:GLU:HG2	2.13	0.49
1:H:360:ILE:HD11	1:H:446:ASP:CB	2.42	0.49
1:C:1092:GLU:CD	1:C:1092:GLU:H	2.15	0.49
1:D:406:HIS:HE1	1:D:408:CYS:HB2	1.78	0.49
1:D:879:GLY:HA3	1:D:972:TYR:CD2	2.47	0.49
1:D:943:TYR:OH	1:D:1027:VAL:HG22	2.12	0.49
1:F:919:ILE:O	1:F:923:LEU:HG	2.13	0.49
1:F:1046:LEU:O	1:F:1049:LEU:HG	2.12	0.49
1:G:352:LEU:HD22	1:G:1095:ARG:HH12	1.77	0.49
1:G:376:MET:HB3	1:G:381:LEU:HD13	1.94	0.49
1:G:675:GLN:NE2	1:G:1104:TYR:CD2	2.81	0.49
1:G:744:HIS:HD2	1:G:749:HIS:NE2	2.10	0.49
1:G:895:ALA:HB3	1:G:1006:SER:CB	2.43	0.49
1:H:462:SER:HB3	1:H:465:GLU:OE1	2.12	0.49
1:B:613:GLU:OE2	1:B:859:LYS:NZ	2.46	0.49
1:B:981:SER:CB	1:B:1008:GLY:H	2.25	0.49
1:D:437:GLN:NE2	1:D:438:ASP:OD1	2.40	0.49
1:D:641:THR:N	1:D:644:THR:OG1	2.46	0.49
1:D:650:GLN:HB3	1:D:707:VAL:CG1	2.42	0.49
1:D:888:GLY:HA2	1:D:976:SER:O	2.13	0.49
1:E:752:MET:CE	1:E:1033:GLU:HA	2.43	0.49
1:F:719:HIS:CE1	1:F:721:GLN:HB2	2.47	0.49
1:F:984:ASN:HA	1:F:987:PRO:HD2	1.95	0.49
1:F:1083:VAL:HA	1:F:1086:LYS:HD2	1.95	0.49
1:G:763:ALA:O	1:G:766:TYR:HD2	1.95	0.49
1:H:408:CYS:SG	1:H:415:ALA:HB2	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:598:ALA:O	1:H:602:ILE:HG12	2.13	0.49
1:H:697:THR:HG22	1:H:701:MET:SD	2.52	0.49
1:H:789:THR:OG1	1:H:790:GLN:N	2.44	0.49
1:H:1043:PHE:HB2	1:H:1076:PHE:HD1	1.78	0.49
1:A:685:GLN:HG3	1:A:746:ASP:OD2	2.13	0.49
1:B:703:ALA:O	1:B:707:VAL:HG22	2.13	0.49
1:B:773:GLU:CD	1:B:980:LEU:HD22	2.33	0.49
1:C:679:ASN:OD1	1:C:680:LEU:N	2.46	0.49
1:D:632:GLU:HG2	1:D:636:ARG:NE	2.27	0.49
1:D:879:GLY:HA3	1:D:972:TYR:CE2	2.48	0.49
1:D:971:LEU:HB3	1:D:972:TYR:CD1	2.48	0.49
1:D:1033:GLU:HB2	1:E:760:PHE:CE2	2.47	0.49
1:E:888:GLY:HA2	1:E:976:SER:O	2.13	0.49
1:E:894:LEU:O	1:E:898:VAL:HG22	2.12	0.49
1:A:785:SER:HB2	3:A:1302:HOH:O	2.12	0.48
1:C:650:GLN:HB3	1:C:707:VAL:CG1	2.42	0.48
1:D:511:GLY:O	1:D:515:ILE:HG13	2.13	0.48
1:F:428:GLU:O	1:F:432:MET:HB2	2.13	0.48
1:G:592:PRO:HA	1:G:597:GLU:HG2	1.95	0.48
1:G:708:LYS:HA	1:G:738:MET:SD	2.53	0.48
1:H:666:LEU:HG	1:H:667:GLY:N	2.28	0.48
1:B:1021:THR:HG22	1:B:1025:LYS:HE2	1.96	0.48
1:F:756:LYS:HZ3	1:F:782:GLN:NE2	2.11	0.48
1:G:863:SER:OG	1:G:875:ASP:HB2	2.13	0.48
1:G:966:ARG:HA	1:G:974:THR:CG2	2.43	0.48
1:H:360:ILE:HG22	1:H:363:ALA:HB3	1.95	0.48
1:H:407:PRO:HD3	1:H:607:SER:HB2	1.95	0.48
1:C:351:TYR:CE1	1:C:412:ARG:HD2	2.48	0.48
1:C:738:MET:HG2	1:C:1098:ILE:HB	1.95	0.48
1:E:657:ALA:HA	1:E:711:GLN:HB2	1.94	0.48
1:E:813:LEU:HD12	1:E:837:HIS:HB2	1.95	0.48
1:E:904:ILE:O	1:E:908:VAL:HB	2.13	0.48
1:F:448:LYS:NZ	1:F:452:GLU:OE1	2.34	0.48
1:F:486:SER:CB	1:F:789:THR:HB	2.43	0.48
1:F:657:ALA:HA	1:F:711:GLN:HB2	1.94	0.48
1:H:355:ARG:HG2	1:H:355:ARG:HH11	1.79	0.48
1:H:370:VAL:HG23	1:H:371:LYS:N	2.27	0.48
1:H:387:ARG:O	1:H:391:GLU:HG3	2.12	0.48
1:F:435:ARG:HG2	1:F:436:PRO:HD2	1.94	0.48
1:F:995:THR:HG23	1:F:999:ARG:HH11	1.77	0.48
1:H:379:ILE:HG23	1:H:380:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:753:MET:HE1	1:H:776:LYS:HB2	1.94	0.48
1:A:504:ASP:OD1	1:A:505:VAL:N	2.45	0.48
1:B:731:VAL:HG11	1:B:1056:ARG:HG2	1.95	0.48
1:C:735:LYS:HD3	1:C:1050:LEU:HB3	1.96	0.48
1:D:435:ARG:HD2	1:D:665:GLU:HB2	1.95	0.48
1:D:1044:LYS:HD2	1:D:1124:VAL:HG22	1.94	0.48
1:E:393:ALA:O	1:E:556:ARG:NH2	2.46	0.48
1:G:587:VAL:HG21	1:G:597:GLU:O	2.14	0.48
1:G:616:THR:HB	1:G:661:TRP:CD1	2.49	0.48
1:H:532:GLU:H	1:H:532:GLU:HG3	1.34	0.48
1:H:551:VAL:O	1:H:554:ALA:HB3	2.13	0.48
1:A:641:THR:H	1:A:644:THR:HG1	1.56	0.48
1:B:498:ASP:HA	1:B:769:MET:CE	2.44	0.48
1:D:483:THR:OG1	1:D:485:VAL:HG23	2.14	0.48
1:E:508:PHE:O	1:E:591:PRO:HB3	2.14	0.48
1:F:764:ARG:HH11	1:G:1031:ASN:ND2	2.11	0.48
1:A:1025:LYS:O	1:A:1028:SER:HB3	2.13	0.48
1:B:1100:ARG:HH12	1:B:1103:GLY:CA	2.18	0.48
1:C:428:GLU:O	1:C:432:MET:HB2	2.13	0.48
1:C:491:HIS:HB2	1:C:786:THR:HG23	1.95	0.48
1:D:789:THR:O	1:D:891:PHE:HA	2.14	0.48
1:D:1057:HIS:O	1:D:1061:THR:HG23	2.14	0.48
1:E:641:THR:N	1:E:644:THR:OG1	2.27	0.48
1:E:1043:PHE:CE1	1:E:1074:MET:HG2	2.48	0.48
1:F:443:SER:O	1:F:447:LYS:HG3	2.13	0.48
1:F:444:GLU:HA	1:F:447:LYS:HD2	1.94	0.48
1:F:1058:GLY:HA3	1:F:1128:PHE:CD2	2.48	0.48
1:A:411:PRO:HB3	1:A:658:GLU:HG2	1.95	0.48
1:A:1084:LEU:HD22	1:A:1108:PHE:CD1	2.48	0.48
1:C:984:ASN:HA	1:C:987:PRO:HD2	1.96	0.48
1:D:364:LEU:HD23	1:D:454:ILE:HD11	1.96	0.48
1:D:989:GLY:CA	1:D:1005:LEU:HD13	2.43	0.48
1:E:817:ASP:HB2	1:E:819:ARG:HG3	1.95	0.48
1:F:504:ASP:HB3	1:F:626:TYR:CG	2.49	0.48
1:G:651:ALA:HA	1:G:654:ILE:CD1	2.44	0.48
1:G:914:TYR:CD1	1:G:933:LEU:HD12	2.48	0.48
1:G:1127:LYS:O	1:G:1128:PHE:CD1	2.66	0.48
1:H:666:LEU:HG	1:H:667:GLY:H	1.78	0.48
1:C:769:MET:SD	1:C:770:GLY:N	2.87	0.48
1:F:780:ILE:HG12	1:F:781:TYR:H	1.79	0.48
1:H:805:VAL:HG11	1:H:993:ASN:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:LEU:HD13	1:A:994:ALA:O	2.14	0.48
1:B:357:SER:O	1:B:413:ALA:HA	2.14	0.48
1:B:983:SER:HB2	1:B:1104:TYR:OH	2.14	0.48
1:G:625:GLN:OE1	1:G:692:ALA:HB1	2.14	0.48
1:H:437:GLN:NE2	1:H:1111:LEU:HA	2.27	0.48
1:A:769:MET:SD	1:A:770:GLY:N	2.87	0.47
1:D:498:ASP:HA	1:D:769:MET:SD	2.54	0.47
1:D:555:ARG:HD3	1:D:585:GLU:OE2	2.14	0.47
1:E:426:ARG:NE	1:E:427:ASP:OD1	2.45	0.47
1:F:792:PRO:HG2	1:F:1005:LEU:HD23	1.95	0.47
1:F:871:GLU:OE1	1:F:871:GLU:N	2.31	0.47
1:F:1112:CYS:CB	1:F:1115:VAL:H	2.25	0.47
1:G:347:LEU:HD21	1:G:399:ASP:O	2.14	0.47
1:G:634:ASP:HB3	1:G:640:LEU:CG	2.42	0.47
1:G:999:ARG:NH1	1:G:1004:PRO:O	2.41	0.47
1:H:406:HIS:HE1	1:H:408:CYS:HB2	1.79	0.47
1:H:446:ASP:HA	1:H:449:THR:OG1	2.13	0.47
1:H:691:ASP:OD2	1:H:723:PRO:HD3	2.13	0.47
1:A:463:LEU:HG	1:A:852:VAL:HG12	1.96	0.47
1:A:1044:LYS:HE3	1:A:1124:VAL:HG22	1.95	0.47
1:C:343:ARG:NE	1:C:647:GLU:OE2	2.42	0.47
1:C:905:ARG:HG2	1:C:910:GLU:HG3	1.97	0.47
1:D:815:THR:HG21	1:D:830:ALA:O	2.14	0.47
1:D:935:ARG:O	1:D:939:ASN:HB2	2.14	0.47
1:E:718:ILE:HD11	1:E:743:CYS:HB3	1.96	0.47
1:E:823:THR:HG23	1:E:826:GLU:HB2	1.95	0.47
1:F:671:PHE:CE1	1:F:982:ILE:HD12	2.48	0.47
1:F:831:VAL:HG21	1:F:901:MET:HE1	1.95	0.47
1:H:781:TYR:HB2	1:H:881:ALA:HB2	1.97	0.47
1:A:1099:VAL:HG21	1:A:1108:PHE:CD1	2.49	0.47
1:B:705:ARG:HG2	1:B:705:ARG:O	2.13	0.47
1:B:728:GLU:OE2	1:B:1056:ARG:NE	2.33	0.47
1:C:1007:ASP:OD1	1:C:1042:ASN:HB2	2.14	0.47
1:D:343:ARG:NH1	1:D:402:LEU:HD11	2.29	0.47
1:D:779:ARG:HB3	1:D:882:MET:HE1	1.96	0.47
1:G:649:LEU:HD11	1:G:696:LEU:HD12	1.96	0.47
1:G:990:GLU:HG3	1:G:1002:TRP:HB3	1.96	0.47
1:G:1024:ILE:HD12	1:G:1069:LEU:HD12	1.97	0.47
1:A:393:ALA:O	1:A:556:ARG:NH2	2.48	0.47
1:A:620:LEU:HD12	1:A:680:LEU:HD12	1.97	0.47
1:B:419:ASP:HB3	1:B:458:TRP:CH2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:GLN:CD	1:B:793:ILE:HB	2.35	0.47
1:B:1092:GLU:HG2	1:B:1093:LYS:HG2	1.95	0.47
1:C:375:GLY:HA3	1:G:466:ILE:HA	1.97	0.47
1:C:813:LEU:HD22	1:C:837:HIS:HB2	1.96	0.47
1:E:347:LEU:HD21	1:E:399:ASP:O	2.14	0.47
1:E:988:ILE:HA	1:E:991:LEU:HD12	1.96	0.47
1:E:1100:ARG:HD2	1:E:1104:TYR:C	2.34	0.47
1:G:680:LEU:HD23	1:G:681:THR:N	2.30	0.47
1:H:577:LEU:HG	1:H:580:ILE:HD12	1.97	0.47
1:A:444:GLU:OE1	1:A:447:LYS:HD2	2.14	0.47
1:B:630:MET:N	1:B:630:MET:SD	2.87	0.47
1:B:799:LEU:HA	1:B:818:LEU:HD21	1.95	0.47
1:B:888:GLY:HA2	1:B:976:SER:O	2.14	0.47
1:B:894:LEU:CD1	1:B:957:ILE:HD11	2.45	0.47
1:C:369:VAL:O	1:C:373:ASN:HB2	2.15	0.47
1:C:888:GLY:HA3	1:C:1037:ILE:HG13	1.96	0.47
1:D:897:TYR:CD2	1:D:957:ILE:HD13	2.50	0.47
1:D:1013:GLN:O	1:D:1013:GLN:HG2	2.15	0.47
1:D:1040:VAL:HG23	1:D:1075:GLN:OE1	2.14	0.47
1:F:437:GLN:HE22	1:F:1112:CYS:H	1.61	0.47
1:F:730:ILE:HG23	1:F:741:PRO:CG	2.43	0.47
1:G:595:LEU:O	1:G:648:LEU:HD13	2.15	0.47
1:H:504:ASP:HB3	1:H:626:TYR:CG	2.49	0.47
1:H:508:PHE:O	1:H:591:PRO:HB3	2.14	0.47
1:H:536:ARG:HG3	1:H:873:GLY:HA3	1.95	0.47
1:A:416:PHE:CE1	1:A:425:VAL:HG21	2.49	0.47
1:C:919:ILE:O	1:C:923:LEU:HG	2.14	0.47
1:E:896:THR:OG1	1:E:1006:SER:N	2.46	0.47
1:E:1100:ARG:HD2	1:E:1104:TYR:O	2.15	0.47
1:F:470:GLN:O	1:F:848:ILE:HD13	2.15	0.47
1:F:784:THR:O	1:F:888:GLY:HA3	2.15	0.47
1:F:944:GLY:HA2	1:F:1023:ILE:HG23	1.96	0.47
1:G:710:TYR:CD1	1:G:1107:TYR:HE1	2.32	0.47
1:G:847:VAL:HG12	1:G:850:GLN:OE1	2.14	0.47
1:G:871:GLU:OE1	1:G:871:GLU:N	2.44	0.47
1:H:623:VAL:HA	1:H:626:TYR:CE1	2.49	0.47
1:H:1095:ARG:HG2	1:H:1095:ARG:NH1	2.30	0.47
1:A:362:ARG:NH1	1:A:417:SER:HA	2.30	0.47
1:A:657:ALA:HA	1:A:711:GLN:HB2	1.96	0.47
1:A:788:TYR:CE2	1:A:890:ILE:HG13	2.50	0.47
1:B:416:PHE:HE2	1:B:454:ILE:HG21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:824:PHE:CE1	1:B:905:ARG:HB2	2.48	0.47
1:B:927:PHE:CD1	1:B:934:ARG:HB2	2.49	0.47
1:C:344:MET:CE	1:C:647:GLU:HG2	2.41	0.47
1:C:506:LEU:HD23	1:C:506:LEU:HA	1.77	0.47
1:C:641:THR:N	1:C:644:THR:OG1	2.42	0.47
1:D:876:VAL:HG12	1:D:881:ALA:HB2	1.97	0.47
1:D:940:ALA:O	1:D:942:LYS:NZ	2.37	0.47
1:D:1039:MET:SD	1:D:1072:GLY:HA3	2.54	0.47
1:E:460:GLY:N	1:E:465:GLU:OE2	2.41	0.47
1:E:649:LEU:HD22	1:E:700:ILE:HD12	1.97	0.47
1:E:995:THR:OG1	1:E:997:ASN:OD1	2.32	0.47
1:F:796:GLU:CD	1:F:993:ASN:HB3	2.34	0.47
1:F:970:MET:SD	1:F:975:LEU:HD23	2.54	0.47
1:F:1013:GLN:HG2	1:F:1121:SER:OG	2.14	0.47
1:F:1127:LYS:CD	1:F:1128:PHE:H	2.28	0.47
1:G:499:THR:O	1:G:501:PRO:HD3	2.15	0.47
1:G:620:LEU:HD12	1:G:620:LEU:N	2.30	0.47
1:H:405:GLY:H	1:H:655:LYS:NZ	2.12	0.47
1:H:491:HIS:HB2	1:H:786:THR:HG23	1.96	0.47
1:H:519:ALA:O	1:H:523:LEU:N	2.47	0.47
1:H:744:HIS:HD2	1:H:749:HIS:HE1	1.62	0.47
1:A:463:LEU:HD11	1:A:853:HIS:CD2	2.49	0.47
1:C:398:GLN:HB2	1:C:401:GLU:OE2	2.14	0.47
1:D:646:LEU:HD12	1:D:699:LEU:HD23	1.96	0.47
1:E:948:ASN:OD1	1:E:1029:LYS:HG2	2.15	0.47
1:E:1107:TYR:HD2	1:E:1110:GLU:OE1	1.98	0.47
1:F:655:LYS:HD2	1:F:655:LYS:HA	1.74	0.47
1:F:727:MET:HB3	1:F:1060:ILE:HG13	1.96	0.47
1:F:940:ALA:O	1:F:942:LYS:HE2	2.14	0.47
1:G:616:THR:HB	1:G:661:TRP:CG	2.50	0.47
1:G:1075:GLN:NE2	1:G:1100:ARG:HH21	2.13	0.47
1:H:748:SER:O	1:H:752:MET:HG2	2.14	0.47
1:A:762:ASP:OD1	1:A:779:ARG:NH1	2.46	0.47
1:C:544:ILE:O	1:C:548:GLU:HG3	2.15	0.47
1:C:1025:LYS:O	1:C:1028:SER:OG	2.24	0.47
1:E:1099:VAL:HG21	1:E:1108:PHE:CD1	2.50	0.47
1:F:369:VAL:HG11	1:F:385:ALA:HB2	1.97	0.47
1:F:612:GLU:HG3	1:F:860:PRO:HD2	1.96	0.47
1:F:685:GLN:HG3	1:F:690:GLY:O	2.14	0.47
1:G:393:ALA:O	1:G:556:ARG:NH2	2.34	0.47
1:G:478:ALA:HA	1:G:482:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:962:GLU:HB2	1:H:977:HIS:CE1	2.49	0.47
1:B:424:TRP:CD2	1:B:664:SER:HA	2.49	0.47
1:D:504:ASP:HB3	1:D:626:TYR:CG	2.49	0.47
1:D:1042:ASN:ND2	1:D:1101:VAL:O	2.41	0.47
1:G:889:LEU:O	1:G:977:HIS:HA	2.15	0.47
1:H:552:ASN:O	1:H:556:ARG:HB2	2.14	0.47
1:H:1032:VAL:HB	1:H:1039:MET:HE1	1.96	0.47
1:A:359:SER:OG	1:A:408:CYS:HB3	2.15	0.46
1:E:394:PRO:HB2	1:E:409:GLY:HA2	1.97	0.46
1:F:934:ARG:HA	1:F:937:CYS:SG	2.55	0.46
1:H:616:THR:OG1	1:H:617:GLY:N	2.47	0.46
1:H:729:LYS:HA	1:H:732:ASP:HB2	1.97	0.46
1:A:487:ASP:O	1:A:787:GLY:HA2	2.15	0.46
1:C:900:SER:OG	1:C:995:THR:HG22	2.15	0.46
1:G:358:VAL:HG12	1:G:441:GLU:O	2.15	0.46
1:G:512:MET:HG2	1:G:550:VAL:HB	1.98	0.46
1:G:686:LYS:HE3	1:G:689:GLY:O	2.15	0.46
1:G:698:TYR:HB3	1:G:729:LYS:HD3	1.96	0.46
1:G:1097:LEU:O	1:G:1107:TYR:HA	2.15	0.46
1:H:423:ARG:NH1	1:H:465:GLU:HA	2.30	0.46
1:A:396:LEU:HD21	1:A:398:GLN:HG3	1.97	0.46
1:A:1084:LEU:HD22	1:A:1108:PHE:CE1	2.50	0.46
1:B:771:CYS:SG	2:B:1201:A1H9I:O1	2.73	0.46
1:C:348:ARG:NE	1:C:707:VAL:O	2.45	0.46
1:C:565:ALA:O	1:C:574:ARG:HG3	2.15	0.46
1:C:913:LYS:HE2	1:C:914:TYR:CE2	2.50	0.46
1:D:416:PHE:CZ	1:D:425:VAL:HG11	2.50	0.46
1:D:487:ASP:O	1:D:787:GLY:HA2	2.15	0.46
1:D:801:ARG:HG2	1:D:816:GLY:O	2.15	0.46
1:E:483:THR:OG1	1:E:485:VAL:HG23	2.15	0.46
1:F:464:ASP:OD1	1:F:492:GLN:NE2	2.48	0.46
1:F:467:CYS:HB3	1:F:492:GLN:HG3	1.98	0.46
1:F:598:ALA:HB2	1:F:630:MET:HE2	1.96	0.46
1:H:522:HIS:HB3	1:H:540:TYR:CE2	2.50	0.46
1:H:724:GLN:O	1:H:728:GLU:HG2	2.15	0.46
1:E:1032:VAL:HA	1:E:1035:MET:HE3	1.97	0.46
1:F:926:ASN:C	1:F:926:ASN:HD22	2.19	0.46
1:F:971:LEU:HD23	1:F:972:TYR:CE2	2.50	0.46
1:F:984:ASN:O	1:F:988:ILE:HG13	2.16	0.46
1:F:1047:LYS:HG3	1:F:1078:TYR:O	2.14	0.46
1:G:348:ARG:HH22	1:G:1096:ASP:CG	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:698:TYR:HE1	1:G:726:TYR:HA	1.80	0.46
1:G:840:ARG:HG2	1:G:968:TYR:OH	2.16	0.46
1:H:416:PHE:HE1	1:H:425:VAL:HG21	1.80	0.46
1:A:587:VAL:HG12	1:A:590:ASN:O	2.15	0.46
1:A:984:ASN:C	1:A:987:PRO:HD2	2.36	0.46
1:D:894:LEU:HD23	1:D:1009:ILE:HB	1.97	0.46
1:G:1058:GLY:O	1:G:1061:THR:OG1	2.30	0.46
1:H:358:VAL:HG21	1:H:432:MET:CE	2.45	0.46
1:H:553:TYR:O	1:H:557:ILE:HG12	2.16	0.46
1:A:568:GLU:HG3	1:A:574:ARG:HB2	1.98	0.46
1:A:1041:HIS:O	1:A:1075:GLN:HG2	2.16	0.46
1:B:393:ALA:N	1:B:556:ARG:HH22	2.14	0.46
1:B:806:LEU:HB2	1:B:1002:TRP:CZ3	2.51	0.46
1:C:670:TYR:HE2	1:C:988:ILE:HD11	1.81	0.46
1:D:471:TYR:OH	1:D:849:SER:HB3	2.15	0.46
1:D:622:ARG:NH2	1:D:685:GLN:O	2.48	0.46
1:E:946:ASP:OD2	1:E:1025:LYS:HE2	2.15	0.46
1:F:815:THR:HG21	1:F:830:ALA:O	2.16	0.46
1:H:739:GLY:HA3	1:H:1100:ARG:CG	2.43	0.46
1:H:805:VAL:HG11	1:H:993:ASN:ND2	2.30	0.46
1:A:403:ILE:HG13	1:A:652:PHE:HB2	1.97	0.46
1:A:640:LEU:HD23	1:A:644:THR:HB	1.98	0.46
1:A:755:ARG:NE	1:B:759:ASP:OD1	2.43	0.46
1:A:948:ASN:O	1:A:952:GLN:HG2	2.15	0.46
1:A:1071:ASN:HB3	3:A:1317:HOH:O	2.15	0.46
1:B:464:ASP:OD1	1:B:492:GLN:NE2	2.49	0.46
1:B:989:GLY:HA3	1:B:1004:PRO:HA	1.96	0.46
1:C:546:THR:HG21	1:C:860:PRO:CB	2.44	0.46
1:C:835:ILE:CD1	1:C:957:ILE:HD11	2.46	0.46
1:C:966:ARG:NH1	1:C:974:THR:HG23	2.29	0.46
1:C:980:LEU:HD12	1:C:980:LEU:O	2.15	0.46
1:D:348:ARG:O	1:D:351:TYR:HB3	2.16	0.46
1:E:740:PHE:HA	1:E:741:PRO:HA	1.68	0.46
1:F:803:ARG:HB2	1:F:810:TYR:CZ	2.50	0.46
1:A:477:TRP:O	1:A:481:GLY:N	2.43	0.46
1:C:739:GLY:HA2	1:C:1076:PHE:O	2.16	0.46
1:D:507:LEU:HD21	1:D:605:VAL:HG21	1.98	0.46
1:D:1108:PHE:CZ	1:D:1116:GLN:HG2	2.50	0.46
1:D:1127:LYS:HG2	1:D:1128:PHE:H	1.81	0.46
1:F:337:MET:HG3	1:F:340:LEU:HD12	1.97	0.46
1:F:422:TRP:CH2	1:F:459:GLU:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:TRP:CD1	1:F:664:SER:OG	2.68	0.46
1:F:639:ARG:O	1:F:640:LEU:HD23	2.15	0.46
1:G:699:LEU:HD12	1:G:699:LEU:HA	1.64	0.46
1:G:817:ASP:OD1	1:G:818:LEU:N	2.48	0.46
1:G:980:LEU:CD1	1:G:982:ILE:CG1	2.94	0.46
1:G:1050:LEU:HD12	1:G:1078:TYR:CD1	2.51	0.46
1:H:340:LEU:HB3	1:H:344:MET:HB3	1.98	0.46
1:H:640:LEU:CD2	1:H:648:LEU:HD13	2.44	0.46
1:C:382:ARG:HG2	1:C:382:ARG:HH11	1.80	0.46
1:D:398:GLN:HG3	1:D:401:GLU:CD	2.36	0.46
1:E:420:ILE:CD1	1:E:614:ASN:HB3	2.45	0.46
1:E:512:MET:HG3	1:E:550:VAL:HG11	1.98	0.46
1:E:513:ASN:ND2	1:E:589:ALA:HB1	2.31	0.46
1:E:847:VAL:O	1:E:851:ARG:HG3	2.16	0.46
1:F:444:GLU:O	1:F:447:LYS:HB2	2.15	0.46
1:F:980:LEU:HA	1:F:1040:VAL:HG12	1.97	0.46
1:H:388:HIS:HA	1:H:391:GLU:HB2	1.98	0.46
1:H:404:VAL:H	1:H:600:GLN:NE2	2.14	0.46
1:H:987:PRO:O	1:H:990:GLU:HB2	2.15	0.46
1:H:1101:VAL:O	1:H:1122:ARG:NH2	2.49	0.46
1:A:985:ASN:OD1	1:A:985:ASN:N	2.49	0.46
1:B:445:ALA:O	1:B:449:THR:HG23	2.16	0.46
1:B:848:ILE:O	1:B:852:VAL:HG23	2.16	0.46
1:B:917:GLU:HG2	1:B:920:ARG:NH2	2.30	0.46
1:C:806:LEU:HD22	1:C:991:LEU:HA	1.98	0.46
1:D:1084:LEU:HD12	1:D:1108:PHE:CE1	2.50	0.46
1:E:542:ALA:O	1:E:545:GLU:HB2	2.16	0.46
1:E:805:VAL:HG13	1:E:806:LEU:N	2.31	0.46
1:E:1047:LYS:HD3	1:E:1047:LYS:HA	1.58	0.46
1:E:1092:GLU:H	1:E:1092:GLU:CD	2.19	0.46
1:G:669:LYS:O	1:G:983:SER:OG	2.33	0.46
1:G:738:MET:HA	1:G:1098:ILE:O	2.16	0.46
1:H:796:GLU:OE1	1:H:993:ASN:HB3	2.15	0.46
1:A:572:GLN:H	1:A:572:GLN:HG2	1.53	0.45
1:A:1106:ALA:HB3	1:A:1111:LEU:HD11	1.97	0.45
1:D:813:LEU:CD1	1:D:837:HIS:HB2	2.46	0.45
1:D:1046:LEU:HD22	1:D:1126:GLU:CG	2.46	0.45
1:E:803:ARG:HB3	1:E:810:TYR:CZ	2.51	0.45
1:E:904:ILE:HG23	1:E:908:VAL:HG21	1.99	0.45
1:E:983:SER:O	1:E:983:SER:OG	2.34	0.45
1:F:366:PHE:O	1:F:370:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:669:LYS:NZ	1:F:1114:GLU:HG2	2.31	0.45
1:G:1114:GLU:H	1:G:1114:GLU:CD	2.20	0.45
1:H:734:VAL:HG23	1:H:741:PRO:HD2	1.98	0.45
1:A:407:PRO:HG3	1:A:608:LEU:HD23	1.98	0.45
1:A:1087:ALA:HA	1:A:1094:TYR:CD2	2.51	0.45
1:B:398:GLN:HG2	1:B:401:GLU:CD	2.37	0.45
1:B:479:PHE:CG	1:B:841:LEU:HD23	2.52	0.45
1:B:506:LEU:HD23	1:B:510:LYS:HD2	1.99	0.45
1:C:361:TYR:O	1:C:364:LEU:N	2.49	0.45
1:C:1093:LYS:CD	1:C:1094:TYR:CZ	2.99	0.45
1:D:718:ILE:O	1:D:745:PHE:HA	2.16	0.45
1:E:729:LYS:O	1:E:733:VAL:HG23	2.16	0.45
1:F:1040:VAL:HA	1:F:1073:GLN:OE1	2.17	0.45
1:G:941:PRO:HG2	1:G:949:TYR:CD2	2.51	0.45
1:H:1007:ASP:OD1	1:H:1007:ASP:N	2.44	0.45
1:A:426:ARG:O	1:A:429:LEU:HG	2.16	0.45
1:B:1049:LEU:N	1:B:1078:TYR:OH	2.47	0.45
1:C:510:LYS:HB3	1:C:514:GLY:HA3	1.96	0.45
1:C:522:HIS:O	1:C:525:SER:N	2.43	0.45
1:D:710:TYR:O	1:D:711:GLN:HG2	2.17	0.45
1:D:955:LEU:HB2	1:D:1029:LYS:O	2.16	0.45
1:E:579:THR:O	1:E:583:VAL:HG13	2.16	0.45
1:F:778:GLY:O	1:F:867:GLU:N	2.44	0.45
1:F:944:GLY:O	1:F:1023:ILE:HG12	2.16	0.45
1:H:357:SER:HB3	1:H:413:ALA:CB	2.46	0.45
1:H:403:ILE:HD13	1:H:596:GLN:HB2	1.98	0.45
1:H:1047:LYS:HA	1:H:1078:TYR:CE1	2.51	0.45
1:B:362:ARG:HH21	1:B:417:SER:HB3	1.79	0.45
1:D:491:HIS:CE1	1:D:783:TRP:CD2	3.05	0.45
1:D:993:ASN:CG	1:D:994:ALA:H	2.20	0.45
1:E:444:GLU:HA	1:E:447:LYS:HG3	1.97	0.45
1:E:753:MET:O	1:E:756:LYS:HB2	2.16	0.45
1:E:803:ARG:HB3	1:E:810:TYR:CE2	2.51	0.45
1:F:1016:ASP:OD1	1:F:1016:ASP:N	2.48	0.45
1:H:894:LEU:O	1:H:898:VAL:HG12	2.16	0.45
1:H:896:THR:CG2	1:H:1006:SER:H	2.29	0.45
1:B:355:ARG:HD2	1:B:441:GLU:OE2	2.16	0.45
1:E:428:GLU:CD	1:E:665:GLU:HB2	2.37	0.45
1:E:435:ARG:HG2	1:E:437:GLN:O	2.16	0.45
1:E:520:GLU:HG2	1:E:544:ILE:CD1	2.47	0.45
1:E:1043:PHE:HE1	1:E:1074:MET:HG2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:HIS:CE1	1:F:408:CYS:HB2	2.50	0.45
1:F:411:PRO:O	1:F:412:ARG:HG2	2.16	0.45
1:F:887:PRO:O	1:F:975:LEU:HD22	2.16	0.45
1:G:698:TYR:CE1	1:G:725:LYS:HD3	2.52	0.45
1:A:1085:LYS:O	1:A:1089:GLN:HG2	2.16	0.45
1:D:463:LEU:HG	1:D:852:VAL:HG12	1.98	0.45
1:F:920:ARG:NE	1:F:921:ASP:OD1	2.50	0.45
1:F:1088:GLN:HG3	1:F:1116:GLN:OE1	2.16	0.45
1:H:346:ARG:HH21	1:H:400:ASP:HB3	1.82	0.45
1:H:463:LEU:HD12	1:H:492:GLN:O	2.17	0.45
1:H:834:GLN:O	1:H:838:ILE:HG13	2.16	0.45
1:H:1047:LYS:CE	1:H:1079:VAL:HA	2.44	0.45
1:A:966:ARG:HA	1:A:974:THR:CG2	2.47	0.45
1:B:623:VAL:HG12	1:B:626:TYR:CZ	2.51	0.45
1:C:599:LEU:HD11	1:C:649:LEU:HD23	1.97	0.45
1:D:512:MET:N	1:D:589:ALA:O	2.49	0.45
1:D:1048:GLY:N	1:D:1078:TYR:OH	2.43	0.45
1:F:462:SER:OG	1:F:465:GLU:HG3	2.16	0.45
1:F:1013:GLN:HG3	1:F:1122:ARG:HA	1.98	0.45
1:G:1090:GLU:HA	1:G:1092:GLU:OE1	2.16	0.45
1:H:376:MET:HG3	1:H:377:PRO:HD2	1.99	0.45
1:H:624:ASP:HB3	1:H:682:VAL:CG2	2.45	0.45
1:H:1086:LYS:O	1:H:1094:TYR:HE2	2.00	0.45
1:A:597:GLU:O	1:A:601:SER:HB2	2.16	0.45
1:A:682:VAL:CG1	1:A:697:THR:HG23	2.47	0.45
1:B:594:THR:C	1:B:630:MET:HB3	2.36	0.45
1:D:934:ARG:CZ	1:D:938:LEU:HD21	2.47	0.45
1:F:412:ARG:HH12	1:F:710:TYR:HE1	1.64	0.45
1:F:489:SER:OG	1:F:490:TYR:N	2.50	0.45
1:F:490:TYR:O	1:F:494:ASN:ND2	2.49	0.45
1:F:806:LEU:HD13	1:F:806:LEU:C	2.37	0.45
1:F:930:TYR:O	1:F:933:LEU:N	2.24	0.45
1:F:1041:HIS:NE2	1:F:1043:PHE:HE1	2.14	0.45
1:H:1063:LEU:HD21	1:H:1076:PHE:CZ	2.30	0.45
1:H:1063:LEU:HD11	1:H:1076:PHE:HE2	1.82	0.45
1:H:1097:LEU:HD23	1:H:1098:ILE:N	2.32	0.45
1:B:612:GLU:OE2	1:B:860:PRO:HD2	2.17	0.45
1:B:616:THR:HB	1:B:661:TRP:CG	2.52	0.45
1:C:804:MET:CE	1:C:807:PHE:HD2	2.30	0.45
1:E:790:GLN:HB2	1:E:792:PRO:HD2	1.98	0.45
1:F:887:PRO:HD2	1:F:970:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:435:ARG:NH1	1:G:663:SER:O	2.45	0.45
1:H:401:GLU:HB3	1:H:404:VAL:CG1	2.40	0.45
1:H:596:GLN:CG	1:H:648:LEU:HD11	2.46	0.45
1:D:425:VAL:HG13	1:D:426:ARG:N	2.32	0.45
1:D:507:LEU:CD2	1:D:605:VAL:HG21	2.47	0.45
1:E:1013:GLN:H	1:E:1013:GLN:CD	2.16	0.45
1:F:686:LYS:HB3	1:F:686:LYS:HE3	1.77	0.45
1:G:995:THR:OG1	1:G:999:ARG:HB3	2.17	0.45
1:G:1112:CYS:HB2	1:G:1114:GLU:OE2	2.16	0.45
1:H:732:ASP:HA	1:H:735:LYS:HG2	1.99	0.45
1:H:850:GLN:CD	1:H:971:LEU:HB2	2.38	0.45
1:H:1099:VAL:HG11	1:H:1119:ILE:HG21	1.98	0.45
1:A:510:LYS:HB3	1:A:514:GLY:HA3	1.99	0.44
1:C:739:GLY:HA3	1:C:1100:ARG:HB2	1.99	0.44
1:C:802:GLY:O	1:C:810:TYR:HA	2.18	0.44
1:D:824:PHE:HZ	1:D:953:TYR:CE2	2.35	0.44
1:D:954:ALA:O	1:D:958:THR:HG23	2.17	0.44
1:E:586:ASN:O	1:E:590:ASN:HB2	2.17	0.44
1:F:718:ILE:O	1:F:745:PHE:HA	2.17	0.44
1:H:362:ARG:NH1	1:H:366:PHE:CZ	2.85	0.44
1:H:526:LEU:HD22	1:H:533:ASP:HB3	1.98	0.44
1:H:622:ARG:HA	1:H:681:THR:O	2.17	0.44
1:A:586:ASN:ND2	1:A:597:GLU:OE2	2.42	0.44
1:B:984:ASN:HA	1:B:987:PRO:HD2	1.99	0.44
1:D:797:PHE:CE1	1:D:804:MET:HB2	2.50	0.44
1:D:984:ASN:C	1:D:987:PRO:HD2	2.38	0.44
1:F:380:LEU:HD12	1:F:380:LEU:HA	1.79	0.44
1:F:854:ARG:HA	1:F:877:ALA:HB1	1.97	0.44
1:G:650:GLN:O	1:G:654:ILE:HG13	2.17	0.44
1:G:971:LEU:HB3	1:G:972:TYR:CE2	2.52	0.44
1:G:974:THR:HG22	1:G:975:LEU:N	2.32	0.44
1:H:741:PRO:HG2	1:H:743:CYS:SG	2.57	0.44
1:H:835:ILE:O	1:H:839:VAL:HG23	2.18	0.44
1:B:745:PHE:CD1	1:B:1067:SER:HB2	2.52	0.44
1:D:823:THR:HG22	1:D:824:PHE:N	2.33	0.44
1:D:1049:LEU:HD21	1:D:1127:LYS:HA	1.99	0.44
1:E:424:TRP:CZ2	1:E:425:VAL:HG22	2.52	0.44
1:E:748:SER:O	1:E:752:MET:HG2	2.18	0.44
1:F:375:GLY:HA3	1:H:466:ILE:HA	1.98	0.44
1:F:488:LEU:HD13	1:F:845:GLY:HA3	1.99	0.44
1:G:515:ILE:O	1:G:518:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:657:ALA:HA	1:G:711:GLN:HB2	1.99	0.44
1:G:724:GLN:OE1	1:G:1060:ILE:HG21	2.17	0.44
1:H:370:VAL:HG12	1:H:381:LEU:HD21	2.00	0.44
1:H:477:TRP:CZ3	1:H:482:GLU:HG3	2.53	0.44
1:H:897:TYR:CZ	1:H:901:MET:HG3	2.52	0.44
1:B:561:ALA:HB3	1:B:581:ALA:HB2	1.99	0.44
1:B:1043:PHE:HB2	1:B:1075:GLN:O	2.18	0.44
1:D:351:TYR:CZ	1:D:657:ALA:HB1	2.52	0.44
1:D:822:ARG:HG2	1:D:822:ARG:HH11	1.83	0.44
1:E:913:LYS:HG3	1:E:914:TYR:CE2	2.52	0.44
1:E:993:ASN:CG	1:E:994:ALA:H	2.17	0.44
1:F:771:CYS:HB2	1:F:772:VAL:HG22	1.99	0.44
1:G:402:LEU:HA	1:G:580:ILE:HD11	1.99	0.44
1:G:527:SER:HB3	1:G:529:GLU:HG2	1.99	0.44
1:G:686:LYS:HA	1:G:692:ALA:HB2	1.99	0.44
1:H:635:ILE:HA	1:H:640:LEU:O	2.16	0.44
1:H:888:GLY:HA2	1:H:976:SER:O	2.18	0.44
1:A:993:ASN:OD1	1:A:994:ALA:N	2.51	0.44
1:B:705:ARG:HB2	1:B:733:VAL:HG22	1.98	0.44
1:B:803:ARG:HD2	1:B:808:ASP:OD1	2.18	0.44
1:C:937:CYS:O	1:C:942:LYS:NZ	2.49	0.44
1:D:501:PRO:O	1:D:777:SER:HB2	2.17	0.44
1:D:708:LYS:HA	1:D:738:MET:SD	2.58	0.44
1:D:1020:PRO:HB2	1:D:1062:LEU:CD2	2.44	0.44
1:E:424:TRP:CE2	1:E:425:VAL:HG22	2.52	0.44
1:E:573:ARG:NH2	1:E:577:LEU:HD21	2.33	0.44
1:F:803:ARG:HB2	1:F:810:TYR:CE1	2.52	0.44
1:F:965:CYS:SG	1:F:975:LEU:HD12	2.57	0.44
1:H:1050:LEU:HD12	1:H:1078:TYR:CE1	2.53	0.44
1:B:343:ARG:CG	1:B:400:ASP:HB3	2.47	0.44
1:B:743:CYS:O	1:B:1073:GLN:HA	2.17	0.44
1:C:579:THR:O	1:C:583:VAL:HG23	2.18	0.44
1:C:694:ASN:O	1:C:697:THR:HB	2.17	0.44
1:C:1046:LEU:HB2	1:C:1126:GLU:HG2	1.98	0.44
1:D:471:TYR:HE1	1:D:848:ILE:HB	1.83	0.44
1:F:687:ARG:HG2	1:F:765:ASP:HB2	1.99	0.44
1:F:716:CYS:HB3	1:F:726:TYR:OH	2.16	0.44
1:F:930:TYR:HB3	1:F:933:LEU:HB3	1.99	0.44
1:G:431:THR:O	1:G:434:THR:N	2.48	0.44
1:G:1042:ASN:HD21	1:G:1102:ALA:HA	1.83	0.44
1:H:1117:ASP:O	1:H:1121:SER:OG	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:VAL:HG21	1:B:779:ARG:NH2	2.32	0.44
1:D:568:GLU:HG2	1:D:569:GLN:N	2.33	0.44
1:E:655:LYS:HD2	1:E:658:GLU:OE1	2.17	0.44
1:E:760:PHE:O	1:E:763:ALA:N	2.51	0.44
1:E:1013:GLN:HB3	1:E:1121:SER:O	2.17	0.44
1:F:386:PHE:CZ	1:F:861:LEU:HD22	2.52	0.44
1:F:719:HIS:O	1:F:721:GLN:N	2.50	0.44
1:F:739:GLY:HA3	1:F:1100:ARG:HD3	2.00	0.44
1:F:761:GLU:HA	1:F:764:ARG:HH21	1.83	0.44
1:F:846:THR:O	1:F:849:SER:OG	2.31	0.44
1:F:874:LYS:HE3	1:F:880:GLY:HA2	1.99	0.44
1:G:700:ILE:O	1:G:703:ALA:HB3	2.18	0.44
1:G:779:ARG:HD3	1:G:882:MET:SD	2.57	0.44
1:H:422:TRP:CZ2	1:H:423:ARG:HG2	2.53	0.44
1:H:920:ARG:NE	1:H:921:ASP:OD1	2.43	0.44
1:A:386:PHE:CE2	1:A:546:THR:HG23	2.53	0.44
1:B:806:LEU:HD23	1:B:807:PHE:CE2	2.53	0.44
1:C:984:ASN:ND2	3:C:1309:HOH:O	2.44	0.44
1:C:1039:MET:SD	1:C:1072:GLY:HA3	2.57	0.44
1:E:341:THR:O	1:E:345:GLN:HG3	2.17	0.44
1:E:618:LEU:H	1:E:618:LEU:HD22	1.82	0.44
1:E:1058:GLY:O	1:E:1061:THR:OG1	2.34	0.44
1:F:789:THR:OG1	1:F:790:GLN:N	2.48	0.44
1:F:823:THR:HG23	3:F:1328:HOH:O	2.17	0.44
1:F:915:THR:HG22	1:F:916:LEU:N	2.33	0.44
1:G:512:MET:CE	1:G:550:VAL:HG11	2.47	0.44
1:G:739:GLY:HA3	1:G:1100:ARG:HD3	2.00	0.44
1:B:341:THR:CG2	1:B:647:GLU:HG3	2.48	0.44
1:D:544:ILE:O	1:D:548:GLU:HG2	2.18	0.44
1:D:806:LEU:HD23	1:D:807:PHE:CZ	2.53	0.44
1:E:650:GLN:HB2	1:E:707:VAL:CG1	2.48	0.44
1:E:791:TRP:HD1	1:E:835:ILE:HD13	1.83	0.44
1:E:1001:ALA:HB1	1:E:1002:TRP:CE2	2.53	0.44
1:F:746:ASP:C	1:F:750:ILE:HG13	2.36	0.44
1:G:885:HIS:HA	1:G:973:SER:OG	2.17	0.44
1:H:362:ARG:HD3	1:H:415:ALA:HB1	2.00	0.44
1:H:485:VAL:HG22	1:H:804:MET:SD	2.58	0.44
1:H:1086:LYS:CG	1:H:1089:GLN:OE1	2.66	0.44
1:A:941:PRO:HG2	1:A:949:TYR:CD2	2.53	0.43
1:B:797:PHE:HE1	1:B:804:MET:HB2	1.83	0.43
1:D:982:ILE:O	1:D:1102:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:803:ARG:HB3	1:E:810:TYR:CD2	2.53	0.43
1:F:813:LEU:CD1	1:F:837:HIS:HB2	2.48	0.43
1:H:550:VAL:HG23	1:H:551:VAL:H	1.82	0.43
1:C:368:GLU:OE2	1:C:388:HIS:NE2	2.44	0.43
1:C:654:ILE:O	1:C:658:GLU:HG3	2.18	0.43
1:C:818:LEU:HD13	1:C:916:LEU:HB3	2.00	0.43
1:C:866:VAL:HG22	3:C:1337:HOH:O	2.18	0.43
1:E:747:ASP:HB2	3:E:1320:HOH:O	2.17	0.43
1:E:790:GLN:CD	1:E:793:ILE:HB	2.39	0.43
1:F:503:TYR:HA	1:F:507:LEU:HB3	1.99	0.43
1:F:1040:VAL:HG23	1:F:1075:GLN:NE2	2.33	0.43
1:G:506:LEU:HA	1:G:506:LEU:HD23	1.81	0.43
1:H:1080:ASP:HB3	1:H:1083:VAL:HG12	2.00	0.43
1:A:758:PHE:CE2	1:A:883:VAL:HG11	2.54	0.43
1:A:848:ILE:O	1:A:849:SER:C	2.56	0.43
1:B:633:ALA:O	1:B:637:GLU:HB2	2.19	0.43
1:D:532:GLU:H	1:D:532:GLU:HG2	1.51	0.43
1:F:343:ARG:CG	1:F:400:ASP:HB3	2.48	0.43
1:G:397:ILE:HG23	1:G:404:VAL:HG11	1.99	0.43
1:H:360:ILE:O	1:H:362:ARG:N	2.51	0.43
1:H:934:ARG:NH1	1:H:1000:LEU:HD11	2.33	0.43
1:H:971:LEU:HB3	1:H:972:TYR:CE2	2.53	0.43
1:H:1114:GLU:N	1:H:1114:GLU:OE2	2.52	0.43
1:B:653:ILE:HD13	1:B:704:VAL:HG12	2.00	0.43
1:C:836:ALA:HB2	1:C:960:TRP:HH2	1.83	0.43
1:C:934:ARG:O	1:C:938:LEU:HG	2.18	0.43
1:D:982:ILE:HG23	1:D:1104:TYR:CE1	2.52	0.43
1:E:373:ASN:HB3	1:E:376:MET:HE3	2.00	0.43
1:F:772:VAL:HG11	1:F:1040:VAL:HB	2.00	0.43
1:G:727:MET:O	1:G:731:VAL:HG23	2.18	0.43
1:G:941:PRO:HB3	1:G:947:ASP:OD2	2.19	0.43
1:H:423:ARG:HH12	1:H:465:GLU:HA	1.83	0.43
1:A:532:GLU:H	1:A:532:GLU:HG2	1.47	0.43
1:A:577:LEU:O	1:A:580:ILE:HB	2.18	0.43
1:D:360:ILE:HG21	1:D:450:ILE:HD11	2.00	0.43
1:E:370:VAL:HG12	1:E:457:PHE:HZ	1.83	0.43
1:F:412:ARG:NH1	1:F:657:ALA:O	2.52	0.43
1:F:1080:ASP:HB3	1:F:1083:VAL:CG2	2.48	0.43
1:F:1115:VAL:O	1:F:1119:ILE:HG13	2.18	0.43
1:G:516:LYS:O	1:G:520:GLU:HG3	2.19	0.43
1:G:635:ILE:HA	1:G:640:LEU:O	2.19	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:401:GLU:OE1	1:H:404:VAL:HG11	2.17	0.43
1:H:444:GLU:HA	1:H:447:LYS:HG3	1.99	0.43
1:H:531:PRO:HA	1:H:534:ILE:CD1	2.49	0.43
1:A:943:TYR:O	1:A:1011:PRO:HB3	2.18	0.43
1:B:794:ALA:HB1	1:B:834:GLN:HB2	1.99	0.43
1:D:356:PRO:HA	1:D:412:ARG:O	2.19	0.43
1:D:396:LEU:HD22	1:D:409:GLY:O	2.19	0.43
1:D:573:ARG:O	1:D:576:GLU:HB2	2.18	0.43
1:D:724:GLN:O	1:D:728:GLU:N	2.46	0.43
1:D:785:SER:HB3	1:D:890:ILE:HG12	2.00	0.43
1:D:895:ALA:HA	1:D:898:VAL:HG12	2.00	0.43
1:E:941:PRO:HB3	1:E:947:ASP:OD2	2.18	0.43
1:E:1020:PRO:HA	1:E:1023:ILE:HD12	2.00	0.43
1:F:728:GLU:O	1:F:731:VAL:HB	2.18	0.43
1:F:756:LYS:HA	1:F:885:HIS:CD2	2.54	0.43
1:F:1093:LYS:HD2	1:F:1093:LYS:N	2.33	0.43
1:G:422:TRP:HZ2	1:G:459:GLU:HA	1.81	0.43
1:G:531:PRO:HA	1:G:534:ILE:HD12	2.00	0.43
1:G:595:LEU:O	1:G:595:LEU:HG	2.18	0.43
1:G:624:ASP:OD1	1:G:625:GLN:HG2	2.18	0.43
1:A:984:ASN:CA	1:A:987:PRO:HD2	2.46	0.43
1:B:398:GLN:HG2	1:B:401:GLU:OE1	2.19	0.43
1:C:532:GLU:CD	1:C:532:GLU:H	2.21	0.43
1:E:796:GLU:OE2	1:E:805:VAL:HG12	2.18	0.43
1:F:971:LEU:HB3	1:F:972:TYR:CD2	2.54	0.43
1:G:608:LEU:HG	1:G:611:ILE:HG13	2.00	0.43
1:H:376:MET:HE3	1:H:384:LYS:HD3	2.01	0.43
1:H:650:GLN:HA	1:H:653:ILE:CG1	2.46	0.43
1:H:896:THR:HG21	1:H:1005:LEU:HD22	2.00	0.43
1:A:421:ALA:HA	3:A:1313:HOH:O	2.17	0.43
1:A:508:PHE:CE1	1:A:592:PRO:HG3	2.53	0.43
1:A:594:THR:C	1:A:630:MET:HB3	2.39	0.43
1:A:768:LEU:HD13	1:A:774:PRO:HA	2.01	0.43
1:B:346:ARG:HD2	1:B:400:ASP:OD2	2.18	0.43
1:C:791:TRP:HB2	1:C:792:PRO:HD3	2.00	0.43
1:D:1068:ILE:HG23	1:E:720:ASN:HD22	1.83	0.43
1:E:437:GLN:HA	1:E:437:GLN:NE2	2.34	0.43
1:E:616:THR:HB	1:E:661:TRP:CG	2.54	0.43
1:F:539:TYR:O	1:F:542:ALA:HB3	2.18	0.43
1:F:723:PRO:HG2	1:F:726:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1023:ILE:O	1:F:1027:VAL:HG22	2.18	0.43
1:G:1049:LEU:O	1:G:1055:GLY:HA3	2.19	0.43
1:A:565:ALA:HA	1:A:568:GLU:HB3	1.99	0.43
1:A:681:THR:O	1:A:682:VAL:HG23	2.19	0.43
1:B:394:PRO:HB2	1:B:409:GLY:HA2	2.01	0.43
1:B:397:ILE:HD13	1:B:404:VAL:HB	2.01	0.43
1:B:424:TRP:O	1:B:428:GLU:HG3	2.19	0.43
1:C:382:ARG:HG2	1:C:382:ARG:NH1	2.34	0.43
1:D:1054:GLU:H	1:D:1054:GLU:HG2	1.61	0.43
1:G:507:LEU:HB2	1:G:865:LEU:HD21	2.01	0.43
1:G:686:LYS:CA	1:G:692:ALA:HB2	2.49	0.43
1:G:938:LEU:HD23	1:G:938:LEU:HA	1.79	0.43
1:H:506:LEU:N	1:H:506:LEU:CD2	2.82	0.43
1:H:803:ARG:HD2	1:H:808:ASP:OD1	2.19	0.43
1:H:1016:ASP:OD1	1:H:1016:ASP:N	2.43	0.43
1:A:560:HIS:HA	1:A:563:GLU:HB3	2.00	0.43
1:A:890:ILE:HD12	1:A:980:LEU:HD21	2.00	0.43
1:C:471:TYR:O	1:C:476:VAL:HG22	2.19	0.43
1:D:627:CYS:HA	1:D:630:MET:CE	2.46	0.43
1:D:710:TYR:CD1	1:D:1107:TYR:CE2	3.07	0.43
1:D:743:CYS:O	1:D:1073:GLN:HA	2.18	0.43
1:D:1050:LEU:HA	1:D:1050:LEU:HD13	1.83	0.43
1:E:716:CYS:SG	1:E:741:PRO:HG3	2.59	0.43
1:F:654:ILE:O	1:F:658:GLU:HG3	2.19	0.43
1:G:795:ILE:HG21	1:G:996:PRO:HG2	1.99	0.43
1:H:343:ARG:NH2	1:H:576:GLU:OE2	2.52	0.43
1:H:432:MET:O	1:H:435:ARG:HG3	2.18	0.43
1:H:546:THR:O	1:H:550:VAL:HG22	2.19	0.43
1:H:804:MET:HE1	1:H:807:PHE:CD2	2.54	0.43
1:H:868:GLY:HA2	1:H:871:GLU:OE2	2.18	0.43
1:H:1063:LEU:HD11	1:H:1076:PHE:CE2	2.53	0.43
1:A:984:ASN:C	1:A:984:ASN:OD1	2.57	0.42
1:B:478:ALA:HA	1:B:482:GLU:HG3	2.01	0.42
1:B:776:LYS:HD2	1:B:779:ARG:HD2	2.00	0.42
1:B:801:ARG:HD3	1:B:814:ASP:OD2	2.18	0.42
1:B:828:ASP:OD2	1:B:832:LYS:HE2	2.19	0.42
1:B:838:ILE:O	1:B:842:SER:HB2	2.19	0.42
1:C:371:LYS:HG3	1:C:372:ALA:N	2.33	0.42
1:E:383:ALA:HB2	1:E:542:ALA:HB1	2.00	0.42
1:G:648:LEU:HA	1:G:648:LEU:HD23	1.85	0.42
1:A:832:LYS:HB3	1:A:960:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ARG:NE	1:B:707:VAL:O	2.46	0.42
1:B:504:ASP:HB3	1:B:626:TYR:CD2	2.54	0.42
1:C:619:SER:HB3	1:C:679:ASN:HB3	2.01	0.42
1:D:429:LEU:HB3	1:D:447:LYS:HD3	2.01	0.42
1:D:720:ASN:HB2	1:D:721:GLN:OE1	2.18	0.42
1:D:813:LEU:O	1:D:834:GLN:NE2	2.38	0.42
1:F:376:MET:SD	1:F:380:LEU:HD23	2.58	0.42
1:F:719:HIS:H	1:F:722:SER:HG	1.64	0.42
1:F:982:ILE:HA	3:F:1326:HOH:O	2.19	0.42
1:F:1080:ASP:OD1	1:F:1082:GLU:N	2.52	0.42
1:G:1035:MET:HE2	1:G:1035:MET:HB2	1.87	0.42
1:G:1092:GLU:H	1:G:1092:GLU:CD	2.21	0.42
1:A:908:VAL:HG12	3:A:1310:HOH:O	2.20	0.42
1:B:772:VAL:CG2	1:B:773:GLU:OE2	2.66	0.42
1:C:675:GLN:CD	1:C:1104:TYR:CD2	2.92	0.42
1:D:623:VAL:HB	1:D:680:LEU:HD21	2.01	0.42
1:E:639:ARG:O	1:E:640:LEU:HD23	2.18	0.42
1:E:653:ILE:HD13	1:E:704:VAL:HG22	2.01	0.42
1:E:798:VAL:HG13	1:E:834:GLN:HG2	2.01	0.42
1:F:722:SER:HB3	1:F:726:TYR:CD2	2.55	0.42
1:F:894:LEU:HD22	1:F:1009:ILE:HG22	2.02	0.42
1:F:1082:GLU:O	1:F:1086:LYS:HG3	2.18	0.42
1:G:386:PHE:CZ	1:G:861:LEU:HD22	2.53	0.42
1:H:355:ARG:HG2	1:H:355:ARG:NH1	2.34	0.42
1:H:422:TRP:CE2	1:H:423:ARG:HG2	2.54	0.42
1:A:894:LEU:CD1	1:A:957:ILE:HD11	2.49	0.42
1:A:990:GLU:HG2	3:A:1324:HOH:O	2.19	0.42
1:A:1007:ASP:OD2	1:A:1042:ASN:HB2	2.18	0.42
1:A:1024:ILE:HG21	1:A:1074:MET:HE3	2.00	0.42
1:A:1088:GLN:O	1:A:1091:PRO:HD3	2.19	0.42
1:C:394:PRO:HD2	1:C:407:PRO:O	2.19	0.42
1:C:699:LEU:HA	1:C:699:LEU:HD23	1.54	0.42
1:E:580:ILE:O	1:E:583:VAL:HG22	2.19	0.42
1:E:850:GLN:NE2	1:E:887:PRO:HD3	2.34	0.42
1:F:701:MET:HE2	1:F:729:LYS:HG2	2.01	0.42
1:F:867:GLU:HB3	1:F:882:MET:HE3	2.01	0.42
1:F:1035:MET:HE3	1:F:1039:MET:HB2	2.01	0.42
1:G:345:GLN:O	1:G:349:ASN:ND2	2.50	0.42
1:G:760:PHE:O	1:G:764:ARG:HG3	2.19	0.42
1:G:1095:ARG:HA	1:G:1109:VAL:CG2	2.42	0.42
1:H:986:THR:HB	1:H:1115:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:TYR:CD1	1:A:933:LEU:HD12	2.54	0.42
1:B:623:VAL:O	1:B:627:CYS:HB2	2.19	0.42
1:D:708:LYS:HE3	1:D:736:ALA:O	2.19	0.42
1:E:573:ARG:O	1:E:577:LEU:HG	2.19	0.42
1:F:599:LEU:HD13	1:F:652:PHE:HB2	2.01	0.42
1:G:561:ALA:HB3	1:G:581:ALA:HB2	2.02	0.42
1:G:608:LEU:O	1:G:611:ILE:N	2.51	0.42
1:G:610:GLU:HA	1:G:613:GLU:O	2.19	0.42
1:G:806:LEU:CD2	1:G:991:LEU:HA	2.49	0.42
1:G:813:LEU:HD11	1:G:837:HIS:CB	2.45	0.42
1:H:386:PHE:CD1	1:H:611:ILE:HG22	2.54	0.42
1:H:400:ASP:HA	1:H:573:ARG:CZ	2.43	0.42
1:H:512:MET:HE2	1:H:588:PRO:HB2	2.01	0.42
1:H:744:HIS:CE1	1:H:1073:GLN:HE21	2.38	0.42
1:H:907:LEU:HD13	1:H:914:TYR:CD2	2.45	0.42
1:H:914:TYR:CZ	1:H:933:LEU:HB3	2.55	0.42
1:A:573:ARG:HG2	1:A:576:GLU:OE1	2.18	0.42
1:B:694:ASN:OD1	1:B:694:ASN:C	2.57	0.42
1:C:446:ASP:O	1:C:450:ILE:HG13	2.19	0.42
1:D:359:SER:HB2	1:D:361:TYR:CD2	2.54	0.42
1:D:771:CYS:SG	1:D:982:ILE:HG12	2.60	0.42
1:D:1033:GLU:H	1:D:1033:GLU:HG2	1.65	0.42
1:E:359:SER:HB3	1:E:408:CYS:HB3	2.02	0.42
1:E:790:GLN:HG3	1:E:793:ILE:HG22	2.02	0.42
1:F:487:ASP:OD2	1:F:489:SER:OG	2.32	0.42
1:F:1042:ASN:HD21	1:F:1102:ALA:HA	1.84	0.42
1:H:536:ARG:CG	1:H:873:GLY:HA3	2.49	0.42
1:H:739:GLY:HA2	1:H:1076:PHE:O	2.19	0.42
1:A:919:ILE:HD13	1:A:933:LEU:HD11	2.02	0.42
1:A:1043:PHE:HB2	1:A:1076:PHE:CD1	2.54	0.42
1:B:618:LEU:HD13	1:B:618:LEU:HA	1.84	0.42
1:B:906:LYS:HE3	1:B:911:GLU:HG3	2.01	0.42
1:D:748:SER:HB2	1:D:749:HIS:HD1	1.85	0.42
1:F:493:ILE:O	1:F:493:ILE:HG22	2.19	0.42
1:F:498:ASP:O	1:F:775:GLN:NE2	2.45	0.42
1:F:655:LYS:NZ	3:F:1305:HOH:O	2.51	0.42
1:F:671:PHE:CD1	1:F:982:ILE:HD12	2.55	0.42
1:F:915:THR:HG22	1:F:916:LEU:H	1.85	0.42
1:F:1050:LEU:HB2	1:F:1078:TYR:CZ	2.54	0.42
1:F:1050:LEU:HG	1:F:1078:TYR:CE1	2.55	0.42
1:F:1127:LYS:HD2	1:F:1127:LYS:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:694:ASN:H	1:G:697:THR:CB	2.31	0.42
1:H:340:LEU:O	1:H:345:GLN:NE2	2.51	0.42
1:H:639:ARG:H	1:H:639:ARG:HD2	1.85	0.42
1:H:854:ARG:HA	1:H:877:ALA:CB	2.47	0.42
1:H:1086:LYS:O	1:H:1094:TYR:CE2	2.72	0.42
1:A:983:SER:HB3	1:A:1104:TYR:OH	2.20	0.42
1:A:1099:VAL:HG21	1:A:1108:PHE:HD1	1.85	0.42
1:B:610:GLU:HG2	1:B:659:LEU:HD11	2.01	0.42
1:C:888:GLY:HA2	1:C:976:SER:O	2.20	0.42
1:D:502:GLY:HA3	1:D:505:VAL:HG22	2.02	0.42
1:E:1075:GLN:OE1	1:E:1100:ARG:NE	2.51	0.42
1:F:366:PHE:HA	1:F:369:VAL:HG12	2.00	0.42
1:G:377:PRO:HG2	1:G:538:TYR:CE1	2.55	0.42
1:G:619:SER:HB3	1:G:679:ASN:O	2.20	0.42
1:G:859:LYS:O	1:G:863:SER:OG	2.24	0.42
1:H:584:ASN:HD21	1:H:600:GLN:NE2	2.17	0.42
1:H:675:GLN:HG2	1:H:1104:TYR:CD2	2.55	0.42
1:A:758:PHE:CE2	1:A:780:ILE:HD12	2.54	0.42
1:B:768:LEU:HD22	1:B:768:LEU:N	2.35	0.42
1:C:432:MET:HE2	1:C:442:ILE:HB	2.02	0.42
1:C:824:PHE:CD2	1:C:905:ARG:HD3	2.55	0.42
1:C:1080:ASP:HB3	1:C:1083:VAL:HG23	2.02	0.42
1:D:616:THR:HB	1:D:661:TRP:CD1	2.54	0.42
1:D:1062:LEU:HD12	1:D:1062:LEU:HA	1.93	0.42
1:E:489:SER:O	1:E:492:GLN:N	2.53	0.42
1:E:568:GLU:HB3	1:E:574:ARG:HB2	2.01	0.42
1:E:980:LEU:HD12	1:E:982:ILE:HG13	2.02	0.42
1:E:1059:LEU:HD21	1:E:1076:PHE:CE1	2.55	0.42
1:G:850:GLN:CD	1:G:971:LEU:HB2	2.41	0.42
1:G:907:LEU:O	1:G:911:GLU:HB3	2.19	0.42
1:H:729:LYS:O	1:H:733:VAL:HG12	2.20	0.42
1:H:992:THR:HB	1:H:999:ARG:HH22	1.84	0.42
1:A:784:THR:HG22	1:A:890:ILE:HD11	2.02	0.42
1:C:861:LEU:O	1:C:864:LEU:HB2	2.20	0.42
1:D:724:GLN:HG3	1:D:1064:ARG:NH2	2.35	0.42
1:D:731:VAL:HG13	1:D:1059:LEU:HD22	2.01	0.42
1:D:951:ASP:OD1	1:D:1026:SER:OG	2.37	0.42
1:E:618:LEU:H	1:E:618:LEU:CD2	2.33	0.42
1:E:914:TYR:HD1	1:E:918:GLN:NE2	2.18	0.42
1:F:682:VAL:HG13	1:F:697:THR:HB	2.02	0.42
1:F:850:GLN:HE22	1:F:887:PRO:CD	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1068:ILE:HG23	1:G:1068:ILE:HG12	2.01	0.42
1:F:1075:GLN:NE2	1:F:1100:ARG:HH21	2.18	0.42
1:A:632:GLU:HG2	1:A:636:ARG:HH11	1.85	0.41
1:B:362:ARG:NH2	1:B:419:ASP:OD1	2.52	0.41
1:B:596:GLN:HA	1:B:648:LEU:HD21	2.01	0.41
1:B:758:PHE:HZ	1:B:780:ILE:HD12	1.85	0.41
1:C:343:ARG:HH11	1:C:343:ARG:HD3	1.71	0.41
1:C:857:ALA:O	1:C:859:LYS:NZ	2.40	0.41
1:C:959:GLU:O	1:C:963:LYS:HG3	2.20	0.41
1:C:1019:GLY:O	1:C:1023:ILE:HG13	2.20	0.41
1:D:671:PHE:CE2	1:D:982:ILE:HD13	2.55	0.41
1:D:966:ARG:NH1	1:D:974:THR:HG23	2.34	0.41
1:D:1084:LEU:HD11	1:D:1099:VAL:HG21	2.02	0.41
1:E:943:TYR:HE2	1:E:1009:ILE:O	2.02	0.41
1:F:341:THR:O	1:F:345:GLN:HG3	2.20	0.41
1:F:1117:ASP:O	1:F:1121:SER:N	2.46	0.41
1:G:894:LEU:O	1:G:898:VAL:HG13	2.20	0.41
1:H:502:GLY:CA	1:H:778:GLY:HA3	2.50	0.41
1:H:583:VAL:HB	1:H:597:GLU:HG2	2.02	0.41
1:H:934:ARG:HH12	1:H:1000:LEU:HD11	1.85	0.41
1:A:401:GLU:N	1:A:573:ARG:HH22	2.19	0.41
1:B:735:LYS:HD2	1:B:1050:LEU:O	2.20	0.41
1:B:1047:LYS:HD2	1:B:1047:LYS:HA	1.78	0.41
1:C:738:MET:HG2	1:C:1098:ILE:CG2	2.50	0.41
1:D:985:ASN:OD1	1:D:986:THR:N	2.52	0.41
1:E:512:MET:HG3	1:E:550:VAL:CG1	2.49	0.41
1:E:1048:GLY:HA2	1:E:1051:ASP:OD2	2.20	0.41
1:F:538:TYR:HE1	1:H:473:GLU:OE1	2.04	0.41
1:F:1081:ASN:OD1	1:F:1120:ILE:HA	2.19	0.41
1:G:388:HIS:NE2	1:G:392:THR:HG21	2.34	0.41
1:G:487:ASP:O	1:G:787:GLY:HA2	2.19	0.41
1:G:614:ASN:ND2	1:G:662:MET:HB2	2.36	0.41
1:G:902:ALA:CB	1:G:950:VAL:HG23	2.49	0.41
1:G:916:LEU:O	1:G:920:ARG:HB2	2.20	0.41
1:B:775:GLN:HB3	1:B:780:ILE:HG21	2.01	0.41
1:B:1100:ARG:HA	1:B:1105:SER:HA	2.02	0.41
1:D:380:LEU:HA	1:D:542:ALA:HB2	2.03	0.41
1:D:935:ARG:HA	1:D:938:LEU:HD23	2.03	0.41
1:E:927:PHE:CD2	1:E:934:ARG:HD2	2.54	0.41
1:F:703:ALA:O	1:F:707:VAL:HG22	2.20	0.41
1:F:977:HIS:CE1	1:F:1035:MET:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:733:VAL:HB	1:G:741:PRO:HD3	2.01	0.41
1:H:341:THR:HB	1:H:344:MET:H	1.85	0.41
1:H:401:GLU:CB	1:H:404:VAL:HG11	2.40	0.41
1:H:541:LYS:O	1:H:545:GLU:HG3	2.19	0.41
1:H:937:CYS:HB3	1:H:996:PRO:O	2.19	0.41
1:A:1092:GLU:OE1	1:A:1092:GLU:N	2.43	0.41
1:B:971:LEU:HA	1:B:971:LEU:HD12	1.83	0.41
1:C:424:TRP:O	1:C:428:GLU:HG3	2.21	0.41
1:E:656:CYS:HB3	1:E:678:ILE:HD13	2.03	0.41
1:E:1092:GLU:CD	1:E:1092:GLU:N	2.74	0.41
1:F:719:HIS:HE1	1:F:721:GLN:HB2	1.86	0.41
1:H:355:ARG:HA	1:H:356:PRO:HD3	1.93	0.41
1:H:934:ARG:CZ	1:H:1000:LEU:HD21	2.50	0.41
1:H:941:PRO:HG2	1:H:949:TYR:CD1	2.54	0.41
1:H:1043:PHE:HB2	1:H:1076:PHE:CD1	2.54	0.41
1:C:528:MET:HG3	1:G:844:ILE:HG23	2.02	0.41
1:C:698:TYR:CE2	1:C:725:LYS:HD3	2.55	0.41
1:C:840:ARG:HG2	1:C:968:TYR:HE2	1.86	0.41
1:D:984:ASN:O	1:D:988:ILE:HG13	2.19	0.41
1:E:850:GLN:HB3	1:E:971:LEU:HD22	2.03	0.41
1:F:681:THR:HA	1:F:715:ALA:O	2.21	0.41
1:F:780:ILE:HG12	1:F:781:TYR:N	2.35	0.41
1:F:824:PHE:HE2	1:F:953:TYR:HH	1.65	0.41
1:F:971:LEU:HB3	1:F:972:TYR:CE2	2.54	0.41
1:F:982:ILE:HG23	1:F:1104:TYR:CE1	2.55	0.41
1:G:592:PRO:CA	1:G:597:GLU:HG2	2.49	0.41
1:H:360:ILE:HD13	1:H:360:ILE:HG21	1.82	0.41
1:H:1119:ILE:HA	1:H:1122:ARG:HD2	2.01	0.41
1:A:1073:GLN:O	1:A:1074:MET:HG3	2.20	0.41
1:B:412:ARG:NH1	1:B:1095:ARG:HH22	2.19	0.41
1:B:617:GLY:HA3	1:B:769:MET:CE	2.51	0.41
1:C:618:LEU:HD13	1:C:618:LEU:HA	1.74	0.41
1:C:760:PHE:HB3	1:C:764:ARG:NH1	2.35	0.41
1:E:953:TYR:N	1:E:953:TYR:CD1	2.88	0.41
1:F:414:GLY:N	1:F:660:MET:HB3	2.35	0.41
1:F:490:TYR:HD1	1:F:494:ASN:HD22	1.67	0.41
1:F:739:GLY:CA	1:F:1100:ARG:HB2	2.47	0.41
1:F:749:HIS:HA	1:F:752:MET:CG	2.46	0.41
1:F:781:TYR:CZ	1:F:876:VAL:HB	2.56	0.41
1:G:748:SER:O	1:G:752:MET:HG3	2.19	0.41
1:G:1003:MET:SD	1:G:1004:PRO:HD2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:622:ARG:O	1:H:626:TYR:HD1	2.04	0.41
1:H:870:MET:O	1:H:870:MET:HG3	2.19	0.41
1:H:1064:ARG:O	1:H:1068:ILE:HG13	2.21	0.41
1:B:439:PRO:HD2	1:B:674:TYR:OH	2.21	0.41
1:B:450:ILE:O	1:B:455:VAL:HG23	2.21	0.41
1:D:753:MET:HE3	1:D:774:PRO:HB2	2.01	0.41
1:E:804:MET:HE1	1:E:807:PHE:CD2	2.54	0.41
1:E:899:ASP:OD1	1:E:943:TYR:N	2.51	0.41
1:E:908:VAL:HA	1:E:914:TYR:O	2.21	0.41
1:F:1068:ILE:H	1:F:1068:ILE:HG13	1.65	0.41
1:G:513:ASN:HB2	1:G:589:ALA:O	2.21	0.41
1:H:1075:GLN:CD	1:H:1100:ARG:HH21	2.20	0.41
1:A:540:TYR:O	1:A:544:ILE:HG13	2.19	0.41
1:B:1084:LEU:HD22	1:B:1108:PHE:CD1	2.56	0.41
1:C:344:MET:HG3	1:C:650:GLN:OE1	2.20	0.41
1:C:387:ARG:HH11	1:C:545:GLU:CD	2.24	0.41
1:C:758:PHE:HZ	1:C:780:ILE:HB	1.85	0.41
1:C:923:LEU:HD11	1:C:996:PRO:HD3	2.02	0.41
1:D:349:ASN:O	1:D:353:THR:HG23	2.20	0.41
1:D:832:LYS:HB3	1:D:960:TRP:CZ2	2.56	0.41
1:D:1127:LYS:HG2	1:D:1128:PHE:N	2.35	0.41
1:E:965:CYS:HB3	1:E:975:LEU:HG	2.03	0.41
1:F:397:ILE:HG23	1:F:404:VAL:CG1	2.51	0.41
1:F:507:LEU:HD13	1:F:512:MET:CE	2.51	0.41
1:F:820:ASP:HA	1:F:822:ARG:HE	1.86	0.41
1:F:859:LYS:HA	1:F:860:PRO:HD3	1.91	0.41
1:F:1041:HIS:N	1:F:1073:GLN:OE1	2.54	0.41
1:G:653:ILE:HG21	1:G:707:VAL:HG21	2.01	0.41
1:H:345:GLN:HA	1:H:348:ARG:HB3	2.02	0.41
1:H:347:LEU:CD2	1:H:400:ASP:HB2	2.50	0.41
1:H:356:PRO:HB2	1:H:440:PHE:HD2	1.86	0.41
1:H:359:SER:HB3	1:H:414:GLY:O	2.20	0.41
1:H:429:LEU:O	1:H:442:ILE:HD11	2.20	0.41
1:H:634:ASP:HA	1:H:639:ARG:HD3	2.03	0.41
1:H:702:ASP:OD1	1:H:705:ARG:NE	2.48	0.41
1:H:1116:GLN:O	1:H:1120:ILE:HG13	2.20	0.41
1:A:660:MET:CE	1:A:674:TYR:HB3	2.50	0.41
1:A:714:LEU:HD12	1:A:714:LEU:HA	1.87	0.41
1:A:890:ILE:HD12	1:A:980:LEU:CD2	2.50	0.41
1:B:696:LEU:HA	1:B:696:LEU:HD12	1.72	0.41
1:B:864:LEU:C	1:B:865:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:LEU:O	1:B:977:HIS:HA	2.20	0.41
1:B:969:LYS:HA	1:B:974:THR:HG22	2.02	0.41
1:C:913:LYS:HE2	1:C:914:TYR:HE2	1.85	0.41
1:C:925:ALA:O	1:C:928:GLU:HB2	2.20	0.41
1:D:608:LEU:HD23	1:D:611:ILE:HG13	2.02	0.41
1:D:799:LEU:HA	1:D:799:LEU:HD23	1.79	0.41
1:D:803:ARG:HE	1:D:803:ARG:HB3	1.53	0.41
1:F:395:ILE:HD13	1:F:395:ILE:HA	1.90	0.41
1:F:940:ALA:O	1:F:941:PRO:C	2.60	0.41
1:G:728:GLU:CG	1:G:1056:ARG:HH21	2.34	0.41
1:G:843:ALA:O	1:G:847:VAL:HG22	2.21	0.41
1:H:379:ILE:HG23	1:H:380:LEU:N	2.36	0.41
1:H:402:LEU:O	1:H:580:ILE:HG12	2.20	0.41
1:H:790:GLN:CD	1:H:793:ILE:HB	2.41	0.41
1:H:790:GLN:HA	1:H:892:SER:H	1.86	0.41
1:H:854:ARG:HE	1:H:854:ARG:HB3	1.74	0.41
1:H:966:ARG:HD3	1:H:974:THR:HG23	2.03	0.41
1:A:356:PRO:HG2	1:A:674:TYR:CZ	2.56	0.41
1:B:370:VAL:HA	1:B:381:LEU:HD11	2.02	0.41
1:B:411:PRO:HA	1:B:658:GLU:HB3	2.03	0.41
1:B:510:LYS:NZ	1:B:518:ASP:OD2	2.52	0.41
1:B:587:VAL:HB	1:B:601:SER:HB2	2.03	0.41
1:C:968:TYR:HB3	3:G:1312:HOH:O	2.20	0.41
1:D:463:LEU:HD23	1:D:463:LEU:O	2.21	0.41
1:D:504:ASP:HB3	1:D:626:TYR:CD2	2.56	0.41
1:D:937:CYS:O	1:D:942:LYS:NZ	2.42	0.41
1:E:795:ILE:HG22	1:E:799:LEU:HG	2.03	0.41
1:F:349:ASN:O	1:F:353:THR:OG1	2.37	0.41
1:F:701:MET:CE	1:F:729:LYS:HG2	2.51	0.41
1:F:770:GLY:HA3	2:F:1201:A1H9I:C1	2.50	0.41
1:F:1084:LEU:HD21	1:F:1099:VAL:HG11	2.03	0.41
1:G:686:LYS:HG3	1:G:692:ALA:HA	2.03	0.41
1:H:450:ILE:O	1:H:455:VAL:HG23	2.21	0.41
1:H:531:PRO:HA	1:H:534:ILE:HD12	2.03	0.41
1:H:1047:LYS:HB2	1:H:1047:LYS:HE3	1.68	0.41
1:B:831:VAL:HG11	1:B:901:MET:CE	2.50	0.40
1:B:993:ASN:OD1	1:B:994:ALA:N	2.47	0.40
1:C:343:ARG:HD3	1:C:400:ASP:O	2.21	0.40
1:C:344:MET:HE2	1:C:647:GLU:HG3	2.04	0.40
1:C:419:ASP:OD1	1:C:419:ASP:N	2.52	0.40
1:C:523:LEU:CD1	1:C:537:ILE:HG23	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:752:MET:O	1:C:756:LYS:HG3	2.21	0.40
1:C:794:ALA:O	1:C:798:VAL:HG23	2.22	0.40
1:C:1043:PHE:HB2	1:C:1076:PHE:HD1	1.87	0.40
1:D:894:LEU:O	1:D:898:VAL:HG12	2.21	0.40
1:E:963:LYS:O	1:E:967:LYS:HG3	2.20	0.40
1:F:786:THR:HG23	1:F:846:THR:HG23	2.02	0.40
1:F:836:ALA:N	3:F:1308:HOH:O	2.54	0.40
1:F:957:ILE:O	1:F:961:THR:OG1	2.17	0.40
1:G:340:LEU:CB	1:G:345:GLN:OE1	2.67	0.40
1:H:630:MET:H	1:H:630:MET:HG2	1.59	0.40
1:A:349:ASN:O	1:A:353:THR:HG23	2.21	0.40
1:A:382:ARG:NH2	1:A:613:GLU:OE1	2.54	0.40
1:A:935:ARG:O	1:A:939:ASN:N	2.42	0.40
1:B:477:TRP:CZ2	1:B:481:GLY:HA3	2.57	0.40
1:B:1098:ILE:HG12	1:B:1107:TYR:CD1	2.56	0.40
1:D:359:SER:HB2	1:D:361:TYR:HD2	1.87	0.40
1:D:599:LEU:HD22	1:D:652:PHE:CD1	2.55	0.40
1:D:767:CYS:O	1:D:774:PRO:HA	2.21	0.40
1:D:832:LYS:NZ	1:D:956:ASP:OD2	2.38	0.40
1:E:769:MET:HE3	1:E:769:MET:O	2.20	0.40
1:E:803:ARG:HB3	1:E:810:TYR:CE1	2.56	0.40
1:E:888:GLY:HA3	1:E:1037:ILE:HG13	2.02	0.40
1:F:422:TRP:CZ2	1:F:459:GLU:HG2	2.56	0.40
1:F:1084:LEU:O	1:F:1087:ALA:HB3	2.20	0.40
1:G:348:ARG:NE	1:G:707:VAL:O	2.45	0.40
1:G:383:ALA:CB	1:G:542:ALA:HB1	2.52	0.40
1:H:416:PHE:CE1	1:H:425:VAL:HG21	2.56	0.40
1:H:612:GLU:OE2	1:H:860:PRO:HD2	2.21	0.40
1:A:376:MET:HE1	1:A:384:LYS:HG3	2.03	0.40
1:A:419:ASP:HB3	1:A:458:TRP:CH2	2.56	0.40
1:A:619:SER:HB3	1:A:679:ASN:CB	2.42	0.40
1:B:676:PRO:HD2	1:B:711:GLN:HG3	2.02	0.40
1:B:940:ALA:HB3	1:B:942:LYS:NZ	2.36	0.40
1:B:1044:LYS:HZ3	1:B:1122:ARG:HB2	1.87	0.40
1:D:599:LEU:HD23	1:D:599:LEU:HA	1.91	0.40
1:D:608:LEU:O	1:D:611:ILE:HB	2.21	0.40
1:E:655:LYS:O	1:E:658:GLU:HB2	2.20	0.40
1:E:824:PHE:HZ	1:E:953:TYR:HE2	1.65	0.40
1:H:362:ARG:NH2	1:H:419:ASP:OD1	2.54	0.40
1:H:376:MET:HB3	1:H:376:MET:HE2	1.97	0.40
1:H:397:ILE:HG13	1:H:560:HIS:ND1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:404:VAL:CA	1:H:655:LYS:HE2	2.49	0.40
1:H:419:ASP:N	1:H:419:ASP:OD1	2.54	0.40
1:H:499:THR:O	1:H:501:PRO:HD3	2.21	0.40
1:H:570:ASN:O	1:H:574:ARG:N	2.37	0.40
1:H:946:ASP:HA	1:H:951:ASP:OD2	2.21	0.40
1:A:430:ASP:OD1	1:A:447:LYS:NZ	2.43	0.40
1:A:621:GLY:HA2	1:A:767:CYS:CB	2.52	0.40
1:A:622:ARG:HH11	1:A:765:ASP:HA	1.86	0.40
1:A:1081:ASN:O	1:A:1084:LEU:N	2.55	0.40
1:B:587:VAL:HG11	1:B:597:GLU:HB3	2.04	0.40
1:B:948:ASN:OD1	1:B:1029:LYS:HE2	2.22	0.40
1:C:608:LEU:O	1:C:611:ILE:N	2.53	0.40
1:D:397:ILE:HG12	1:D:404:VAL:HB	2.03	0.40
1:D:446:ASP:O	1:D:450:ILE:HG13	2.22	0.40
1:E:558:ALA:HB1	1:E:585:GLU:HG2	2.03	0.40
1:E:744:HIS:CD2	1:E:768:LEU:HD13	2.57	0.40
1:E:805:VAL:CG1	1:E:993:ASN:HB2	2.37	0.40
1:E:829:ALA:O	1:E:833:GLN:HB2	2.21	0.40
1:E:889:LEU:HD12	1:E:889:LEU:HA	1.92	0.40
1:E:895:ALA:HB2	1:E:943:TYR:HD2	1.86	0.40
1:E:933:LEU:O	1:E:934:ARG:C	2.59	0.40
1:F:1042:ASN:ND2	1:F:1122:ARG:HH12	2.19	0.40
1:G:553:TYR:O	1:G:557:ILE:HG12	2.21	0.40
1:G:572:GLN:O	1:G:576:GLU:N	2.54	0.40
1:H:410:LYS:HB3	1:H:413:ALA:HB2	2.04	0.40
1:H:540:TYR:O	1:H:544:ILE:HG13	2.21	0.40
1:H:587:VAL:HG11	1:H:597:GLU:O	2.21	0.40
1:A:450:ILE:O	1:A:455:VAL:HG23	2.22	0.40
1:A:926:ASN:O	1:A:927:PHE:HB2	2.22	0.40
1:A:1024:ILE:CG2	1:A:1074:MET:HE3	2.52	0.40
1:B:362:ARG:NH1	1:B:612:GLU:O	2.55	0.40
1:B:393:ALA:O	1:B:556:ARG:NH2	2.52	0.40
1:B:745:PHE:HD1	1:B:1067:SER:HB2	1.85	0.40
1:B:1069:LEU:HD23	1:B:1069:LEU:HA	1.82	0.40
1:C:792:PRO:HG3	1:C:897:TYR:HB2	2.04	0.40
1:C:948:ASN:OD1	1:C:1029:LYS:HD3	2.22	0.40
1:D:567:LYS:HD2	1:D:567:LYS:HA	1.88	0.40
1:E:980:LEU:HD12	1:E:980:LEU:O	2.22	0.40
1:F:424:TRP:O	1:F:428:GLU:HG3	2.22	0.40
1:F:601:SER:O	1:F:605:VAL:HG22	2.21	0.40
1:F:795:ILE:HG12	1:F:901:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:895:ALA:HB2	1:F:1010:SER:O	2.21	0.40
1:G:544:ILE:O	1:G:548:GLU:HG2	2.21	0.40
1:H:608:LEU:HD23	1:H:608:LEU:HA	1.82	0.40

All (1) 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:C:574:ARG:CD	1:C:819:ARG:NH2[1_655]	1.92	0.28

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	790/1150 (69%)	732 (93%)	56 (7%)	2 (0%)	41	66
1	B	790/1150 (69%)	737 (93%)	52 (7%)	1 (0%)	51	78
1	C	790/1150 (69%)	723 (92%)	66 (8%)	1 (0%)	51	78
1	D	790/1150 (69%)	733 (93%)	55 (7%)	2 (0%)	41	66
1	E	790/1150 (69%)	720 (91%)	69 (9%)	1 (0%)	51	78
1	F	790/1150 (69%)	700 (89%)	89 (11%)	1 (0%)	51	78
1	G	790/1150 (69%)	713 (90%)	76 (10%)	1 (0%)	51	78
1	H	790/1150 (69%)	699 (88%)	89 (11%)	2 (0%)	41	66
All	All	6320/9200 (69%)	5757 (91%)	552 (9%)	11 (0%)	47	73

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	ILE
1	A	983	SER

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Mol	Chain	Res	Type
1	B	982	ILE
1	C	982	ILE
1	F	982	ILE
1	H	778	GLY
1	D	982	ILE
1	E	982	ILE
1	G	982	ILE
1	H	946	ASP
1	D	481	GLY

5.3.2 Protein sidechains (i)

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%)	656 (98%)	12 (2%)	59	83
1	B	668/955 (70%)	661 (99%)	7 (1%)	76	91
1	C	668/955 (70%)	655 (98%)	13 (2%)	57	82
1	D	668/955 (70%)	653 (98%)	15 (2%)	52	79
1	E	668/955 (70%)	655 (98%)	13 (2%)	57	82
1	F	668/955 (70%)	650 (97%)	18 (3%)	44	74
1	G	668/955 (70%)	650 (97%)	18 (3%)	44	74
1	H	668/955 (70%)	643 (96%)	25 (4%)	34	63
All	All	5344/7640 (70%)	5223 (98%)	121 (2%)	50	78

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ARG
1	A	371	LYS
1	A	527	SER
1	A	573	ARG
1	A	710	TYR
1	A	747	ASP

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Mol	Chain	Res	Type
1	A	791	TRP
1	A	801	ARG
1	A	859	LYS
1	A	980	LEU
1	A	983	SER
1	A	1026	SER
1	B	705	ARG
1	B	710	TYR
1	B	725	LYS
1	B	769	MET
1	B	819	ARG
1	B	1095	ARG
1	B	1100	ARG
1	C	362	ARG
1	C	371	LYS
1	C	433	SER
1	C	435	ARG
1	C	555	ARG
1	C	606	GLU
1	C	819	ARG
1	C	840	ARG
1	C	851	ARG
1	C	859	LYS
1	C	993	ASN
1	C	1093	LYS
1	C	1095	ARG
1	D	574	ARG
1	D	642	HIS
1	D	663	SER
1	D	695	ASP
1	D	710	TYR
1	D	754	LEU
1	D	819	ARG
1	D	859	LYS
1	D	900	SER
1	D	935	ARG
1	D	936	ASP
1	D	980	LEU
1	D	1029	LYS
1	D	1089	GLN
1	D	1095	ARG
1	E	362	ARG

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Mol	Chain	Res	Type
1	E	437	GLN
1	E	486	SER
1	E	574	ARG
1	E	636	ARG
1	E	699	LEU
1	E	710	TYR
1	E	728	GLU
1	E	822	ARG
1	E	905	ARG
1	E	983	SER
1	E	1039	MET
1	E	1095	ARG
1	F	355	ARG
1	F	362	ARG
1	F	671	PHE
1	F	713	SER
1	F	729	LYS
1	F	809	SER
1	F	819	ARG
1	F	875	ASP
1	F	921	ASP
1	F	924	LEU
1	F	926	ASN
1	F	943	TYR
1	F	976	SER
1	F	999	ARG
1	F	1028	SER
1	F	1093	LYS
1	F	1095	ARG
1	F	1113	LYS
1	G	345	GLN
1	G	359	SER
1	G	362	ARG
1	G	433	SER
1	G	448	LYS
1	G	569	GLN
1	G	639	ARG
1	G	705	ARG
1	G	710	TYR
1	G	761	GLU
1	G	767	CYS
1	G	819	ARG

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Mol	Chain	Res	Type
1	G	820	ASP
1	G	892	SER
1	G	948	ASN
1	G	999	ARG
1	G	1073	GLN
1	G	1128	PHE
1	H	352	LEU
1	H	359	SER
1	H	382	ARG
1	H	462	SER
1	H	472	ARG
1	H	535	ASP
1	H	562	ARG
1	H	573	ARG
1	H	601	SER
1	H	639	ARG
1	H	655	LYS
1	H	666	LEU
1	H	721	GLN
1	H	722	SER
1	H	752	MET
1	H	789	THR
1	H	809	SER
1	H	851	ARG
1	H	963	LYS
1	H	980	LEU
1	H	1033	GLU
1	H	1095	ARG
1	H	1105	SER
1	H	1113	LYS
1	H	1128	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	437	GLN
1	B	685	GLN
1	B	749	HIS
1	B	1075	GLN
1	C	711	GLN
1	C	721	GLN
1	C	993	ASN

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Mol	Chain	Res	Type
1	D	811	GLN
1	D	1036	ASN
1	D	1073	GLN
1	D	1075	GLN
1	E	437	GLN
1	E	650	GLN
1	E	749	HIS
1	F	345	GLN
1	F	675	GLN
1	F	721	GLN
1	F	926	ASN
1	F	1042	ASN
1	G	437	GLN
1	G	650	GLN
1	G	675	GLN
1	G	711	GLN
1	G	744	HIS
1	G	833	GLN
1	G	1042	ASN
1	H	530	ASN
1	H	572	GLN
1	H	584	ASN
1	H	744	HIS
1	H	749	HIS
1	H	850	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	A1H9I	A	1201	-	6,7,7	1.67	2 (33%)	7,9,9	0.91	0
2	A1H9I	E	1201	-	6,7,7	1.37	2 (33%)	7,9,9	0.74	0
2	A1H9I	C	1201	-	6,7,7	1.77	2 (33%)	7,9,9	0.86	0
2	A1H9I	H	1201	-	6,7,7	1.67	2 (33%)	7,9,9	0.60	0
2	A1H9I	D	1201	-	6,7,7	1.59	1 (16%)	7,9,9	0.90	0
2	A1H9I	F	1201	-	6,7,7	1.40	1 (16%)	7,9,9	0.91	0
2	A1H9I	B	1201	-	6,7,7	1.59	2 (33%)	7,9,9	1.13	0
2	A1H9I	G	1201	-	6,7,7	1.36	1 (16%)	7,9,9	0.61	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	A1H9I	A	1201	-	-	1/4/7/7	-
2	A1H9I	E	1201	-	-	4/4/7/7	-
2	A1H9I	C	1201	-	-	3/4/7/7	-
2	A1H9I	H	1201	-	-	3/4/7/7	-
2	A1H9I	D	1201	-	-	4/4/7/7	-
2	A1H9I	F	1201	-	-	0/4/7/7	-
2	A1H9I	B	1201	-	-	0/4/7/7	-
2	A1H9I	G	1201	-	-	3/4/7/7	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1H9I	C2-N1	-2.57	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1201	A1H9I	C5-N1	-2.55	1.46	1.50
2	C	1201	A1H9I	C5-N1	-2.54	1.46	1.50
2	H	1201	A1H9I	C2-N1	-2.51	1.47	1.52
2	D	1201	A1H9I	C5-N1	-2.50	1.46	1.50
2	F	1201	A1H9I	C2-N1	-2.49	1.47	1.52
2	B	1201	A1H9I	C2-N1	-2.46	1.47	1.52
2	C	1201	A1H9I	C2-N1	-2.36	1.47	1.52
2	E	1201	A1H9I	C2-N1	-2.28	1.47	1.52
2	G	1201	A1H9I	C2-N1	-2.22	1.47	1.52
2	B	1201	A1H9I	C5-N1	-2.22	1.47	1.50
2	A	1201	A1H9I	C5-N1	-2.16	1.47	1.50
2	E	1201	A1H9I	C5-N1	-2.02	1.47	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1201	A1H9I	C1-C2-N1-C4
2	C	1201	A1H9I	C1-C2-N1-C5
2	C	1201	A1H9I	C1-C2-N1-C3
2	D	1201	A1H9I	C1-C2-N1-C4
2	D	1201	A1H9I	C1-C2-N1-C5
2	D	1201	A1H9I	C1-C2-N1-C3
2	E	1201	A1H9I	C1-C2-N1-C4
2	E	1201	A1H9I	C1-C2-N1-C5
2	E	1201	A1H9I	C1-C2-N1-C3
2	D	1201	A1H9I	O1-C1-C2-N1
2	G	1201	A1H9I	O1-C1-C2-N1
2	H	1201	A1H9I	C1-C2-N1-C3
2	A	1201	A1H9I	O1-C1-C2-N1
2	E	1201	A1H9I	O1-C1-C2-N1
2	G	1201	A1H9I	C1-C2-N1-C5
2	H	1201	A1H9I	C1-C2-N1-C4
2	H	1201	A1H9I	C1-C2-N1-C5
2	G	1201	A1H9I	C1-C2-N1-C3

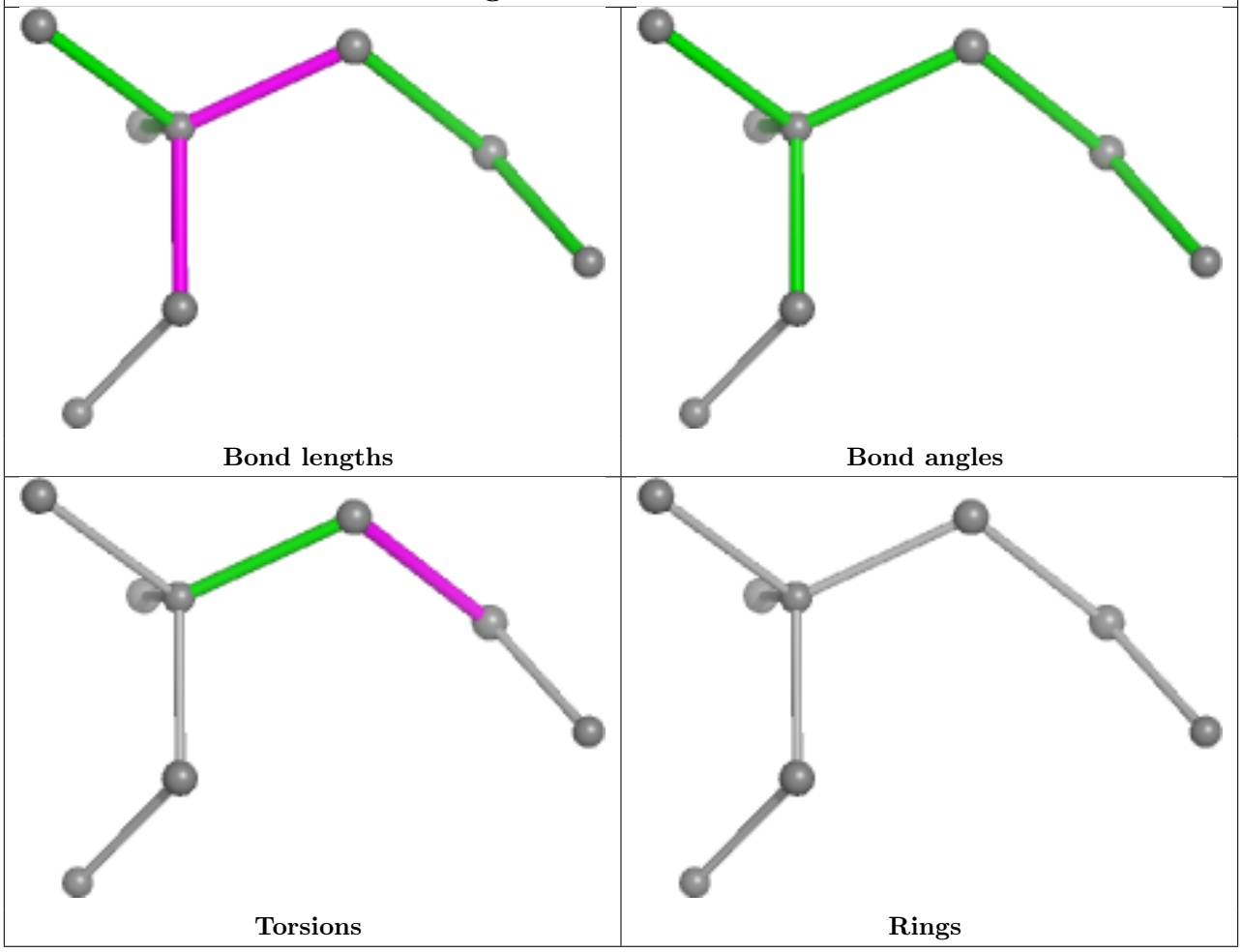
There are no ring outliers.

2 monomers are involved in 3 short contacts:

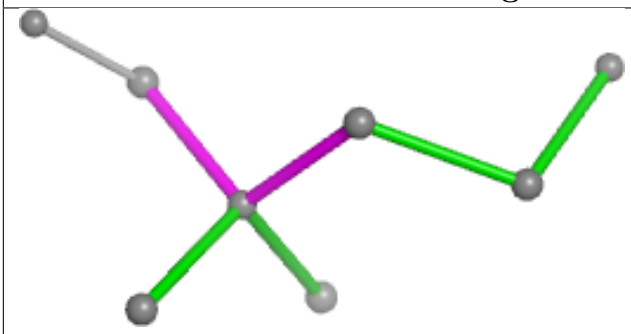
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1201	A1H9I	2	0
2	B	1201	A1H9I	1	0

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 then 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.

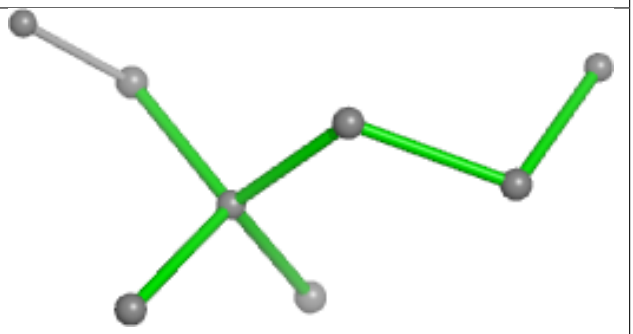
Ligand A1H9I A 1201



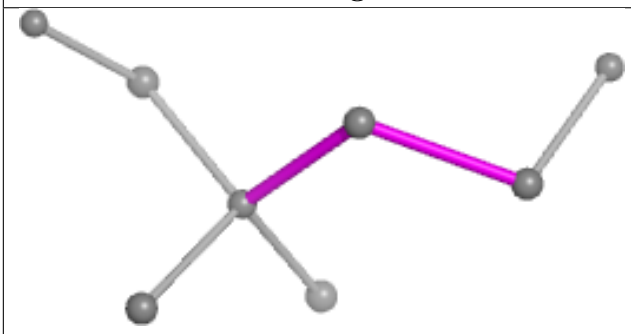
Ligand A1H9I E 1201



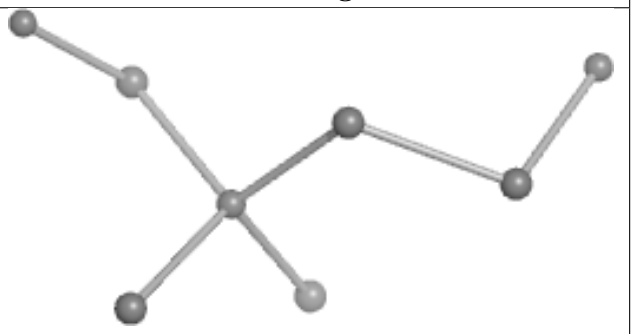
Bond lengths



Bond angles

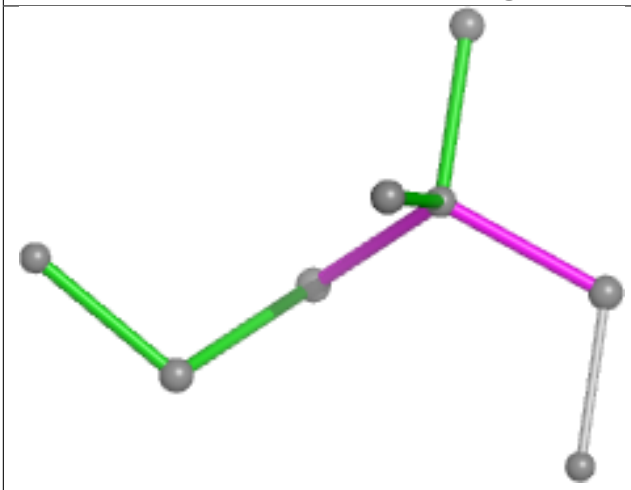


Torsions

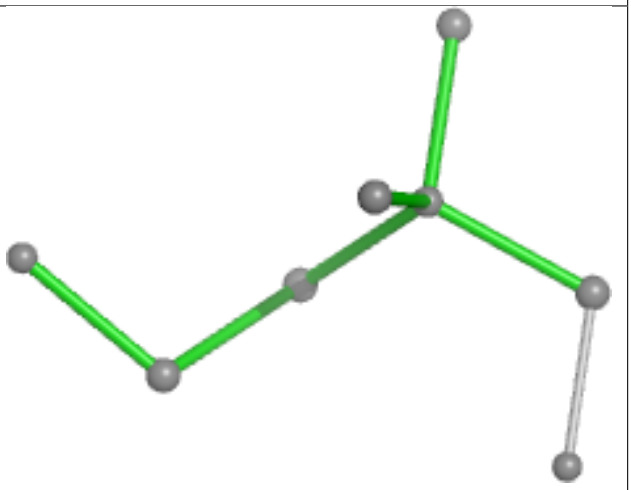


Rings

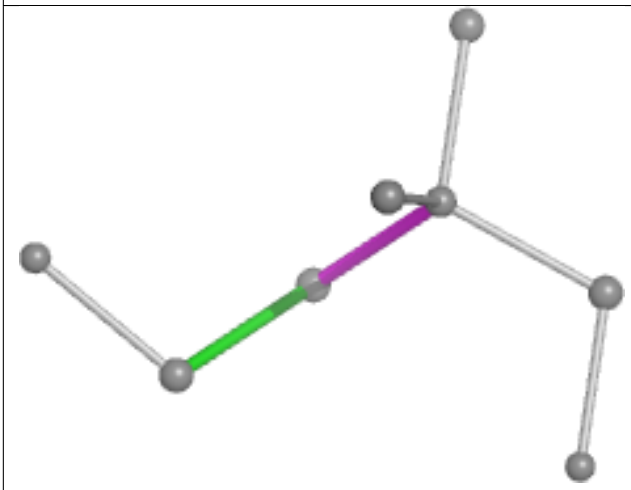
Ligand A1H9I C 1201



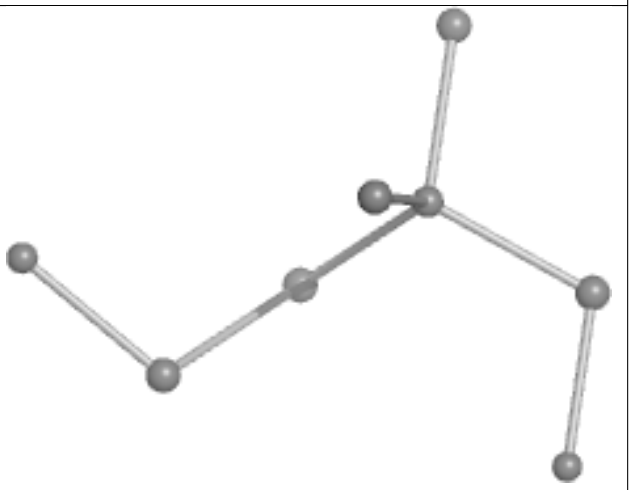
Bond lengths



Bond angles

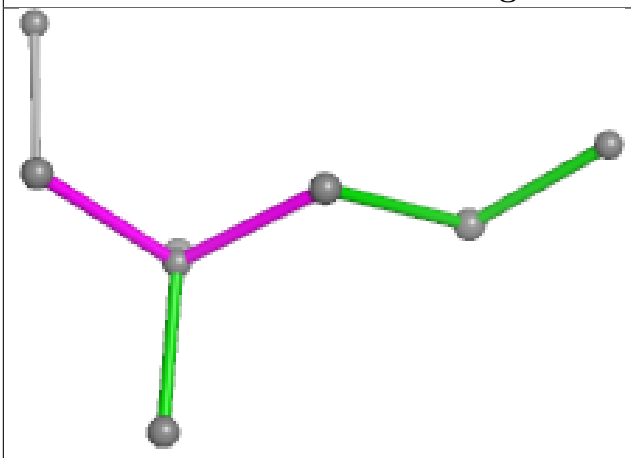


Torsions

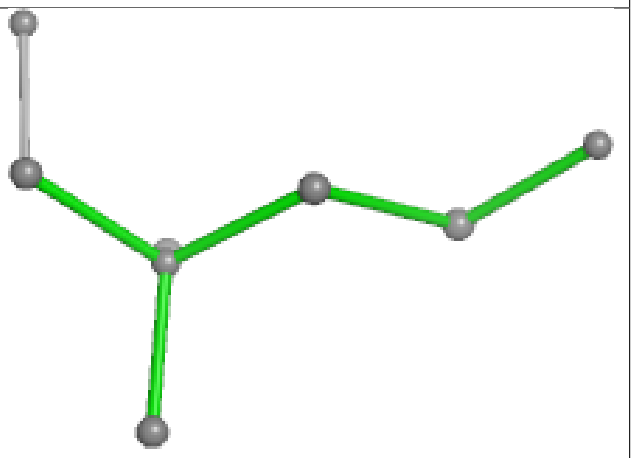


Rings

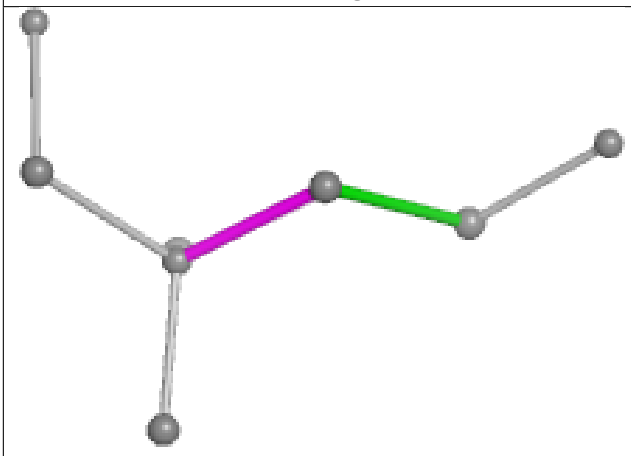
Ligand A1H9I H 1201



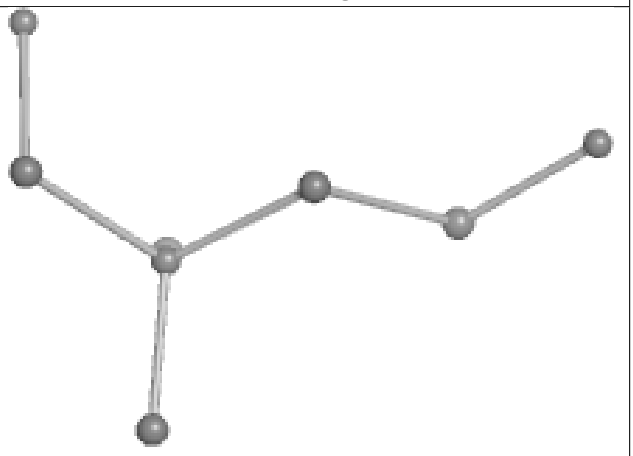
Bond lengths



Bond angles

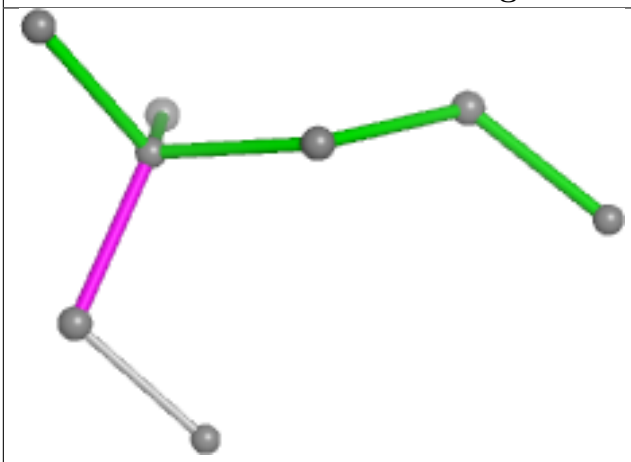


Torsions

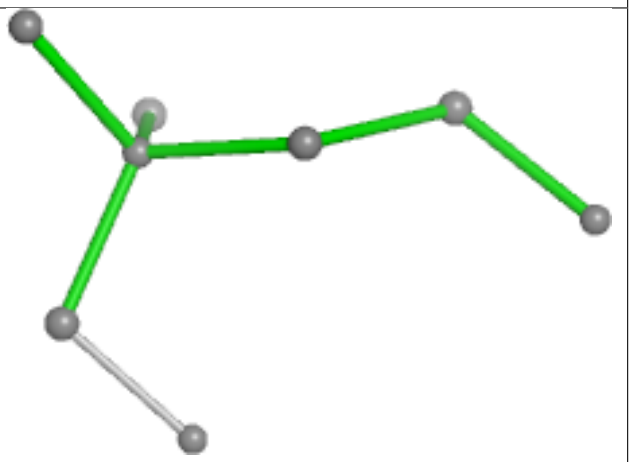


Rings

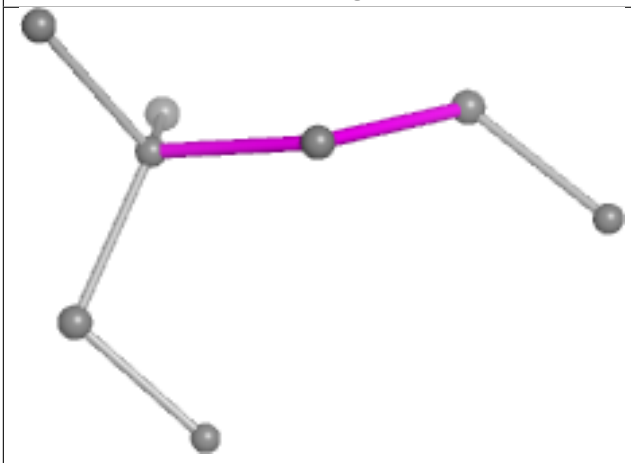
Ligand A1H9I D 1201



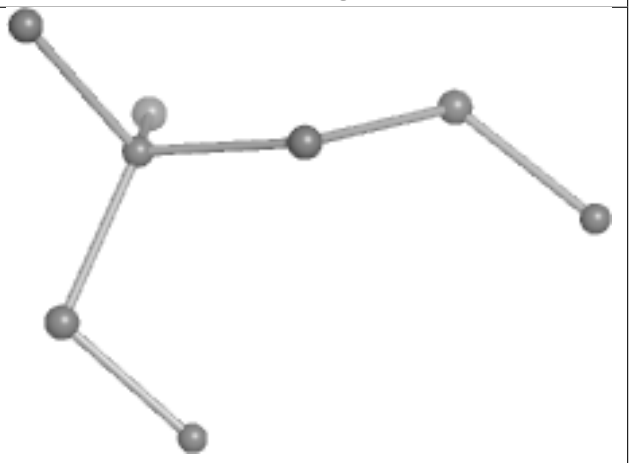
Bond lengths



Bond angles

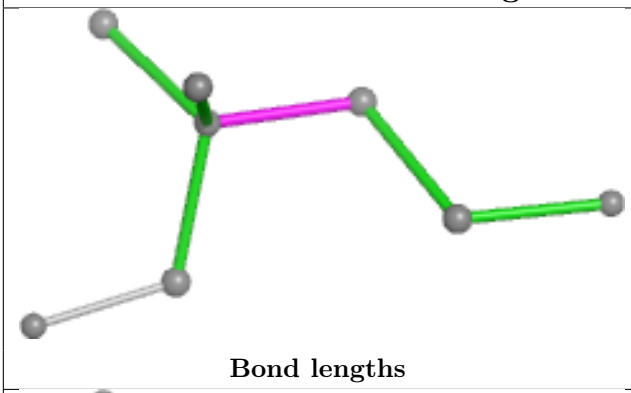


Torsions

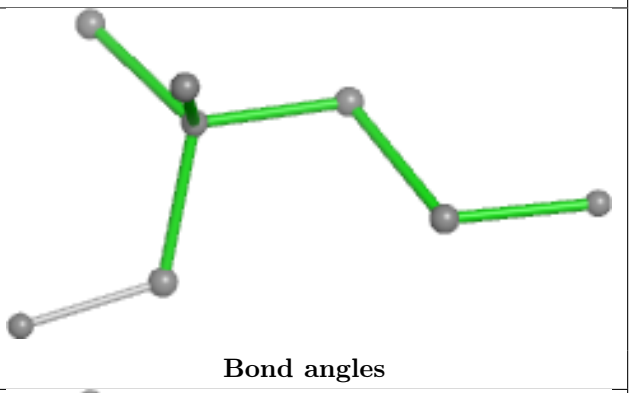


Rings

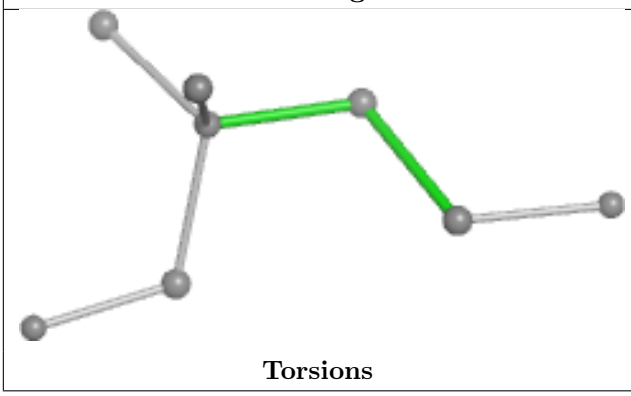
Ligand A1H9I F 1201



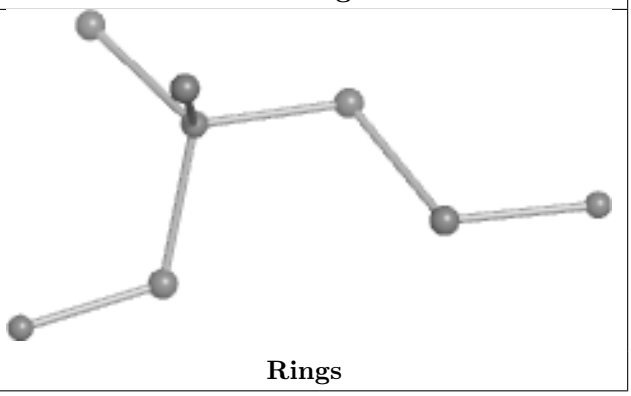
Bond lengths



Bond angles

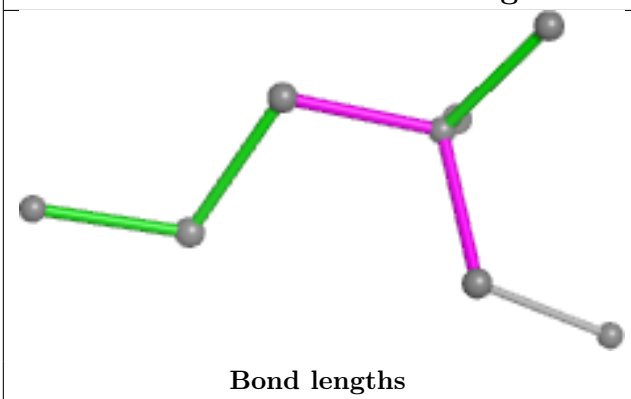


Torsions

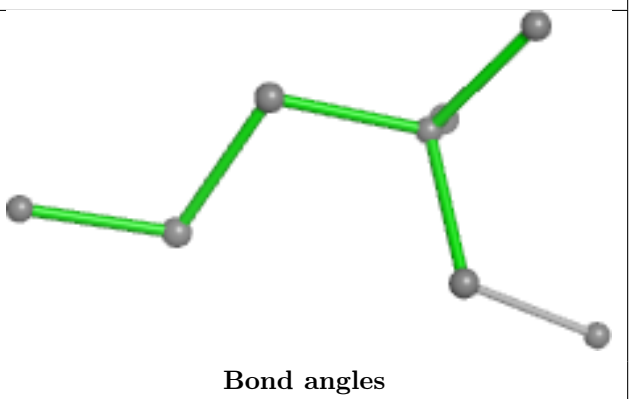


Rings

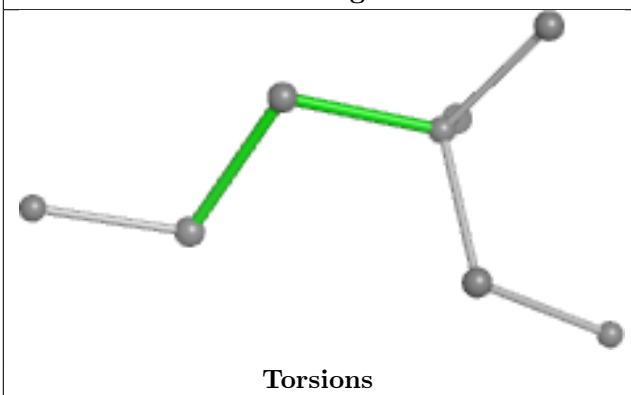
Ligand A1H9I B 1201



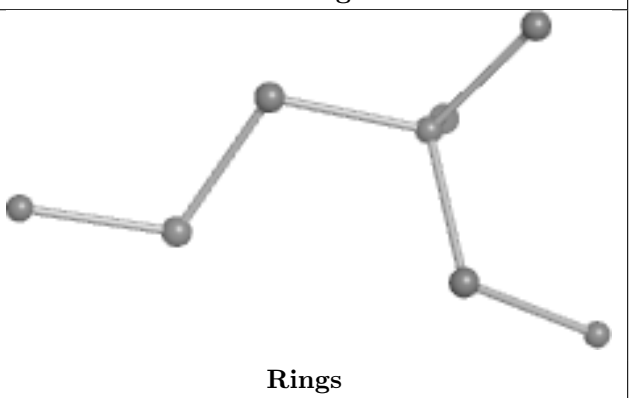
Bond lengths



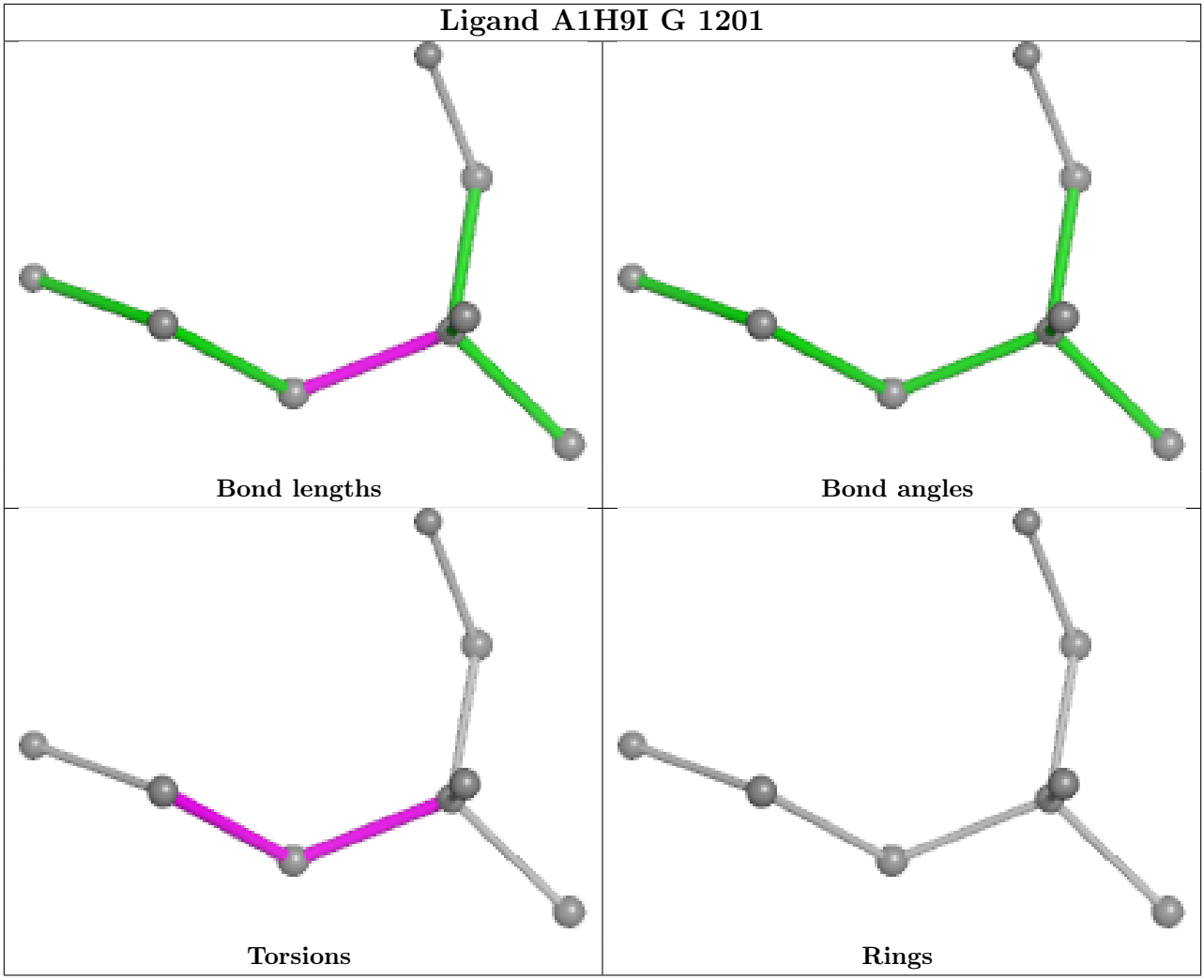
Bond angles



Torsions



Rings



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, 95^{th} 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%)	-0.35	0 100 100	13, 25, 45, 73	0
1	B	792/1150 (68%)	-0.33	0 100 100	11, 26, 43, 57	0
1	C	792/1150 (68%)	-0.23	1 (0%) 95 96	15, 32, 51, 86	0
1	D	792/1150 (68%)	-0.08	1 (0%) 95 96	17, 43, 62, 80	0
1	E	792/1150 (68%)	-0.06	6 (0%) 86 87	17, 49, 76, 95	0
1	F	792/1150 (68%)	0.02	10 (1%) 77 78	19, 45, 71, 92	0
1	G	792/1150 (68%)	0.27	27 (3%) 45 45	25, 51, 76, 102	0
1	H	792/1150 (68%)	0.46	55 (6%) 16 15	32, 61, 87, 102	0
All	All	6336/9200 (68%)	-0.04	100 (1%) 72 74	11, 40, 74, 102	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	MET	6.7
1	G	339	GLY	5.0
1	H	405	GLY	5.0
1	G	340	LEU	4.7
1	G	645	ALA	4.6
1	H	450	ILE	4.2
1	H	706	PHE	4.2
1	H	709	VAL	4.1
1	H	454	ILE	4.1
1	H	337	MET	4.0
1	H	561	ALA	4.0
1	G	337	MET	4.0
1	H	1046	LEU	3.4
1	H	1097	LEU	3.4
1	H	651	ALA	3.3
1	G	659	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	1091	PRO	3.2
1	E	1038	GLY	3.2
1	H	440	PHE	3.2
1	H	1020	PRO	3.2
1	H	340	LEU	3.1
1	H	575	ALA	3.1
1	H	663	SER	3.1
1	H	1050	LEU	3.1
1	H	554	ALA	3.1
1	H	565	ALA	3.1
1	G	602	ILE	3.1
1	H	710	TYR	3.0
1	G	981	SER	3.0
1	F	914	TYR	3.0
1	G	550	VAL	3.0
1	H	907	LEU	3.0
1	H	1124	VAL	3.0
1	H	740	PHE	2.9
1	H	602	ILE	2.9
1	F	943	TYR	2.8
1	G	743	CYS	2.8
1	H	402	LEU	2.7
1	H	551	VAL	2.7
1	G	338	GLU	2.7
1	H	932	ALA	2.7
1	E	1000	LEU	2.7
1	D	566	ALA	2.6
1	G	646	LEU	2.6
1	H	366	PHE	2.6
1	H	1109	VAL	2.5
1	H	654	ILE	2.5
1	F	953	TYR	2.4
1	H	418	PRO	2.4
1	E	1115	VAL	2.4
1	G	706	PHE	2.4
1	G	1106	ALA	2.4
1	H	1094	TYR	2.4
1	H	906	LYS	2.4
1	H	1096	ASP	2.4
1	G	440	PHE	2.4
1	H	1120	ILE	2.3
1	H	1095	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	338	GLU	2.3
1	H	795	ILE	2.3
1	H	1101	VAL	2.3
1	G	1059	LEU	2.3
1	G	633	ALA	2.3
1	H	442	ILE	2.3
1	H	411	PRO	2.2
1	G	656	CYS	2.2
1	H	704	VAL	2.2
1	G	712	PRO	2.2
1	G	604	THR	2.2
1	H	666	LEU	2.2
1	H	558	ALA	2.2
1	H	572	GLN	2.2
1	G	351	TYR	2.2
1	G	356	PRO	2.2
1	F	802	GLY	2.2
1	G	1046	LEU	2.2
1	H	1093	LYS	2.2
1	H	361	TYR	2.2
1	F	907	LEU	2.2
1	G	583	VAL	2.1
1	H	933	LEU	2.1
1	H	935	ARG	2.1
1	H	1051	ASP	2.1
1	G	1027	VAL	2.1
1	H	490	TYR	2.1
1	H	1048	GLY	2.1
1	E	838	ILE	2.1
1	H	1106	ALA	2.1
1	F	897	TYR	2.0
1	H	726	TYR	2.0
1	E	922	ALA	2.0
1	H	581	ALA	2.0
1	F	824	PHE	2.0
1	G	1047	LYS	2.0
1	F	938	LEU	2.0
1	F	792	PRO	2.0
1	F	1046	LEU	2.0
1	G	578	LEU	2.0
1	H	649	LEU	2.0
1	G	805	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 monosaccharides in this entry.

6.4 Ligands (i)

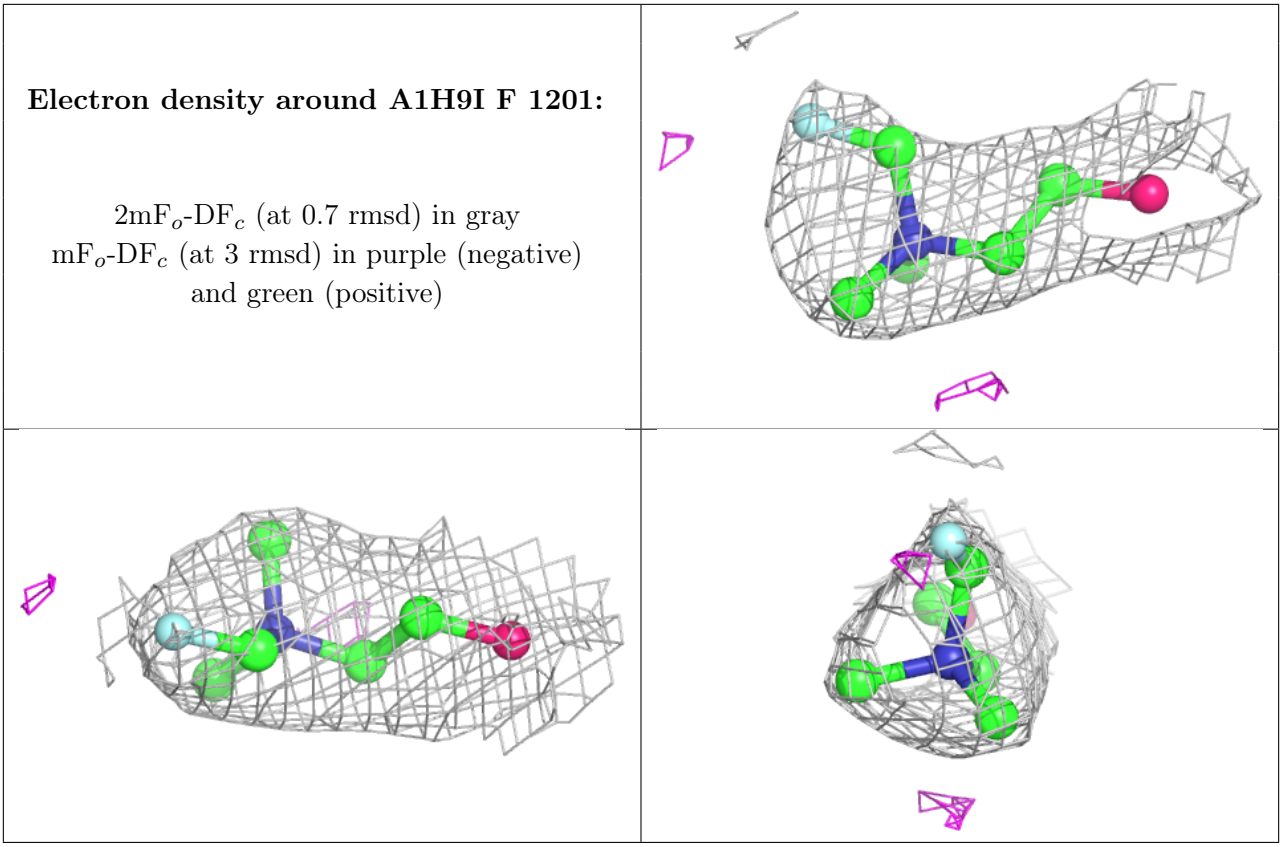
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1H9I	F	1201	8/8	0.92	0.24	34,40,49,49	0
2	A1H9I	E	1201	8/8	0.93	0.22	34,40,45,47	0
2	A1H9I	H	1201	8/8	0.93	0.28	54,63,65,65	0
2	A1H9I	D	1201	8/8	0.96	0.18	32,35,37,38	0
2	A1H9I	G	1201	8/8	0.96	0.23	32,34,42,46	0
2	A1H9I	C	1201	8/8	0.96	0.19	19,24,29,29	0
2	A1H9I	A	1201	8/8	0.98	0.18	16,21,25,26	0
2	A1H9I	B	1201	8/8	0.98	0.16	18,23,25,29	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.

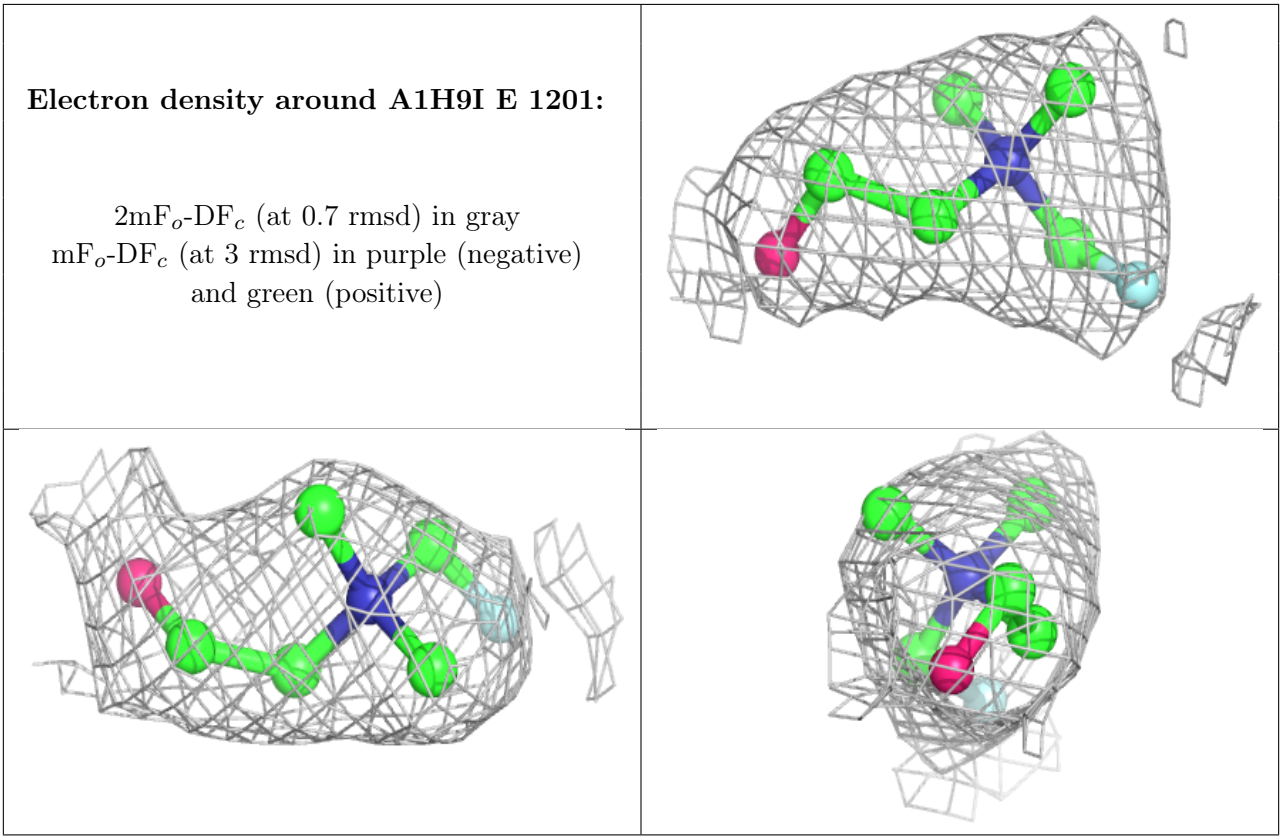
Electron density around A1H9I F 1201:

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



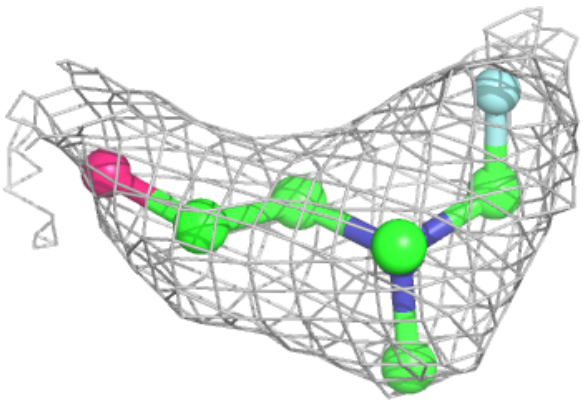
Electron density around A1H9I E 1201:

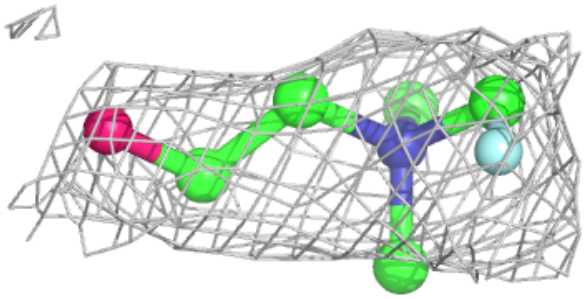
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

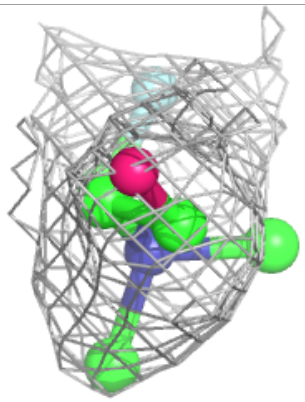


Electron density around A1H9I H 1201:

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

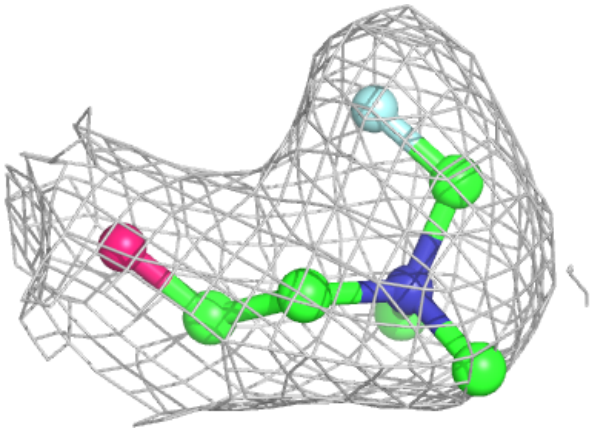


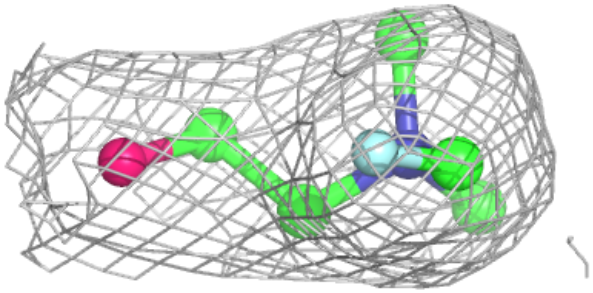


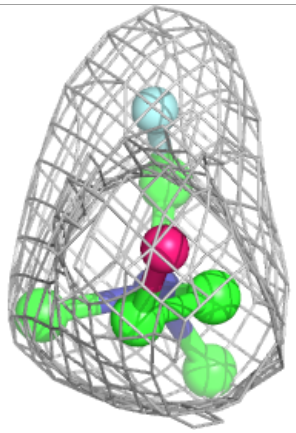


Electron density around A1H9I D 1201:

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

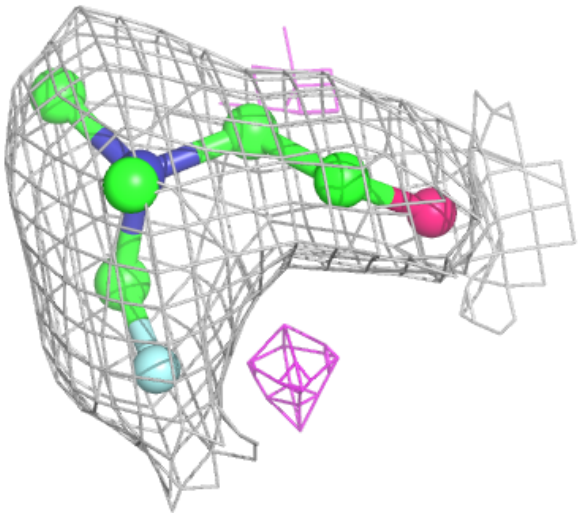


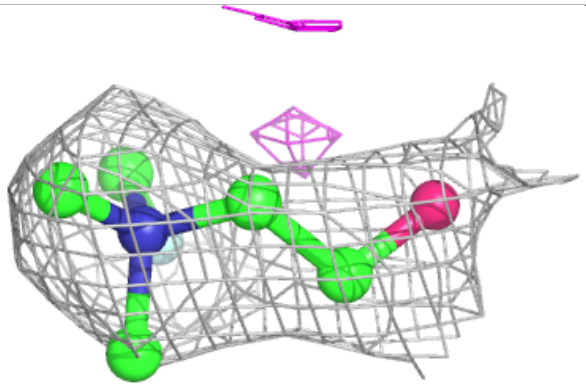


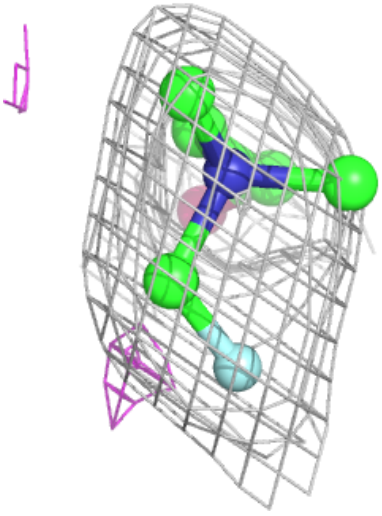


Electron density around A1H9I G 1201:

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

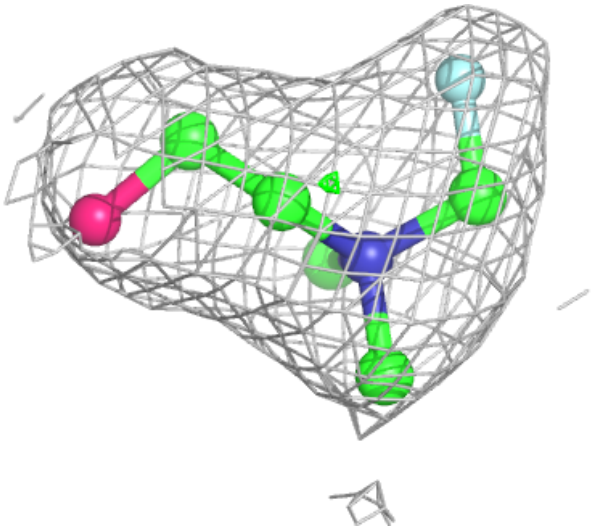


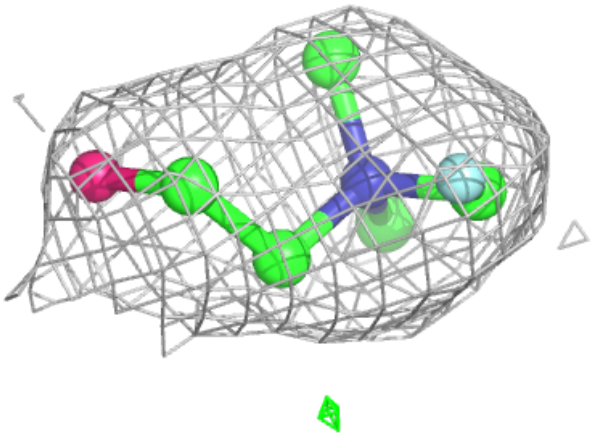


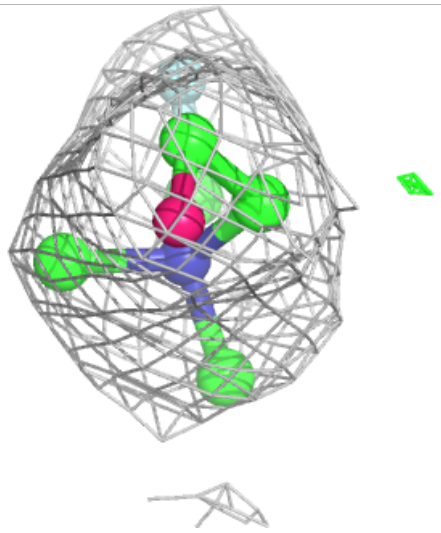


Electron density around A1H9I C 1201:

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

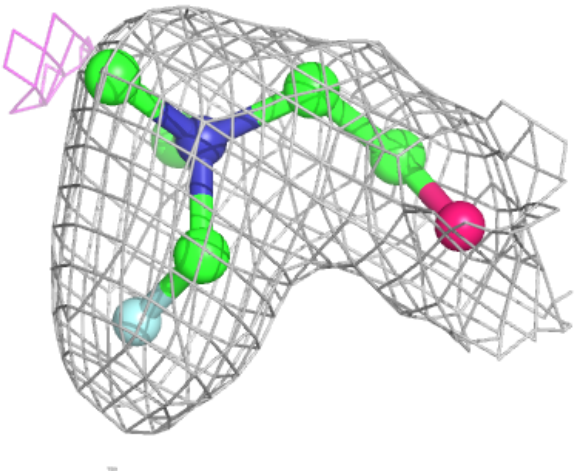


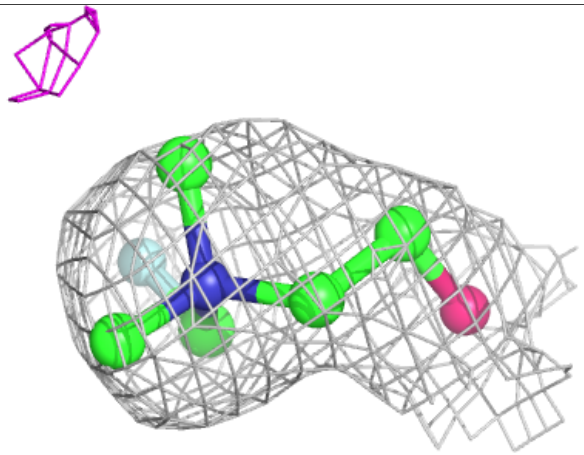


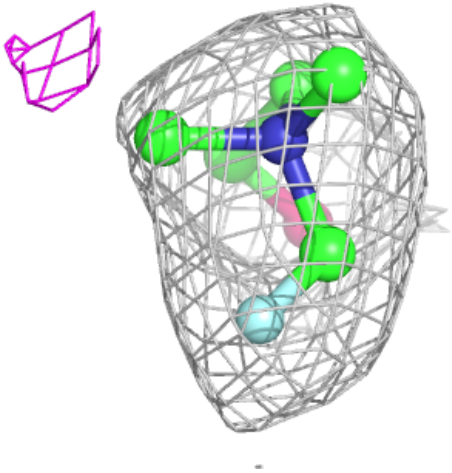


Electron density around A1H9I A 1201:

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

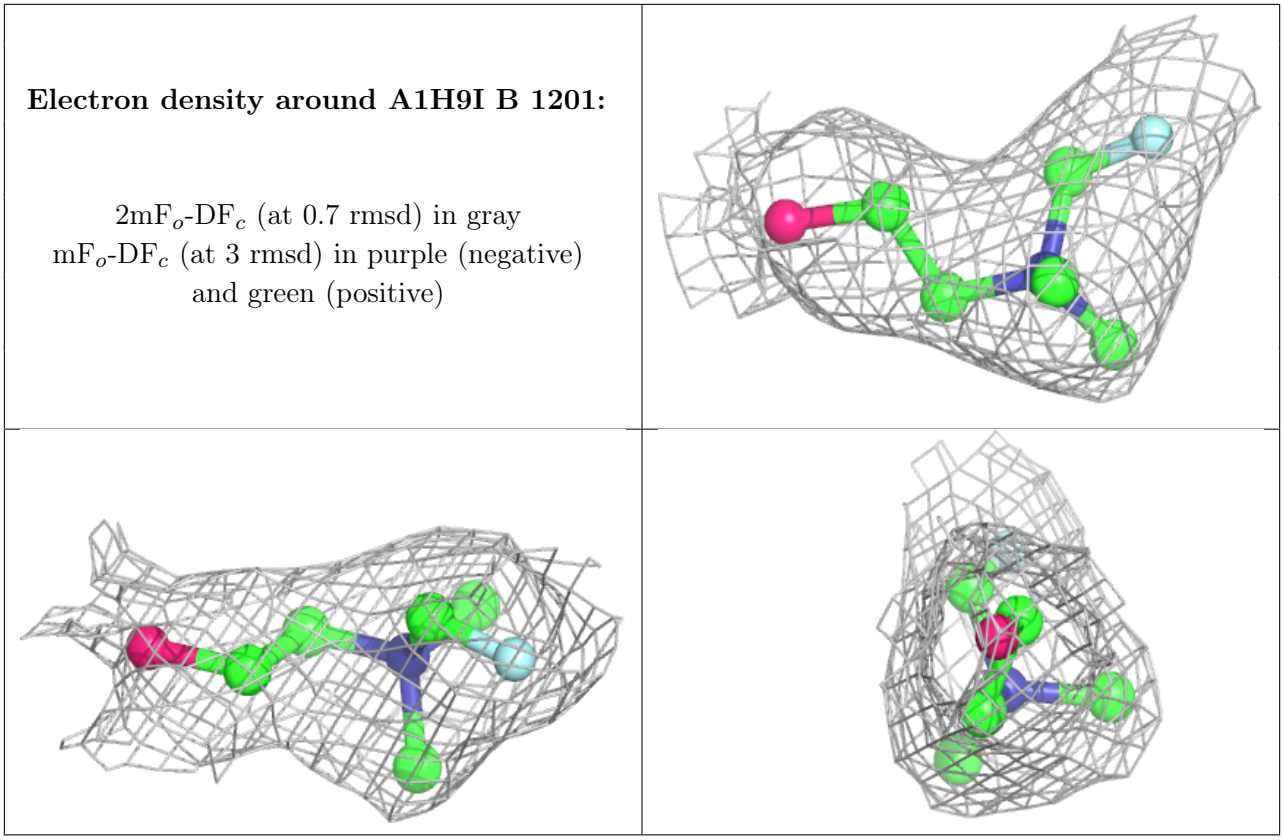






Electron density around A1H9I B 1201:

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



6.5 Other polymers (i)

There are no such residues in this entry.