



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:21 AM UTC

PDB ID : 9F3W / pdb_00009f3w
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

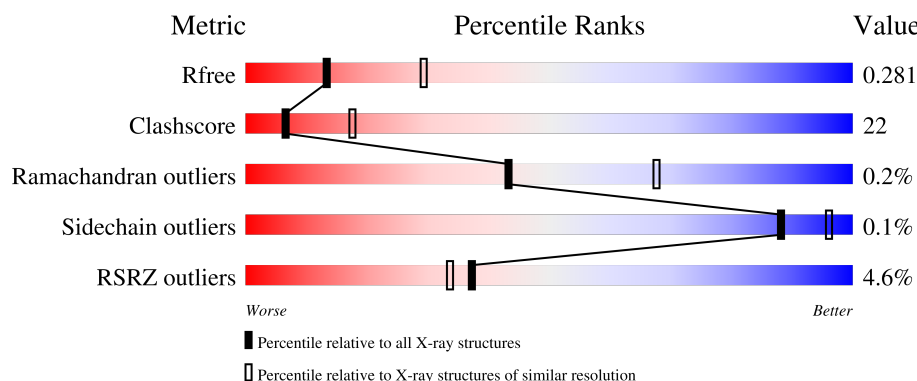
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1150	
1	B	1150	
1	C	1150	
1	D	1150	
1	E	1150	

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Mol	Chain	Length	Quality of chain
1	F	1150	5% 37% 32% 31%
1	G	1150	6% 36% 32% 31%
1	H	1150	10% 32% 36% 31%

2 Entry composition

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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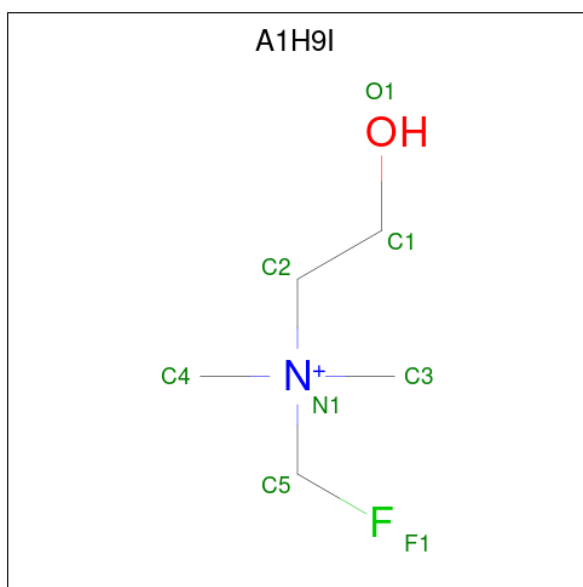
Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP A0A486V7R5
E	-11	SER	-	expression tag	UNP A0A486V7R5
E	-10	GLN	-	expression tag	UNP A0A486V7R5
E	-9	ASP	-	expression tag	UNP A0A486V7R5
E	-8	HIS	-	expression tag	UNP A0A486V7R5
E	-7	GLU	-	expression tag	UNP A0A486V7R5
E	-6	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 (CCD ID: A1H9I) (formula: C₅H₁₃FNO) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

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

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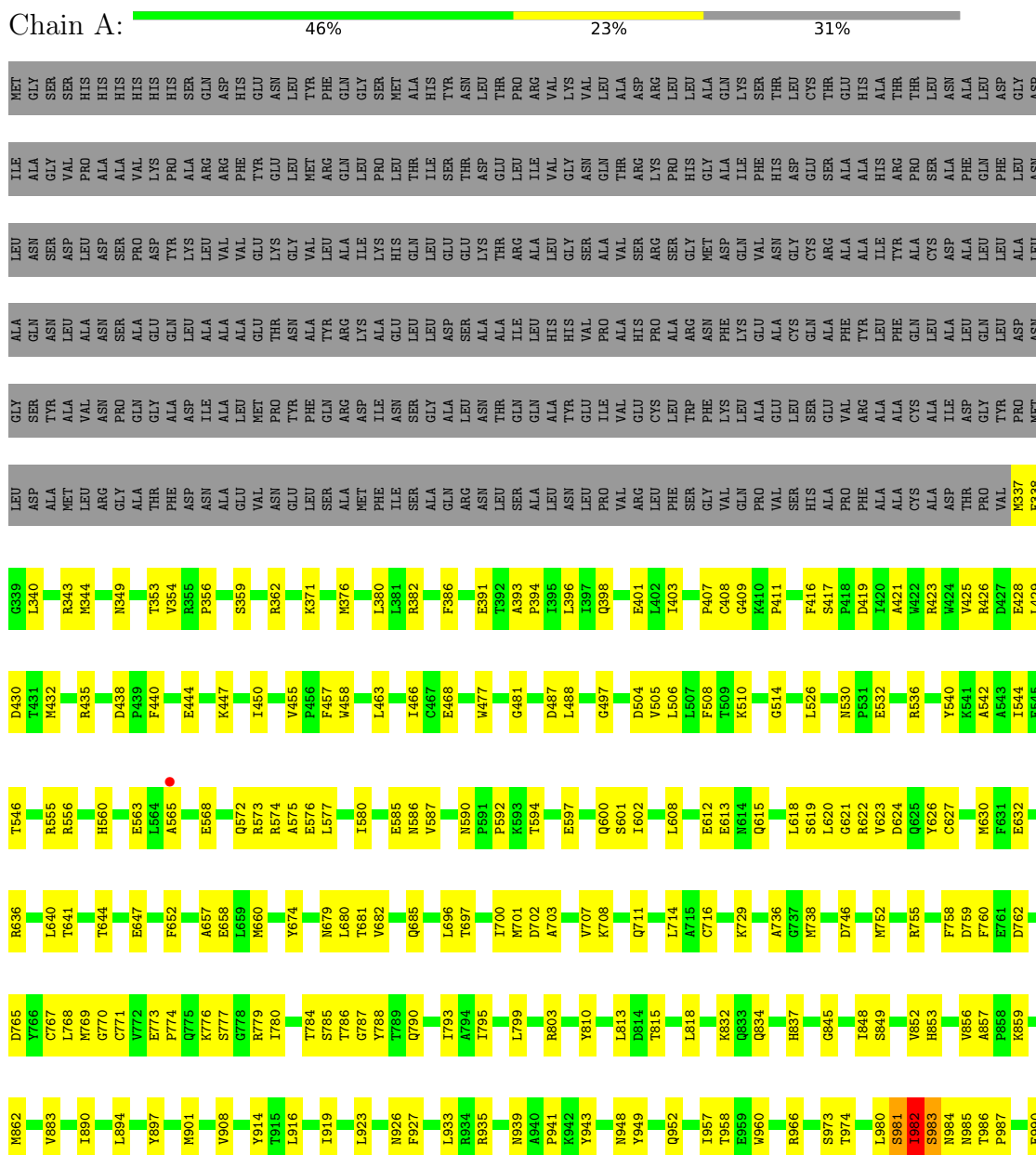
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	27	Total 27	O 27	0	0
3	F	31	Total 31	O 31	0	0
3	G	23	Total 23	O 23	0	0
3	H	9	Total 9	O 9	0	0

3 Residue-property plots

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

- Molecule 1: Choline trimethylamine-lyase





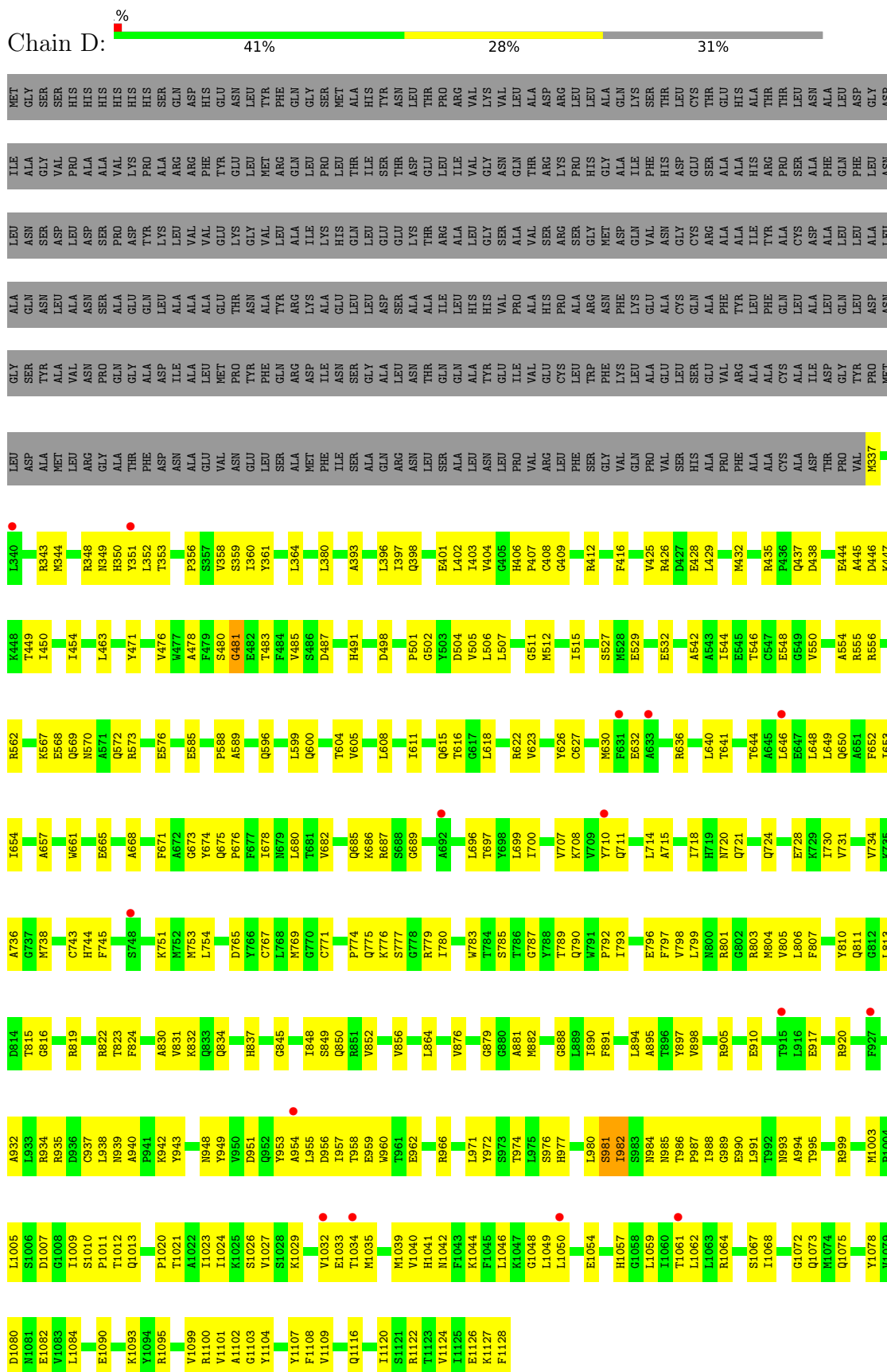
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K1127
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● Molecule 1: Choline trimethylamine-lyase

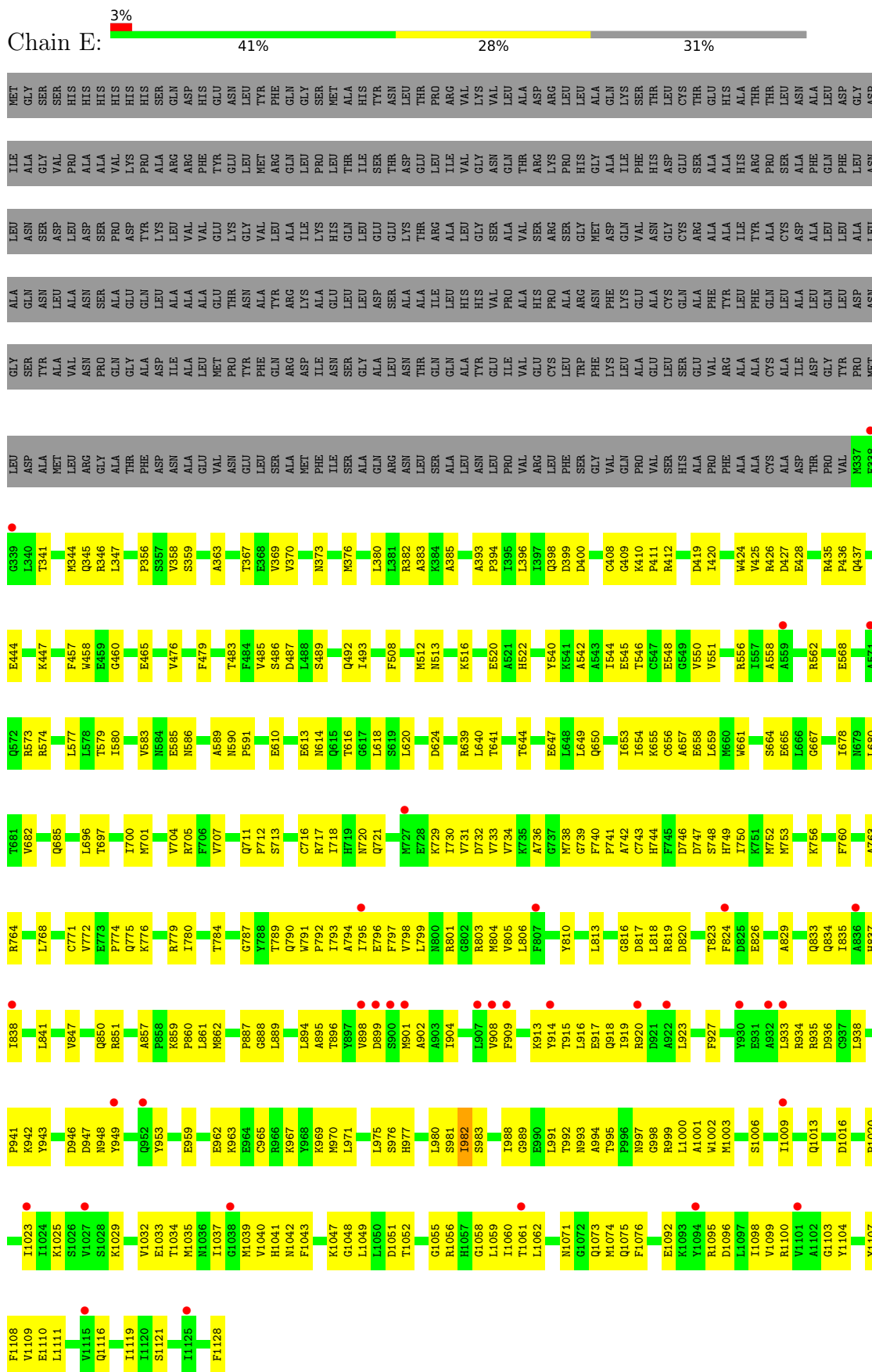
Chain C: 44% 24% 31%

MET	ILE	LEU	ALA	GLY	R343	D446	E548	V682	T786	H862	R966	R1066
GLY	ALA	ASN	GLN	TYR	M344	K447	A561	M694	G787	S863	R967	R1067
SER	VAL	SER	ASN	ALA	R348	I450	A565	T697	Y788	L864	Y968	G1072
LEU	PRO	ASP	ALA	VAL	Y351	W458	R574	L699	T790	V866	M970	Q1075
HIS	ALA	ASP	SER	PRO	Y361	L463	R579	I700	W791	H882	T974	F1076
HIS	VAL	SER	ALA	GLN	R362	D464	I580	M701	P792	V883	L975	S1077
HIS	PRO	ASP	GLN	ALA	L364	Y471	A581	A703	A794	P887	S976	Y1078
ASP	LEU	TYR	LEU	ASP	Y471	Y471	E582	A703	A794	C888	D1080	D1080
GLN	ARG	LEU	ALA	ILE	E368	V476	V583	V707	V798	Y897	L980	V1083
ASP	ARG	VAL	ALA	ALA	V369	W477	E583	K708	R801	S900	S981	L1084
HIS	PHE	VAL	ALA	LEU	V370	A478	P592	P712	R802	S900	I982	E1092
GLU	TYR	GLU	GLU	MET	K371	F479	L599	C716	R803	R905	N984	K1093
ASN	GLU	PRO	THR	GLY	A372	S480	L599	C716	M804	R906	P987	Y1094
LEU	LEU	GLY	ASN	TYR	N373	C481	L608	R717	V805	K906	I988	R1095
MET	MET	VAL	ALA	PHE	P374	E482	L608	I718	L806	E910	L991	I1098
ARG	ARG	LEU	GLN	GLN	G375	T483	L611	Q721	F807	E911	T992	V1099
GLN	LEU	ALA	TYR	ARG	M376	F484	E612	Q721	S809	K912	N993	R1100
GLY	GLY	ILE	LEU	LYS	P377	V485	E613	K725	Y810	K913	A994	G1103
LEU	PRO	ALA	GLN	GLU	R382	D487	E613	M738	Y810	Y914	T995	Y1104
LEU	THR	LEU	LEU	ASP	K384	S489	S619	Q739	L813	L916	P996	V1109
THR	SER	GLU	LEU	SER	R387	T490	R622	C743	G816	E917	R999	E1110
ASN	LEU	LYS	ALA	ALA	H388	I493	R622	C743	D817	Q918	L999	L1111
LEU	GLU	THR	ALA	ALA	P394	I493	M630	H749	R819	R920	M1003	E1126
THR	ARG	ILE	ILE	LEU	E401	I493	M630	I750	F824	D921	D1007	K1127
VAL	VAL	ALA	GLN	ALA	P407	D504	E637	G751	F824	A922	T1012	F1128
LYS	ARG	VAL	GLN	GLY	Q398	V505	G638	G751	R831	E928	G1019	
ARG	PRO	LYS	LYS	TRP	D399	L506	R639	M752	K832	R934	P1020	
LEU	LEU	ASP	ASP	GLY	E401	L507	L640	M753	I835	R935	T1021	
ASP	ARG	ARG	ARG	GLY	P407	K510	T641	M753	A836	I1023	A1022	
PRO	LEU	LEU	LEU	LEU	R412	G511	D643	K756	H837	D936	K1024	
LEU	LEU	GLY	GLY	LEU	D419	M512	T644	K756	R840	C937	S1025	
HIS	GLY	ASP	ASP	LEU	R423	G514	E647	G757	I844	L938	V1027	
GLY	ALA	GLN	GLN	LEU	W424	H522	L648	G757	G845	K942	S1028	
LYS	ILE	VAL	VAL	GLN	E428	L523	Q650	G757	T846	D946	K1029	
SER	HIS	VAL	VAL	GLN	L429	S525	A651	F758	I847	D947	I1037	
THR	ASP	ARG	ARG	GLY	L429	L526	F652	D759	I848	N948	G1038	
GLU	GLY	ALA	ALA	ASP	M432	S527	I654	R764	S849	D951	M1039	
THR	THR	ALA	ALA	ALA	M432	M528	E529	D765	E658	P951	N1042	
HIS	ALA	TYR	TYR	LEU	R435	E529	E658	M769	Q850	D951	F1043	
ALA	HIS	LEU	LEU	LEU	P436	M530	M662	G770	R851	L955	K1044	
ALA	ARG	THR	THR	ALA	Q437	E532	Y670	Q775	V852	D956	F1045	
ASP	ALA	ALA	ALA	ALA	F440	I537	Q675	K776	H853	N957	L1046	
LEU	PHE	LEU	LEU	LEU	E441	I544	Q675	R779	P856	E959	L1049	
LEU	GLN	LEU	LEU	LEU	S443	T546	N679	I780	R859	W960	L1050	
ASP	PHE	LEU	LEU	LEU	I442	C547	L680	Y781	P860	K963	D1051	
GLY	LEU	ALA	ALA	ASP	M337			Q782	L861			
PRO	GLY	PRO	PRO	ASP								
ASP	ASP	ASP	ASP	ASP								

● Molecule 1: Choline trimethylamine-lyase



- Molecule 1: Choline trimethylamine-lyase

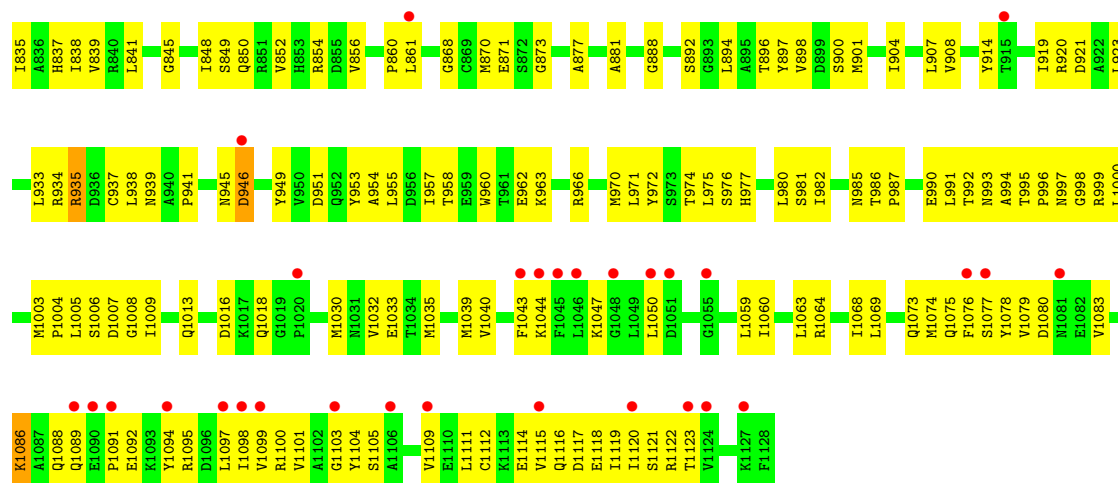


Chain F:









4 Data and refinement statistics

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 83.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.7 (83.54-2.70) 85.8 (83.54-2.70)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.223 , 0.282 0.224 , 0.281	Depositor DCC
R_{free} test set	9643 reflections (4.32%)	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)	0.36 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/6385	0.71	0/8640
1	B	0.48	0/6385	0.72	1/8640 (0.0%)
1	C	0.44	0/6385	0.68	0/8640
1	D	0.42	0/6385	0.69	0/8640
1	E	0.38	0/6385	0.65	0/8640
1	F	0.44	0/6385	0.72	1/8640 (0.0%)
1	G	0.41	1/6385 (0.0%)	0.69	2/8640 (0.0%)
1	H	0.38	0/6385	0.73	2/8640 (0.0%)
All	All	0.43	1/51080 (0.0%)	0.70	6/69120 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	986	THR	C-N	5.75	1.41	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	823	THR	OG1-CB-CG2	-6.00	97.31	109.30
1	H	453	GLU	CA-C-N	-5.65	117.17	123.16
1	H	453	GLU	C-N-CA	-5.65	117.17	123.16
1	B	801	ARG	CB-CG-CD	-5.46	98.73	111.30
1	G	819	ARG	CA-C-N	-5.18	114.05	122.65
1	G	819	ARG	C-N-CA	-5.18	114.05	122.65

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	184	0
1	B	6254	0	6171	201	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6254	0	6171	216	1
1	D	6254	0	6171	249	0
1	E	6254	0	6171	265	0
1	F	6254	0	6171	344	0
1	G	6254	0	6171	311	0
1	H	6254	0	6171	402	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	2159	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 22.

All (2159) 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	1.22
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
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:H:752:MET:HE2	1:H:1033:GLU:HA	1.36	1.04
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:B:1100:ARG:NH1	1:B:1103:GLY:C	2.18	1.00
1:C:1075:GLN:HE22	1:C:1103:GLY:H	1.07	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:424:TRP:CG	1:F:664:SER:HG	1.81	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:E:731:VAL:HG21	1:E:1060:ILE:HD11	1.50	0.93
1:C:344:MET:HE3	1:C:647:GLU:CG	1.99	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:C:483:THR:HB	1:C:804:MET:HE1	1.50	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:H:344:MET:HE3	1:H:650:GLN:HB2	1.54	0.88
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:C:344:MET:HE3	1:C:647:GLU:HG2	1.55	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:G:480:SER:HB2	1:G:488:LEU:HD12	1.58	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:804:MET:HE3	1:C:807:PHE:HD2	1.47	0.80
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:D:1032:VAL:HB	1:D:1039:MET:HE1	1.62	0.79
1:F:701:MET:HE2	1:F:729:LYS:HG2	1.65	0.79
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:B:592:PRO:HG2	1:B:630:MET:HE2	1.65	0.79
1:F:905:ARG:HD3	1:F:953:TYR:OH	1.83	0.79
1:H:804:MET:HE2	1:H:807:PHE:HD2	1.48	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:B:752:MET:HE3	1:B:774:PRO:HG2	1.64	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: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:H:505:VAL:C	1:H:506:LEU:HD22	2.09	0.77
1:G:403:ILE:HG23	1:G:600:GLN:HG3	1.66	0.77
1:H:376:MET:HE3	1:H:381:LEU:HA	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:831:VAL:HG21	1:B:901:MET:HE1	1.67	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:C:970:MET:HE3	1:C:975:LEU:HB2	1.67	0.75
1:F:592:PRO:HG2	1:F:630:MET:HE3	1.68	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:C:344:MET:HE3	1:C:647:GLU:HG3	1.68	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:H:528:MET:HE3	1:H:534:ILE:HG23	1.70	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:F:382:ARG:NH2	1:F:613:GLU:OE1	2.20	0.74
1:F:660:MET:HE1	1:F:674:TYR:HB3	1.68	0.73
1:C:618:LEU:HD11	1:C:862:MET:HE1	1.69	0.73
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:H:1032:VAL:HB	1:H:1039:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:512:MET:HE3	1:G:550:VAL:HG11	1.69	0.73
1:A:555:ARG:NH1	1:A:585:GLU:O	2.22	0.73
1:E:752:MET:HE1	1:E:1039:MET:HE1	1.70	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
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: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:C:592:PRO:HG2	1:C:630:MET:HE2	1.72	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:D:483:THR:HB	1:D:804:MET:HE1	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:804:MET:HE2	1:H:807:PHE:CD2	2.27	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
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:660:MET:HE1	1:A:674:TYR:HB3	1.74	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:G:536:ARG:NH1	1:G:872:SER:O	2.26	0.68
1:A:752:MET:HE3	1:A:774:PRO:HG3	1.76	0.68
1:F:1009:ILE:HG21	1:F:1035:MET:HE1	1.74	0.68
1:A:435:ARG:NH2	1:A:438:ASP:O	2.25	0.68
1:F:831:VAL:HG21	1:F:901:MET:HE1	1.75	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:G:618:LEU:HD11	1:G:862:MET:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:701:MET:HE1	1:G:726:TYR:HE2	1.60	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:F:752:MET:HE2	1:F:774:PRO:HG3	1.77	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:E:970:MET:HE3	1:E:975:LEU:HB2	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:618:LEU:HD11	1:B:862:MET:HE1	1.78	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
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:E:753:MET:HE3	1:E:774:PRO:HB2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:804:MET:HE3	1:C:807:PHE:CD2	2.31	0.63
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: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
1:D:627:CYS:HA	1:D:630:MET:HE2	1.80	0.63
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:C:801:ARG:HE	1:C:816:GLY:C	2.06	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: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:A:958:THR:HG21	1:A:1030:MET:HE3	1.82	0.62
1:C:485:VAL:O	1:C:789:THR:OG1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:453:GLU:O	1:H:453:GLU:CD	2.43	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
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:B:701:MET:HE2	1:B:729:LYS:HG3	1.82	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: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:F:1052:THR:CG2	1:F:1054:GLU:HG2	2.30	0.61
1:H:828:ASP:CG	1:H:832:LYS:HZ3	2.09	0.61
1:C:432:MET:HA	1:C:435:ARG:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:851:ARG:HH22	1:G:535:ASP:CG	2.08	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:G:1043:PHE:CE2	1:G:1074:MET:HE3	2.36	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: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
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:E:752:MET:HE2	1:E:1033:GLU:HA	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:753:MET:HE3	1:D:774:PRO:HB2	1.82	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
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:F:1127:LYS:HZ3	1:F:1128:PHE:HB2	1.66	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: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:G:701:MET:HE1	1:G:726:TYR:CE2	2.36	0.59
1:H:512:MET:HE3	1:H:588:PRO:HG2	1.82	0.59
1:H:852:VAL:O	1:H:856:VAL:HG12	2.01	0.59
1:H:970:MET:HE3	1:H:975:LEU:HB2	1.83	0.59
1:C:528:MET:HE2	1:C:537:ILE:HD13	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:341:THR:HG22	1:H:343:ARG:H	1.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:1063:LEU:HD22	1:H:1074:MET:HE1	1.86	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: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:G:1032:VAL:HB	1:G:1039:MET:HE2	1.86	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1058:GLY:C	1:G:1128:PHE:CE2	2.82	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:F:748:SER:OG	1:F:1071:ASN:O	2.16	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:B:752:MET:CE	1:B:774:PRO:HG2	2.33	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
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:C:1093:LYS:NZ	1:C:1094:TYR:CZ	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:LEU:HD21	1:H:400:ASP:C	2.31	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:F:641:THR:H	1:F:644:THR:HG1	1.54	0.56
1:F:958:THR:HG21	1:F:1030:MET:HE2	1.88	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: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: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:H:594:THR:OG1	1:H:595:LEU:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1114:GLU:CD	1:F:1114:GLU:H	2.10	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:358:VAL:HG21	1:H:432:MET:HE1	1.89	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
1:G:624:ASP:O	1:G:694:ASN:ND2	2.39	0.55
1:B:356:PRO:HB3	1:B:660:MET:HE3	1.88	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:A:337:MET:HE1	1:A:708:LYS:HD2	1.89	0.55
1:B:380:LEU:HA	1:B:542:ALA:HB2	1.87	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:G:598:ALA:HB2	1:G:630:MET:HE3	1.88	0.55
1:F:418:PRO:HA	1:F:421:ALA:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:749:HIS:HA	1:C:752:MET:HG2	1.89	0.54
1:E:818:LEU:C	1:E:820:ASP:H	2.15	0.54
1:G:351:TYR:OH	1:G:657:ALA:O	2.19	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:701:MET:HE1	1:B:730:ILE:HG13	1.90	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: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:776:LYS:C	1:E:776:LYS:HD3	2.32	0.54
1:G:1020:PRO:HD3	1:G:1127:LYS:HB2	1.88	0.54
1:G:1043:PHE:HE2	1:G:1074:MET:HE3	1.71	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
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:H:753:MET:HE1	1:H:776:LYS:HB2	1.90	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:483:THR:O	1:H:804:MET:HE1	2.07	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:773:GLU:CD	1:B:980:LEU:HD22	2.33	0.54
1:B:1075:GLN:OE1	1:B:1100:ARG:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1092:GLU:CD	1:C:1092:GLU:H	2.15	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
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:E:1032:VAL:HB	1:E:1039:MET:HE2	1.91	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:H:785:SER:OG	1:H:787:GLY:O	2.26	0.53
1:F:882:MET:HG2	1:F:883:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:536:ARG:HG2	1:G:873:GLY:HA3	1.89	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:B:749:HIS:CG	1:B:752:MET:HE2	2.43	0.53
1:C:376:MET:HE1	1:C:384:LYS:HD3	1.90	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: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
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:E:344:MET:HE1	1:E:654:ILE:HD11	1.91	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:1085:LYS:O	1:G:1089:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:352:LEU:HG	1:H:1095:ARG:HE	1.74	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: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:B:790:GLN:CD	1:B:793:ILE:HB	2.35	0.52
1:E:1100:ARG:HD2	1:E:1104:TYR:C	2.34	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
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:A:1003:MET:HE3	1:A:1004:PRO:HD2	1.92	0.52
1:E:373:ASN:HB3	1:E:376:MET:HE3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:993:ASN:CG	1:E:994:ALA:H	2.17	0.52
1:F:796:GLU:CD	1:F:993:ASN:HB3	2.34	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:752:MET:HE3	1:G:774:PRO:HG3	1.91	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: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:A:432:MET:HE3	1:A:440:PHE:HB2	1.91	0.51
1:A:701:MET:HE3	1:A:716:CYS:SG	2.51	0.51
1:D:344:MET:HE3	1:D:650:GLN:HB2	1.91	0.51
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:348:ARG:HH22	1:G:1096:ASP:CG	2.19	0.51
1:G:694:ASN:O	1:G:697:THR:HB	2.11	0.51
1:H:512:MET:HE2	1:H:588:PRO:HB2	1.91	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:A:984:ASN:C	1:A:987:PRO:HD2	2.36	0.51
1:E:824:PHE:CZ	1:E:953:TYR:HE2	2.29	0.51
1:F:926:ASN:C	1:F:926:ASN:HD22	2.19	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:C:507:LEU:HD13	1:C:512:MET:HE2	1.93	0.51
1:E:793:ILE:HG13	1:E:797:PHE:CZ	2.46	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:795:ILE:HG12	1:B:901:MET:HE2	1.92	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: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: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:D:398:GLN:HG3	1:D:401:GLU:CD	2.36	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:E:1092:GLU:H	1:E:1092:GLU:CD	2.19	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:G:1114:GLU:H	1:G:1114:GLU:CD	2.20	0.50
1:A:419:ASP:OD1	1:A:419:ASP:N	2.44	0.50
1:B:398:GLN:HG2	1:B:401:GLU:CD	2.37	0.50
1:B:428:GLU:O	1:B:432:MET:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:GLN:HG3	1:D:668:ALA:HB1	1.93	0.50
1:F:396:LEU:HD22	1:F:409:GLY:O	2.12	0.50
1:F:746:ASP:C	1:F:750:ILE:HG13	2.36	0.50
1:F:1039:MET:SD	1:F:1072:GLY:HA3	2.52	0.50
1:H:1075:GLN:CD	1:H:1100:ARG:HH21	2.20	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:594:THR:C	1:B:630:MET:HB3	2.36	0.50
1:B:660:MET:SD	1:B:674:TYR:HB3	2.51	0.50
1:E:428:GLU:CD	1:E:665:GLU:HB2	2.37	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:D:993:ASN:CG	1:D:994:ALA:H	2.20	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:1032:VAL:HA	1:E:1035:MET:HE3	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:F:806:LEU:HD13	1:F:806:LEU:C	2.37	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: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:E:1013:GLN:H	1:E:1013:GLN:CD	2.16	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:F:1032:VAL:HB	1:F:1035:MET:HE2	1.94	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:850:GLN:CD	1:H:971:LEU:HB2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:745:PHE:HE2	1:H:1074:MET:HE2	1.77	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
1:D:984:ASN:C	1:D:987:PRO:HD2	2.38	0.49
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:598:ALA:HB2	1:F:630:MET:HE2	1.93	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: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: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:H:745:PHE:CE2	1:H:1074:MET:HE2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:GLN:NE2	1:D:438:ASP:OD1	2.40	0.49
1:D:480:SER:OG	1:D:481:GLY:N	2.44	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
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: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: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:D:1035:MET:HE3	1:D:1039:MET:HE3	1.93	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:532:GLU:CD	1:C:532:GLU:H	2.21	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: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:H:660:MET:HE1	1:H:674:TYR:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:790:GLN:CD	1:E:793:ILE:HB	2.39	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
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:848:ILE:O	1:A:849:SER:C	2.56	0.48
1:B:498:ASP:HA	1:B:769:MET:CE	2.44	0.48
1:C:483:THR:HB	1:C:804:MET:CE	2.32	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:G:337:MET:HE3	1:G:340:LEU:HD12	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:753:MET:HE2	1:E:756:LYS:HD2	1.96	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
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:594:THR:C	1:A:630:MET:HB3	2.39	0.47
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:675:GLN:CD	1:C:1104:TYR:CD2	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:781:TYR:HB2	1:H:881:ALA:HB2	1.97	0.47
1:A:984:ASN:C	1:A:984:ASN:OD1	2.57	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: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:G:1092:GLU:H	1:G:1092:GLU:CD	2.21	0.47
1:H:958:THR:HG21	1:H:1035:MET:HE2	1.96	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
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: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:500:CYS:HG	1:B:767:CYS:HG	1.63	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:1032:VAL:CB	1:D:1039:MET:HE1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:H:789:THR:OG1	1:H:790:GLN:N	2.44	0.47
1:A:463:LEU:HD11	1:A:853:HIS:CD2	2.49	0.47
1:B:694:ASN:C	1:B:694:ASN:OD1	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:832:LYS:NZ	1:D:956:ASP:OD2	2.38	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:804:MET:HE2	1:E:804:MET:HB3	1.78	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
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: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:G:850:GLN:CD	1:G:971:LEU:HB2	2.41	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:1058:GLY:O	1:G:1061:THR:OG1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:973:SER:OG	1:A:974:THR:N	2.40	0.46
1:D:894:LEU:HD23	1:D:1009:ILE:HB	1.97	0.46
1:F:487:ASP:OD2	1:F:489:SER:OG	2.32	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:E:1092:GLU:CD	1:E:1092:GLU:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:862:MET:HE2	1:B:862:MET:HB2	1.89	0.46
1:C:382:ARG:HG2	1:C:382:ARG:HH11	1.80	0.46
1:C:387:ARG:HH11	1:C:545:GLU:CD	2.24	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:344:MET:HE1	1:F:651:ALA:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:669:LYS:NZ	1:F:1114:GLU:HG2	2.31	0.45
1:F:887:PRO:HD2	1:F:970:MET:HE2	1.98	0.45
1:H:734:VAL:HG23	1:H:741:PRO:HD2	1.98	0.45
1:H:790:GLN:CD	1:H:793:ILE:HB	2.41	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: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:B:864:LEU:C	1:B:865:LEU:HD23	2.41	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:940:ALA:O	1:F:941:PRO:C	2.60	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:627:CYS:HA	1:D:630:MET:CE	2.46	0.45
1:D:710:TYR:O	1:D:711:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:1074:MET:HE3	1:H:1074:MET:HB2	1.55	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: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:A:897:TYR:CE2	1:A:901:MET:HE3	2.51	0.45
1:B:355:ARG:HD2	1:B:441:GLU:OE2	2.16	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
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:B:1007:ASP:OD1	1:B:1010:SER:OG	2.28	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:E:933:LEU:O	1:E:934:ARG:C	2.59	0.45
1:F:462:SER:OG	1:F:465:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1013:GLN:HG3	1:F:1122:ARG:HA	1.98	0.45
1:G:749:HIS:CG	1:G:752:MET:HE2	2.51	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:D:934:ARG:CZ	1:D:938:LEU:HD21	2.47	0.45
1:E:701:MET:HE2	1:E:733:VAL:HG21	1.99	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: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:701:MET:HE3	1:C:716:CYS:SG	2.57	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
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: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:1107:TYR:HB2	1:G:1110:GLU:CD	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1035:MET:HE3	1:F:1039:MET:HB3	1.98	0.44
1:G:604:THR:C	1:G:607:SER:HG	2.24	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:376:MET:HE1	1:A:380:LEU:HG	1.98	0.44
1:A:586:ASN:ND2	1:A:597:GLU:OE2	2.42	0.44
1:A:795:ILE:HG12	1:A:901:MET:HE1	1.99	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: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:B:1043:PHE:CE1	1:B:1074:MET:HE3	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
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:C:432:MET:HE1	1:C:442:ILE:HD12	2.00	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:1032:VAL:HG12	1:E:1035:MET:HE1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:630:MET:HE2	1:G:630:MET:HB2	1.74	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:E:919:ILE:O	1:E:920:ARG:C	2.60	0.44
1:F:803:ARG:HB2	1:F:810:TYR:CE1	2.52	0.44
1:F:846:THR:HG22	1:F:970:MET:HE2	1.99	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
1:B:505:VAL:HG21	1:B:779:ARG:NH2	2.32	0.44
1:B:1074:MET:HE2	1:B:1076:PHE:CZ	2.53	0.44
1:C:432:MET:HE3	1:C:440:PHE:HB2	1.98	0.44
1:D:568:GLU:HG2	1:D:569:GLN:N	2.33	0.44
1:E:344:MET:HE1	1:E:654:ILE:CD1	2.47	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:694:ASN:CG	1:F:697:THR:HG23	2.43	0.44
1:F:719:HIS:O	1:F:721:GLN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:401:GLU:CD	1:H:404:VAL:HG11	2.43	0.44
1:H:405:GLY:H	1:H:655:LYS:HZ1	1.66	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:B:859:LYS:O	1:B:863:SER:OG	2.29	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: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: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:B:1033:GLU:H	1:B:1033:GLU:CD	2.25	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: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:600:GLN:O	1:A:601:SER:C	2.60	0.43
1:A:941:PRO:HG2	1:A:949:TYR:CD2	2.53	0.43
1:B:498:ASP:HA	1:B:769:MET:HE3	1.99	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
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:F:1075:GLN:CD	1:F:1100:ARG:HH21	2.26	0.43
1:H:432:MET:C	1:H:434:THR:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:818:LEU:C	1:E:820:ASP:N	2.76	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: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:432:MET:HE1	1:C:442:ILE:HB	1.99	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:779:ARG:CG	1:D:882:MET:HE1	2.48	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:857:ALA:O	1:A:859:LYS:NZ	2.50	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:E:796:GLU:OE2	1:E:805:VAL:HG12	2.18	0.43
1:E:923:LEU:HD22	1:E:994:ALA:C	2.43	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: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:768:LEU:HD13	1:A:774:PRO:HA	2.01	0.43
1:A:982:ILE:C	1:A:984:ASN:H	2.26	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:E:795:ILE:HD11	1:E:901:MET:HE3	1.99	0.43
1:E:861:LEU:O	1:E:862:MET:C	2.60	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:736:ALA:HB1	1:F:738:MET:HE2	2.01	0.43
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: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: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: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:C:662:MET:HE2	1:C:662:MET:HB3	1.94	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
1:B:348:ARG:NE	1:B:707:VAL:O	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:O	1:B:411:PRO:C	2.62	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: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:867:GLU:OE2	1:G:882:MET:HE1	2.19	0.42
1:H:512:MET:HE1	1:H:550:VAL:HB	2.01	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: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:430:ASP:OD1	1:A:447:LYS:NZ	2.43	0.42
1:A:618:LEU:HD11	1:A:862:MET:HE1	2.00	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: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: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
1:A:914:TYR:CD1	1:A:933:LEU:HD12	2.54	0.42
1:A:1033:GLU:H	1:A:1033:GLU:CD	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:717:ARG:C	1:E:718:ILE:HG13	2.44	0.42
1:E:790:GLN:HG3	1:E:793:ILE:HG22	2.02	0.42
1:E:795:ILE:C	1:E:797:PHE:N	2.78	0.42
1:F:707:VAL:O	1:F:708:LYS:C	2.62	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:337:MET:HE3	1:D:337:MET:HB3	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:984:ASN:C	1:C:987:PRO:HD2	2.44	0.42
1:D:502:GLY:HA3	1:D:505:VAL:HG22	2.02	0.42
1:E:791:TRP:O	1:E:792:PRO:C	2.62	0.42
1:E:993:ASN:CG	1:E:994:ALA:N	2.78	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: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:1011:PRO:O	1:D:1012:THR:C	2.63	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: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:D:1035:MET:HE3	1:D:1039:MET:CE	2.50	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:A:897:TYR:CZ	1:A:901:MET:HE3	2.55	0.41
1:B:362:ARG:NH2	1:B:419:ASP:OD1	2.52	0.41
1:B:564:LEU:C	1:B:577:LEU:HD13	2.45	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:736:ALA:CB	1:F:738:MET:HE2	2.50	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:870:MET:HE2	1:H:870:MET:HB2	1.84	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:H:403:ILE:C	1:H:404:VAL:HG13	2.45	0.41
1:H:460:GLY:H	1:H:465:GLU:CD	2.27	0.41
1:B:775:GLN:HB3	1:B:780:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:733:VAL:HB	1:G:741:PRO:HD3	2.01	0.41
1:G:746:ASP:O	1:G:747:ASP:C	2.63	0.41
1:G:768:LEU:HD12	1:G:772:VAL:C	2.45	0.41
1:H:337:MET:HE1	1:H:348:ARG:HE	1.85	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:F:719:HIS:HE1	1:F:721:GLN:HB2	1.86	0.41
1:F:1032:VAL:CG1	1:F:1035:MET:HE2	2.51	0.41
1:H:351:TYR:OH	1:H:657:ALA:O	2.32	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:605:VAL:O	1:F:606:GLU:C	2.63	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: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:G:984:ASN:C	1:G:987:PRO:HD2	2.45	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:343:ARG:HH21	1:A:647:GLU:CD	2.28	0.41
1:A:897:TYR:CD1	1:A:897:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:1030:MET:HE3	1:B:1030:MET:HB2	1.89	0.41
1:C:862:MET:HE2	1:C:862:MET:HB2	1.80	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:E:701:MET:HE3	1:E:716:CYS:SG	2.61	0.41
1:E:989:GLY:C	1:E:991:LEU:H	2.28	0.41
1:F:395:ILE:HD13	1:F:395:ILE:HA	1.90	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: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:D:981:SER:O	1:D:982:ILE:C	2.64	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:424:TRP:CD1	1:F:664:SER:HG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:624:ASP:CG	1:G:625:GLN:HE21	2.29	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:A:1094:TYR:O	1:A:1095:ARG:C	2.64	0.40
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: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
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:850:GLN:OE1	1:F:970:MET:HE3	2.21	0.40
1:G:340:LEU:CB	1:G:345:GLN:OE1	2.67	0.40
1:G:862:MET:HE2	1:G:862:MET:HB2	1.91	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:C:946:ASP:H	1:C:1026:SER:HG	1.64	0.40
1:D:359:SER:HB2	1:D:361:TYR:HD2	1.87	0.40
1:D:444:GLU:CD	1:D:447:LYS:HE3	2.46	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: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:428:GLU:CD	1:F:665:GLU:HG3	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:397:ILE:HG13	1:H:560:HIS:ND1	2.37	0.40
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: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:B:1114:GLU:H	1:B:1114:GLU:CD	2.30	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:D:993:ASN:CG	1:D:994:ALA:N	2.78	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: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:1074:MET:HE2	1:A:1076:PHE:CZ	2.57	0.40
1:B:362:ARG:NH1	1:B:612:GLU:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:897:TYR:CD1	1:B:897:TYR:C	2.99	0.40
1:B:1069:LEU:HD23	1:B:1069:LEU:HA	1.82	0.40
1:C:738:MET:HE3	1:C:738:MET:HB2	1.94	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:358:VAL:HG11	1:D:432:MET:HE1	2.03	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:769:MET:HE3	1:F:769:MET:HB3	1.77	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	790/1150 (69%)	732 (93%)	56 (7%)	2 (0%)	36	60
1	B	790/1150 (69%)	737 (93%)	52 (7%)	1 (0%)	48	73
1	C	790/1150 (69%)	723 (92%)	66 (8%)	1 (0%)	48	73
1	D	790/1150 (69%)	733 (93%)	55 (7%)	2 (0%)	36	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	790/1150 (69%)	720 (91%)	69 (9%)	1 (0%)	48	73
1	F	790/1150 (69%)	700 (89%)	89 (11%)	1 (0%)	48	73
1	G	790/1150 (69%)	713 (90%)	76 (10%)	1 (0%)	48	73
1	H	790/1150 (69%)	699 (88%)	89 (11%)	2 (0%)	36	60
All	All	6320/9200 (69%)	5757 (91%)	552 (9%)	11 (0%)	43	68

All (11) Ramachandran outliers are listed below:

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	668/955 (70%)	668 (100%)	0	100	100
1	B	668/955 (70%)	668 (100%)	0	100	100
1	C	668/955 (70%)	667 (100%)	1 (0%)	88	96
1	D	668/955 (70%)	668 (100%)	0	100	100
1	E	668/955 (70%)	668 (100%)	0	100	100
1	F	668/955 (70%)	668 (100%)	0	100	100
1	G	668/955 (70%)	666 (100%)	2 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	668/955 (70%)	667 (100%)	1 (0%)	88	96
All	All	5344/7640 (70%)	5340 (100%)	4 (0%)	88	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1012	THR
1	G	654	ILE
1	G	819	ARG
1	H	789	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	A	470	GLN
1	A	513	ASN
1	A	590	ASN
1	A	600	GLN
1	A	625	GLN
1	A	719	HIS
1	A	811	GLN
1	A	952	GLN
1	B	373	ASN
1	B	437	GLN
1	B	560	HIS
1	B	590	ASN
1	B	685	GLN
1	B	749	HIS
1	B	1057	HIS
1	C	724	GLN
1	C	850	GLN
1	C	885	HIS
1	C	993	ASN
1	D	373	ASN
1	D	590	ASN
1	D	811	GLN
1	D	977	HIS
1	D	1073	GLN
1	D	1075	GLN
1	E	437	GLN

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Mol	Chain	Res	Type
1	E	492	GLN
1	E	590	ASN
1	E	650	GLN
1	E	749	HIS
1	E	790	GLN
1	E	811	GLN
1	E	837	HIS
1	E	1031	ASN
1	F	345	GLN
1	F	437	GLN
1	F	494	ASN
1	F	721	GLN
1	F	749	HIS
1	F	800	ASN
1	F	926	ASN
1	F	1031	ASN
1	F	1042	ASN
1	G	437	GLN
1	G	650	GLN
1	G	675	GLN
1	G	685	GLN
1	G	711	GLN
1	G	744	HIS
1	G	811	GLN
1	G	833	GLN
1	G	884	ASN
1	G	1031	ASN
1	G	1042	ASN
1	H	530	ASN
1	H	572	GLN
1	H	584	ASN
1	H	586	ASN
1	H	600	GLN
1	H	744	HIS
1	H	749	HIS
1	H	850	GLN
1	H	1042	ASN
1	H	1075	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1H9I	H	1201	-	7,7,7	1.26	1 (14%)	7,9,9	0.61	0
2	A1H9I	B	1201	-	7,7,7	1.21	1 (14%)	7,9,9	1.05	0
2	A1H9I	G	1201	-	7,7,7	1.05	0	7,9,9	0.56	0
2	A1H9I	D	1201	-	7,7,7	1.20	0	7,9,9	0.82	0
2	A1H9I	C	1201	-	7,7,7	1.35	1 (14%)	7,9,9	0.84	0
2	A1H9I	E	1201	-	7,7,7	1.01	0	7,9,9	0.70	0
2	A1H9I	F	1201	-	7,7,7	1.09	1 (14%)	7,9,9	0.86	0
2	A1H9I	A	1201	-	7,7,7	1.29	1 (14%)	7,9,9	0.88	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	H	1201	-	-	3/6/7/7	-
2	A1H9I	B	1201	-	-	0/6/7/7	-
2	A1H9I	G	1201	-	-	4/6/7/7	-
2	A1H9I	D	1201	-	-	5/6/7/7	-
2	A1H9I	C	1201	-	-	3/6/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H9I	E	1201	-	-	4/6/7/7	-
2	A1H9I	F	1201	-	-	0/6/7/7	-
2	A1H9I	A	1201	-	-	3/6/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1H9I	C2-N1	-2.22	1.47	1.52
2	H	1201	A1H9I	C2-N1	-2.16	1.47	1.52
2	F	1201	A1H9I	C2-N1	-2.15	1.47	1.52
2	B	1201	A1H9I	C2-N1	-2.12	1.47	1.52
2	C	1201	A1H9I	C2-N1	-2.04	1.47	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	A1H9I	F1-C5-N1-C4
2	A	1201	A1H9I	F1-C5-N1-C3
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	D	1201	A1H9I	F1-C5-N1-C4
2	G	1201	A1H9I	F1-C5-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-C5
2	G	1201	A1H9I	C1-C2-N1-C3
2	H	1201	A1H9I	C1-C2-N1-C4

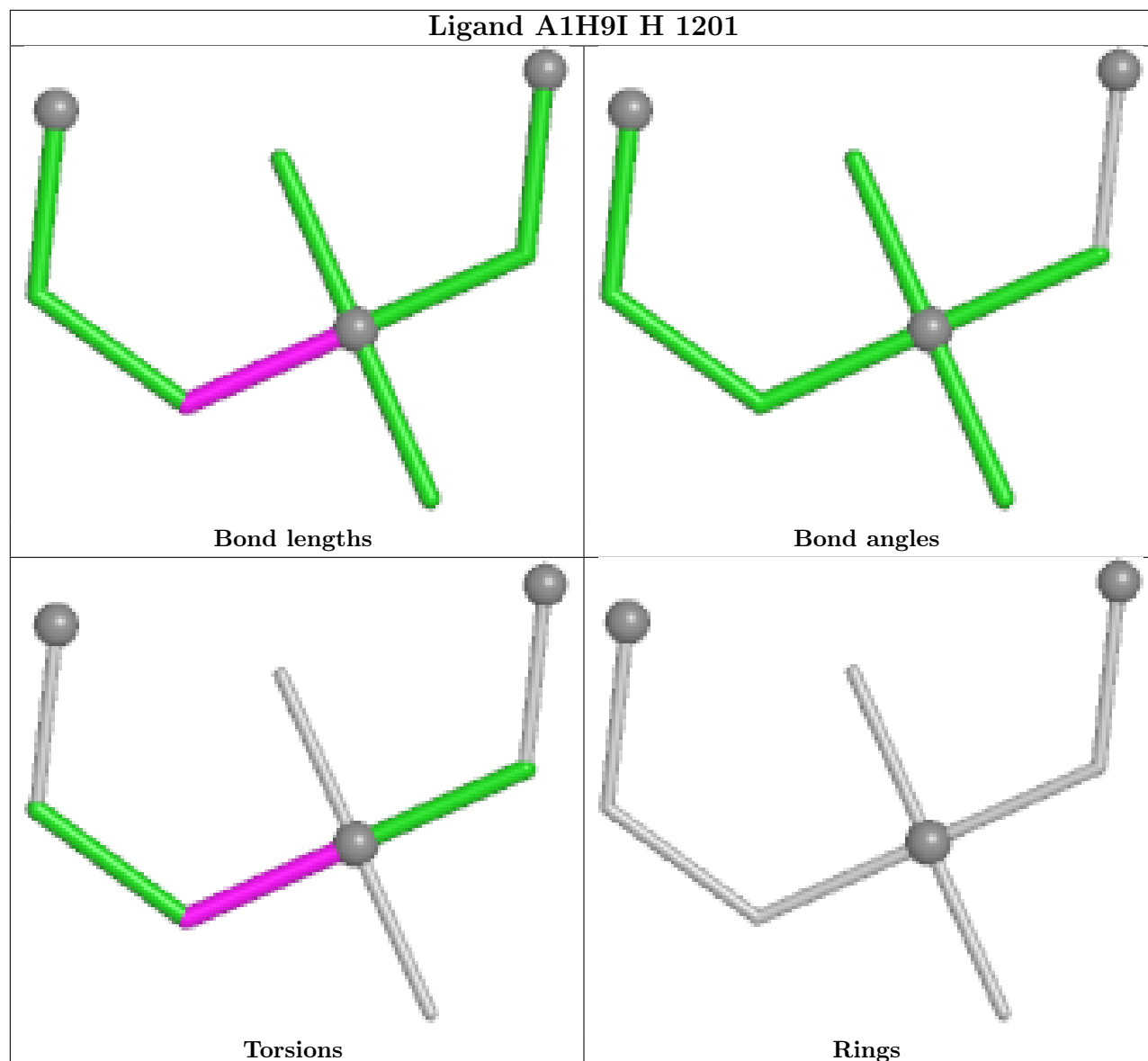
There are no ring outliers.

2 monomers are involved in 3 short contacts:

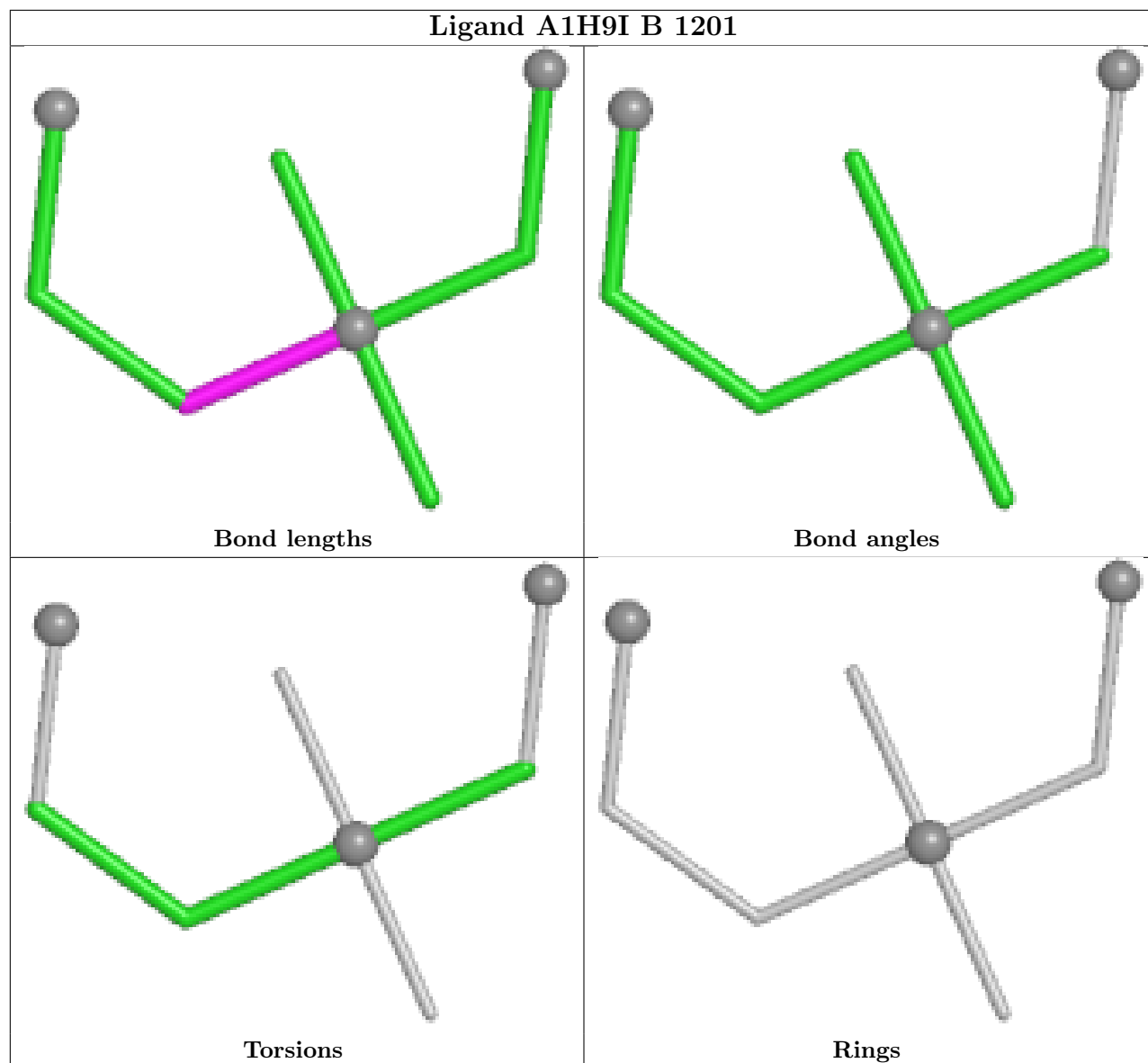
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	A1H9I	1	0
2	F	1201	A1H9I	2	0

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

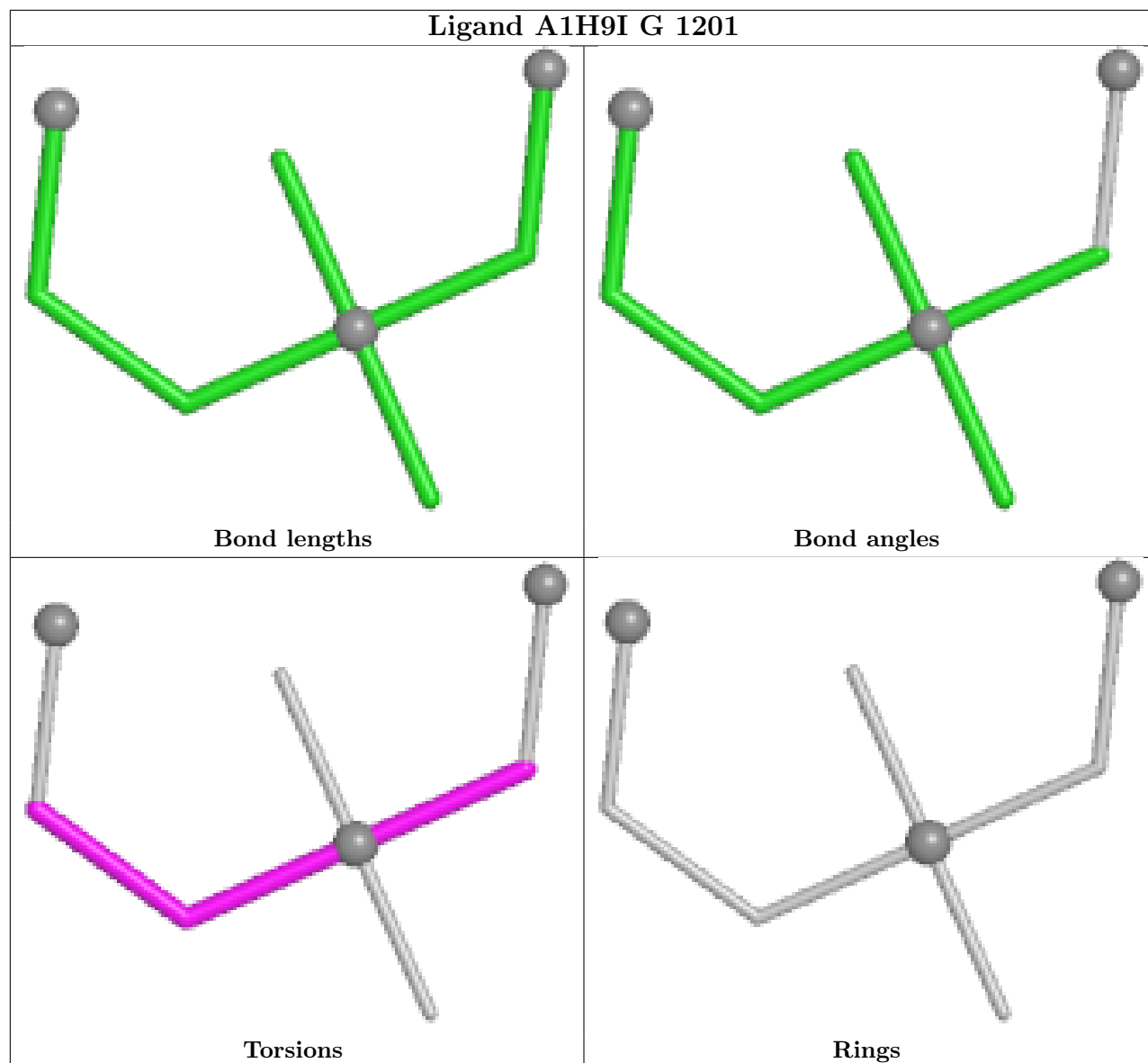
Ligand A1H9I H 1201



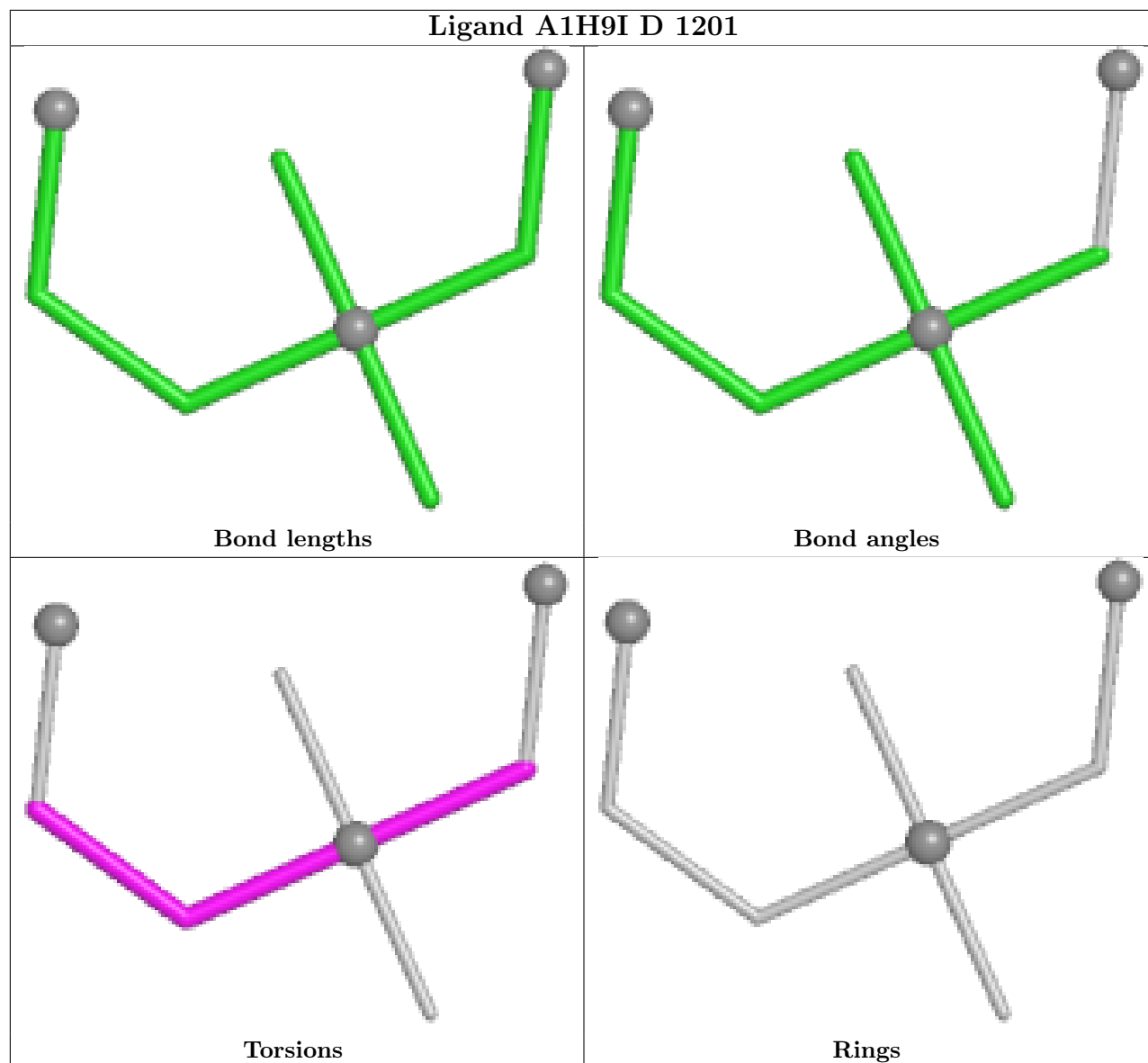
Ligand A1H9I B 1201



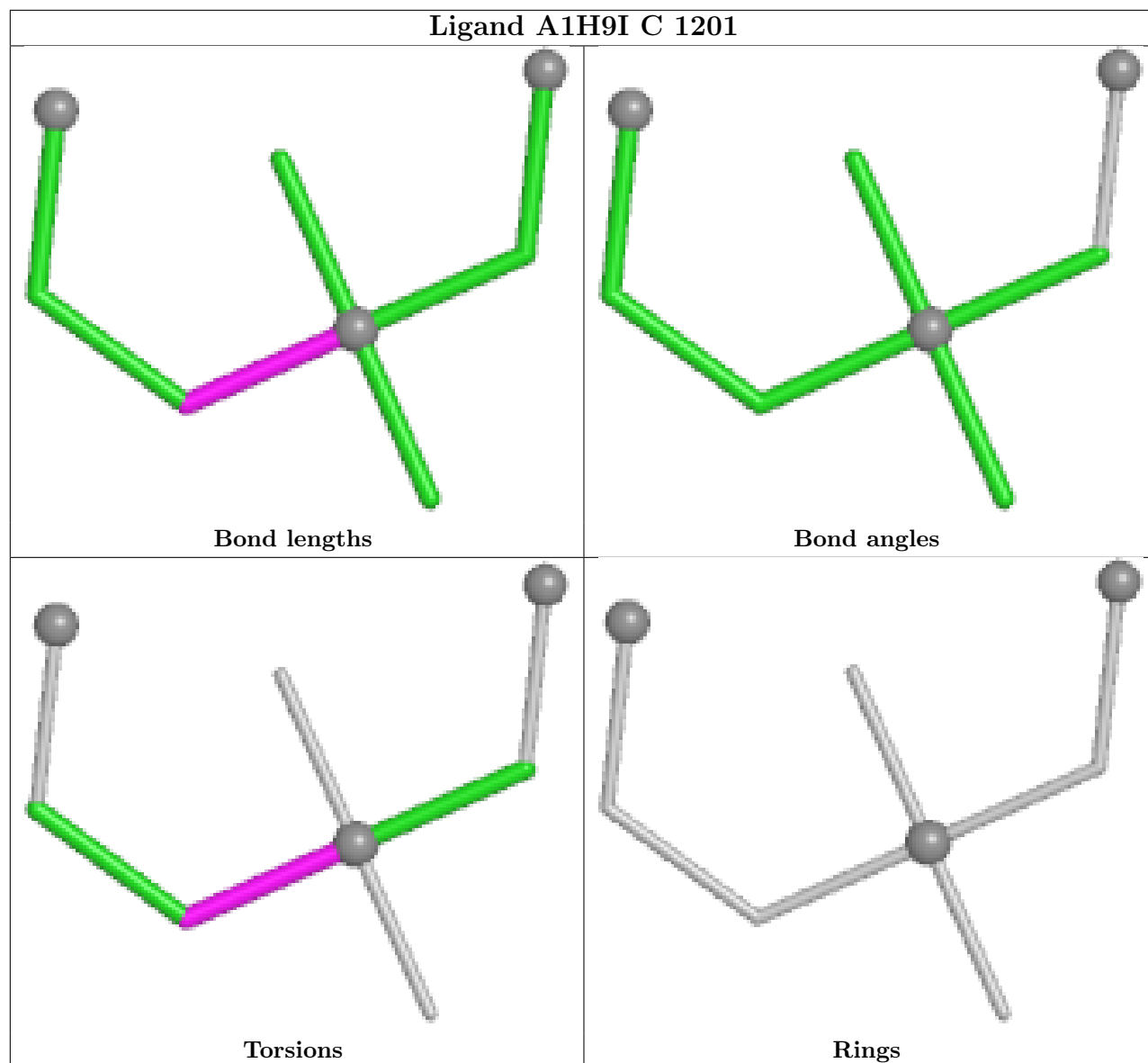
Ligand A1H9I G 1201



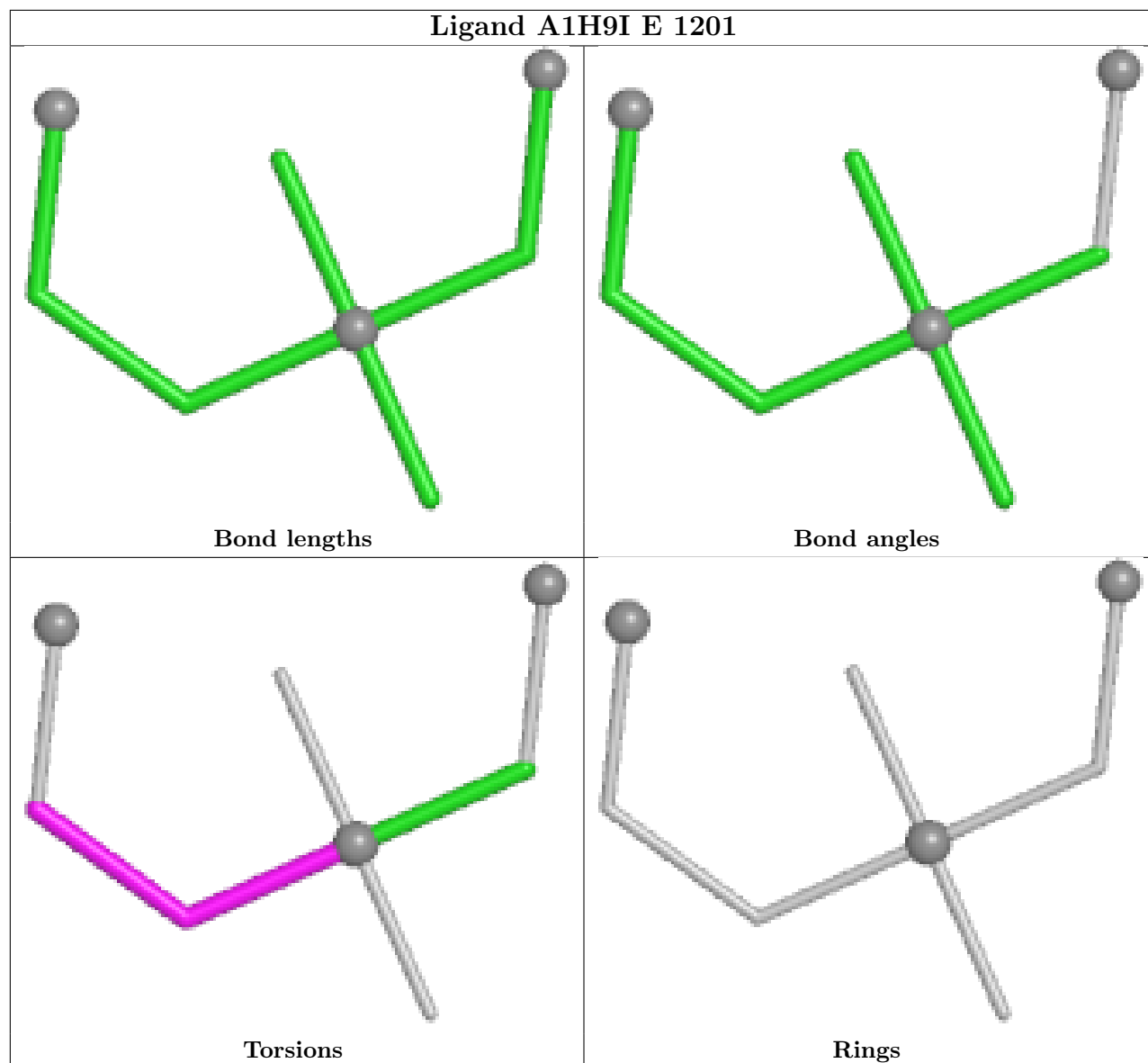
Ligand A1H9I D 1201



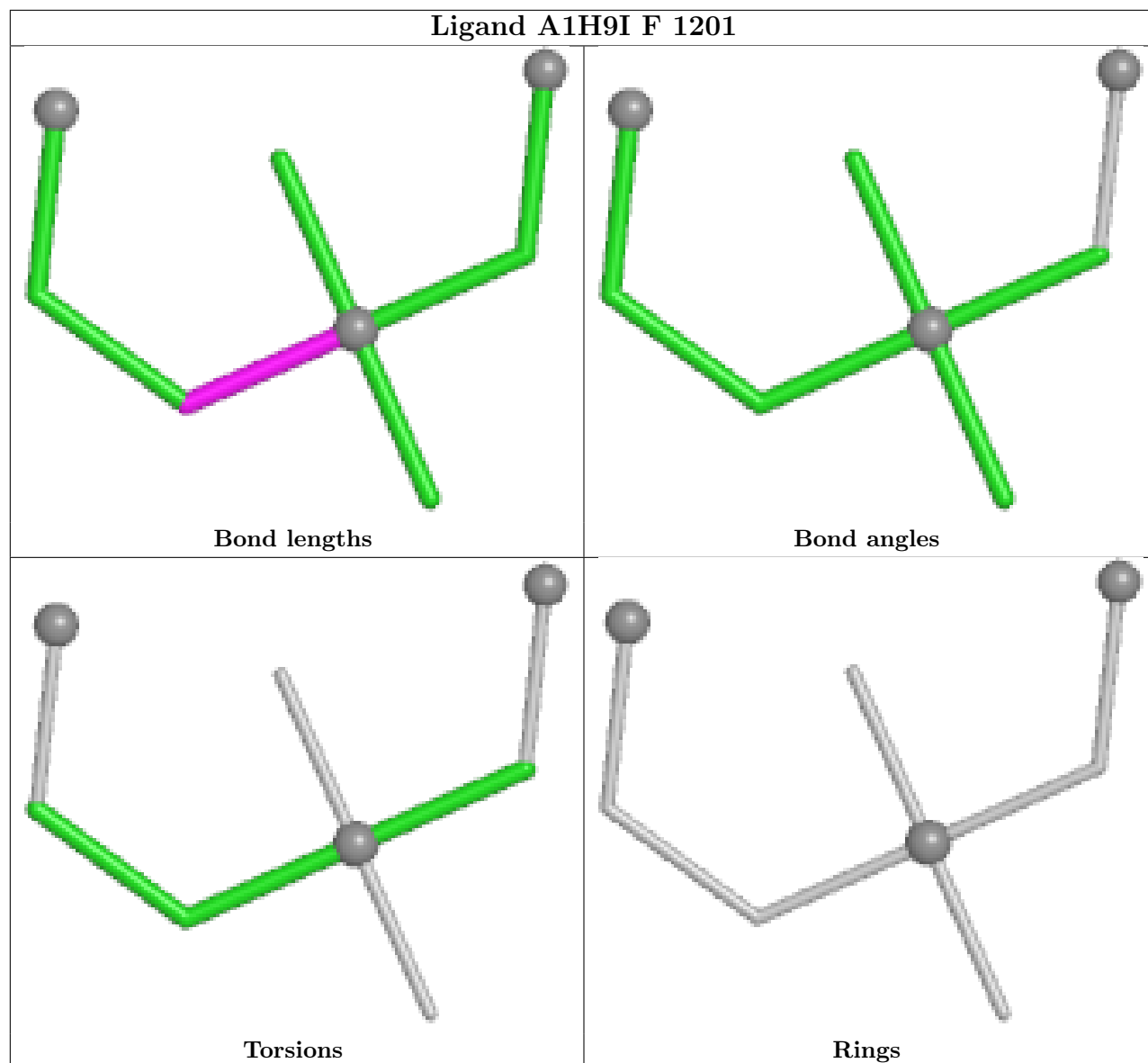
Ligand A1H9I C 1201

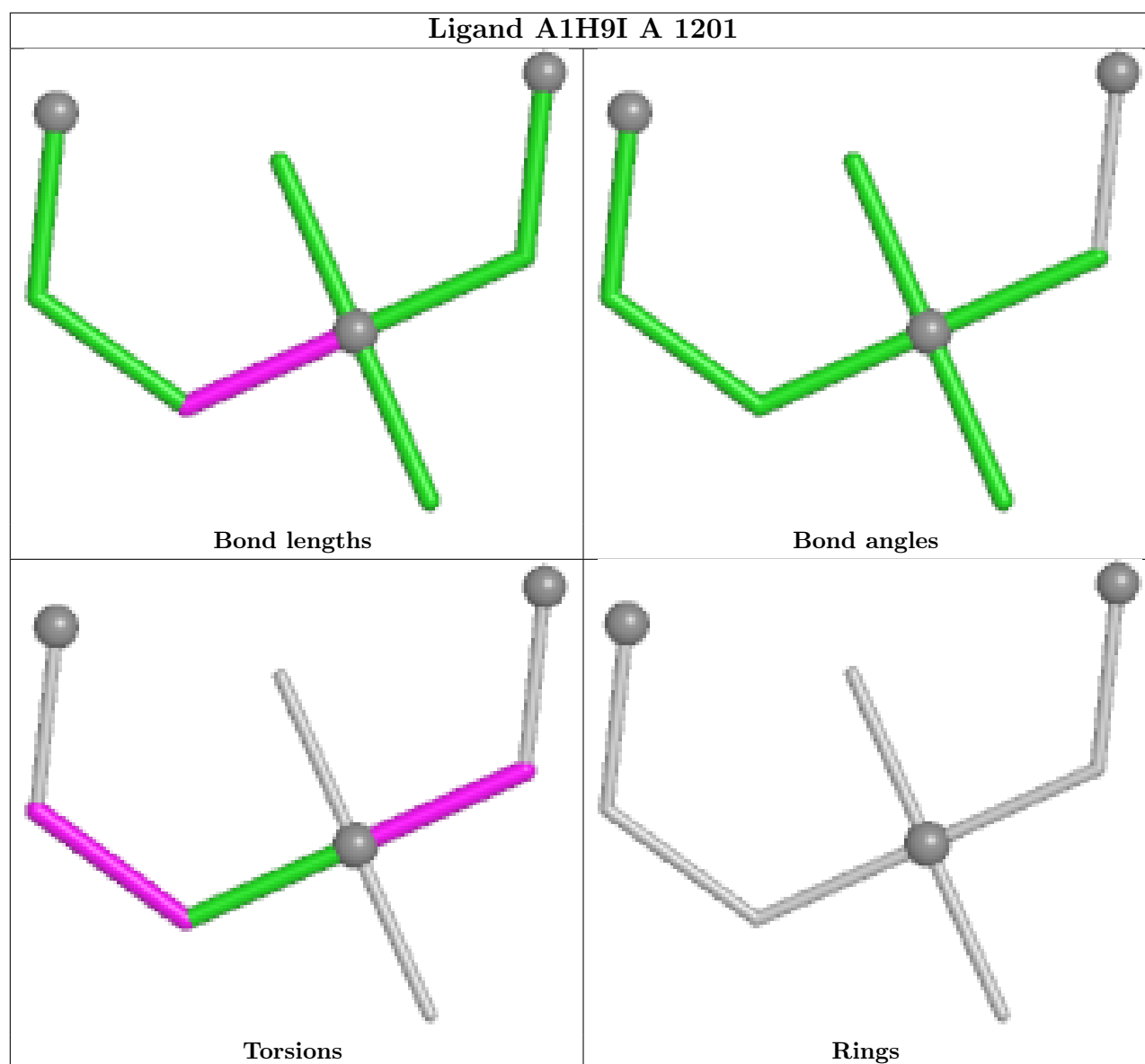


Ligand A1H9I E 1201



Ligand A1H9I F 1201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	792/1150 (68%)	-0.37	1 (0%) 92 91	13, 25, 45, 73	0
1	B	792/1150 (68%)	-0.30	0 100 100	11, 26, 43, 57	0
1	C	792/1150 (68%)	-0.01	3 (0%) 88 87	15, 32, 51, 86	0
1	D	792/1150 (68%)	0.34	15 (1%) 66 63	17, 43, 62, 80	0
1	E	792/1150 (68%)	0.52	34 (4%) 40 36	17, 49, 76, 95	0
1	F	792/1150 (68%)	0.58	57 (7%) 21 18	19, 45, 71, 92	0
1	G	792/1150 (68%)	0.75	66 (8%) 17 14	25, 51, 76, 102	0
1	H	792/1150 (68%)	1.08	115 (14%) 6 5	32, 61, 87, 102	0
All	All	6336/9200 (68%)	0.32	291 (4%) 37 34	11, 40, 74, 102	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1038	GLY	5.4
1	G	981	SER	5.1
1	H	558	ALA	5.1
1	H	403	ILE	4.8
1	G	633	ALA	4.7
1	H	405	GLY	4.6
1	H	454	ILE	4.5
1	H	737	GLY	4.4
1	H	651	ALA	4.4
1	H	554	ALA	4.2
1	H	440	PHE	3.8
1	H	450	ILE	3.8
1	H	566	ALA	3.7
1	H	671	PHE	3.6
1	H	709	VAL	3.6
1	H	577	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	922	ALA	3.5
1	H	706	PHE	3.5
1	H	418	PRO	3.4
1	G	566	ALA	3.4
1	H	351	TYR	3.4
1	F	916	LEU	3.4
1	E	898	VAL	3.4
1	G	583	VAL	3.4
1	H	404	VAL	3.3
1	H	654	ILE	3.3
1	H	1106	ALA	3.3
1	H	602	ILE	3.3
1	H	649	LEU	3.2
1	G	339	GLY	3.2
1	G	820	ASP	3.2
1	F	897	TYR	3.2
1	H	1046	LEU	3.1
1	E	932	ALA	3.1
1	H	672	ALA	3.1
1	F	929	GLY	3.1
1	E	571	ALA	3.1
1	H	416	PHE	3.1
1	E	1125	ILE	3.1
1	H	1098	ILE	3.1
1	F	1083	VAL	3.1
1	H	361	TYR	3.0
1	H	565	ALA	3.0
1	H	547	CYS	3.0
1	C	819	ARG	3.0
1	E	1061	THR	3.0
1	D	1032	VAL	3.0
1	F	806	LEU	3.0
1	F	914	TYR	3.0
1	G	403	ILE	3.0
1	G	908	VAL	3.0
1	D	1050	LEU	3.0
1	H	1050	LEU	3.0
1	E	930	TYR	3.0
1	H	538	TYR	3.0
1	E	727	MET	3.0
1	E	920	ARG	3.0
1	F	932	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	598	ALA	3.0
1	H	354	VAL	3.0
1	G	340	LEU	2.9
1	H	666	LEU	2.9
1	G	1098	ILE	2.9
1	G	1042	ASN	2.9
1	G	397	ILE	2.9
1	H	710	TYR	2.9
1	F	943	TYR	2.8
1	H	1020	PRO	2.8
1	H	1077	SER	2.8
1	G	716	CYS	2.8
1	F	909	PHE	2.8
1	F	1053	PRO	2.8
1	G	817	ASP	2.8
1	H	1045	PHE	2.8
1	H	1099	VAL	2.8
1	F	793	ILE	2.7
1	F	1046	LEU	2.7
1	H	339	GLY	2.7
1	F	1079	VAL	2.7
1	G	1043	PHE	2.7
1	H	342	PRO	2.7
1	H	653	ILE	2.7
1	H	1097	LEU	2.7
1	F	799	LEU	2.7
1	G	396	LEU	2.7
1	F	1002	TRP	2.7
1	H	1103	GLY	2.7
1	E	1115	VAL	2.7
1	F	671	PHE	2.7
1	G	608	LEU	2.7
1	H	578	LEU	2.7
1	G	647	GLU	2.7
1	D	1034	THR	2.7
1	G	575	ALA	2.7
1	G	644	THR	2.7
1	H	645	ALA	2.7
1	H	1091	PRO	2.7
1	H	603	TRP	2.6
1	E	949	TYR	2.6
1	H	402	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1072	GLY	2.6
1	H	1109	VAL	2.6
1	G	944	GLY	2.6
1	D	692	ALA	2.6
1	F	926	ASN	2.6
1	F	1081	ASN	2.6
1	H	366	PHE	2.6
1	H	1076	PHE	2.6
1	G	580	ILE	2.6
1	H	506	LEU	2.6
1	H	646	LEU	2.6
1	F	468	GLU	2.6
1	H	665	GLU	2.6
1	G	592	PRO	2.6
1	F	900	SER	2.5
1	H	573	ARG	2.5
1	E	914	TYR	2.5
1	E	338	GLU	2.5
1	H	401	GLU	2.5
1	H	563	GLU	2.5
1	C	337	MET	2.5
1	H	661	TRP	2.5
1	E	838	ILE	2.5
1	G	1078	TYR	2.5
1	H	490	TYR	2.5
1	F	667	GLY	2.5
1	E	908	VAL	2.5
1	D	631	PHE	2.5
1	E	909	PHE	2.5
1	H	1123	THR	2.5
1	G	551	VAL	2.5
1	H	630	MET	2.5
1	G	627	CYS	2.5
1	H	1044	LYS	2.5
1	G	620	LEU	2.5
1	E	901	MET	2.5
1	F	794	ALA	2.5
1	F	906	LYS	2.4
1	G	602	ILE	2.4
1	G	654	ILE	2.4
1	G	734	VAL	2.4
1	H	707	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	633	ALA	2.4
1	H	740	PHE	2.4
1	F	896	THR	2.4
1	G	659	LEU	2.4
1	H	494	ASN	2.4
1	F	1038	GLY	2.4
1	G	818	LEU	2.4
1	H	635	ILE	2.4
1	H	432	MET	2.4
1	G	741	PRO	2.4
1	G	733	VAL	2.4
1	H	561	ALA	2.4
1	F	907	LEU	2.4
1	G	819	ARG	2.4
1	H	556	ARG	2.4
1	H	609	PHE	2.4
1	H	763	ALA	2.4
1	F	670	TYR	2.3
1	H	350	HIS	2.3
1	H	1055	GLY	2.3
1	E	1027	VAL	2.3
1	D	633	ALA	2.3
1	E	807	PHE	2.3
1	G	413	ALA	2.3
1	G	1108	PHE	2.3
1	F	890	ILE	2.3
1	D	351	TYR	2.3
1	E	899	ASP	2.3
1	H	356	PRO	2.3
1	F	1019	GLY	2.3
1	F	908	VAL	2.3
1	G	682	VAL	2.3
1	H	550	VAL	2.3
1	H	733	VAL	2.3
1	E	907	LEU	2.3
1	H	861	LEU	2.3
1	F	930	TYR	2.3
1	H	607	SER	2.3
1	G	356	PRO	2.3
1	F	1032	VAL	2.3
1	F	824	PHE	2.3
1	F	927	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	640	LEU	2.3
1	E	559	ALA	2.3
1	F	830	ALA	2.3
1	F	978	GLY	2.3
1	D	340	LEU	2.3
1	F	1005	LEU	2.3
1	G	699	LEU	2.3
1	H	587	VAL	2.3
1	F	1123	THR	2.2
1	H	915	THR	2.2
1	H	1090	GLU	2.2
1	H	553	TYR	2.2
1	F	993	ASN	2.2
1	H	590	ASN	2.2
1	D	646	LEU	2.2
1	F	791	TRP	2.2
1	G	799	LEU	2.2
1	E	836	ALA	2.2
1	G	1024	ILE	2.2
1	H	442	ILE	2.2
1	F	917	GLU	2.2
1	H	407	PRO	2.2
1	H	596	GLN	2.2
1	D	748	SER	2.2
1	G	739	GLY	2.2
1	F	1102	ALA	2.2
1	H	543	ALA	2.2
1	D	1061	THR	2.2
1	G	705	ARG	2.2
1	H	373	ASN	2.2
1	F	792	PRO	2.2
1	E	339	GLY	2.2
1	G	1048	GLY	2.2
1	E	900	SER	2.2
1	G	1079	VAL	2.2
1	E	824	PHE	2.2
1	D	954	ALA	2.2
1	G	353	THR	2.2
1	E	1094	TYR	2.2
1	F	788	TYR	2.2
1	H	628	TYR	2.2
1	E	933	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	414	GLY	2.2
1	G	1049	LEU	2.2
1	G	1062	LEU	2.2
1	H	429	LEU	2.2
1	H	659	LEU	2.2
1	H	1048	GLY	2.2
1	E	1101	VAL	2.2
1	G	740	PHE	2.2
1	F	668	ALA	2.1
1	G	645	ALA	2.1
1	F	915	THR	2.1
1	H	1127	LYS	2.1
1	E	1023	ILE	2.1
1	G	866	VAL	2.1
1	H	1051	ASP	2.1
1	D	927	PHE	2.1
1	G	677	PHE	2.1
1	A	565	ALA	2.1
1	D	915	THR	2.1
1	G	676	PRO	2.1
1	F	821	LEU	2.1
1	G	590	ASN	2.1
1	H	584	ASN	2.1
1	H	1094	TYR	2.1
1	E	1009	ILE	2.1
1	H	358	VAL	2.1
1	H	1115	VAL	2.1
1	H	1124	VAL	2.1
1	H	417	SER	2.1
1	H	742	ALA	2.1
1	F	822	ARG	2.1
1	H	1089	GLN	2.1
1	F	813	LEU	2.1
1	G	907	LEU	2.1
1	H	714	LEU	2.1
1	G	710	TYR	2.1
1	F	487	ASP	2.1
1	G	571	ALA	2.1
1	G	579	THR	2.1
1	G	595	LEU	2.1
1	H	364	LEU	2.1
1	H	640	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	1081	ASN	2.1
1	F	845	GLY	2.1
1	H	627	CYS	2.1
1	D	710	TYR	2.1
1	F	805	VAL	2.1
1	F	1045	PHE	2.1
1	H	562	ARG	2.0
1	F	483	THR	2.0
1	F	337	MET	2.0
1	H	406	HIS	2.0
1	E	795	ILE	2.0
1	H	795	ILE	2.0
1	G	698	TYR	2.0
1	G	1099	VAL	2.0
1	G	386	PHE	2.0
1	H	1043	PHE	2.0
1	H	581	ALA	2.0
1	H	946	ASP	2.0
1	E	952	GLN	2.0
1	F	924	LEU	2.0
1	G	1103	GLY	2.0
1	H	1120	ILE	2.0
1	F	485	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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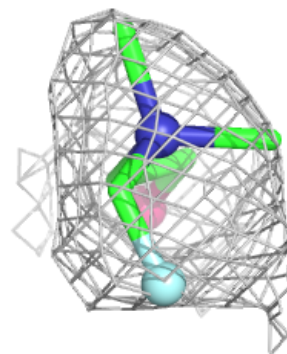
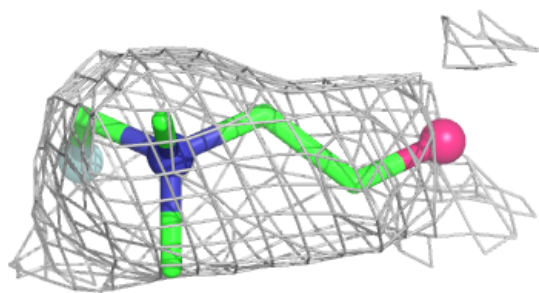
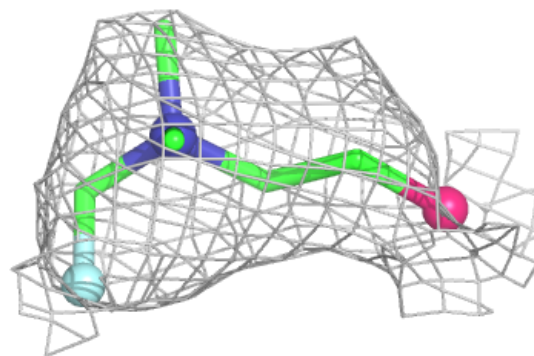
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1H9I	H	1201	8/8	0.89	0.14	54,63,65,65	0
2	A1H9I	F	1201	8/8	0.90	0.12	34,40,49,49	0
2	A1H9I	E	1201	8/8	0.91	0.13	34,40,45,47	0
2	A1H9I	D	1201	8/8	0.93	0.12	32,35,37,38	0
2	A1H9I	C	1201	8/8	0.93	0.12	19,24,29,29	0
2	A1H9I	G	1201	8/8	0.94	0.11	32,34,42,46	0
2	A1H9I	B	1201	8/8	0.97	0.07	18,23,25,29	0
2	A1H9I	A	1201	8/8	0.98	0.06	16,21,25,26	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.

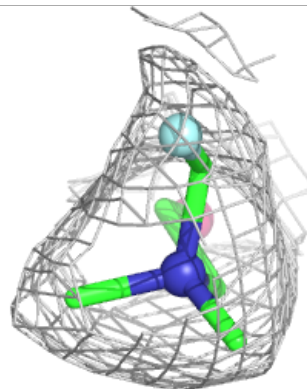
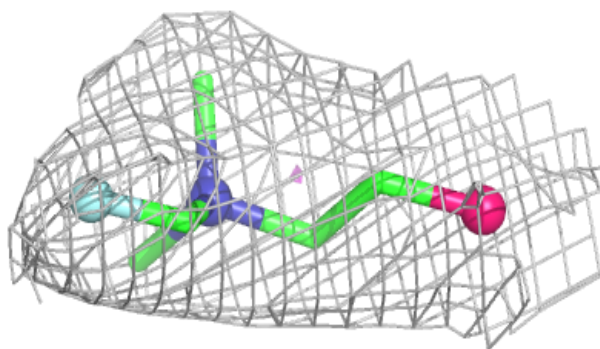
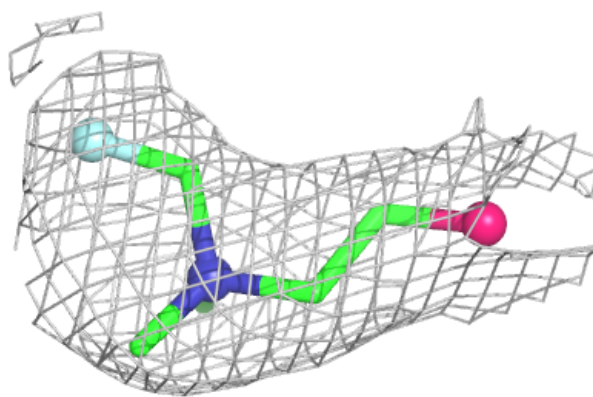
Electron density around A1H9I H 1201:

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



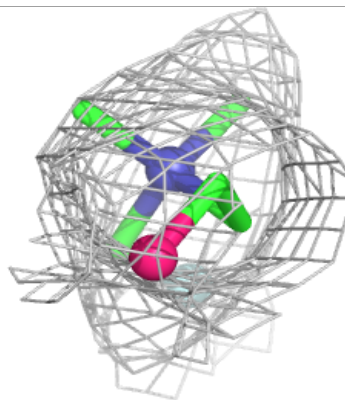
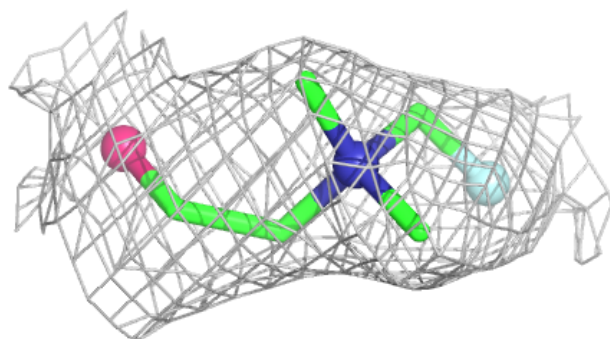
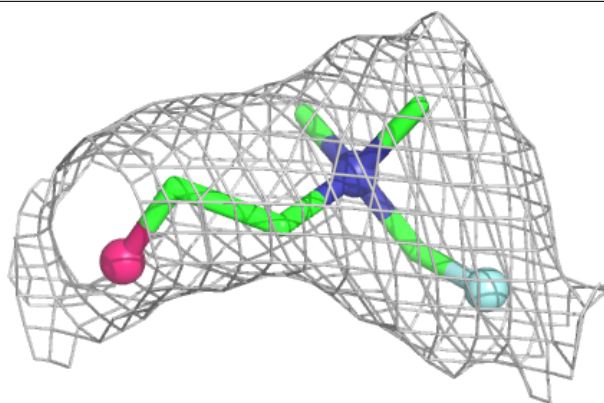
Electron density around A1H9I F 1201:

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

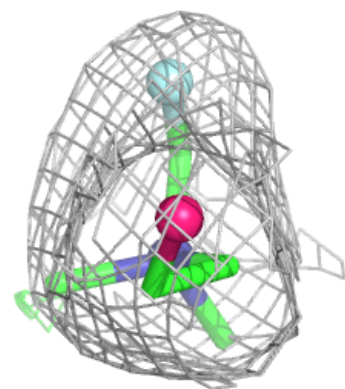
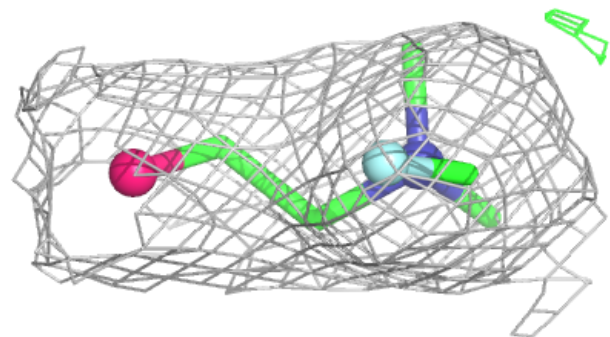
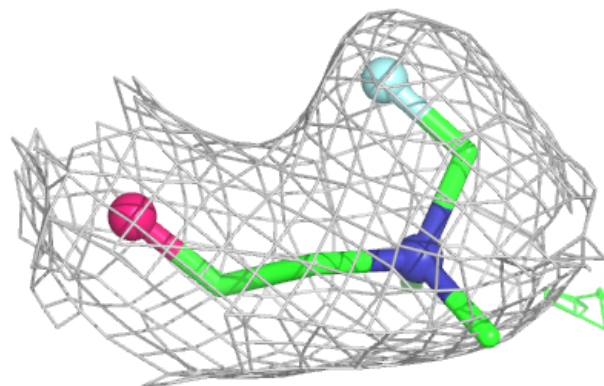


Electron density around A1H9I E 1201:

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

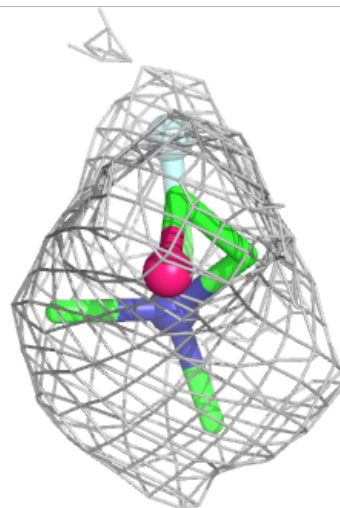
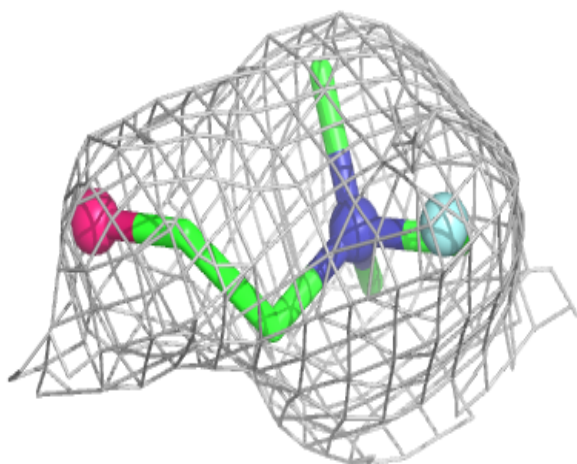
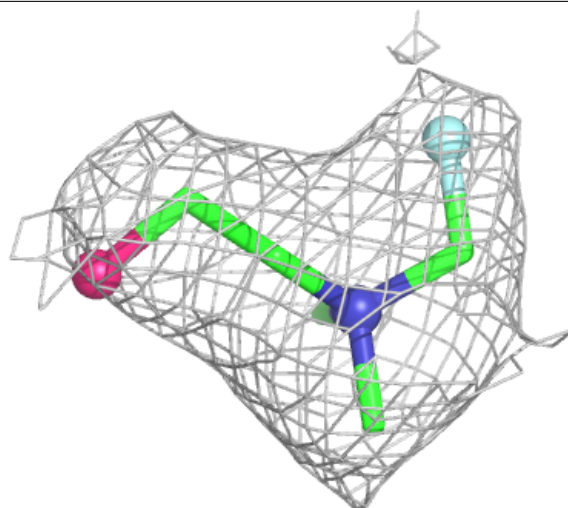
**Electron density around A1H9I D 1201:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



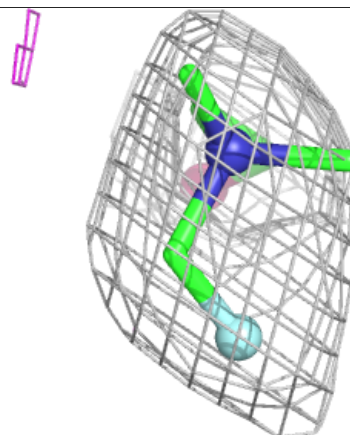
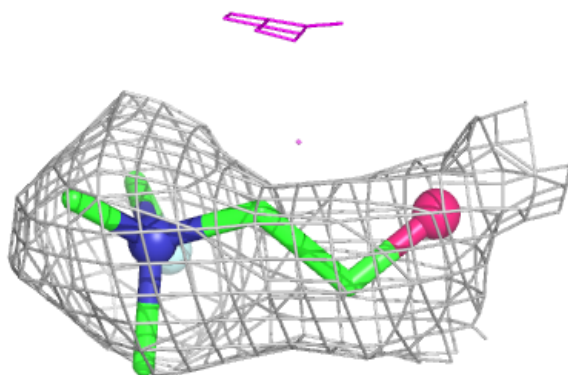
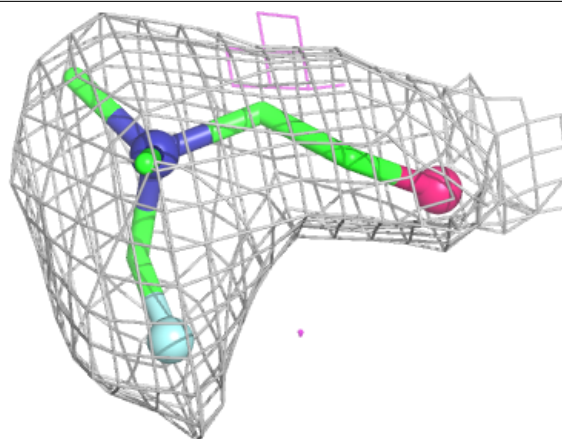
Electron density around A1H9I C 1201:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

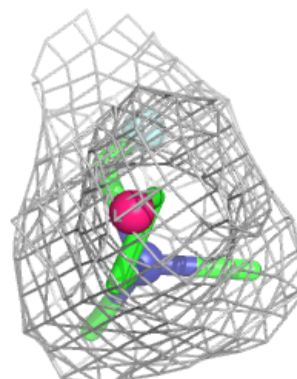
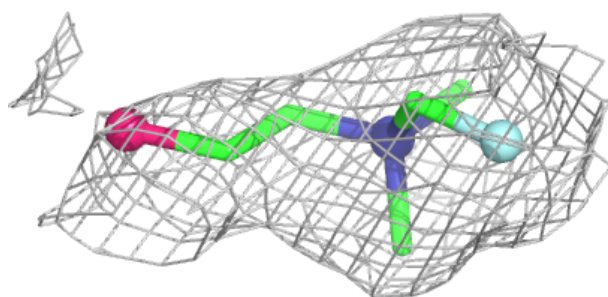
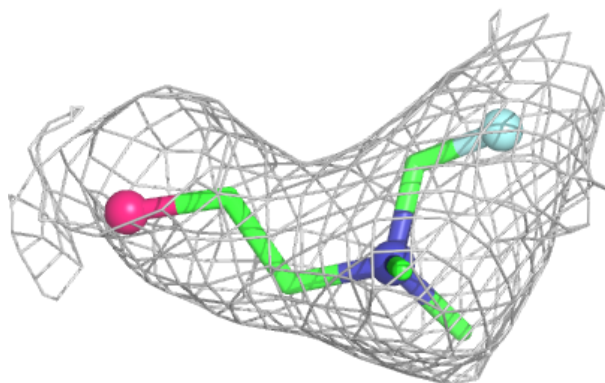


Electron density around A1H9I G 1201:

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

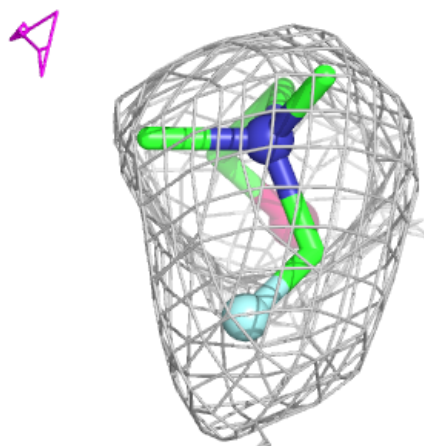
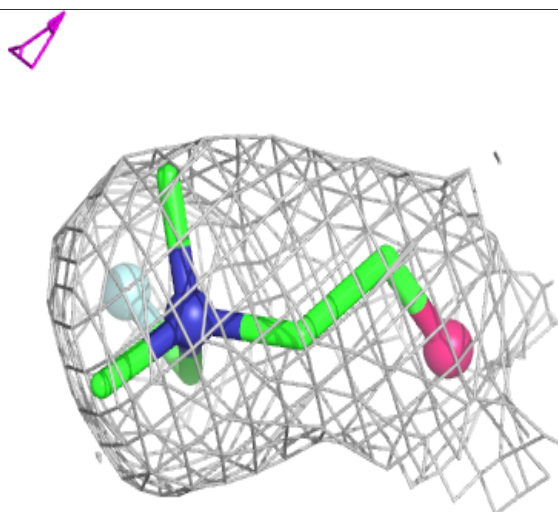
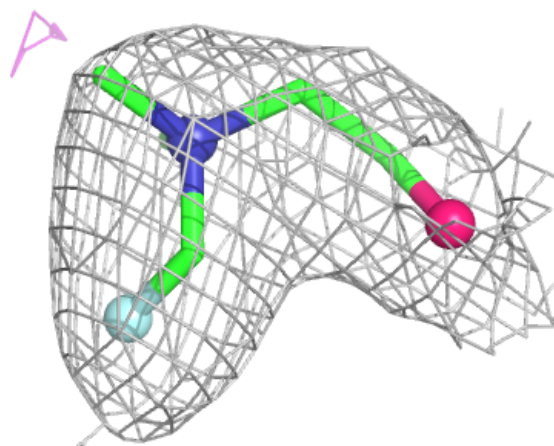
**Electron density around A1H9I B 1201:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.