



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 9F3X / pdb_00009f3x
Title : CutC choline lyase in complex with cyclopropylcholine
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

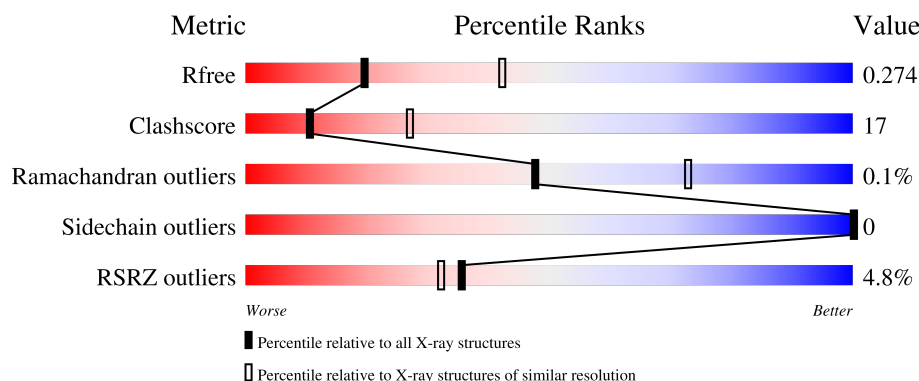
1 Overall quality at a glance

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.



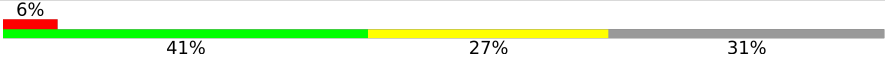
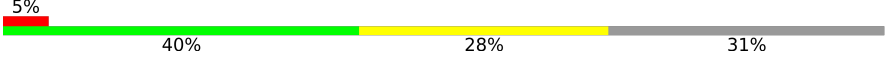
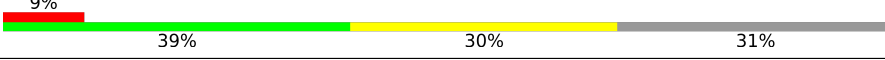
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	 6% 41% 27% 31%
1	G	1150	 5% 40% 28% 31%
1	H	1150	 9% 39% 30% 31%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 50434 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	791	Total	C	N	O	S	0	0	0
			6246	3949	1076	1180	41			
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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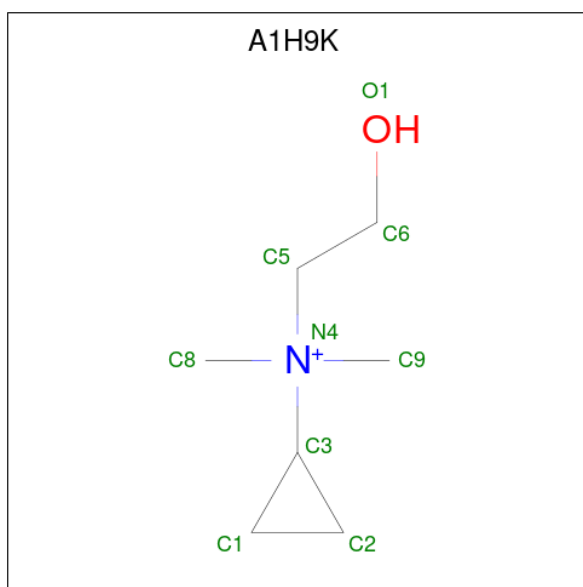
Chain	Residue	Modelled	Actual	Comment	Reference
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E	-11	SER	-	expression tag	UNP A0A486V7R5
E	-10	GLN	-	expression tag	UNP A0A486V7R5
E	-9	ASP	-	expression tag	UNP A0A486V7R5
E	-8	HIS	-	expression tag	UNP A0A486V7R5
E	-7	GLU	-	expression tag	UNP A0A486V7R5
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 cyclopropylcholine (CCD ID: A1H9K) (formula: C₇H₁₆NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	7	1	1		
2	B	1	Total	C	N	O	0	0
			9	7	1	1		
2	C	1	Total	C	N	O	0	0
			9	7	1	1		
2	D	1	Total	C	N	O	0	0
			9	7	1	1		
2	E	1	Total	C	N	O	0	0
			9	7	1	1		
2	F	1	Total	C	N	O	0	0
			9	7	1	1		
2	G	1	Total	C	N	O	0	0
			9	7	1	1		
2	H	1	Total	C	N	O	0	0
			9	7	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	71	Total	O	0	0
			71	71		
3	C	65	Total	O	0	0
			65	65		
3	D	31	Total	O	0	0
			31	31		

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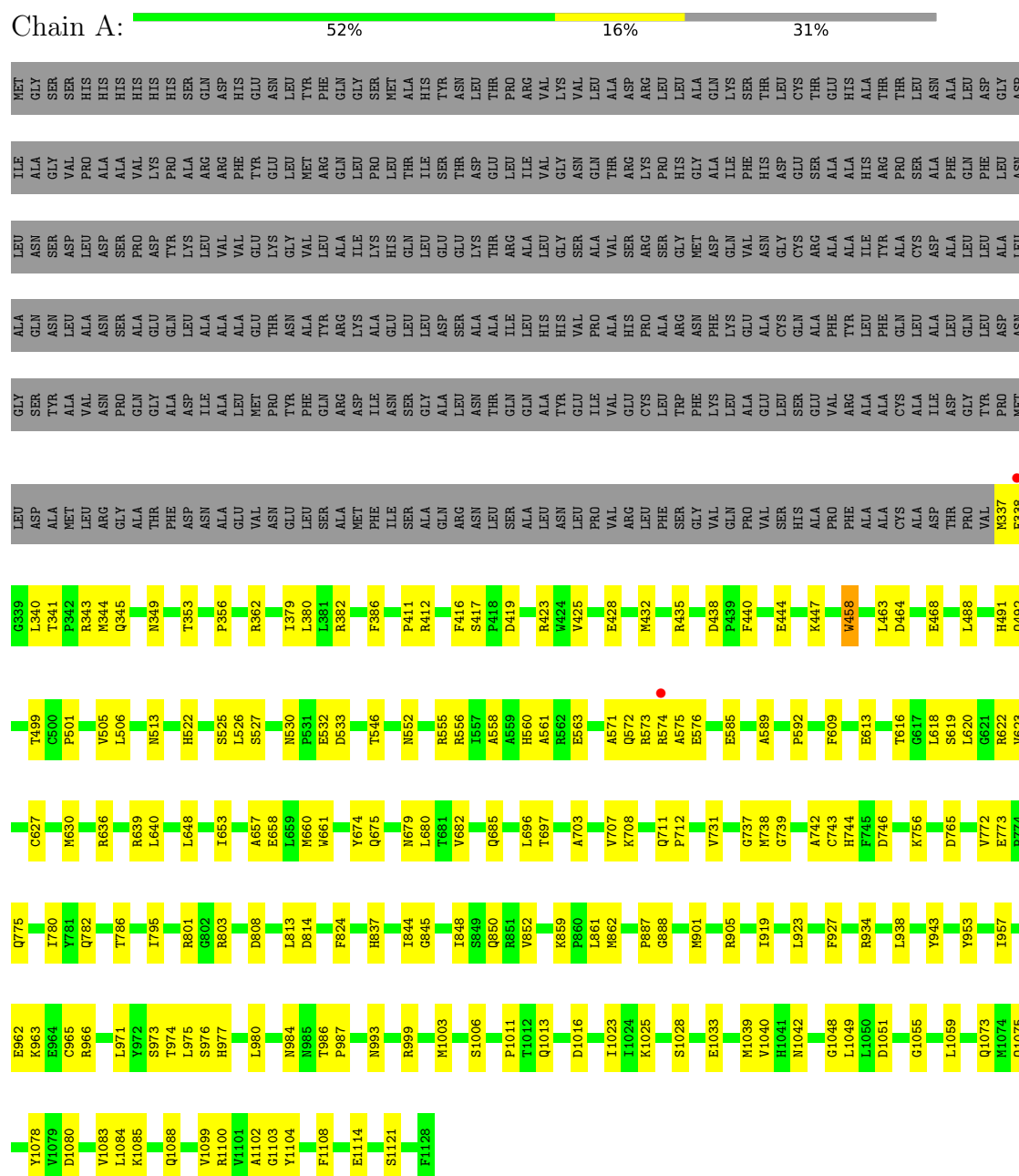
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	29	Total 29	O 29	0	0
3	F	24	Total 24	O 24	0	0
3	G	20	Total 20	O 20	0	0
3	H	11	Total 11	O 11	0	0

3 Residue-property plots

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

• Molecule 1: Choline trimethylamine-lyase

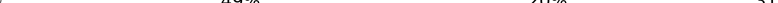


- Molecule 1: Choline trimethylamine-lyase

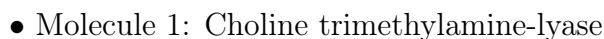
Chain B:  53% 16% 31%

L1084	F927	M738	T616	L463	L340	LEU	GLY	ALA	LEU	ALA	GLN	ASN	GLY	MET
Q1088	R934	C743	G617	D464	T341	ASP	SER	TYR	ASP	ASN	GLN	ASN	GLY	GLY
K1093	R934	C743	L618	E465	P342	ALA	ALA	TYR	ALA	ASN	GLN	ASN	VAL	SER
Y1094	P941	H744	S619	I466	R343	MET	ALA	ALA	LEU	ALA	GLN	LEU	PRO	HIS
R1095	P941	F758	G621	D487	N344	ARG	ASN	ASN	ARG	ASN	ASN	ASP	ALA	HIS
R1100	G944	F758	R622	L506	R348	GLY	PRO	PRO	GLY	SER	SER	SER	ALA	HIS
V1101	Y949	W772	R623	L507	R349	ALA	ALA	GLN	ALA	PRO	GLN	PRO	VAL	HIS
A1102	Y949	E773	Y626	L507	H350	PHE	GLY	GLY	THR	GLN	GLN	TYR	VAL	HIS
G1103	V950	W772	Y626	K510	L352	ASP	ALA	ALA	ASP	GLN	GLN	TYR	PRO	HIS
Y1104	Y953	K776	M630	G511	T353	ASN	ILE	ALA	ILE	ALA	ALA	LYS	ALA	SER
F1108	W960	R779	D634	H512	V369	ALA	ASN	ALA	ASN	VAL	VAL	LYS	ARG	GLN
V1109	W960	I780	E637	N513	K371	GLU	ASN	THR	GLU	GLY	GLU	ASN	GLY	ASN
E1114	R966	G787	G638	D518	R376	LEU	TYR	PHE	VAL	VAL	ALA	VAL	LEU	TYR
V1115	S973	Q790	R639	H528	K376	SER	GLN	GLN	ALA	TYR	ALA	VAL	MET	PHE
Q1116	T974	E647	E529	E529	I379	ALA	ARG	ARG	GLN	GLN	GLN	ALA	ARG	GLN
D1117	I793	L648	P531	N530	L380	MET	ASP	ASP	ILE	LYS	ILE	LYS	LEU	GLY
E1118	L980	A794	E532	E532	L381	PHE	ILE	ILE	ALA	GLY	GLY	HIS	LEU	SER
S1121	S981	I795	I653	I537	R382	SER	SER	SER	LEU	GLN	LEU	GLN	THR	ALA
V1124	I982	T823	A657	I537	A386	ALA	GLY	GLY	LEU	LEU	LEU	GLN	ILE	HIS
F1128	T986	F824	E658	V551	I395	GLN	ALA	ALA	GLN	ASP	GLU	GLU	THR	TYR
	P987	D825	E658	N552	D400	ARG	ASN	ASN	ASN	SER	GLY	LYS	THR	ASN
	I988	V661	G662	V563	P411	ASN	THR	ALA	ALA	ALA	ALA	LYS	GLU	LEU
	L991	K832	S663	I557	F416	LEU	GLN	GLN	ILE	ARG	ARG	THR	GLU	THR
	T992	Q850	S664	A561	P411	ALA	GLN	GLN	ILE	ARG	ILE	LEU	VAL	PRO
A994	N993	P858	E665	E561	F416	ASN	TYR	ALA	HIS	LEU	HIS	LEU	VAL	ARG
	R999	M862	Q675	E568	P418	PRO	ILE	VAL	PRO	ALA	VAL	ALA	ASN	LEU
M1003	L864	S863	P676	D569	D419	ARG	VAL	VAL	ALA	VAL	ALA	VAL	THR	ALA
S1006	L865	W866	F677	N570	R423	LEU	CYS	CYS	PRO	HIS	HIS	SER	THR	ALA
	E867	L680	L680	E576	W424	PHE	TRP	TRP	GLY	GLY	GLY	GLY	GLY	ASP
P1011	T700	M701	L699	T579	E428	GLY	PHE	PHE	ASN	MET	ASN	MET	GLY	ALA
T1012	T1012	E581	M701	A581	E428	VAL	LYS	LYS	ASN	ASP	ASN	ASP	ALA	GLN
Q1013	A703	E582	Y702	E583	M432	GLN	LEU	LEU	GLN	GLN	GLN	GLN	ILE	LYS
V1040	W704	E583	A703	E583	M432	PRO	ALA	ALA	VAL	VAL	VAL	VAL	PHE	SER
K1044	R705	V587	R705	V587	R435	SER	LEU	LEU	CYS	GLY	CYS	CYS	GLY	THR
G1048	F706	P588	F706	P588	Q437	HIS	SER	SER	GLN	GLN	GLN	ARG	SER	CYS
D1051	W707	A589	W707	A589	D438	ALA	GLU	VAL	ALA	ALA	PHE	ALA	GLU	THR
L1059	Q711	P592	Q711	P592	F440	PHE	VAL	ARG	ALA	ALA	TYR	ALA	GLU	HIS
Q1073	L714	L	L714	L	K448	ALA	ALA	ALA	ALA	ALA	PHE	TYR	ALA	HIS
M1074	L	L	L	L	E482	CYS	CYS	CYS	ALA	ALA	GLN	ALA	PRO	ALA
Q1075	I718	V605	I718	V605	E453	ASP	ILE	ILE	ALA	ASP	LEU	ALA	ALA	SER
V1079	K729	E613	K729	E613	T454	THR	GLY	GLY	GLN	LEU	LEU	GLN	PHE	THR
	Y1919	E613	Y1919	E613	W458	PRO	TYR	TYR	LEU	LEU	LEU	LEU	PHE	LEU
	Y1079	Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	GLY
		Y731	Y731	Y731	W458	VAL	PRO	PRO	ASP	ASP	ASP	ASP	PHE	

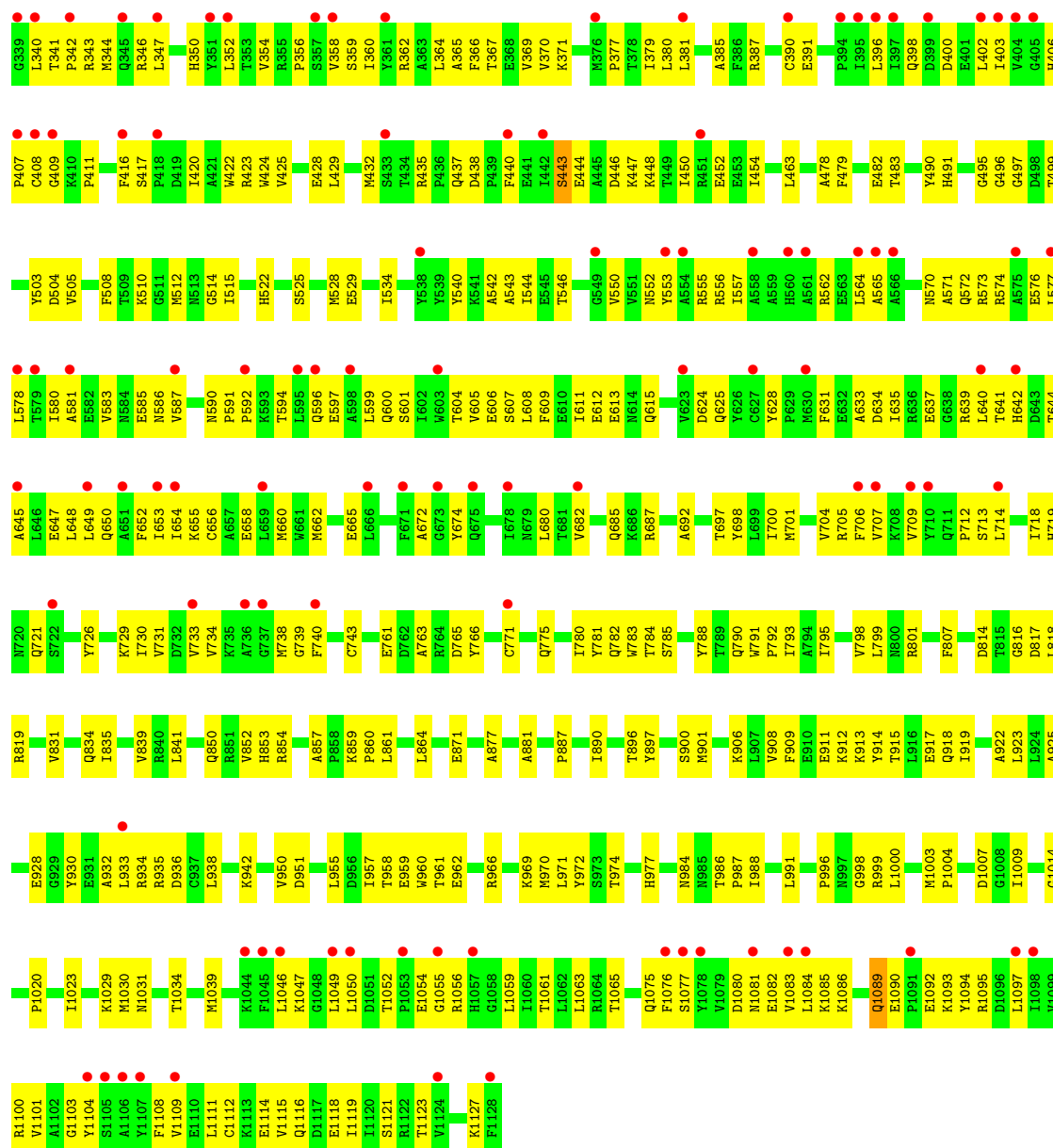
- Molecule 1: Choline trimethylamine-lyase

Chain C:  49% 20% 31%

[illegible]







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.27Å 119.66Å 214.70Å 77.86° 85.18° 69.32°	Depositor
Resolution (Å)	44.64 – 2.70 44.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.64-2.70) 95.7 (44.64-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.218 , 0.273 0.220 , 0.274	Depositor DCC
R_{free} test set	10759 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50434	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H9K

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	0.51	0/6385	0.74	1/8640 (0.0%)
1	B	0.50	0/6385	0.74	2/8640 (0.0%)
1	C	0.45	0/6377	0.70	0/8630
1	D	0.45	0/6385	0.72	0/8640
1	E	0.46	0/6385	0.70	1/8640 (0.0%)
1	F	0.50	4/6385 (0.1%)	0.83	9/8640 (0.1%)
1	G	0.50	6/6385 (0.1%)	0.73	13/8640 (0.2%)
1	H	0.41	0/6385	0.71	0/8640
All	All	0.47	10/51072 (0.0%)	0.73	26/69110 (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	1
1	C	0	1
1	E	0	1
1	F	0	2
1	G	0	2
1	H	0	2
All	All	0	9

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	820	ASP	CB-CG	-11.59	1.23	1.52
1	F	822	ARG	CZ-NH1	10.47	1.47	1.32
1	G	820	ASP	CG-OD2	9.56	1.43	1.25
1	G	820	ASP	C-N	-7.13	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	820	ASP	CG-OD1	-6.45	1.13	1.25
1	F	591	PRO	CA-C	6.38	1.55	1.51
1	G	820	ASP	CA-CB	-6.12	1.45	1.54
1	F	822	ARG	CB-CG	-5.31	1.36	1.52
1	G	1127	LYS	CD-CE	5.18	1.68	1.52
1	F	822	ARG	CD-NE	5.09	1.53	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	822	ARG	NE-CZ-NH2	24.09	140.88	119.20
1	F	822	ARG	NH1-CZ-NH2	-18.82	94.84	119.30
1	G	819	ARG	CA-C-O	-9.21	107.33	120.51
1	F	822	ARG	CB-CG-CD	-8.89	90.85	111.30
1	G	820	ASP	CA-CB-CG	-7.35	105.25	112.60
1	G	819	ARG	CA-C-N	7.25	133.60	122.23
1	G	819	ARG	C-N-CA	7.25	133.60	122.23
1	F	822	ARG	CG-CD-NE	-7.06	96.48	112.00
1	G	820	ASP	CB-CG-OD1	-7.03	102.24	118.40
1	G	820	ASP	CB-CA-C	-6.78	97.99	109.38
1	F	822	ARG	N-CA-CB	-6.50	99.51	110.49
1	G	821	LEU	N-CA-C	-6.46	97.29	108.52
1	F	905	ARG	CA-C-N	-6.12	110.68	122.06
1	F	905	ARG	C-N-CA	-6.12	110.68	122.06
1	G	820	ASP	N-CA-C	5.99	122.44	114.12
1	G	819	ARG	O-C-N	5.85	130.37	122.59
1	G	821	LEU	CA-CB-CG	-5.58	96.76	116.30
1	G	821	LEU	CB-CA-C	5.55	120.71	111.83
1	A	458	TRP	CA-CB-CG	-5.27	103.59	113.60
1	E	626	TYR	CA-CB-CG	5.23	123.32	113.90
1	F	591	PRO	O-C-N	5.15	123.68	121.31
1	F	912	LYS	CD-CE-NZ	-5.15	95.43	111.90
1	B	663	SER	CA-C-N	5.14	128.38	120.82
1	B	663	SER	C-N-CA	5.14	128.38	120.82
1	G	905	ARG	CA-C-N	-5.04	111.75	121.58
1	G	905	ARG	C-N-CA	-5.04	111.75	121.58

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	981	SER	Peptide
1	E	338	GLU	Peptide
1	F	826	GLU	Peptide
1	F	981	SER	Peptide
1	G	569	GLN	Peptide
1	G	981	SER	Peptide
1	H	1089	GLN	Peptide
1	H	443	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6254	0	6171	129	0
1	B	6254	0	6171	138	0
1	C	6246	0	6162	155	0
1	D	6254	0	6171	217	1
1	E	6254	0	6171	204	1
1	F	6254	0	6171	276	1
1	G	6254	0	6171	250	1
1	H	6254	0	6171	308	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	1	0
2	E	9	0	0	0	0
2	F	9	0	0	1	0
2	G	9	0	0	2	0
2	H	9	0	0	0	0
3	A	87	0	0	5	0
3	B	71	0	0	3	0
3	C	65	0	0	4	0
3	D	31	0	0	5	0
3	E	29	0	0	1	0
3	F	24	0	0	1	0
3	G	20	0	0	0	0
3	H	11	0	0	1	0
All	All	50434	0	49359	1668	2

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 17.

All (1668) 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:E:979:THR:HG21	1:E:1035:MET:CE	1.53	1.35
1:E:979:THR:CG2	1:E:1035:MET:HE3	1.81	1.11
1:F:803:ARG:NH1	1:F:808:ASP:OD1	1.85	1.08
1:B:435:ARG:NH2	1:B:438:ASP:HB2	1.69	1.07
1:D:343:ARG:NE	1:D:647:GLU:OE2	1.89	1.05
1:E:979:THR:CG2	1:E:1035:MET:CE	2.35	1.04
1:F:908:VAL:O	1:F:912:LYS:HE3	1.57	1.04
1:H:791:TRP:HE1	1:H:961:THR:HG21	1.23	1.01
1:G:728:GLU:HG3	1:G:1056:ARG:HH21	1.24	1.01
1:E:979:THR:HG21	1:E:1035:MET:HE3	0.98	0.97
1:C:483:THR:HB	1:C:804:MET:HE1	1.44	0.97
1:E:1075:GLN:HE22	1:E:1103:GLY:H	1.06	0.97
1:F:1075:GLN:HE22	1:F:1103:GLY:HA2	1.29	0.96
1:G:821:LEU:HB3	1:G:827:PHE:HB2	1.44	0.95
1:G:1056:ARG:O	1:G:1060:ILE:HD12	1.65	0.95
1:D:935:ARG:O	1:D:939:ASN:HB2	1.68	0.93
1:D:343:ARG:NH2	1:D:647:GLU:OE1	2.06	0.89
1:F:906:LYS:HB2	1:F:949:TYR:OH	1.72	0.89
1:H:999:ARG:NH1	1:H:1003:MET:O	2.05	0.88
1:D:341:THR:O	1:D:345:GLN:OE1	1.92	0.88
1:F:1073:GLN:HE22	1:F:1075:GLN:HG3	1.39	0.87
1:F:915:THR:HG22	1:F:917:GLU:H	1.38	0.87
1:C:910:GLU:OE1	1:C:949:TYR:OH	1.92	0.86
1:F:1082:GLU:CD	1:F:1085:LYS:HE3	2.00	0.85
1:H:713:SER:HA	1:H:740:PHE:HE1	1.39	0.84
1:E:906:LYS:HA	1:E:910:GLU:HB2	1.59	0.84
1:E:771:CYS:HB3	1:E:1103:GLY:HA3	1.59	0.84
1:B:435:ARG:HH22	1:B:438:ASP:HB2	1.42	0.84
1:H:587:VAL:HB	1:H:601:SER:HB2	1.59	0.84
1:F:739:GLY:HA3	1:F:1100:ARG:HG2	1.60	0.84
1:D:1063:LEU:HD23	1:D:1074:MET:HE3	1.60	0.84
1:F:993:ASN:OD1	1:F:994:ALA:N	2.10	0.83
1:G:352:LEU:HD23	1:G:1095:ARG:HH21	1.42	0.83
1:G:429:LEU:HD21	1:G:450:ILE:HD11	1.58	0.83
1:F:938:LEU:HD21	1:F:998:GLY:HA3	1.61	0.83
1:C:850:GLN:HB3	1:C:971:LEU:HD22	1.57	0.82
1:F:847:VAL:HG23	1:F:970:MET:HE1	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:999:ARG:NH1	1:E:1003:MET:O	2.13	0.82
1:H:934:ARG:O	1:H:938:LEU:HD12	1.80	0.81
1:E:979:THR:HG21	1:E:1035:MET:HE2	1.61	0.81
1:D:393:ALA:O	1:D:556:ARG:NH2	2.13	0.80
1:H:1052:THR:HG22	1:H:1054:GLU:H	1.46	0.80
1:E:1009:ILE:HG21	1:E:1035:MET:HE1	1.62	0.80
1:G:546:THR:HG21	1:G:860:PRO:HB2	1.63	0.80
1:G:350:HIS:O	1:G:353:THR:OG1	2.00	0.79
1:E:1020:PRO:HA	1:E:1023:ILE:HD12	1.64	0.79
1:B:592:PRO:HG2	1:B:630:MET:HE2	1.64	0.79
1:G:702:ASP:OD1	1:G:705:ARG:NH2	2.15	0.79
1:G:995:THR:HG23	1:G:999:ARG:HH21	1.47	0.79
1:B:435:ARG:NH2	1:B:437:GLN:O	2.16	0.79
1:F:789:THR:HG22	1:F:790:GLN:H	1.46	0.79
1:G:775:GLN:HG3	1:G:780:ILE:HG21	1.64	0.79
1:G:587:VAL:HB	1:G:601:SER:HB2	1.63	0.79
1:G:906:LYS:HB3	1:G:949:TYR:OH	1.82	0.79
1:E:857:ALA:O	1:E:859:LYS:NZ	2.12	0.79
1:G:850:GLN:HB3	1:G:971:LEU:HD22	1.65	0.79
1:F:847:VAL:HG23	1:F:970:MET:CE	2.13	0.78
1:D:813:LEU:O	1:D:834:GLN:NE2	2.16	0.78
1:H:403:ILE:HA	1:H:600:GLN:HE22	1.49	0.78
1:F:906:LYS:HG3	1:F:910:GLU:HB3	1.64	0.78
1:H:801:ARG:HG2	1:H:801:ARG:HH11	1.48	0.78
1:F:979:THR:HG21	1:F:1035:MET:HE2	1.64	0.78
1:F:1052:THR:HG23	1:F:1055:GLY:H	1.49	0.78
1:D:640:LEU:HD22	1:D:644:THR:HB	1.65	0.77
1:E:1009:ILE:CG2	1:E:1035:MET:HE1	2.14	0.77
1:E:979:THR:CG2	1:E:1035:MET:HE2	2.13	0.77
1:H:396:LEU:HD21	1:H:398:GLN:HG2	1.66	0.77
1:C:823:THR:HG1	1:C:826:GLU:H	1.30	0.77
1:A:962:GLU:HB2	1:A:977:HIS:CE1	2.19	0.77
1:A:491:HIS:HB2	1:A:786:THR:HG23	1.67	0.76
1:B:424:TRP:O	1:B:428:GLU:HB2	1.85	0.76
1:H:771:CYS:HB3	1:H:1103:GLY:HA3	1.68	0.76
1:D:1020:PRO:HB2	1:D:1062:LEU:HD21	1.68	0.76
1:H:337:MET:HB3	1:H:340:LEU:HD12	1.67	0.76
1:E:818:LEU:HA	1:E:821:LEU:HD23	1.67	0.75
1:E:640:LEU:HD22	1:E:644:THR:HB	1.67	0.75
1:H:512:MET:HE1	1:H:605:VAL:HG11	1.69	0.75
1:H:1112:CYS:O	1:H:1116:GLN:NE2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:771:CYS:HB3	1:G:1103:GLY:HA3	1.68	0.75
1:B:395:ILE:HG23	1:B:557:ILE:HD13	1.67	0.74
1:H:951:ASP:HB3	1:H:1029:LYS:HG3	1.68	0.74
1:E:653:ILE:HG23	1:E:712:PRO:HD2	1.66	0.74
1:H:785:SER:HB3	1:H:890:ILE:HD12	1.69	0.74
1:G:859:LYS:O	1:G:863:SER:OG	2.05	0.74
1:A:962:GLU:OE1	1:A:977:HIS:ND1	2.20	0.74
1:B:1075:GLN:HE22	1:B:1103:GLY:HA2	1.53	0.74
1:A:618:LEU:HD11	1:A:862:MET:HE1	1.68	0.73
1:G:980:LEU:HD12	1:G:980:LEU:O	1.88	0.73
1:E:813:LEU:HD11	1:E:837:HIS:HB2	1.68	0.73
1:C:653:ILE:HG23	1:C:712:PRO:HD2	1.70	0.73
1:C:948:ASN:HA	1:C:951:ASP:HB2	1.71	0.73
1:G:376:MET:HB3	1:G:381:LEU:HD13	1.69	0.73
1:G:966:ARG:HH11	1:G:974:THR:HG23	1.52	0.73
1:H:546:THR:HG23	1:H:864:LEU:HD11	1.71	0.73
1:F:480:SER:HB3	1:F:486:SER:O	1.87	0.73
1:F:813:LEU:HD11	1:F:837:HIS:HB2	1.70	0.73
1:F:505:VAL:HG12	1:F:506:LEU:HD12	1.71	0.73
1:F:857:ALA:O	1:F:859:LYS:NZ	2.22	0.73
1:H:352:LEU:HD21	1:H:1095:ARG:HG3	1.69	0.73
1:G:337:MET:HG3	1:G:340:LEU:HD12	1.70	0.73
1:G:550:VAL:HG23	1:G:608:LEU:HD12	1.71	0.73
1:D:773:GLU:OE2	1:D:980:LEU:HD22	1.89	0.72
1:C:592:PRO:HG2	1:C:630:MET:HE2	1.71	0.72
1:H:1081:ASN:HA	1:H:1084:LEU:HD12	1.71	0.72
1:C:428:GLU:HG2	3:C:1311:HOH:O	1.89	0.72
1:F:948:ASN:HB3	1:F:952:GLN:HE22	1.54	0.72
1:H:738:MET:HB2	1:H:740:PHE:HD2	1.53	0.72
1:A:1075:GLN:HE22	1:A:1103:GLY:H	1.34	0.72
1:D:739:GLY:HA3	1:D:1100:ARG:HB2	1.71	0.72
1:D:776:LYS:HD2	1:D:779:ARG:HD2	1.71	0.72
1:G:1108:PHE:CZ	1:G:1116:GLN:HB2	2.24	0.72
1:B:823:THR:HG22	1:B:825:ASP:H	1.55	0.72
1:G:900:SER:HB2	1:G:996:PRO:HG2	1.72	0.71
1:H:713:SER:OG	1:H:1100:ARG:NH1	2.22	0.71
1:G:631:PHE:HE2	1:G:645:ALA:CB	2.03	0.71
1:B:999:ARG:NH1	1:B:1003:MET:O	2.23	0.71
1:A:703:ALA:O	1:A:707:VAL:HG23	1.90	0.71
1:F:813:LEU:O	1:F:834:GLN:NE2	2.20	0.71
1:G:1099:VAL:HG11	1:G:1108:PHE:HD1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:823:THR:OG1	1:C:826:GLU:N	2.15	0.71
1:E:882:MET:HG2	1:E:883:VAL:HG23	1.72	0.71
1:H:1101:VAL:HG13	1:H:1119:ILE:HD11	1.71	0.71
1:A:660:MET:HE1	1:A:674:TYR:HB3	1.72	0.71
1:F:704:VAL:HG21	1:F:714:LEU:HD22	1.70	0.71
1:H:1075:GLN:HE22	1:H:1103:GLY:H	1.39	0.71
1:C:970:MET:HE3	1:C:975:LEU:HB2	1.73	0.70
1:F:943:TYR:CE1	1:F:1026:SER:HB3	2.26	0.70
1:B:435:ARG:NH2	1:B:438:ASP:CB	2.53	0.70
1:D:749:HIS:HA	1:D:752:MET:HG2	1.74	0.70
1:G:516:LYS:HB3	1:G:547:CYS:SG	2.32	0.70
1:G:1035:MET:HE3	1:G:1039:MET:HE2	1.74	0.70
1:G:1101:VAL:HG13	1:G:1119:ILE:HD11	1.74	0.70
1:H:801:ARG:NH1	1:H:814:ASP:OD1	2.25	0.70
1:C:343:ARG:HG3	1:C:400:ASP:HB3	1.74	0.70
1:D:793:ILE:HD11	1:D:804:MET:HG3	1.73	0.70
1:G:604:THR:O	1:G:607:SER:OG	2.10	0.70
1:G:634:ASP:HB3	1:G:640:LEU:HD13	1.73	0.70
1:F:382:ARG:NH2	1:F:613:GLU:OE1	2.25	0.70
1:C:703:ALA:O	1:C:707:VAL:HG23	1.92	0.69
1:A:343:ARG:NH2	1:A:576:GLU:OE2	2.25	0.69
1:G:569:GLN:HA	1:G:574:ARG:NH1	2.07	0.69
1:D:428:GLU:HB3	1:D:432:MET:HG3	1.73	0.69
1:G:599:LEU:HD23	1:G:652:PHE:HB2	1.74	0.69
1:G:730:ILE:O	1:G:734:VAL:HG23	1.91	0.69
1:G:771:CYS:SG	2:G:1201:A1H9K:O1	2.50	0.69
1:C:937:CYS:O	1:C:942:LYS:NZ	2.26	0.69
1:B:448:LYS:HG3	1:B:452:GLU:OE1	1.92	0.68
1:C:488:LEU:HD23	1:C:787:GLY:HA3	1.74	0.68
1:E:935:ARG:HA	1:E:938:LEU:HB2	1.75	0.68
1:B:772:VAL:N	1:B:773:GLU:OE2	2.16	0.68
1:F:805:VAL:HG21	1:F:993:ASN:HD22	1.57	0.68
1:H:594:THR:HG23	1:H:597:GLU:H	1.59	0.68
1:G:937:CYS:O	1:G:942:LYS:NZ	2.24	0.68
1:H:416:PHE:HE1	1:H:425:VAL:HG21	1.59	0.68
1:H:429:LEU:HD11	1:H:450:ILE:HD11	1.76	0.68
1:C:920:ARG:O	1:C:924:LEU:HD23	1.93	0.68
1:D:731:VAL:HG22	1:D:1059:LEU:HD23	1.74	0.68
1:D:980:LEU:O	1:D:980:LEU:HD12	1.94	0.68
1:D:681:THR:HG21	1:D:768:LEU:H	1.59	0.68
1:D:985:ASN:ND2	3:D:1303:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:913:LYS:HD2	1:H:914:TYR:CZ	2.28	0.68
1:E:1047:LYS:HD2	1:E:1080:ASP:HB2	1.76	0.68
1:G:731:VAL:HG21	1:G:1060:ILE:HD11	1.75	0.67
1:E:739:GLY:HA3	1:E:1100:ARG:HG3	1.77	0.67
1:D:446:ASP:OD2	3:D:1301:HOH:O	2.12	0.67
1:D:850:GLN:HB3	1:D:971:LEU:HD22	1.76	0.67
1:C:361:TYR:CE1	1:C:394:PRO:HG3	2.29	0.67
1:G:771:CYS:N	2:G:1201:A1H9K:O1	2.26	0.67
1:C:873:GLY:O	1:C:874:LYS:HE2	1.94	0.67
1:G:703:ALA:O	1:G:707:VAL:HG23	1.95	0.67
1:G:1085:LYS:HA	1:G:1088:GLN:HG3	1.76	0.67
1:H:400:ASP:H	1:H:573:ARG:HH12	1.43	0.67
1:C:908:VAL:HG11	1:C:916:LEU:HD23	1.75	0.67
1:F:1075:GLN:HE22	1:F:1103:GLY:CA	2.07	0.67
1:G:442:ILE:HG23	1:G:447:LYS:NZ	2.10	0.67
1:F:488:LEU:HD13	1:F:845:GLY:HA3	1.77	0.67
1:F:911:GLU:HG3	1:F:913:LYS:NZ	2.10	0.67
1:A:382:ARG:NH2	1:A:613:GLU:OE1	2.27	0.66
1:C:341:THR:O	1:C:345:GLN:HG3	1.95	0.66
1:F:467:CYS:HB3	1:F:492:GLN:HG3	1.78	0.66
1:D:428:GLU:OE2	1:D:435:ARG:NH1	2.26	0.66
1:H:396:LEU:HD23	1:H:396:LEU:O	1.96	0.66
1:H:396:LEU:CD2	1:H:398:GLN:HG2	2.26	0.66
1:D:355:ARG:HH11	1:H:1052:THR:HG21	1.60	0.66
1:E:745:PHE:HD2	1:E:1067:SER:HB2	1.60	0.66
1:A:349:ASN:O	1:A:353:THR:HG23	1.95	0.66
1:F:783:TRP:HH2	1:F:853:HIS:CD2	2.13	0.66
1:H:1050:LEU:HD21	1:H:1059:LEU:HD22	1.78	0.66
1:D:355:ARG:NH1	1:H:1052:THR:HG21	2.11	0.65
1:E:395:ILE:HG23	1:E:557:ILE:HD13	1.78	0.65
1:F:915:THR:HG22	1:F:917:GLU:N	2.08	0.65
1:F:739:GLY:HA3	1:F:1100:ARG:CG	2.26	0.65
1:D:641:THR:N	1:D:644:THR:OG1	2.29	0.65
1:E:803:ARG:HB2	1:E:810:TYR:CZ	2.31	0.65
1:G:499:THR:HA	1:G:775:GLN:HE22	1.62	0.65
1:D:1075:GLN:HE22	1:D:1103:GLY:H	1.45	0.65
1:E:980:LEU:HD12	1:E:982:ILE:HG13	1.78	0.65
1:F:848:ILE:O	1:F:852:VAL:HG23	1.97	0.65
1:F:744:HIS:HE2	1:F:772:VAL:HG12	1.62	0.65
1:B:462:SER:O	1:B:466:ILE:HG13	1.97	0.65
1:G:1064:ARG:O	1:G:1068:ILE:HG12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:674:TYR:HE2	1:E:1110:GLU:HG2	1.62	0.65
1:F:882:MET:HG2	1:F:883:VAL:HG23	1.79	0.65
1:H:366:PHE:O	1:H:370:VAL:HG22	1.97	0.64
1:H:857:ALA:O	1:H:859:LYS:NZ	2.29	0.64
1:D:926:ASN:HD21	1:D:1000:LEU:HB3	1.61	0.64
1:D:1115:VAL:O	1:D:1119:ILE:HG13	1.98	0.64
1:G:395:ILE:HG23	1:G:557:ILE:HD13	1.80	0.64
1:G:1003:MET:HE3	1:G:1004:PRO:HD2	1.80	0.64
1:H:358:VAL:HG21	1:H:432:MET:HE1	1.78	0.64
1:H:784:THR:HG22	1:H:890:ILE:HD11	1.78	0.64
1:H:1014:GLY:H	1:H:1123:THR:HG23	1.62	0.64
1:D:640:LEU:HB3	1:D:644:THR:OG1	1.98	0.64
1:H:634:ASP:OD1	1:H:639:ARG:NE	2.30	0.64
1:C:348:ARG:HH21	1:C:708:LYS:HB2	1.63	0.64
1:G:917:GLU:HB3	1:G:920:ARG:HH12	1.61	0.64
1:E:629:PRO:HB2	1:E:630:MET:HE3	1.79	0.64
1:H:437:GLN:NE2	1:H:1111:LEU:HA	2.12	0.64
1:D:599:LEU:HD22	1:D:652:PHE:CD1	2.32	0.64
1:F:1116:GLN:O	1:F:1120:ILE:HG13	1.98	0.64
1:G:993:ASN:O	1:G:999:ARG:NH2	2.30	0.64
1:G:450:ILE:HG22	1:G:454:ILE:HG13	1.80	0.64
1:H:350:HIS:NE2	1:H:398:GLN:OE1	2.31	0.64
1:H:801:ARG:NH1	1:H:816:GLY:C	2.56	0.64
1:B:435:ARG:HH21	1:B:438:ASP:HB2	1.58	0.64
1:B:507:LEU:HD13	1:B:512:MET:HE2	1.80	0.64
1:D:914:TYR:CD1	1:D:933:LEU:HD12	2.33	0.64
1:B:432:MET:HE3	1:B:440:PHE:HB2	1.80	0.64
1:F:905:ARG:HD2	1:F:953:TYR:OH	1.97	0.64
1:H:416:PHE:CE1	1:H:425:VAL:HG21	2.32	0.64
1:H:450:ILE:HA	1:H:454:ILE:HB	1.80	0.64
1:A:682:VAL:HB	1:A:697:THR:HG23	1.78	0.64
1:D:893:GLY:HA3	1:D:1005:LEU:HD23	1.78	0.64
1:E:942:LYS:O	1:E:945:ASN:ND2	2.31	0.64
1:E:995:THR:OG1	1:E:997:ASN:OD1	2.16	0.64
1:H:403:ILE:HG22	1:H:655:LYS:HD2	1.79	0.63
1:F:489:SER:O	1:F:493:ILE:HG12	1.98	0.63
1:F:744:HIS:HE2	1:F:772:VAL:CG1	2.11	0.63
1:F:960:TRP:CH2	1:F:964:GLU:HG3	2.33	0.63
1:G:354:VAL:HG11	1:G:411:PRO:HB2	1.79	0.63
1:H:596:GLN:HB3	1:H:648:LEU:HD21	1.79	0.63
1:E:487:ASP:O	1:E:787:GLY:HA2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:HG23	1:A:506:LEU:HG	1.81	0.63
1:F:837:HIS:CE1	1:F:841:LEU:HD21	2.34	0.63
1:H:962:GLU:HB2	1:H:977:HIS:CE1	2.33	0.63
1:B:528:MET:HE2	1:B:537:ILE:HG21	1.80	0.63
1:G:651:ALA:O	1:G:654:ILE:HG22	1.98	0.63
1:G:906:LYS:HE2	1:G:941:PRO:HD3	1.80	0.63
1:B:599:LEU:HD12	1:B:648:LEU:HD23	1.80	0.63
1:E:700:ILE:O	1:E:704:VAL:HG23	1.98	0.63
1:E:904:ILE:O	1:E:908:VAL:HG22	1.98	0.63
1:H:698:TYR:HD2	1:H:729:LYS:HE3	1.64	0.63
1:E:1099:VAL:HG11	1:E:1108:PHE:HD1	1.64	0.63
1:D:730:ILE:O	1:D:734:VAL:HG23	1.99	0.62
1:F:730:ILE:O	1:F:734:VAL:HG23	1.99	0.62
1:E:806:LEU:HD22	1:E:991:LEU:HA	1.80	0.62
1:H:775:GLN:HB3	1:H:780:ILE:HG21	1.82	0.62
1:C:382:ARG:NH2	1:C:613:GLU:OE1	2.33	0.62
1:F:789:THR:HG21	1:F:838:ILE:CG2	2.29	0.62
1:F:1058:GLY:HA3	1:F:1128:PHE:CD1	2.34	0.62
1:F:852:VAL:O	1:F:856:VAL:HG22	1.99	0.62
1:A:423:ARG:HH21	1:A:464:ASP:CG	2.07	0.62
1:D:775:GLN:HB3	1:D:780:ILE:HG21	1.82	0.62
1:H:790:GLN:HG3	1:H:792:PRO:HD2	1.79	0.62
1:H:831:VAL:HG21	1:H:901:MET:HE1	1.82	0.62
1:H:1000:LEU:HB2	1:H:1003:MET:HE2	1.81	0.62
1:D:940:ALA:O	1:D:942:LYS:NZ	2.32	0.62
1:D:980:LEU:HA	1:D:1040:VAL:HG12	1.82	0.62
1:H:411:PRO:HB3	1:H:658:GLU:HG2	1.81	0.62
1:H:573:ARG:HE	1:H:577:LEU:CD2	2.13	0.62
1:D:685:GLN:HG3	1:D:746:ASP:OD2	2.00	0.61
1:D:758:PHE:HZ	1:D:780:ILE:HB	1.63	0.61
1:F:744:HIS:HE1	1:F:772:VAL:HB	1.66	0.61
1:A:653:ILE:HG23	1:A:712:PRO:HD2	1.82	0.61
1:E:411:PRO:HB3	1:E:658:GLU:HG2	1.83	0.61
1:F:837:HIS:O	1:F:841:LEU:HD23	2.00	0.61
1:F:587:VAL:HB	1:F:601:SER:HB2	1.81	0.61
1:F:618:LEU:HD11	1:F:862:MET:HE1	1.82	0.61
1:F:970:MET:HE2	1:F:970:MET:HA	1.81	0.61
1:G:863:SER:OG	1:G:875:ASP:HB2	2.00	0.61
1:E:775:GLN:HB3	1:E:780:ILE:HG21	1.82	0.61
1:F:899:ASP:HB3	1:F:942:LYS:HE3	1.81	0.61
1:A:435:ARG:NH2	1:A:438:ASP:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:GLU:OE2	1:B:665:GLU:HB2	2.01	0.61
1:D:943:TYR:OH	1:D:1027:VAL:HG22	2.01	0.61
1:F:488:LEU:HD23	1:F:787:GLY:HA3	1.83	0.61
1:A:1042:ASN:O	3:A:1301:HOH:O	2.16	0.61
1:E:1101:VAL:HG22	1:E:1119:ILE:HD11	1.82	0.61
1:F:487:ASP:O	1:F:787:GLY:HA2	2.01	0.61
1:A:999:ARG:NH1	1:A:1003:MET:O	2.34	0.61
1:E:738:MET:HG2	1:E:1098:ILE:HB	1.82	0.61
1:E:941:PRO:HB2	1:E:950:VAL:HB	1.82	0.61
1:E:1013:GLN:HG2	1:E:1121:SER:OG	2.01	0.61
1:F:1114:GLU:OE1	1:F:1114:GLU:N	2.34	0.61
1:E:467:CYS:HB2	1:E:852:VAL:HG21	1.83	0.61
1:G:595:LEU:HD13	1:G:631:PHE:HB2	1.82	0.61
1:G:895:ALA:HB3	1:G:1006:SER:HB2	1.83	0.61
1:C:423:ARG:HD2	1:C:465:GLU:HG3	1.83	0.60
1:F:943:TYR:HE1	1:F:1026:SER:HB3	1.66	0.60
1:H:791:TRP:NE1	1:H:961:THR:HG21	2.05	0.60
1:D:599:LEU:HD22	1:D:652:PHE:CG	2.36	0.60
1:F:406:HIS:CE1	1:F:408:CYS:HB2	2.36	0.60
1:G:806:LEU:HD23	1:G:991:LEU:HD23	1.82	0.60
1:H:528:MET:HG3	1:H:534:ILE:HG12	1.83	0.60
1:E:908:VAL:HG23	1:E:909:PHE:CD2	2.37	0.60
1:F:847:VAL:CG2	1:F:970:MET:CE	2.80	0.60
1:B:579:THR:O	1:B:582:GLU:HG2	2.01	0.60
1:E:674:TYR:CE2	1:E:1110:GLU:HG2	2.36	0.60
1:C:823:THR:HG1	1:C:826:GLU:N	1.97	0.60
1:E:620:LEU:HD12	1:E:680:LEU:HD12	1.84	0.60
1:E:970:MET:HE3	1:E:975:LEU:HB2	1.83	0.60
1:G:343:ARG:HG3	1:G:400:ASP:HB3	1.83	0.60
1:C:964:GLU:HA	1:C:967:LYS:HD2	1.84	0.60
1:A:444:GLU:OE2	1:C:342:PRO:HB3	2.02	0.60
1:F:927:PHE:CD2	1:F:934:ARG:HB2	2.37	0.60
1:H:422:TRP:CE3	1:H:423:ARG:HA	2.36	0.60
1:D:790:GLN:HB2	1:D:792:PRO:HD2	1.84	0.60
1:E:749:HIS:NE2	3:E:1301:HOH:O	2.32	0.60
1:F:955:LEU:HD13	1:F:1030:MET:HA	1.84	0.60
1:D:1073:GLN:HE22	1:D:1075:GLN:NE2	2.00	0.60
1:H:341:THR:HG22	1:H:343:ARG:H	1.67	0.60
1:H:364:LEU:HD23	1:H:454:ILE:HD11	1.84	0.60
1:H:396:LEU:HD13	1:H:409:GLY:O	2.01	0.60
1:E:428:GLU:O	1:E:432:MET:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:MET:HE1	1:E:442:ILE:HB	1.84	0.60
1:F:944:GLY:HA3	1:F:1011:PRO:HG3	1.84	0.60
1:B:1095:ARG:HA	1:B:1109:VAL:HG21	1.84	0.59
1:A:341:THR:HG22	1:A:343:ARG:H	1.66	0.59
1:H:407:PRO:HD3	1:H:607:SER:HB2	1.83	0.59
1:F:756:LYS:NZ	1:F:782:GLN:OE1	2.33	0.59
1:G:340:LEU:HB2	1:G:345:GLN:HE22	1.67	0.59
1:A:795:ILE:HG12	1:A:901:MET:HE3	1.83	0.59
1:F:744:HIS:CE1	1:F:772:VAL:HB	2.38	0.59
1:F:999:ARG:NH1	1:F:1003:MET:O	2.35	0.59
1:D:487:ASP:O	1:D:787:GLY:HA2	2.02	0.59
1:F:536:ARG:HG3	1:F:873:GLY:HA3	1.85	0.59
1:G:1060:ILE:O	1:G:1064:ARG:HG3	2.02	0.59
1:B:744:HIS:CE1	1:B:1073:GLN:HG3	2.37	0.59
1:C:496:GLY:HA3	1:C:859:LYS:HE3	1.83	0.59
1:G:595:LEU:HG	1:G:599:LEU:HD13	1.84	0.59
1:H:478:ALA:HA	1:H:482:GLU:HB3	1.84	0.59
1:F:622:ARG:NH2	1:F:685:GLN:O	2.27	0.59
1:H:424:TRP:O	1:H:428:GLU:HG3	2.02	0.59
1:H:570:ASN:O	1:H:573:ARG:N	2.36	0.59
1:C:1075:GLN:HE22	1:C:1103:GLY:HA2	1.67	0.59
1:D:1075:GLN:HE22	1:D:1103:GLY:N	2.00	0.59
1:E:419:ASP:HB3	1:E:458:TRP:CH2	2.38	0.59
1:F:429:LEU:HD13	1:F:447:LYS:HB2	1.84	0.59
1:H:390:CYS:HB3	1:H:553:TYR:HB2	1.85	0.59
1:D:337:MET:HE2	1:D:340:LEU:HD13	1.85	0.59
1:E:696:LEU:O	1:E:700:ILE:HG12	2.03	0.59
1:H:416:PHE:HE2	1:H:454:ILE:HG21	1.68	0.59
1:D:479:PHE:HZ	1:D:838:ILE:HD13	1.67	0.58
1:G:407:PRO:HG3	1:G:608:LEU:HD23	1.85	0.58
1:H:570:ASN:O	1:H:572:GLN:N	2.36	0.58
1:H:573:ARG:HH21	1:H:577:LEU:HD21	1.67	0.58
1:D:1095:ARG:HA	1:D:1109:VAL:HG21	1.86	0.58
1:E:713:SER:HB3	1:E:1100:ARG:NH2	2.18	0.58
1:E:1075:GLN:HE22	1:E:1103:GLY:N	1.90	0.58
1:A:432:MET:HE3	1:A:440:PHE:HB2	1.84	0.58
1:G:687:ARG:HD2	1:G:765:ASP:OD2	2.04	0.58
1:E:792:PRO:HG2	1:E:1005:LEU:HD13	1.83	0.58
1:E:913:LYS:HE2	1:E:914:TYR:OH	2.03	0.58
1:F:748:SER:OG	1:F:1071:ASN:O	2.17	0.58
1:H:416:PHE:CE1	1:H:425:VAL:HG11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1084:LEU:HD21	1:C:1099:VAL:HG21	1.85	0.58
1:E:817:ASP:OD1	1:E:819:ARG:HG2	2.03	0.58
1:F:742:ALA:HB2	1:F:1100:ARG:NH2	2.19	0.58
1:H:400:ASP:HA	1:H:573:ARG:HH12	1.69	0.58
1:A:337:MET:O	1:A:345:GLN:NE2	2.37	0.58
1:A:966:ARG:HH11	1:A:974:THR:CG2	2.16	0.58
1:D:337:MET:HG3	1:D:340:LEU:HD22	1.85	0.58
1:E:634:ASP:OD1	1:E:639:ARG:HD2	2.04	0.58
1:A:592:PRO:HG2	1:A:630:MET:HE2	1.85	0.58
1:C:795:ILE:HG12	1:C:901:MET:HE3	1.85	0.58
1:D:1039:MET:HE1	1:D:1072:GLY:HA3	1.84	0.58
1:E:703:ALA:O	1:E:707:VAL:HG22	2.04	0.58
1:E:730:ILE:O	1:E:734:VAL:HG23	2.04	0.58
1:F:1055:GLY:HA2	1:F:1128:PHE:HE1	1.68	0.58
1:B:966:ARG:HH11	1:B:974:THR:HG23	1.68	0.58
1:C:966:ARG:HH11	1:C:974:THR:HG23	1.68	0.58
1:F:432:MET:HA	1:F:435:ARG:HG3	1.84	0.58
1:F:657:ALA:HA	1:F:711:GLN:HB2	1.86	0.58
1:H:739:GLY:HA3	1:H:1100:ARG:HB2	1.85	0.58
1:H:640:LEU:HB2	1:H:644:THR:OG1	2.04	0.58
1:D:728:GLU:OE2	1:D:1056:ARG:NH2	2.35	0.57
1:H:555:ARG:HG3	1:H:585:GLU:HG3	1.86	0.57
1:B:704:VAL:HG21	1:B:714:LEU:HD22	1.86	0.57
1:D:640:LEU:HD11	1:D:648:LEU:HD22	1.85	0.57
1:F:1108:PHE:CZ	1:F:1116:GLN:HG2	2.39	0.57
1:H:432:MET:CE	1:H:440:PHE:HB2	2.34	0.57
1:H:553:TYR:O	1:H:557:ILE:HG12	2.04	0.57
1:H:633:ALA:O	1:H:637:GLU:HG3	2.04	0.57
1:D:803:ARG:NH1	1:D:808:ASP:OD1	2.37	0.57
1:H:705:ARG:HD3	1:H:733:VAL:HG22	1.86	0.57
1:B:898:VAL:HG13	1:B:953:TYR:HB2	1.86	0.57
1:D:905:ARG:HD2	1:D:953:TYR:OH	2.04	0.57
1:H:713:SER:HA	1:H:740:PHE:CE1	2.28	0.57
1:G:342:PRO:O	1:G:346:ARG:HG2	2.05	0.57
1:G:895:ALA:HA	1:G:898:VAL:HG22	1.85	0.57
1:F:835:ILE:HA	1:F:838:ILE:HD12	1.85	0.57
1:D:419:ASP:OD1	1:D:419:ASP:N	2.38	0.57
1:F:938:LEU:CD2	1:F:998:GLY:HA3	2.35	0.57
1:G:568:GLU:HG2	1:G:573:ARG:HD3	1.87	0.57
1:A:973:SER:OG	1:A:974:THR:N	2.37	0.57
1:C:1092:GLU:HG2	1:C:1093:LYS:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:745:PHE:CD2	1:E:1067:SER:HB2	2.40	0.57
1:F:822:ARG:O	1:F:909:PHE:HE1	1.88	0.57
1:H:962:GLU:OE1	1:H:977:HIS:ND1	2.30	0.57
1:A:813:LEU:HD11	1:A:837:HIS:HB2	1.86	0.57
1:B:966:ARG:HH11	1:B:974:THR:CG2	2.18	0.57
1:D:743:CYS:O	1:D:1073:GLN:HA	2.05	0.57
1:F:343:ARG:NH2	1:F:576:GLU:OE2	2.31	0.57
1:F:685:GLN:HG3	1:F:746:ASP:OD2	2.05	0.57
1:F:783:TRP:CH2	1:F:853:HIS:CD2	2.93	0.57
1:G:348:ARG:O	1:G:352:LEU:HD12	2.05	0.57
1:B:731:VAL:HG22	1:B:1059:LEU:HD23	1.86	0.57
1:G:616:THR:HB	1:G:661:TRP:CG	2.40	0.57
1:H:871:GLU:OE1	1:H:871:GLU:N	2.35	0.57
1:D:650:GLN:HB3	1:D:707:VAL:HG21	1.87	0.56
1:D:1010:SER:HA	1:D:1041:HIS:CE1	2.39	0.56
1:H:367:THR:O	1:H:371:LYS:HB3	2.05	0.56
1:A:744:HIS:CE1	1:A:1073:GLN:HG3	2.41	0.56
1:B:507:LEU:CD1	1:B:512:MET:HE2	2.35	0.56
1:B:530:ASN:HB3	1:B:532:GLU:OE1	2.05	0.56
1:B:1075:GLN:CD	1:B:1100:ARG:HE	2.12	0.56
1:H:403:ILE:HA	1:H:600:GLN:NE2	2.20	0.56
1:B:341:THR:HG21	1:B:647:GLU:CD	2.31	0.56
1:B:1100:ARG:NH2	3:B:1303:HOH:O	2.38	0.56
1:D:1080:ASP:O	1:D:1083:VAL:HG22	2.05	0.56
1:E:640:LEU:HD11	1:E:648:LEU:HD12	1.86	0.56
1:F:907:LEU:O	1:F:912:LYS:HA	2.04	0.56
1:F:931:GLU:O	1:F:935:ARG:HG3	2.06	0.56
1:G:599:LEU:HD21	1:G:649:LEU:HD23	1.87	0.56
1:H:400:ASP:CA	1:H:573:ARG:HH12	2.18	0.56
1:H:650:GLN:HB3	1:H:707:VAL:HG21	1.87	0.56
1:B:382:ARG:NH2	1:B:613:GLU:OE1	2.39	0.56
1:E:894:LEU:O	1:E:898:VAL:HG22	2.05	0.56
1:G:710:TYR:HD2	1:G:1106:ALA:HA	1.69	0.56
1:H:788:TYR:CE2	1:H:890:ILE:HD13	2.40	0.56
1:H:1020:PRO:HA	1:H:1023:ILE:HD12	1.88	0.56
1:A:775:GLN:HB3	1:A:780:ILE:HG21	1.88	0.56
1:D:608:LEU:O	1:D:611:ILE:N	2.36	0.56
1:G:902:ALA:HB2	1:G:950:VAL:HG23	1.88	0.56
1:H:934:ARG:HG2	1:H:938:LEU:CD1	2.35	0.56
1:D:905:ARG:HD3	1:D:949:TYR:OH	2.05	0.56
1:H:906:LYS:HE2	1:H:911:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1052:THR:HG22	1:H:1054:GLU:N	2.19	0.56
1:D:937:CYS:C	1:D:939:ASN:H	2.12	0.56
1:H:835:ILE:O	1:H:839:VAL:HG23	2.05	0.56
1:C:637:GLU:OE1	1:C:639:ARG:NH1	2.34	0.56
1:D:774:PRO:HD2	1:D:1037:ILE:O	2.06	0.56
1:D:1100:ARG:HG3	1:D:1101:VAL:N	2.21	0.56
1:E:993:ASN:ND2	1:E:994:ALA:H	2.03	0.56
1:E:756:LYS:NZ	1:E:782:GLN:OE1	2.37	0.56
1:F:914:TYR:OH	1:F:936:ASP:OD1	2.18	0.56
1:G:919:ILE:HD13	1:G:933:LEU:HD11	1.87	0.56
1:C:894:LEU:N	3:C:1302:HOH:O	2.23	0.56
1:C:959:GLU:OE2	1:C:1034:THR:HG21	2.06	0.56
1:F:465:GLU:O	1:F:468:GLU:HB3	2.06	0.56
1:G:631:PHE:HE2	1:G:645:ALA:HB1	1.71	0.56
1:G:744:HIS:HD2	1:G:749:HIS:HE1	1.55	0.56
1:A:428:GLU:HB3	1:A:432:MET:HG3	1.89	0.55
1:E:840:ARG:HG3	1:E:968:TYR:OH	2.05	0.55
1:F:448:LYS:HE2	1:F:452:GLU:CD	2.31	0.55
1:A:560:HIS:HA	1:A:563:GLU:HG2	1.89	0.55
1:B:927:PHE:CD1	1:B:934:ARG:HB2	2.41	0.55
1:E:637:GLU:OE1	1:E:639:ARG:NH2	2.38	0.55
1:F:346:ARG:NH1	1:F:400:ASP:OD1	2.38	0.55
1:F:382:ARG:HD3	1:F:858:PRO:HD2	1.87	0.55
1:F:1059:LEU:HD11	1:F:1076:PHE:CE2	2.41	0.55
1:G:896:THR:HA	1:G:997:ASN:ND2	2.21	0.55
1:H:360:ILE:HG22	1:H:364:LEU:HG	1.87	0.55
1:H:599:LEU:HB3	1:H:652:PHE:CD2	2.41	0.55
1:H:1112:CYS:O	1:H:1116:GLN:HG2	2.07	0.55
1:C:346:ARG:NH1	1:C:400:ASP:OD1	2.39	0.55
1:C:685:GLN:H	1:C:717:ARG:NH2	2.04	0.55
1:E:554:ALA:HB2	1:E:588:PRO:HD2	1.87	0.55
1:H:1089:GLN:HB2	1:H:1090:GLU:HG3	1.88	0.55
1:C:797:PHE:O	1:C:802:GLY:N	2.31	0.55
1:G:546:THR:OG1	1:G:864:LEU:HD11	2.06	0.55
1:G:897:TYR:CE1	1:G:901:MET:HE2	2.42	0.55
1:G:1074:MET:HE2	1:G:1076:PHE:HZ	1.70	0.55
1:H:400:ASP:N	1:H:573:ARG:HH12	2.04	0.55
1:A:1114:GLU:OE1	1:A:1114:GLU:N	2.40	0.55
1:E:945:ASN:OD1	1:E:1016:ASP:HA	2.07	0.55
1:G:1088:GLN:OE1	1:G:1116:GLN:HG3	2.06	0.55
1:H:400:ASP:H	1:H:573:ARG:NH1	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:850:GLN:CD	1:H:971:LEU:HB2	2.32	0.55
1:C:491:HIS:HB2	1:C:786:THR:HG23	1.89	0.55
1:E:905:ARG:HH11	1:E:949:TYR:HE2	1.55	0.55
1:F:776:LYS:HD2	1:F:779:ARG:HD2	1.87	0.55
1:H:1108:PHE:CZ	1:H:1116:GLN:HB2	2.42	0.55
1:C:355:ARG:HD2	1:C:441:GLU:OE2	2.05	0.55
1:C:804:MET:HE3	1:C:807:PHE:HD2	1.71	0.55
1:D:583:VAL:HG21	1:D:596:GLN:OE1	2.07	0.55
1:C:1080:ASP:HB3	1:C:1083:VAL:HG23	1.88	0.55
1:E:480:SER:HB3	1:E:486:SER:O	2.07	0.55
1:F:844:ILE:HG22	1:F:848:ILE:HD11	1.89	0.55
1:A:558:ALA:O	1:A:561:ALA:HB3	2.06	0.55
1:A:613:GLU:OE2	1:A:859:LYS:NZ	2.35	0.55
1:B:528:MET:CE	1:B:537:ILE:HG21	2.36	0.55
1:B:973:SER:OG	1:B:974:THR:N	2.39	0.55
1:F:923:LEU:HD11	1:F:996:PRO:HG3	1.88	0.55
1:G:439:PRO:O	1:G:674:TYR:OH	2.22	0.55
1:H:343:ARG:NH1	1:H:402:LEU:HD11	2.22	0.55
1:C:646:LEU:O	1:C:650:GLN:HG3	2.07	0.55
1:A:993:ASN:O	1:A:999:ARG:NH2	2.40	0.54
1:B:349:ASN:O	1:B:353:THR:HG23	2.07	0.54
1:D:1044:LYS:HE3	1:D:1124:VAL:HG22	1.88	0.54
1:G:831:VAL:HG11	1:G:901:MET:HE1	1.88	0.54
1:H:600:GLN:O	1:H:604:THR:OG1	2.24	0.54
1:D:437:GLN:HA	1:D:437:GLN:HE21	1.73	0.54
1:F:539:TYR:O	1:F:542:ALA:HB3	2.06	0.54
1:C:982:ILE:HG23	1:C:1104:TYR:CE1	2.42	0.54
1:C:999:ARG:NH1	1:C:1003:MET:O	2.39	0.54
1:F:432:MET:HA	1:F:435:ARG:CG	2.38	0.54
1:H:687:ARG:NH1	1:H:765:ASP:OD2	2.35	0.54
1:H:984:ASN:HB2	1:H:988:ILE:HG13	1.89	0.54
1:C:803:ARG:HD2	1:C:808:ASP:OD1	2.07	0.54
1:E:817:ASP:OD1	1:E:818:LEU:N	2.39	0.54
1:E:1021:THR:HA	1:E:1024:ILE:HG12	1.89	0.54
1:E:1075:GLN:NE2	1:E:1103:GLY:H	1.89	0.54
1:F:789:THR:HG21	1:F:838:ILE:HG23	1.88	0.54
1:G:422:TRP:CZ2	1:G:459:GLU:HA	2.42	0.54
1:G:790:GLN:NE2	1:G:793:ILE:HB	2.22	0.54
1:A:1084:LEU:HD22	1:A:1108:PHE:CE1	2.42	0.54
1:B:1044:LYS:HE3	1:B:1124:VAL:HG22	1.89	0.54
1:G:682:VAL:HG22	1:G:714:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:917:GLU:HB3	1:G:920:ARG:NH1	2.21	0.54
1:G:1095:ARG:HA	1:G:1109:VAL:HG21	1.88	0.54
1:H:416:PHE:HA	1:H:662:MET:HE1	1.90	0.54
1:B:618:LEU:HB2	3:B:1356:HOH:O	2.08	0.54
1:G:886:GLY:O	1:G:973:SER:HB3	2.07	0.54
1:C:654:ILE:O	1:C:658:GLU:HG3	2.08	0.54
1:E:982:ILE:O	1:E:1102:ALA:HB3	2.08	0.54
1:H:1114:GLU:H	1:H:1114:GLU:CD	2.15	0.54
1:B:513:ASN:OD1	1:B:589:ALA:HB1	2.07	0.54
1:D:520:GLU:HG3	1:D:544:ILE:HD11	1.90	0.54
1:F:914:TYR:CD1	1:F:933:LEU:HD12	2.43	0.54
1:C:908:VAL:HG11	1:C:916:LEU:CD2	2.38	0.54
1:F:653:ILE:HG23	1:F:712:PRO:HD2	1.90	0.54
1:G:487:ASP:O	1:G:787:GLY:HA2	2.08	0.54
1:H:346:ARG:HE	1:H:400:ASP:CG	2.16	0.54
1:H:680:LEU:HD23	1:H:714:LEU:HD12	1.90	0.54
1:D:941:PRO:HB3	1:D:947:ASP:OD2	2.08	0.53
1:E:562:ARG:HH12	1:E:585:GLU:HG3	1.73	0.53
1:E:1111:LEU:O	1:E:1116:GLN:NE2	2.40	0.53
1:D:905:ARG:HD3	1:D:949:TYR:CZ	2.43	0.53
1:G:593:LYS:N	1:G:597:GLU:OE1	2.40	0.53
1:G:726:TYR:CE2	1:G:730:ILE:HD11	2.43	0.53
1:H:522:HIS:O	1:H:525:SER:HB3	2.08	0.53
1:H:609:PHE:CD1	1:H:861:LEU:HD23	2.43	0.53
1:D:669:LYS:O	1:D:983:SER:OG	2.26	0.53
1:E:439:PRO:O	1:E:674:TYR:OH	2.25	0.53
1:F:432:MET:HA	1:F:435:ARG:HD3	1.90	0.53
1:F:622:ARG:NH1	1:F:765:ASP:HA	2.23	0.53
1:F:1039:MET:SD	1:F:1072:GLY:HA3	2.48	0.53
1:H:738:MET:HB2	1:H:740:PHE:CD2	2.40	0.53
1:C:375:GLY:HA3	1:G:466:ILE:HA	1.89	0.53
1:E:713:SER:HB3	1:E:1100:ARG:HH21	1.74	0.53
1:G:380:LEU:HA	1:G:542:ALA:HB2	1.89	0.53
1:H:739:GLY:HA2	1:H:1076:PHE:O	2.08	0.53
1:B:705:ARG:NH1	1:B:732:ASP:HB3	2.23	0.53
1:C:962:GLU:OE2	1:C:976:SER:OG	2.26	0.53
1:D:744:HIS:NE2	1:D:1073:GLN:HG3	2.24	0.53
1:E:739:GLY:HA3	1:E:1100:ARG:CG	2.38	0.53
1:F:911:GLU:HG3	1:F:913:LYS:HZ2	1.73	0.53
1:G:1044:LYS:NZ	1:G:1081:ASN:HD21	2.07	0.53
1:H:463:LEU:HG	1:H:852:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:442:ILE:HG23	1:G:447:LYS:HZ2	1.72	0.53
1:G:682:VAL:CG2	1:G:714:LEU:HD11	2.39	0.53
1:H:443:SER:CB	1:H:446:ASP:H	2.22	0.53
1:H:790:GLN:CD	1:H:793:ILE:HB	2.34	0.53
1:C:478:ALA:HA	1:C:482:GLU:HB2	1.91	0.53
1:D:790:GLN:OE1	1:D:792:PRO:HD2	2.09	0.53
1:F:407:PRO:HB2	1:F:611:ILE:HD11	1.89	0.53
1:F:818:LEU:HD23	1:F:821:LEU:HD12	1.89	0.53
1:G:999:ARG:HD2	1:G:1004:PRO:O	2.09	0.53
1:E:639:ARG:O	1:E:640:LEU:HD23	2.09	0.53
1:F:752:MET:O	1:F:756:LYS:HG3	2.09	0.53
1:F:773:GLU:OE1	1:F:784:THR:HG21	2.07	0.53
1:A:685:GLN:HG3	1:A:746:ASP:OD2	2.09	0.53
1:B:379:ILE:HD13	1:B:858:PRO:HB2	1.91	0.53
1:B:510:LYS:NZ	1:B:518:ASP:OD2	2.35	0.53
1:E:803:ARG:HB2	1:E:810:TYR:CE1	2.44	0.53
1:E:1106:ALA:HB3	1:E:1111:LEU:HD11	1.91	0.53
1:F:847:VAL:CG2	1:F:970:MET:HE2	2.38	0.53
1:H:641:THR:N	1:H:644:THR:OG1	2.37	0.53
1:E:1049:LEU:HD21	1:E:1128:PHE:CE2	2.43	0.52
1:F:464:ASP:OD1	1:F:492:GLN:NE2	2.42	0.52
1:H:550:VAL:CG1	1:H:608:LEU:HD13	2.38	0.52
1:H:553:TYR:CZ	1:H:557:ILE:HD11	2.44	0.52
1:B:343:ARG:HH12	1:B:576:GLU:CD	2.17	0.52
1:C:344:MET:HG2	1:C:650:GLN:OE1	2.09	0.52
1:E:774:PRO:HD2	1:E:1037:ILE:O	2.09	0.52
1:H:612:GLU:OE1	1:H:615:GLN:NE2	2.34	0.52
1:H:986:THR:HA	1:H:1004:PRO:HB3	1.91	0.52
1:A:513:ASN:OD1	1:A:589:ALA:HB1	2.09	0.52
1:D:487:ASP:OD1	1:D:489:SER:HB3	2.08	0.52
1:E:1048:GLY:HA2	1:E:1051:ASP:OD2	2.08	0.52
1:H:578:LEU:HD12	1:H:578:LEU:O	2.09	0.52
1:D:1095:ARG:C	1:D:1095:ARG:HD3	2.34	0.52
1:E:576:GLU:O	1:E:579:THR:OG1	2.24	0.52
1:G:432:MET:HE3	1:G:440:PHE:HB2	1.91	0.52
1:G:641:THR:H	1:G:644:THR:HG1	1.53	0.52
1:G:686:LYS:N	1:G:692:ALA:HB2	2.25	0.52
1:H:370:VAL:HG12	1:H:381:LEU:HD21	1.91	0.52
1:A:657:ALA:HA	1:A:711:GLN:HB2	1.92	0.52
1:C:701:MET:HE3	1:C:716:CYS:SG	2.48	0.52
1:C:737:GLY:HA2	1:C:1078:TYR:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:GLY:HA2	1:C:976:SER:O	2.09	0.52
1:E:1032:VAL:HB	1:E:1039:MET:SD	2.50	0.52
1:F:803:ARG:NH2	1:F:924:LEU:HD21	2.24	0.52
1:F:927:PHE:CE2	1:F:933:LEU:HD23	2.45	0.52
1:F:1073:GLN:HE22	1:F:1075:GLN:CG	2.18	0.52
1:H:503:TYR:OH	1:H:606:GLU:OE1	2.23	0.52
1:H:819:ARG:HG3	1:H:917:GLU:OE1	2.08	0.52
1:C:1092:GLU:HG2	1:C:1093:LYS:N	2.24	0.52
1:D:343:ARG:CZ	1:D:647:GLU:OE1	2.58	0.52
1:F:828:ASP:OD1	1:F:832:LYS:HE2	2.10	0.52
1:G:790:GLN:HE21	1:G:793:ILE:H	1.57	0.52
1:H:491:HIS:CE1	1:H:783:TRP:CG	2.97	0.52
1:H:1003:MET:HG2	1:H:1004:PRO:HD2	1.92	0.52
1:A:343:ARG:HH22	1:A:576:GLU:CD	2.18	0.52
1:A:1006:SER:O	3:A:1302:HOH:O	2.18	0.52
1:C:564:LEU:HD23	1:C:567:LYS:NZ	2.24	0.52
1:D:343:ARG:NE	1:D:647:GLU:CD	2.65	0.52
1:D:653:ILE:HG23	1:D:712:PRO:HD2	1.92	0.52
1:F:355:ARG:NH2	1:F:1095:ARG:HE	2.06	0.52
1:C:346:ARG:HH11	1:C:400:ASP:CG	2.18	0.52
1:C:488:LEU:HD13	1:C:845:GLY:HA3	1.90	0.52
1:C:805:VAL:HG21	1:C:993:ASN:ND2	2.25	0.52
1:D:735:LYS:NZ	1:D:1051:ASP:HA	2.25	0.52
1:D:965:CYS:O	1:D:975:LEU:HB3	2.10	0.52
1:F:930:TYR:O	1:F:933:LEU:N	2.42	0.52
1:G:618:LEU:HD11	1:G:862:MET:HE1	1.92	0.52
1:G:624:ASP:OD1	1:G:625:GLN:HG2	2.09	0.52
1:H:660:MET:HE1	1:H:674:TYR:HB3	1.90	0.52
1:H:1009:ILE:HD13	1:H:1039:MET:HG3	1.91	0.52
1:H:1101:VAL:HB	1:H:1104:TYR:CE1	2.44	0.52
1:B:1075:GLN:HE22	1:B:1103:GLY:CA	2.21	0.52
1:D:362:ARG:NH1	1:D:417:SER:HA	2.25	0.52
1:D:681:THR:HG21	1:D:768:LEU:N	2.25	0.52
1:D:923:LEU:HD11	1:D:996:PRO:HG3	1.91	0.52
1:G:641:THR:O	1:G:643:ASP:N	2.43	0.52
1:G:1044:LYS:HZ1	1:G:1081:ASN:HD21	1.58	0.52
1:A:639:ARG:O	1:A:640:LEU:HD12	2.09	0.52
1:E:728:GLU:OE2	1:E:1056:ARG:NE	2.42	0.52
1:G:429:LEU:O	1:G:447:LYS:HE3	2.10	0.52
1:H:785:SER:HB3	1:H:890:ILE:CD1	2.37	0.52
1:B:988:ILE:O	1:B:991:LEU:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:HIS:CE1	1:C:772:VAL:HG12	2.46	0.51
1:C:993:ASN:O	1:C:999:ARG:NH2	2.42	0.51
1:D:503:TYR:HA	1:D:507:LEU:HB3	1.92	0.51
1:D:1073:GLN:NE2	1:D:1075:GLN:HE21	2.08	0.51
1:D:1082:GLU:HA	1:D:1085:LYS:HB2	1.92	0.51
1:E:448:LYS:O	1:E:452:GLU:HG3	2.10	0.51
1:F:934:ARG:O	1:F:938:LEU:HG	2.10	0.51
1:G:798:VAL:HG23	1:G:834:GLN:HG3	1.92	0.51
1:B:718:ILE:HD12	1:B:743:CYS:HB3	1.91	0.51
1:B:832:LYS:HD3	1:B:960:TRP:CE2	2.45	0.51
1:C:769:MET:SD	1:C:770:GLY:N	2.83	0.51
1:C:1041:HIS:HB3	1:C:1073:GLN:O	2.11	0.51
1:F:676:PRO:HD2	1:F:711:GLN:NE2	2.25	0.51
1:F:800:ASN:HD21	1:F:924:LEU:HD11	1.75	0.51
1:C:504:ASP:N	1:C:504:ASP:OD1	2.42	0.51
1:D:785:SER:HA	1:D:888:GLY:O	2.10	0.51
1:F:801:ARG:O	1:F:801:ARG:HG2	2.10	0.51
1:G:779:ARG:HG2	1:G:882:MET:SD	2.50	0.51
1:G:1043:PHE:HB2	1:G:1076:PHE:CD2	2.45	0.51
1:B:428:GLU:HG2	1:B:432:MET:HG3	1.92	0.51
1:C:805:VAL:HG21	1:C:993:ASN:HD22	1.74	0.51
1:G:820:ASP:OD2	1:G:822:ARG:NH2	2.43	0.51
1:A:801:ARG:HG2	1:A:814:ASP:OD1	2.10	0.51
1:B:487:ASP:O	1:B:787:GLY:HA2	2.11	0.51
1:C:346:ARG:HD2	1:C:400:ASP:OD2	2.09	0.51
1:D:986:THR:O	1:D:990:GLU:HG3	2.11	0.51
1:E:486:SER:HG	1:E:842:SER:HG	1.56	0.51
1:G:722:SER:O	1:G:1064:ARG:NH2	2.44	0.51
1:H:1086:LYS:HA	1:H:1086:LYS:HE3	1.92	0.51
1:A:708:LYS:HA	1:A:738:MET:SD	2.51	0.51
1:E:508:PHE:O	1:E:591:PRO:HB3	2.09	0.51
1:E:937:CYS:O	1:E:942:LYS:NZ	2.44	0.51
1:F:1033:GLU:H	1:F:1033:GLU:CD	2.19	0.51
1:F:1084:LEU:HD22	1:F:1108:PHE:CE1	2.45	0.51
1:H:437:GLN:NE2	1:H:672:ALA:HB1	2.25	0.51
1:D:790:GLN:NE2	1:D:793:ILE:HB	2.26	0.51
1:F:369:VAL:O	1:F:373:ASN:ND2	2.44	0.51
1:F:1084:LEU:HD21	1:F:1099:VAL:HG21	1.93	0.51
1:G:605:VAL:HG11	1:G:865:LEU:HD11	1.93	0.51
1:H:352:LEU:HD21	1:H:1095:ARG:HE	1.76	0.51
1:A:773:GLU:OE2	1:A:980:LEU:HD13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:CYS:O	1:A:975:LEU:HB3	2.11	0.51
1:D:727:MET:HE2	1:D:1064:ARG:HG3	1.92	0.51
1:D:771:CYS:O	3:D:1302:HOH:O	2.19	0.51
1:E:979:THR:OG1	1:E:1035:MET:HE2	2.11	0.51
1:F:845:GLY:HA2	1:F:848:ILE:HD12	1.93	0.51
1:F:995:THR:HB	1:F:997:ASN:OD1	2.11	0.51
1:G:348:ARG:HH21	1:G:708:LYS:HB2	1.76	0.51
1:H:564:LEU:HD23	1:H:564:LEU:O	2.10	0.51
1:A:522:HIS:O	1:A:525:SER:OG	2.26	0.51
1:D:785:SER:HB3	1:D:890:ILE:HG12	1.92	0.51
1:E:980:LEU:HA	1:E:1040:VAL:HG12	1.92	0.51
1:G:498:ASP:HA	1:G:769:MET:SD	2.50	0.51
1:H:342:PRO:O	1:H:346:ARG:HG3	2.10	0.51
1:H:510:LYS:HB2	1:H:514:GLY:HA3	1.92	0.51
1:C:523:LEU:HD11	1:C:537:ILE:HG23	1.93	0.51
1:C:618:LEU:HD11	1:C:862:MET:HE1	1.93	0.51
1:D:337:MET:HB3	1:D:340:LEU:HB2	1.92	0.51
1:E:674:TYR:O	1:E:710:TYR:OH	2.23	0.51
1:F:393:ALA:O	1:F:556:ARG:NH2	2.44	0.51
1:H:719:HIS:CD2	1:H:721:GLN:H	2.29	0.51
1:F:872:SER:HB3	1:F:874:LYS:HG2	1.93	0.50
1:F:911:GLU:HG3	1:F:913:LYS:HZ1	1.76	0.50
1:H:522:HIS:HB3	1:H:540:TYR:CE2	2.46	0.50
1:G:343:ARG:NH1	1:G:402:LEU:HD11	2.26	0.50
1:H:379:ILE:HG23	1:H:380:LEU:H	1.76	0.50
1:H:583:VAL:HG22	1:H:597:GLU:HG3	1.92	0.50
1:A:962:GLU:HB2	1:A:977:HIS:HE1	1.74	0.50
1:C:882:MET:HG2	1:C:883:VAL:HG23	1.93	0.50
1:E:783:TRP:HB2	1:E:887:PRO:HB3	1.93	0.50
1:F:920:ARG:HD2	1:F:924:LEU:HD12	1.93	0.50
1:F:999:ARG:HD2	1:F:1004:PRO:O	2.11	0.50
1:G:739:GLY:HA3	1:G:1100:ARG:HD3	1.93	0.50
1:B:416:PHE:HE2	1:B:454:ILE:HG21	1.77	0.50
1:C:965:CYS:O	1:C:975:LEU:HB3	2.10	0.50
1:D:1080:ASP:HB3	1:D:1083:VAL:HG13	1.93	0.50
1:F:1088:GLN:HE21	1:F:1113:LYS:HG3	1.77	0.50
1:G:728:GLU:HG3	1:G:1056:ARG:NH2	2.08	0.50
1:G:1027:VAL:HG21	1:G:1041:HIS:CD2	2.47	0.50
1:H:915:THR:OG1	1:H:918:GLN:HG3	2.11	0.50
1:B:568:GLU:HG3	1:B:570:ASN:H	1.76	0.50
1:F:532:GLU:CD	1:F:532:GLU:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:825:ASP:O	1:F:828:ASP:HB3	2.11	0.50
1:F:915:THR:HB	1:F:918:GLN:HG2	1.93	0.50
1:H:680:LEU:HD23	1:H:714:LEU:CD1	2.42	0.50
1:H:962:GLU:HB2	1:H:977:HIS:HE1	1.74	0.50
1:B:637:GLU:OE1	1:B:639:ARG:NH1	2.43	0.50
1:E:464:ASP:OD1	1:E:493:ILE:HG22	2.10	0.50
1:F:443:SER:O	1:F:447:LYS:HD2	2.12	0.50
1:F:546:THR:HG21	1:F:860:PRO:HB2	1.94	0.50
1:F:1080:ASP:HB3	1:F:1083:VAL:HG23	1.93	0.50
1:F:1082:GLU:HA	1:F:1085:LYS:CG	2.42	0.50
1:H:573:ARG:O	1:H:577:LEU:HD23	2.10	0.50
1:H:586:ASN:O	1:H:590:ASN:HB2	2.10	0.50
1:H:942:LYS:C	1:H:950:VAL:HG11	2.37	0.50
1:A:499:THR:O	1:A:501:PRO:HD3	2.12	0.50
1:B:595:LEU:N	1:B:634:ASP:OD2	2.38	0.50
1:C:1073:GLN:HE22	1:C:1075:GLN:HG3	1.76	0.50
1:D:779:ARG:HG2	1:D:882:MET:SD	2.51	0.50
1:E:435:ARG:NH1	1:E:663:SER:O	2.45	0.50
1:F:546:THR:OG1	1:F:864:LEU:HD11	2.12	0.50
1:F:771:CYS:HB3	1:F:1103:GLY:HA3	1.92	0.50
1:F:906:LYS:HG3	1:F:910:GLU:CB	2.40	0.50
1:H:387:ARG:HG2	1:H:391:GLU:OE1	2.10	0.50
1:A:572:GLN:O	1:A:575:ALA:N	2.45	0.50
1:F:349:ASN:O	1:F:353:THR:HG23	2.10	0.50
1:G:499:THR:O	1:G:501:PRO:HD3	2.12	0.50
1:G:984:ASN:HB2	1:G:988:ILE:HG13	1.94	0.50
1:H:799:LEU:HA	1:H:818:LEU:HD21	1.94	0.50
1:A:850:GLN:NE2	1:A:887:PRO:HD3	2.27	0.50
1:C:387:ARG:NH1	1:C:545:GLU:OE2	2.44	0.50
1:C:657:ALA:HA	1:C:711:GLN:HB2	1.94	0.50
1:F:504:ASP:OD2	1:F:505:VAL:HG23	2.12	0.50
1:G:351:TYR:HB2	1:G:654:ILE:HD11	1.94	0.50
1:H:900:SER:HB3	1:H:996:PRO:HD2	1.94	0.50
1:H:969:LYS:O	1:H:970:MET:HE2	2.12	0.50
1:A:980:LEU:HD23	1:A:980:LEU:H	1.76	0.49
1:D:745:PHE:CD1	1:D:1067:SER:HB2	2.46	0.49
1:E:435:ARG:NH2	1:E:438:ASP:O	2.45	0.49
1:F:670:TYR:CD2	1:F:984:ASN:HB3	2.48	0.49
1:H:914:TYR:CZ	1:H:933:LEU:HB3	2.47	0.49
1:B:370:VAL:HA	1:B:381:LEU:HD11	1.94	0.49
1:B:1079:VAL:HG11	1:B:1084:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:LYS:HA	1:E:672:ALA:HB2	1.93	0.49
1:E:871:GLU:H	1:E:871:GLU:CD	2.19	0.49
1:F:943:TYR:OH	1:F:1027:VAL:HA	2.11	0.49
1:H:450:ILE:HG22	1:H:454:ILE:HG13	1.94	0.49
1:A:966:ARG:HH11	1:A:974:THR:HG23	1.76	0.49
1:D:554:ALA:HB2	1:D:588:PRO:HD2	1.94	0.49
1:F:398:GLN:HB2	1:F:401:GLU:CD	2.38	0.49
1:H:490:TYR:HE2	1:H:491:HIS:CE1	2.30	0.49
1:H:1046:LEU:HD12	1:H:1047:LYS:H	1.77	0.49
1:B:623:VAL:HG21	1:B:680:LEU:HD11	1.93	0.49
1:D:504:ASP:OD1	1:D:504:ASP:N	2.45	0.49
1:E:483:THR:HG21	1:E:811:GLN:NE2	2.27	0.49
1:E:618:LEU:HD11	1:E:862:MET:HE1	1.94	0.49
1:F:773:GLU:OE2	2:F:1201:A1H9K:O1	2.31	0.49
1:F:835:ILE:O	1:F:838:ILE:HB	2.12	0.49
1:G:359:SER:HB3	1:G:414:GLY:O	2.12	0.49
1:H:955:LEU:HD13	1:H:1030:MET:HA	1.95	0.49
1:H:1085:LYS:HD2	1:H:1085:LYS:O	2.13	0.49
1:A:636:ARG:HG2	1:A:636:ARG:HH11	1.78	0.49
1:B:708:LYS:HA	1:B:738:MET:SD	2.53	0.49
1:B:897:TYR:CZ	1:B:901:MET:HE3	2.47	0.49
1:D:720:ASN:OD1	1:D:1067:SER:OG	2.24	0.49
1:D:749:HIS:HA	1:D:752:MET:CG	2.41	0.49
1:H:504:ASP:CG	1:H:505:VAL:HG13	2.38	0.49
1:H:573:ARG:HE	1:H:577:LEU:HD23	1.77	0.49
1:H:790:GLN:OE1	1:H:793:ILE:HB	2.13	0.49
1:A:737:GLY:HA2	1:A:1078:TYR:HB3	1.94	0.49
1:C:396:LEU:HD22	1:C:409:GLY:O	2.12	0.49
1:D:735:LYS:HE2	1:D:1056:ARG:NH1	2.27	0.49
1:F:786:THR:HG21	1:F:849:SER:HB3	1.94	0.49
1:H:540:TYR:O	1:H:544:ILE:HG13	2.13	0.49
1:H:986:THR:HG21	1:H:1115:VAL:HA	1.93	0.49
1:D:866:VAL:HG11	1:D:876:VAL:CG1	2.42	0.49
1:F:898:VAL:HG12	1:F:950:VAL:HG22	1.94	0.49
1:F:966:ARG:HH11	1:F:974:THR:HG23	1.77	0.49
1:G:736:ALA:HB1	1:G:738:MET:HE2	1.94	0.49
1:C:1075:GLN:NE2	1:C:1103:GLY:HA2	2.27	0.49
1:D:732:ASP:O	1:D:735:LYS:HB2	2.12	0.49
1:H:407:PRO:HB2	1:H:611:ILE:CG1	2.43	0.49
1:H:1127:LYS:HD3	1:H:1127:LYS:N	2.27	0.49
1:B:993:ASN:HB3	3:B:1364:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:LEU:HD13	1:C:645:ALA:HB2	1.95	0.49
1:C:931:GLU:O	1:C:935:ARG:HG3	2.13	0.49
1:E:507:LEU:HD13	1:E:512:MET:HE2	1.94	0.49
1:E:758:PHE:HZ	1:E:780:ILE:HD12	1.78	0.49
1:G:573:ARG:O	1:G:577:LEU:HG	2.12	0.49
1:B:743:CYS:O	1:B:1073:GLN:HA	2.12	0.49
1:F:622:ARG:HH11	1:F:765:ASP:HA	1.78	0.49
1:F:805:VAL:HG11	1:F:993:ASN:ND2	2.28	0.49
1:G:488:LEU:HD13	1:G:845:GLY:HA3	1.94	0.49
1:G:603:TRP:CZ2	1:G:655:LYS:HG2	2.48	0.49
1:G:948:ASN:O	1:G:952:GLN:HG2	2.12	0.49
1:H:635:ILE:HD13	1:H:642:HIS:CD2	2.48	0.49
1:H:850:GLN:HB3	1:H:971:LEU:HD22	1.94	0.49
1:H:1063:LEU:HD21	1:H:1076:PHE:HZ	1.78	0.49
1:A:675:GLN:CD	1:A:1104:TYR:CD2	2.91	0.48
1:A:919:ILE:O	1:A:923:LEU:HG	2.13	0.48
1:B:776:LYS:HD3	1:B:776:LYS:C	2.37	0.48
1:D:934:ARG:HE	1:D:938:LEU:HD11	1.77	0.48
1:F:419:ASP:HB3	1:F:458:TRP:CZ3	2.48	0.48
1:F:742:ALA:HB2	1:F:1100:ARG:HH22	1.76	0.48
1:G:1016:ASP:OD1	1:G:1016:ASP:N	2.43	0.48
1:H:437:GLN:HG3	1:H:438:ASP:H	1.77	0.48
1:H:543:ALA:O	1:H:546:THR:HG22	2.12	0.48
1:H:573:ARG:HH21	1:H:577:LEU:CD2	2.26	0.48
1:C:917:GLU:HB3	1:C:920:ARG:NH2	2.28	0.48
1:D:993:ASN:OD1	1:D:994:ALA:N	2.46	0.48
1:D:1075:GLN:OE1	1:D:1100:ARG:HD3	2.13	0.48
1:E:906:LYS:HB2	1:E:949:TYR:OH	2.14	0.48
1:F:844:ILE:O	1:F:848:ILE:HG13	2.13	0.48
1:G:1027:VAL:HG21	1:G:1041:HIS:HD2	1.78	0.48
1:H:761:GLU:O	1:H:765:ASP:HB2	2.12	0.48
1:H:790:GLN:CG	1:H:792:PRO:HD2	2.43	0.48
1:B:701:MET:HE2	1:B:729:LYS:HG3	1.94	0.48
1:C:350:HIS:O	1:C:353:THR:OG1	2.28	0.48
1:D:397:ILE:HG12	1:D:404:VAL:HB	1.94	0.48
1:D:599:LEU:HD11	1:D:649:LEU:HD23	1.94	0.48
1:E:934:ARG:NH1	1:E:1000:LEU:HD21	2.27	0.48
1:A:574:ARG:HD2	3:A:1361:HOH:O	2.12	0.48
1:H:562:ARG:O	1:H:565:ALA:HB3	2.14	0.48
1:H:971:LEU:HB3	1:H:972:TYR:CD2	2.48	0.48
1:A:386:PHE:CE2	1:A:546:THR:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ARG:NE	1:B:437:GLN:O	2.47	0.48
1:B:1013:GLN:CD	1:B:1013:GLN:H	2.21	0.48
1:C:1044:LYS:HE3	1:C:1124:VAL:HG12	1.96	0.48
1:G:364:LEU:O	1:G:368:GLU:HG3	2.13	0.48
1:G:559:ALA:HA	1:G:562:ARG:NH1	2.28	0.48
1:H:1094:TYR:HB3	1:H:1097:LEU:HB2	1.95	0.48
1:E:1118:GLU:O	1:E:1121:SER:OG	2.23	0.48
1:F:1082:GLU:OE2	1:F:1085:LYS:HE3	2.12	0.48
1:G:927:PHE:CD2	1:G:934:ARG:HD2	2.49	0.48
1:A:468:GLU:HB2	1:A:492:GLN:NE2	2.28	0.48
1:D:616:THR:HB	1:D:661:TRP:CG	2.48	0.48
1:D:937:CYS:C	1:D:939:ASN:N	2.72	0.48
1:G:906:LYS:HE2	1:G:941:PRO:CD	2.43	0.48
1:G:1020:PRO:HG3	1:G:1128:PHE:HD1	1.79	0.48
1:A:340:LEU:HB3	1:A:344:MET:HB3	1.94	0.48
1:C:871:GLU:OE1	1:C:871:GLU:N	2.42	0.48
1:D:1042:ASN:ND2	1:D:1122:ARG:NH1	2.61	0.48
1:D:1042:ASN:ND2	1:D:1101:VAL:O	2.46	0.48
1:F:798:VAL:HG12	1:F:799:LEU:HD23	1.95	0.48
1:F:908:VAL:O	1:F:912:LYS:CE	2.46	0.48
1:G:369:VAL:HG21	1:G:385:ALA:HA	1.95	0.48
1:H:573:ARG:HE	1:H:577:LEU:HD21	1.79	0.48
1:A:1080:ASP:HB3	1:A:1083:VAL:HG23	1.96	0.48
1:B:776:LYS:HD2	1:B:779:ARG:HD2	1.96	0.48
1:C:742:ALA:HB2	1:C:1100:ARG:NH2	2.29	0.48
1:C:806:LEU:HB2	1:C:1002:TRP:CH2	2.48	0.48
1:C:995:THR:HG23	1:C:999:ARG:HH21	1.78	0.48
1:D:618:LEU:HD11	1:D:862:MET:HE1	1.95	0.48
1:E:1062:LEU:HG	1:E:1074:MET:HE1	1.96	0.48
1:H:428:GLU:OE1	1:H:665:GLU:HB2	2.14	0.48
1:H:508:PHE:O	1:H:591:PRO:HB3	2.13	0.48
1:H:908:VAL:O	1:H:912:LYS:HE2	2.13	0.48
1:H:1093:LYS:N	1:H:1093:LYS:HD2	2.29	0.48
1:B:376:MET:HB3	1:B:381:LEU:HB2	1.95	0.48
1:D:483:THR:OG1	1:D:485:VAL:HG23	2.14	0.48
1:D:1095:ARG:HH11	1:D:1095:ARG:HG2	1.78	0.48
1:H:653:ILE:HG23	1:H:712:PRO:HD2	1.96	0.48
1:H:1108:PHE:CE1	1:H:1116:GLN:HB2	2.49	0.48
1:C:1095:ARG:HA	1:C:1109:VAL:HG21	1.95	0.47
1:D:654:ILE:O	1:D:658:GLU:HG3	2.13	0.47
1:D:823:THR:OG1	1:D:824:PHE:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:898:VAL:HG13	1:D:953:TYR:HB2	1.96	0.47
1:E:934:ARG:CZ	1:E:1000:LEU:HD21	2.44	0.47
1:F:391:GLU:O	1:F:556:ARG:NH1	2.47	0.47
1:G:708:LYS:HA	1:G:738:MET:SD	2.54	0.47
1:B:941:PRO:HG2	1:B:949:TYR:CD2	2.49	0.47
1:D:491:HIS:CE1	1:D:783:TRP:CD2	3.02	0.47
1:D:594:THR:O	1:D:597:GLU:N	2.47	0.47
1:E:968:TYR:O	1:E:974:THR:OG1	2.27	0.47
1:F:832:LYS:HD3	1:F:960:TRP:CE2	2.49	0.47
1:G:458:TRP:O	1:G:461:ARG:N	2.46	0.47
1:H:795:ILE:HG12	1:H:901:MET:HE3	1.95	0.47
1:H:859:LYS:HD2	3:H:1307:HOH:O	2.15	0.47
1:H:1109:VAL:C	1:H:1111:LEU:H	2.21	0.47
1:D:420:ILE:HD11	1:D:613:GLU:OE1	2.14	0.47
1:D:423:ARG:HH21	1:D:464:ASP:CG	2.22	0.47
1:D:752:MET:HE2	1:D:774:PRO:HG3	1.97	0.47
1:E:854:ARG:HA	1:E:877:ALA:HB1	1.96	0.47
1:F:503:TYR:HA	1:F:507:LEU:HB3	1.96	0.47
1:F:746:ASP:O	1:F:750:ILE:HG13	2.15	0.47
1:B:528:MET:HE2	1:B:537:ILE:CG2	2.43	0.47
1:C:822:ARG:HA	1:C:822:ARG:HD2	1.65	0.47
1:F:785:SER:HA	1:F:888:GLY:O	2.14	0.47
1:G:717:ARG:NH2	1:G:764:ARG:O	2.47	0.47
1:H:925:ALA:O	1:H:928:GLU:HG3	2.14	0.47
1:C:620:LEU:HD12	1:C:680:LEU:HD12	1.96	0.47
1:D:953:TYR:N	1:D:953:TYR:CD2	2.81	0.47
1:E:744:HIS:NE2	1:E:1073:GLN:HG3	2.30	0.47
1:E:979:THR:OG1	1:E:1039:MET:HA	2.14	0.47
1:G:579:THR:HG22	1:G:596:GLN:HE22	1.78	0.47
1:G:906:LYS:HA	1:G:910:GLU:HB2	1.96	0.47
1:H:573:ARG:NH2	1:H:577:LEU:HD21	2.29	0.47
1:H:613:GLU:HG2	1:H:615:GLN:NE2	2.29	0.47
1:H:1090:GLU:HB3	1:H:1093:LYS:HD3	1.95	0.47
1:A:984:ASN:HA	1:A:987:PRO:HD2	1.96	0.47
1:C:716:CYS:HB3	1:C:726:TYR:OH	2.15	0.47
1:H:341:THR:HG21	1:H:647:GLU:OE2	2.15	0.47
1:H:599:LEU:O	1:H:652:PHE:HE2	1.97	0.47
1:A:824:PHE:CG	1:A:905:ARG:HD2	2.50	0.47
1:A:1048:GLY:HA2	1:A:1051:ASP:OD2	2.15	0.47
1:B:423:ARG:HD3	1:B:464:ASP:OD2	2.15	0.47
1:B:1084:LEU:HD22	1:B:1108:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ILE:HA	3:C:1306:HOH:O	2.14	0.47
1:E:419:ASP:HB3	1:E:458:TRP:CZ3	2.49	0.47
1:E:551:VAL:O	1:E:555:ARG:HG2	2.15	0.47
1:E:815:THR:HG23	1:E:834:GLN:HE21	1.79	0.47
1:E:914:TYR:HB3	1:E:918:GLN:OE1	2.15	0.47
1:E:941:PRO:HG2	1:E:949:TYR:CD1	2.50	0.47
1:E:1099:VAL:HG11	1:E:1108:PHE:CD1	2.47	0.47
1:E:1106:ALA:CB	1:E:1111:LEU:HD11	2.44	0.47
1:F:488:LEU:HD23	1:F:787:GLY:CA	2.44	0.47
1:F:753:MET:HE3	1:F:758:PHE:CD2	2.49	0.47
1:F:1084:LEU:HD22	1:F:1108:PHE:CZ	2.50	0.47
1:G:393:ALA:O	1:G:556:ARG:NH2	2.48	0.47
1:G:550:VAL:HG23	1:G:608:LEU:CD1	2.43	0.47
1:H:497:GLY:O	1:H:499:THR:OG1	2.28	0.47
1:H:512:MET:CE	1:H:605:VAL:HG11	2.43	0.47
1:B:599:LEU:HD12	1:B:648:LEU:CD2	2.43	0.47
1:C:351:TYR:CE1	1:C:412:ARG:HD3	2.50	0.47
1:C:596:GLN:HB2	1:C:648:LEU:HD11	1.96	0.47
1:E:483:THR:OG1	1:E:485:VAL:HG23	2.15	0.47
1:F:767:CYS:C	1:F:768:LEU:HD22	2.39	0.47
1:F:849:SER:OG	1:F:850:GLN:N	2.48	0.47
1:G:569:GLN:HA	1:G:574:ARG:HH12	1.78	0.47
1:G:710:TYR:CD2	1:G:1106:ALA:HA	2.50	0.47
1:A:555:ARG:NH1	1:A:585:GLU:O	2.48	0.47
1:F:875:ASP:OD2	1:F:877:ALA:HB3	2.14	0.47
1:G:396:LEU:HD21	1:G:398:GLN:HG2	1.97	0.47
1:A:552:ASN:O	1:A:556:ARG:HG2	2.14	0.47
1:C:487:ASP:O	1:C:787:GLY:HA2	2.14	0.47
1:D:846:THR:O	1:D:849:SER:OG	2.24	0.47
1:E:476:VAL:HG12	1:E:841:LEU:HG	1.95	0.47
1:E:742:ALA:HB2	1:E:1100:ARG:HH12	1.80	0.47
1:F:759:ASP:OD1	1:F:760:PHE:N	2.41	0.47
1:F:905:ARG:HG3	1:F:906:LYS:N	2.30	0.47
1:G:758:PHE:HZ	1:G:780:ILE:HB	1.79	0.47
1:G:803:ARG:HA	1:G:810:TYR:HA	1.96	0.47
1:H:354:VAL:HG11	1:H:411:PRO:O	2.15	0.47
1:C:931:GLU:OE1	1:C:931:GLU:N	2.47	0.46
1:B:1118:GLU:O	1:B:1121:SER:OG	2.31	0.46
1:C:984:ASN:HA	1:C:987:PRO:HD2	1.97	0.46
1:E:758:PHE:CZ	1:E:780:ILE:HD12	2.51	0.46
1:F:437:GLN:HE22	1:F:1111:LEU:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:485:VAL:O	1:F:789:THR:HG23	2.15	0.46
1:F:850:GLN:HB3	1:F:971:LEU:HD22	1.97	0.46
1:F:866:VAL:HG11	1:F:876:VAL:CG1	2.44	0.46
1:F:906:LYS:HE2	1:F:906:LYS:HB3	1.57	0.46
1:H:406:HIS:CE1	1:H:408:CYS:HB2	2.49	0.46
1:H:1003:MET:HG2	1:H:1004:PRO:CD	2.45	0.46
1:C:463:LEU:HD11	1:C:853:HIS:CD2	2.51	0.46
1:C:675:GLN:CD	1:C:1104:TYR:CD2	2.94	0.46
1:E:601:SER:O	1:E:605:VAL:HG22	2.15	0.46
1:E:716:CYS:HB3	1:E:726:TYR:OH	2.15	0.46
1:G:627:CYS:HA	1:G:630:MET:SD	2.55	0.46
1:G:1047:LYS:HA	1:G:1078:TYR:CE1	2.51	0.46
1:A:589:ALA:N	3:A:1304:HOH:O	2.27	0.46
1:B:343:ARG:HG2	1:B:400:ASP:HB3	1.98	0.46
1:B:343:ARG:CG	1:B:400:ASP:HB3	2.45	0.46
1:C:1124:VAL:HG23	1:C:1124:VAL:O	2.15	0.46
1:E:355:ARG:HD3	1:E:355:ARG:HA	1.74	0.46
1:E:1077:SER:OG	1:E:1079:VAL:HG12	2.16	0.46
1:F:356:PRO:HB3	1:F:660:MET:HE3	1.97	0.46
1:F:801:ARG:HG3	1:F:814:ASP:OD1	2.16	0.46
1:F:906:LYS:HG2	1:F:906:LYS:O	2.15	0.46
1:G:532:GLU:H	1:G:532:GLU:CD	2.23	0.46
1:D:447:LYS:O	1:D:451:ARG:HG3	2.16	0.46
1:D:675:GLN:HE22	1:D:711:GLN:HE22	1.64	0.46
1:D:984:ASN:C	1:D:987:PRO:HD2	2.40	0.46
1:E:698:TYR:CE2	1:E:725:LYS:HE2	2.50	0.46
1:F:818:LEU:HA	1:F:821:LEU:HG	1.96	0.46
1:F:979:THR:CG2	1:F:1035:MET:HE2	2.40	0.46
1:F:1118:GLU:O	1:F:1121:SER:HB2	2.16	0.46
1:G:351:TYR:CB	1:G:654:ILE:HD11	2.46	0.46
1:G:354:VAL:HG21	1:G:411:PRO:HB2	1.97	0.46
1:H:365:ALA:O	1:H:369:VAL:HG23	2.15	0.46
1:A:435:ARG:HH21	1:A:438:ASP:HB2	1.81	0.46
1:B:371:LYS:NZ	1:B:453:GLU:OE2	2.49	0.46
1:C:784:THR:HG21	1:C:980:LEU:HD11	1.97	0.46
1:C:874:LYS:NZ	3:C:1301:HOH:O	2.22	0.46
1:F:701:MET:HE1	1:F:726:TYR:HD1	1.80	0.46
1:G:422:TRP:HZ2	1:G:459:GLU:HA	1.80	0.46
1:H:707:VAL:HG12	1:H:709:VAL:HG13	1.97	0.46
1:B:435:ARG:CZ	1:B:438:ASP:O	2.64	0.46
1:D:437:GLN:HA	1:D:437:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:GLN:HG2	1:D:493:ILE:HG23	1.98	0.46
1:D:655:LYS:HD2	1:D:658:GLU:OE2	2.16	0.46
1:F:670:TYR:CD2	1:F:984:ASN:CB	2.99	0.46
1:F:813:LEU:CD1	1:F:837:HIS:HB2	2.44	0.46
1:G:762:ASP:OD1	1:G:779:ARG:NH1	2.49	0.46
1:G:894:LEU:O	1:G:898:VAL:HG13	2.15	0.46
1:D:419:ASP:HB3	1:D:458:TRP:CH2	2.51	0.46
1:F:376:MET:SD	1:F:380:LEU:HD23	2.55	0.46
1:F:650:GLN:HB3	1:F:707:VAL:HG11	1.97	0.46
1:F:1082:GLU:HA	1:F:1085:LYS:CE	2.45	0.46
1:G:539:TYR:CD2	1:G:873:GLY:HA2	2.50	0.46
1:H:763:ALA:O	1:H:766:TYR:HD2	1.98	0.46
1:H:938:LEU:HG	1:H:998:GLY:HA3	1.98	0.46
1:B:703:ALA:O	1:B:707:VAL:HG22	2.15	0.46
1:D:735:LYS:HZ1	1:D:1051:ASP:HA	1.80	0.46
1:D:738:MET:HB3	1:D:1098:ILE:CG2	2.46	0.46
1:G:383:ALA:HB2	1:G:542:ALA:HB1	1.98	0.46
1:B:553:TYR:O	1:B:557:ILE:HG12	2.16	0.46
1:D:718:ILE:O	1:D:745:PHE:HA	2.16	0.46
1:E:435:ARG:HG2	1:E:437:GLN:H	1.81	0.46
1:F:674:TYR:O	1:F:676:PRO:HD3	2.16	0.46
1:F:858:PRO:O	1:F:860:PRO:HD3	2.16	0.46
1:H:909:PHE:O	1:H:912:LYS:HE3	2.15	0.46
1:A:731:VAL:HG22	1:A:1059:LEU:HD23	1.97	0.45
1:A:1099:VAL:HG21	1:A:1108:PHE:CD1	2.51	0.45
1:C:844:ILE:O	1:C:848:ILE:HG13	2.16	0.45
1:D:344:MET:CE	1:D:647:GLU:HG2	2.47	0.45
1:D:641:THR:O	1:D:644:THR:OG1	2.24	0.45
1:F:476:VAL:HG12	1:F:841:LEU:HD12	1.97	0.45
1:F:968:TYR:HE2	1:H:529:GLU:HG2	1.81	0.45
1:G:686:LYS:HE3	1:G:689:GLY:O	2.16	0.45
1:G:829:ALA:O	1:G:833:GLN:HG3	2.15	0.45
1:H:347:LEU:HD21	1:H:400:ASP:HB2	1.97	0.45
1:H:356:PRO:HG2	1:H:674:TYR:CE1	2.51	0.45
1:H:448:LYS:NZ	1:H:452:GLU:OE2	2.46	0.45
1:H:635:ILE:HD13	1:H:642:HIS:HD2	1.80	0.45
1:H:897:TYR:CE2	1:H:957:ILE:HG21	2.51	0.45
1:H:960:TRP:HE3	1:H:961:THR:HG22	1.79	0.45
1:A:1084:LEU:HD22	1:A:1108:PHE:CD1	2.52	0.45
1:B:340:LEU:HD22	1:B:344:MET:CG	2.46	0.45
1:B:622:ARG:O	1:B:626:TYR:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:TRP:CD1	1:D:462:SER:HB3	2.51	0.45
1:D:660:MET:HE1	1:D:674:TYR:HB3	1.99	0.45
1:E:631:PHE:O	1:E:635:ILE:HG12	2.16	0.45
1:E:1047:LYS:CD	1:E:1080:ASP:HB2	2.44	0.45
1:F:906:LYS:CG	1:F:910:GLU:HB3	2.40	0.45
1:H:367:THR:O	1:H:371:LYS:CB	2.65	0.45
1:A:362:ARG:HH11	1:A:417:SER:HA	1.81	0.45
1:A:527:SER:HB3	1:A:530:ASN:OD1	2.17	0.45
1:B:980:LEU:HD12	1:B:980:LEU:O	2.16	0.45
1:B:1048:GLY:HA2	1:B:1051:ASP:OD2	2.15	0.45
1:C:622:ARG:HH11	1:C:765:ASP:HA	1.81	0.45
1:F:536:ARG:HG2	1:F:540:TYR:HE2	1.81	0.45
1:F:1082:GLU:HA	1:F:1085:LYS:HE3	1.98	0.45
1:H:546:THR:CG2	1:H:864:LEU:HD11	2.41	0.45
1:C:906:LYS:NZ	1:C:911:GLU:OE2	2.49	0.45
1:D:498:ASP:HA	1:D:769:MET:SD	2.57	0.45
1:D:618:LEU:HD13	1:D:618:LEU:HA	1.82	0.45
1:D:1075:GLN:NE2	1:D:1103:GLY:H	2.12	0.45
1:E:391:GLU:OE2	1:E:552:ASN:ND2	2.50	0.45
1:F:758:PHE:CE2	1:F:780:ILE:HD12	2.51	0.45
1:F:850:GLN:HG2	3:F:1320:HOH:O	2.16	0.45
1:G:818:LEU:HD23	1:G:818:LEU:HA	1.79	0.45
1:H:352:LEU:HD23	1:H:352:LEU:O	2.17	0.45
1:H:479:PHE:CG	1:H:841:LEU:HD23	2.51	0.45
1:H:957:ILE:HD12	1:H:958:THR:N	2.32	0.45
1:H:966:ARG:HD3	1:H:974:THR:HG23	1.98	0.45
1:E:387:ARG:NH1	1:E:548:GLU:HG3	2.32	0.45
1:F:614:ASN:OD1	1:F:661:TRP:HD1	1.99	0.45
1:F:618:LEU:HD22	1:F:618:LEU:H	1.82	0.45
1:F:1016:ASP:OD1	1:F:1016:ASP:N	2.48	0.45
1:G:803:ARG:HB2	1:G:810:TYR:CE1	2.51	0.45
1:G:984:ASN:O	1:G:988:ILE:HG13	2.17	0.45
1:H:984:ASN:HA	1:H:987:PRO:HG2	1.98	0.45
1:B:506:LEU:HD23	1:B:510:LYS:HE3	1.99	0.45
1:B:758:PHE:CE2	1:B:780:ILE:HD12	2.51	0.45
1:C:561:ALA:HB3	1:C:581:ALA:HB2	1.99	0.45
1:C:608:LEU:O	1:C:611:ILE:N	2.49	0.45
1:F:542:ALA:O	1:F:546:THR:HG23	2.17	0.45
1:G:526:LEU:HB3	1:G:533:ASP:HB3	1.99	0.45
1:G:980:LEU:HD12	1:G:982:ILE:HG13	1.98	0.45
1:G:1099:VAL:HG11	1:G:1108:PHE:CD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:437:GLN:OE1	1:H:1112:CYS:HB3	2.16	0.45
1:A:623:VAL:HG13	1:A:627:CYS:SG	2.56	0.45
1:C:1040:VAL:HG23	1:C:1075:GLN:NE2	2.32	0.45
1:E:650:GLN:HB3	1:E:707:VAL:HG11	1.99	0.45
1:G:356:PRO:HA	1:G:412:ARG:O	2.16	0.45
1:G:729:LYS:O	1:G:733:VAL:HG23	2.16	0.45
1:B:913:LYS:HD3	1:B:914:TYR:CZ	2.52	0.45
1:D:767:CYS:C	1:D:768:LEU:HD22	2.42	0.45
1:E:799:LEU:HA	1:E:818:LEU:HD21	1.99	0.45
1:G:917:GLU:H	1:G:917:GLU:HG3	1.39	0.45
1:A:573:ARG:HD2	1:A:576:GLU:OE1	2.16	0.45
1:A:756:LYS:NZ	1:A:782:GLN:OE1	2.43	0.45
1:B:675:GLN:CD	1:B:1104:TYR:CD2	2.95	0.45
1:C:560:HIS:CE1	1:C:564:LEU:HD11	2.52	0.45
1:C:795:ILE:HD11	1:C:897:TYR:CD2	2.52	0.45
1:D:646:LEU:O	1:D:650:GLN:HG3	2.17	0.45
1:D:971:LEU:HB3	1:D:972:TYR:CD2	2.52	0.45
1:D:1073:GLN:HE22	1:D:1075:GLN:HE21	1.62	0.45
1:E:450:ILE:O	1:E:455:VAL:HG23	2.17	0.45
1:G:776:LYS:HD2	1:G:776:LYS:HA	1.66	0.45
1:G:919:ILE:O	1:G:923:LEU:HG	2.16	0.45
1:G:1042:ASN:OD1	1:G:1122:ARG:NH1	2.50	0.45
1:H:358:VAL:CG2	1:H:432:MET:HE1	2.46	0.45
1:H:515:ILE:HG21	1:H:864:LEU:HB3	1.99	0.45
1:H:934:ARG:HG2	1:H:938:LEU:HD11	1.98	0.45
1:H:1082:GLU:O	1:H:1086:LYS:HG2	2.17	0.45
1:A:416:PHE:CE1	1:A:425:VAL:HG21	2.52	0.44
1:A:419:ASP:HB3	1:A:458:TRP:CH2	2.53	0.44
1:B:790:GLN:CD	1:B:793:ILE:HB	2.42	0.44
1:C:624:ASP:HB3	1:C:700:ILE:HD12	1.98	0.44
1:D:1090:GLU:OE2	1:D:1093:LYS:HD3	2.17	0.44
1:F:621:GLY:HA2	1:F:767:CYS:HB2	1.99	0.44
1:F:832:LYS:HD3	1:F:960:TRP:NE1	2.31	0.44
1:F:872:SER:HB3	1:F:874:LYS:CG	2.47	0.44
1:G:577:LEU:HD23	1:G:580:ILE:HD12	1.99	0.44
1:G:628:TYR:CD1	1:G:694:ASN:ND2	2.84	0.44
1:G:641:THR:O	1:G:644:THR:N	2.50	0.44
1:G:744:HIS:HD2	1:G:749:HIS:CE1	2.34	0.44
1:G:900:SER:N	1:G:997:ASN:HB3	2.32	0.44
1:G:966:ARG:NH1	1:G:974:THR:HG23	2.26	0.44
1:H:406:HIS:HE1	1:H:408:CYS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:443:SER:O	1:H:447:LYS:HG3	2.18	0.44
1:H:682:VAL:HB	1:H:697:THR:HG23	1.99	0.44
1:H:986:THR:HG22	1:H:1004:PRO:CG	2.48	0.44
1:H:1063:LEU:HD21	1:H:1076:PHE:CZ	2.51	0.44
1:H:1090:GLU:HB3	1:H:1093:LYS:CE	2.47	0.44
1:A:362:ARG:NH1	1:A:417:SER:HA	2.32	0.44
1:A:966:ARG:HD3	1:A:975:LEU:O	2.17	0.44
1:B:583:VAL:O	1:B:587:VAL:HG22	2.18	0.44
1:D:686:LYS:N	1:D:692:ALA:HB2	2.33	0.44
1:D:1057:HIS:O	1:D:1061:THR:OG1	2.21	0.44
1:F:885:HIS:ND1	1:F:886:GLY:N	2.65	0.44
1:G:573:ARG:O	1:G:576:GLU:HB3	2.17	0.44
1:G:715:ALA:HB1	1:G:768:LEU:HD12	1.99	0.44
1:H:483:THR:HG22	1:H:807:PHE:CD2	2.51	0.44
1:H:896:THR:O	1:H:900:SER:OG	2.22	0.44
1:A:739:GLY:HA3	1:A:1100:ARG:HD3	1.99	0.44
1:B:824:PHE:CE1	1:B:905:ARG:HB2	2.52	0.44
1:C:1057:HIS:O	1:C:1061:THR:OG1	2.29	0.44
1:D:519:ALA:HB2	1:D:870:MET:HE1	2.00	0.44
1:F:476:VAL:HG12	1:F:841:LEU:CD1	2.47	0.44
1:F:806:LEU:HB2	1:F:1002:TRP:CZ3	2.53	0.44
1:G:634:ASP:CB	1:G:640:LEU:HD22	2.47	0.44
1:H:352:LEU:HD11	1:H:1095:ARG:O	2.17	0.44
1:A:850:GLN:HE22	1:A:887:PRO:HD3	1.81	0.44
1:F:614:ASN:OD1	1:F:661:TRP:CD1	2.70	0.44
1:F:703:ALA:O	1:F:707:VAL:HG22	2.17	0.44
1:F:793:ILE:HD11	1:F:804:MET:SD	2.58	0.44
1:F:915:THR:HG22	1:F:916:LEU:N	2.33	0.44
1:F:1100:ARG:HD3	1:F:1105:SER:OG	2.17	0.44
1:H:1090:GLU:HB3	1:H:1093:LYS:CD	2.47	0.44
1:A:888:GLY:HA2	1:A:976:SER:O	2.18	0.44
1:D:348:ARG:O	1:D:351:TYR:HB3	2.18	0.44
1:D:504:ASP:HB3	1:D:626:TYR:CG	2.53	0.44
1:E:379:ILE:HD13	1:E:858:PRO:HB2	1.99	0.44
1:E:685:GLN:HG3	1:E:746:ASP:OD2	2.17	0.44
1:E:887:PRO:O	1:E:975:LEU:HD12	2.17	0.44
1:F:727:MET:O	1:F:731:VAL:HG23	2.18	0.44
1:F:913:LYS:HB2	1:F:914:TYR:CE2	2.51	0.44
1:G:595:LEU:HG	1:G:595:LEU:O	2.17	0.44
1:D:406:HIS:CE1	1:D:408:CYS:HB2	2.52	0.44
1:E:932:ALA:HA	1:E:935:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:922:ALA:HA	1:F:930:TYR:CE1	2.52	0.44
1:G:660:MET:HE1	1:G:674:TYR:HB3	1.99	0.44
1:G:915:THR:O	1:G:919:ILE:HG12	2.18	0.44
1:H:356:PRO:HB3	1:H:660:MET:HE3	2.00	0.44
1:H:362:ARG:NH1	1:H:417:SER:HA	2.33	0.44
1:H:416:PHE:HA	1:H:662:MET:CE	2.47	0.44
1:A:824:PHE:CD1	1:A:905:ARG:HD2	2.53	0.44
1:B:1040:VAL:HG11	1:B:1102:ALA:HB1	2.00	0.44
1:E:679:ASN:HB2	1:E:770:GLY:O	2.17	0.44
1:E:900:SER:HB3	1:E:996:PRO:HB2	2.00	0.44
1:F:789:THR:HG22	1:F:790:GLN:N	2.24	0.44
1:G:727:MET:HG3	1:G:1064:ARG:NH1	2.32	0.44
1:G:981:SER:O	1:G:982:ILE:C	2.61	0.44
1:H:624:ASP:OD1	1:H:625:GLN:HG2	2.18	0.44
1:H:959:GLU:OE2	1:H:1034:THR:HG21	2.18	0.44
1:B:428:GLU:OE2	1:B:435:ARG:HD2	2.18	0.44
1:B:618:LEU:HD11	1:B:862:MET:HE1	2.00	0.44
1:B:653:ILE:HG21	1:B:707:VAL:HG21	1.99	0.44
1:C:1075:GLN:NE2	1:C:1100:ARG:HH21	2.15	0.44
1:D:1069:LEU:HD23	1:E:721:GLN:NE2	2.32	0.44
1:E:1040:VAL:HA	1:E:1073:GLN:OE1	2.17	0.44
1:F:516:LYS:O	1:F:520:GLU:HG2	2.17	0.44
1:F:1082:GLU:HA	1:F:1085:LYS:HG3	1.99	0.44
1:H:360:ILE:HG23	1:H:360:ILE:HD12	1.76	0.44
1:H:443:SER:HB3	1:H:446:ASP:H	1.83	0.44
1:H:444:GLU:HA	1:H:447:LYS:HG3	2.00	0.44
1:A:772:VAL:HG11	1:A:1039:MET:O	2.18	0.44
1:A:963:LYS:HA	1:A:963:LYS:HD2	1.66	0.44
1:B:561:ALA:HB3	1:B:581:ALA:HB2	1.98	0.44
1:B:795:ILE:HG12	1:B:901:MET:HE1	1.99	0.44
1:C:555:ARG:HG3	1:C:555:ARG:HH11	1.83	0.44
1:C:847:VAL:HG13	1:C:971:LEU:HD13	1.99	0.44
1:C:923:LEU:HD11	1:C:996:PRO:HD3	2.00	0.44
1:D:953:TYR:N	1:D:953:TYR:HD2	2.16	0.44
1:D:1045:PHE:CE2	1:D:1059:LEU:HD13	2.53	0.44
1:E:575:ALA:O	1:E:579:THR:HG23	2.17	0.44
1:F:435:ARG:NH2	1:F:438:ASP:O	2.51	0.44
1:F:1108:PHE:CE2	1:F:1116:GLN:HG2	2.52	0.44
1:G:522:HIS:O	1:G:525:SER:OG	2.26	0.44
1:G:640:LEU:HA	1:G:644:THR:HG21	1.99	0.44
1:G:854:ARG:HA	1:G:877:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:350:HIS:ND1	1:H:350:HIS:O	2.51	0.44
1:H:817:ASP:OD1	1:H:818:LEU:N	2.51	0.44
1:B:411:PRO:HB3	1:B:658:GLU:HG2	2.00	0.43
1:D:850:GLN:CD	1:D:971:LEU:HB2	2.43	0.43
1:D:919:ILE:O	1:D:923:LEU:HG	2.18	0.43
1:F:659:LEU:O	1:F:676:PRO:HG3	2.18	0.43
1:F:895:ALA:HB3	1:F:1006:SER:OG	2.18	0.43
1:G:419:ASP:OD1	1:G:419:ASP:N	2.51	0.43
1:H:440:PHE:HE1	1:H:660:MET:SD	2.41	0.43
1:C:734:VAL:HG11	1:C:1059:LEU:HD21	2.00	0.43
1:C:966:ARG:HD3	1:C:975:LEU:O	2.18	0.43
1:D:748:SER:OG	1:D:1071:ASN:O	2.28	0.43
1:D:1007:ASP:OD1	1:D:1010:SER:OG	2.29	0.43
1:G:790:GLN:HE21	1:G:793:ILE:N	2.16	0.43
1:G:908:VAL:HG11	1:G:916:LEU:HG	2.00	0.43
1:G:1112:CYS:HB3	1:G:1115:VAL:HG23	1.99	0.43
1:H:417:SER:O	1:H:420:ILE:HG13	2.18	0.43
1:H:495:GLY:HA3	1:H:613:GLU:HG3	2.00	0.43
1:H:496:GLY:N	1:H:613:GLU:OE2	2.47	0.43
1:H:1092:GLU:H	1:H:1092:GLU:CD	2.26	0.43
1:A:1025:LYS:O	1:A:1028:SER:HB3	2.18	0.43
1:A:1049:LEU:O	1:A:1055:GLY:HA3	2.18	0.43
1:B:993:ASN:O	1:B:999:ARG:NH2	2.50	0.43
1:C:1016:ASP:OD1	1:C:1016:ASP:N	2.49	0.43
1:E:425:VAL:O	1:E:429:LEU:HG	2.18	0.43
1:G:533:ASP:O	1:G:537:ILE:HG12	2.18	0.43
1:G:698:TYR:HE1	1:G:726:TYR:HA	1.82	0.43
1:G:1058:GLY:HA3	1:G:1128:PHE:CD2	2.53	0.43
1:H:971:LEU:HD12	1:H:971:LEU:HA	1.72	0.43
1:A:444:GLU:OE1	1:A:447:LYS:HD2	2.18	0.43
1:C:953:TYR:O	1:C:957:ILE:HG22	2.18	0.43
1:C:1081:ASN:O	1:C:1085:LYS:HG3	2.19	0.43
1:D:1013:GLN:H	1:D:1013:GLN:CD	2.26	0.43
1:E:632:GLU:O	1:E:636:ARG:HB2	2.17	0.43
1:F:1086:LYS:HA	1:F:1089:GLN:HG3	1.99	0.43
1:G:527:SER:HB3	1:G:529:GLU:HG3	2.00	0.43
1:G:569:GLN:C	1:G:574:ARG:HH12	2.27	0.43
1:G:613:GLU:O	1:G:615:GLN:HG2	2.18	0.43
1:G:914:TYR:CD1	1:G:933:LEU:HD12	2.53	0.43
1:G:941:PRO:HG2	1:G:949:TYR:CD2	2.53	0.43
1:H:850:GLN:NE2	1:H:887:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:914:TYR:OH	1:H:936:ASP:OD2	2.37	0.43
1:A:432:MET:HE3	1:A:440:PHE:CB	2.48	0.43
1:A:488:LEU:HD13	1:A:845:GLY:HA3	2.00	0.43
1:A:1040:VAL:HG11	1:A:1102:ALA:HB1	2.00	0.43
1:A:1080:ASP:HB3	1:A:1083:VAL:CG2	2.48	0.43
1:B:419:ASP:OD1	1:B:419:ASP:N	2.51	0.43
1:D:773:GLU:OE1	1:D:784:THR:HG21	2.19	0.43
1:D:955:LEU:C	1:D:955:LEU:HD23	2.44	0.43
1:E:649:LEU:HD13	1:E:700:ILE:HD13	2.00	0.43
1:E:756:LYS:HG2	1:E:885:HIS:CD2	2.54	0.43
1:E:771:CYS:HA	1:E:1103:GLY:O	2.18	0.43
1:F:655:LYS:HD2	1:F:655:LYS:HA	1.79	0.43
1:F:1084:LEU:CD2	1:F:1099:VAL:HG21	2.48	0.43
1:G:352:LEU:HD12	1:G:352:LEU:H	1.84	0.43
1:G:401:GLU:HG3	1:G:404:VAL:HG12	2.01	0.43
1:G:745:PHE:CD1	1:G:1067:SER:HB2	2.54	0.43
1:H:406:HIS:ND1	1:H:407:PRO:HD2	2.33	0.43
1:H:1031:ASN:O	1:H:1034:THR:HG23	2.18	0.43
1:A:463:LEU:HG	1:A:852:VAL:HG12	2.01	0.43
1:A:803:ARG:NH1	1:A:808:ASP:OD1	2.46	0.43
1:C:555:ARG:HD2	1:C:585:GLU:OE2	2.19	0.43
1:D:823:THR:HG23	1:D:826:GLU:H	1.84	0.43
1:D:1013:GLN:HA	3:D:1325:HOH:O	2.19	0.43
1:E:981:SER:O	1:E:982:ILE:C	2.62	0.43
1:E:1114:GLU:OE1	1:E:1114:GLU:N	2.45	0.43
1:F:685:GLN:H	1:F:717:ARG:NH2	2.17	0.43
1:G:423:ARG:HH11	1:G:465:GLU:HG3	1.83	0.43
1:G:478:ALA:HA	1:G:482:GLU:HB2	2.00	0.43
1:G:1074:MET:HE2	1:G:1076:PHE:CZ	2.51	0.43
1:H:599:LEU:HD22	1:H:652:PHE:CD2	2.54	0.43
1:A:411:PRO:HB3	1:A:658:GLU:HG2	2.00	0.43
1:A:572:GLN:HG3	1:A:573:ARG:N	2.33	0.43
1:B:824:PHE:CD1	1:B:905:ARG:HB2	2.53	0.43
1:C:379:ILE:HD13	1:C:858:PRO:HB2	2.00	0.43
1:C:1020:PRO:HA	1:C:1023:ILE:HD12	2.00	0.43
1:D:348:ARG:NH1	1:D:348:ARG:HG2	2.34	0.43
1:D:760:PHE:CZ	1:E:1033:GLU:HB3	2.54	0.43
1:D:1045:PHE:HE2	1:D:1059:LEU:HD13	1.84	0.43
1:E:435:ARG:HG2	1:E:437:GLN:O	2.19	0.43
1:E:1047:LYS:HD2	1:E:1080:ASP:N	2.33	0.43
1:F:358:VAL:HG23	1:F:440:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1112:CYS:SG	1:H:1115:VAL:HG12	2.59	0.43
1:B:832:LYS:HD3	1:B:960:TRP:NE1	2.34	0.43
1:D:963:LYS:NZ	1:E:761:GLU:OE2	2.40	0.43
1:D:1102:ALA:C	1:D:1104:TYR:H	2.26	0.43
1:F:649:LEU:O	1:F:653:ILE:HG13	2.18	0.43
1:F:846:THR:O	1:F:849:SER:OG	2.22	0.43
1:F:1007:ASP:OD1	1:F:1042:ASN:HB2	2.19	0.43
1:G:982:ILE:O	1:G:1102:ALA:HB3	2.18	0.43
1:H:583:VAL:HG13	1:H:597:GLU:HG2	2.01	0.43
1:C:802:GLY:O	1:C:810:TYR:HA	2.19	0.43
1:D:398:GLN:HG3	1:D:401:GLU:CD	2.43	0.43
1:D:489:SER:O	1:D:492:GLN:HB3	2.19	0.43
1:D:512:MET:HG3	1:D:550:VAL:HG11	2.00	0.43
1:D:703:ALA:O	1:D:707:VAL:HG23	2.18	0.43
1:F:618:LEU:CD1	1:F:862:MET:HE1	2.46	0.43
1:F:960:TRP:CZ3	1:F:964:GLU:HG3	2.53	0.43
1:G:897:TYR:CZ	1:G:901:MET:HE2	2.53	0.43
1:B:913:LYS:HD3	1:B:914:TYR:CE2	2.54	0.43
1:B:1073:GLN:HE22	1:B:1075:GLN:NE2	2.16	0.43
1:C:821:LEU:HD22	1:C:826:GLU:C	2.44	0.43
1:D:348:ARG:HG2	1:D:348:ARG:HH11	1.84	0.43
1:D:752:MET:HB2	1:D:1036:ASN:ND2	2.33	0.43
1:D:1028:SER:HB3	1:D:1069:LEU:HD13	2.01	0.43
1:E:530:ASN:O	1:E:531:PRO:C	2.62	0.43
1:E:908:VAL:O	1:E:912:LYS:HA	2.18	0.43
1:E:1081:ASN:O	1:E:1085:LYS:HG3	2.19	0.43
1:F:769:MET:HE3	1:F:769:MET:HB3	1.78	0.43
1:F:854:ARG:HA	1:F:877:ALA:HB1	2.01	0.43
1:H:700:ILE:O	1:H:704:VAL:HG12	2.19	0.43
1:H:790:GLN:HE21	1:H:792:PRO:HB2	1.84	0.43
1:B:616:THR:HB	1:B:661:TRP:CG	2.54	0.42
1:B:657:ALA:HA	1:B:711:GLN:HB2	2.01	0.42
1:C:444:GLU:OE2	1:C:447:LYS:NZ	2.37	0.42
1:D:361:TYR:CE2	1:D:394:PRO:HG3	2.54	0.42
1:D:438:ASP:HA	1:D:674:TYR:CZ	2.54	0.42
1:E:604:THR:O	1:E:607:SER:OG	2.33	0.42
1:E:1021:THR:HG22	1:E:1025:LYS:HE2	2.00	0.42
1:G:1075:GLN:HE22	1:G:1103:GLY:H	1.67	0.42
1:H:612:GLU:OE2	1:H:860:PRO:HD2	2.19	0.42
1:H:1007:ASP:N	1:H:1007:ASP:OD1	2.52	0.42
1:A:526:LEU:HD22	1:A:533:ASP:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ARG:NH2	1:B:438:ASP:O	2.52	0.42
1:C:748:SER:OG	1:C:1071:ASN:O	2.25	0.42
1:D:686:LYS:HB2	1:D:689:GLY:O	2.19	0.42
1:D:832:LYS:HB3	1:D:960:TRP:CZ2	2.54	0.42
1:D:986:THR:HB	1:D:987:PRO:HD3	2.00	0.42
1:E:452:GLU:O	1:E:456:PRO:HG2	2.19	0.42
1:E:989:GLY:HA2	1:E:1005:LEU:HD21	2.01	0.42
1:F:915:THR:CG2	1:F:916:LEU:N	2.82	0.42
1:F:1085:LYS:H	1:F:1085:LYS:HG2	1.59	0.42
1:H:360:ILE:HG13	1:H:446:ASP:HB3	2.01	0.42
1:H:734:VAL:HA	1:H:740:PHE:O	2.19	0.42
1:B:867:GLU:OE1	1:B:882:MET:HE1	2.20	0.42
1:D:496:GLY:HA3	1:D:859:LYS:HE3	2.01	0.42
1:D:513:ASN:ND2	1:D:589:ALA:HB1	2.34	0.42
1:E:697:THR:O	1:E:701:MET:HG3	2.19	0.42
1:E:1039:MET:SD	1:E:1072:GLY:HA3	2.59	0.42
1:F:1047:LYS:HG3	1:F:1080:ASP:HB2	2.00	0.42
1:G:362:ARG:NH1	1:G:417:SER:HA	2.34	0.42
1:G:380:LEU:O	1:G:384:LYS:HG3	2.19	0.42
1:G:694:ASN:OD1	1:G:697:THR:N	2.37	0.42
1:H:604:THR:O	1:H:607:SER:OG	2.23	0.42
1:B:1093:LYS:O	1:B:1093:LYS:HG2	2.18	0.42
1:C:579:THR:O	1:C:583:VAL:HG23	2.19	0.42
1:C:1063:LEU:HD23	1:C:1063:LEU:HA	1.86	0.42
1:D:343:ARG:HG2	1:D:647:GLU:OE2	2.20	0.42
1:D:685:GLN:NE2	1:D:746:ASP:OD2	2.45	0.42
1:D:835:ILE:O	1:D:838:ILE:HB	2.19	0.42
1:H:680:LEU:HD21	1:H:700:ILE:HG21	2.02	0.42
1:A:337:MET:HB3	1:A:340:LEU:HD12	2.00	0.42
1:A:986:THR:HB	1:A:987:PRO:CD	2.49	0.42
1:B:435:ARG:CZ	1:B:437:GLN:O	2.66	0.42
1:B:623:VAL:HA	1:B:626:TYR:CE2	2.55	0.42
1:C:835:ILE:HD13	1:C:957:ILE:HD11	2.01	0.42
1:D:539:TYR:OH	1:D:869:CYS:HB3	2.20	0.42
1:D:613:GLU:OE2	1:D:859:LYS:NZ	2.43	0.42
1:D:1063:LEU:HD21	1:D:1076:PHE:CZ	2.55	0.42
1:F:443:SER:HB3	1:F:446:ASP:HB2	2.01	0.42
1:F:718:ILE:HD12	1:F:743:CYS:HB3	2.01	0.42
1:F:1044:LYS:NZ	1:F:1119:ILE:O	2.53	0.42
1:G:579:THR:O	1:G:583:VAL:HG22	2.19	0.42
1:G:1009:ILE:HD13	1:G:1039:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:576:GLU:O	1:H:580:ILE:HG13	2.19	0.42
1:B:795:ILE:HD11	1:B:901:MET:HE2	2.01	0.42
1:C:799:LEU:O	1:C:920:ARG:HD3	2.20	0.42
1:C:839:VAL:HG11	1:C:964:GLU:HG3	2.02	0.42
1:D:476:VAL:HG12	1:D:841:LEU:HG	2.01	0.42
1:D:671:PHE:CE2	2:D:1201:A1H9K:C1	3.03	0.42
1:E:659:LEU:HD23	1:E:678:ILE:HD11	2.01	0.42
1:F:803:ARG:HH22	1:F:924:LEU:HD21	1.85	0.42
1:G:676:PRO:HG2	1:G:711:GLN:OE1	2.19	0.42
1:C:489:SER:O	1:C:493:ILE:HG12	2.20	0.42
1:C:687:ARG:HD2	1:C:765:ASP:OD2	2.20	0.42
1:C:879:GLY:O	1:C:884:ASN:ND2	2.51	0.42
1:C:953:TYR:HA	1:C:956:ASP:OD1	2.20	0.42
1:D:359:SER:OG	1:D:408:CYS:HB3	2.20	0.42
1:D:560:HIS:HA	1:D:563:GLU:HG2	2.01	0.42
1:D:1040:VAL:HA	1:D:1073:GLN:OE1	2.19	0.42
1:F:444:GLU:HA	1:F:447:LYS:CD	2.48	0.42
1:F:957:ILE:O	1:F:961:THR:OG1	2.35	0.42
1:F:1115:VAL:O	1:F:1119:ILE:HG13	2.20	0.42
1:G:655:LYS:HA	1:G:658:GLU:HG3	2.00	0.42
1:G:865:LEU:HA	1:G:865:LEU:HD23	1.85	0.42
1:G:1007:ASP:O	1:G:1010:SER:HB2	2.20	0.42
1:H:552:ASN:O	1:H:556:ARG:HB2	2.19	0.42
1:H:781:TYR:HB2	1:H:881:ALA:HB2	2.02	0.42
1:H:782:GLN:O	1:H:782:GLN:HG2	2.17	0.42
1:H:1061:THR:O	1:H:1065:THR:HG23	2.19	0.42
1:C:428:GLU:OE2	1:C:665:GLU:HB2	2.20	0.42
1:C:502:GLY:H	1:C:865:LEU:HB3	1.84	0.42
1:C:850:GLN:NE2	1:C:887:PRO:HD3	2.35	0.42
1:C:1095:ARG:O	1:C:1095:ARG:HD3	2.19	0.42
1:D:504:ASP:OD2	1:D:505:VAL:HG13	2.20	0.42
1:F:390:CYS:HB3	1:F:553:TYR:HB2	2.01	0.42
1:F:943:TYR:HD1	1:F:951:ASP:OD1	2.02	0.42
1:F:1080:ASP:OD1	1:F:1082:GLU:N	2.53	0.42
1:G:428:GLU:HG2	1:G:431:THR:OG1	2.20	0.42
1:G:804:MET:HE2	1:G:807:PHE:CD2	2.55	0.42
1:G:906:LYS:CE	1:G:941:PRO:HD3	2.49	0.42
1:A:530:ASN:HB3	1:A:532:GLU:OE1	2.20	0.42
1:B:369:VAL:HG21	1:B:385:ALA:HA	2.01	0.42
1:B:779:ARG:HG2	1:B:882:MET:SD	2.60	0.42
1:D:971:LEU:HD12	1:D:971:LEU:HA	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:SER:HB3	1:E:408:CYS:HB3	2.02	0.42
1:E:657:ALA:HA	1:E:711:GLN:HB2	2.02	0.42
1:E:850:GLN:HB3	1:E:971:LEU:HD22	2.02	0.42
1:F:470:GLN:HG2	1:H:377:PRO:HD3	2.01	0.42
1:F:900:SER:O	1:F:903:ALA:HB3	2.20	0.42
1:H:1080:ASP:O	1:H:1084:LEU:HD12	2.20	0.42
1:A:850:GLN:HB3	1:A:971:LEU:HD22	2.02	0.42
1:B:599:LEU:HA	1:B:599:LEU:HD23	1.67	0.42
1:B:620:LEU:HD12	1:B:680:LEU:HD13	2.01	0.42
1:B:898:VAL:HG12	1:B:950:VAL:HG22	2.01	0.42
1:D:789:THR:O	1:D:891:PHE:HA	2.20	0.42
1:E:798:VAL:HG21	1:E:831:VAL:HA	2.02	0.42
1:E:835:ILE:HG22	1:E:960:TRP:HZ3	1.85	0.42
1:G:463:LEU:HG	1:G:852:VAL:HG12	2.01	0.42
1:G:1021:THR:O	1:G:1025:LYS:HG3	2.20	0.42
1:H:685:GLN:C	1:H:692:ALA:HB2	2.44	0.42
1:H:988:ILE:O	1:H:991:LEU:HB2	2.20	0.42
1:H:1046:LEU:HD12	1:H:1047:LYS:N	2.35	0.42
1:H:1118:GLU:O	1:H:1121:SER:OG	2.25	0.42
1:A:739:GLY:HA3	1:A:1100:ARG:HB2	2.01	0.41
1:A:1016:ASP:OD1	1:A:1016:ASP:N	2.37	0.41
1:B:435:ARG:HH21	1:B:437:GLN:C	2.19	0.41
1:B:850:GLN:NE2	1:B:887:PRO:HD3	2.35	0.41
1:D:976:SER:HB3	1:D:1037:ILE:HD11	2.02	0.41
1:E:423:ARG:NH1	1:E:468:GLU:OE1	2.53	0.41
1:E:428:GLU:HB3	1:E:432:MET:HG2	2.02	0.41
1:F:1007:ASP:OD2	1:F:1122:ARG:HD3	2.19	0.41
1:F:1113:LYS:HB3	1:F:1113:LYS:HE2	1.62	0.41
1:G:504:ASP:HB3	1:G:626:TYR:CG	2.55	0.41
1:H:798:VAL:HG23	1:H:834:GLN:HG3	2.01	0.41
1:H:919:ILE:HG22	1:H:923:LEU:HD11	2.01	0.41
1:C:813:LEU:O	1:C:834:GLN:NE2	2.34	0.41
1:E:504:ASP:OD1	1:E:504:ASP:N	2.48	0.41
1:F:493:ILE:O	1:F:494:ASN:ND2	2.54	0.41
1:F:550:VAL:O	1:F:553:TYR:HB3	2.21	0.41
1:F:804:MET:O	1:F:808:ASP:HA	2.21	0.41
1:F:941:PRO:HB3	1:F:947:ASP:OD2	2.20	0.41
1:G:350:HIS:HA	1:G:353:THR:HG23	2.02	0.41
1:H:435:ARG:HH21	1:H:438:ASP:HB2	1.84	0.41
1:H:565:ALA:HB1	1:H:574:ARG:HG3	2.01	0.41
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:TYR:CE2	1:E:394:PRO:HG3	2.55	0.41
1:E:896:THR:N	1:E:1006:SER:OG	2.52	0.41
1:E:1009:ILE:HG22	1:E:1035:MET:HE1	1.97	0.41
1:F:477:TRP:CD2	1:F:481:GLY:HA3	2.56	0.41
1:F:623:VAL:HG22	1:F:680:LEU:HD21	2.02	0.41
1:G:362:ARG:NH2	1:G:612:GLU:O	2.44	0.41
1:G:448:LYS:HE2	1:G:452:GLU:OE2	2.20	0.41
1:G:551:VAL:O	1:G:555:ARG:HG2	2.20	0.41
1:G:969:LYS:O	1:G:970:MET:HE2	2.20	0.41
1:H:1077:SER:HB2	1:H:1100:ARG:HB3	2.01	0.41
1:A:609:PHE:CD1	1:A:861:LEU:HD23	2.55	0.41
1:A:957:ILE:HD12	1:A:957:ILE:HA	1.83	0.41
1:B:613:GLU:O	1:B:615:GLN:HG2	2.20	0.41
1:C:398:GLN:HB2	1:C:401:GLU:CD	2.45	0.41
1:C:1019:GLY:O	1:C:1023:ILE:HG13	2.20	0.41
1:E:914:TYR:CZ	1:E:933:LEU:HB3	2.55	0.41
1:E:923:LEU:HD22	1:E:994:ALA:C	2.45	0.41
1:G:450:ILE:HA	1:G:454:ILE:HB	2.01	0.41
1:G:522:HIS:HB3	1:G:540:TYR:CE2	2.56	0.41
1:G:1077:SER:HB2	1:G:1100:ARG:HB3	2.03	0.41
1:H:344:MET:HE1	1:H:654:ILE:HD11	2.02	0.41
1:A:356:PRO:HA	1:A:412:ARG:O	2.21	0.41
1:A:622:ARG:HH11	1:A:765:ASP:HA	1.84	0.41
1:A:743:CYS:O	1:A:1073:GLN:HG2	2.20	0.41
1:B:605:VAL:HG11	1:B:865:LEU:HD11	2.02	0.41
1:B:882:MET:HE3	1:B:882:MET:HB2	1.90	0.41
1:D:676:PRO:HB2	1:D:678:ILE:HG13	2.02	0.41
1:D:797:PHE:HE1	1:D:804:MET:HB2	1.84	0.41
1:D:934:ARG:NE	1:D:938:LEU:HD11	2.35	0.41
1:E:349:ASN:O	1:E:353:THR:HG23	2.21	0.41
1:E:502:GLY:HA3	1:E:505:VAL:HG12	2.03	0.41
1:E:720:ASN:OD1	1:E:1067:SER:OG	2.38	0.41
1:F:927:PHE:HE2	1:F:933:LEU:HD23	1.86	0.41
1:F:984:ASN:HA	1:F:987:PRO:HD2	2.02	0.41
1:F:1082:GLU:CG	1:F:1085:LYS:HE3	2.48	0.41
1:G:775:GLN:CG	1:G:780:ILE:HG21	2.42	0.41
1:G:1086:LYS:O	1:G:1086:LYS:HG3	2.21	0.41
1:H:359:SER:O	1:H:360:ILE:HD13	2.20	0.41
1:H:628:TYR:O	1:H:631:PHE:N	2.54	0.41
1:H:1052:THR:O	1:H:1056:ARG:HG3	2.20	0.41
1:A:696:LEU:HD12	1:A:696:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ILE:O	1:A:848:ILE:HG13	2.20	0.41
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.86	0.41
1:B:905:ARG:CZ	1:B:949:TYR:CE1	3.03	0.41
1:C:796:GLU:OE2	1:C:805:VAL:HG23	2.19	0.41
1:C:953:TYR:O	1:C:956:ASP:OD1	2.38	0.41
1:D:913:LYS:HD3	1:D:913:LYS:HA	1.77	0.41
1:D:973:SER:OG	1:D:974:THR:N	2.48	0.41
1:F:740:PHE:HA	1:F:741:PRO:HA	1.83	0.41
1:F:1009:ILE:HG12	1:F:1040:VAL:O	2.20	0.41
1:F:1075:GLN:NE2	1:F:1103:GLY:HA2	2.12	0.41
1:G:650:GLN:HG2	1:G:707:VAL:HG22	2.01	0.41
1:H:656:CYS:HB2	1:H:712:PRO:HD3	2.03	0.41
1:H:932:ALA:O	1:H:935:ARG:HB2	2.21	0.41
1:A:379:ILE:HG23	1:A:380:LEU:N	2.36	0.41
1:A:1013:GLN:HB3	1:A:1121:SER:O	2.20	0.41
1:B:927:PHE:CG	1:B:934:ARG:HD2	2.55	0.41
1:C:804:MET:HE3	1:C:807:PHE:CD2	2.53	0.41
1:D:558:ALA:O	1:D:561:ALA:HB3	2.21	0.41
1:F:1081:ASN:O	1:F:1085:LYS:HG2	2.20	0.41
1:G:727:MET:O	1:G:731:VAL:HG23	2.20	0.41
1:G:821:LEU:H	1:G:821:LEU:HG	1.50	0.41
1:H:697:THR:HG22	1:H:701:MET:SD	2.61	0.41
1:B:617:GLY:HA2	1:B:677:PHE:HB2	2.03	0.41
1:B:863:SER:OG	1:B:875:ASP:HB2	2.21	0.41
1:C:622:ARG:NH1	1:C:765:ASP:HA	2.36	0.41
1:D:761:GLU:H	1:D:761:GLU:HG2	1.72	0.41
1:D:901:MET:HB3	1:D:953:TYR:HD1	1.85	0.41
1:E:622:ARG:NH2	1:E:685:GLN:O	2.52	0.41
1:E:931:GLU:OE1	1:E:931:GLU:N	2.49	0.41
1:F:913:LYS:HB2	1:F:914:TYR:CD2	2.56	0.41
1:G:393:ALA:N	1:G:556:ARG:HH22	2.18	0.41
1:G:449:THR:O	1:G:453:GLU:HB2	2.21	0.41
1:G:622:ARG:HH11	1:G:622:ARG:HG3	1.86	0.41
1:G:820:ASP:O	1:G:826:GLU:OE1	2.39	0.41
1:H:379:ILE:HG23	1:H:380:LEU:N	2.35	0.41
1:H:550:VAL:HG11	1:H:608:LEU:HD13	2.01	0.41
1:H:587:VAL:HG11	1:H:592:PRO:HB3	2.03	0.41
1:H:635:ILE:HG12	1:H:640:LEU:O	2.21	0.41
1:H:645:ALA:O	1:H:649:LEU:HG	2.21	0.41
1:H:706:PHE:HD1	1:H:706:PHE:HA	1.79	0.41
1:H:726:TYR:CE2	1:H:730:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:734:VAL:HG21	1:H:1076:PHE:HB2	2.03	0.41
1:H:1049:LEU:O	1:H:1055:GLY:HA3	2.21	0.41
1:A:571:ALA:HA	3:A:1361:HOH:O	2.21	0.41
1:A:616:THR:HB	1:A:661:TRP:CG	2.56	0.41
1:A:905:ARG:NH1	1:A:953:TYR:OH	2.48	0.41
1:A:927:PHE:CG	1:A:934:ARG:HD2	2.55	0.41
1:A:943:TYR:O	1:A:1011:PRO:HB3	2.21	0.41
1:A:1085:LYS:O	1:A:1088:GLN:HB2	2.21	0.41
1:B:348:ARG:O	1:B:351:TYR:HB3	2.21	0.41
1:B:944:GLY:HA3	1:B:1011:PRO:HG3	2.03	0.41
1:B:1100:ARG:HG3	1:B:1104:TYR:O	2.20	0.41
1:C:352:LEU:HD23	1:C:352:LEU:HA	1.94	0.41
1:C:495:GLY:HA3	1:C:613:GLU:HG3	2.03	0.41
1:C:794:ALA:CB	1:C:835:ILE:HG13	2.51	0.41
1:C:797:PHE:HD1	1:C:797:PHE:HA	1.79	0.41
1:C:1084:LEU:HD22	1:C:1108:PHE:CE1	2.56	0.41
1:E:904:ILE:HD11	1:E:996:PRO:HG2	2.03	0.41
1:E:906:LYS:HE3	1:E:907:LEU:CD2	2.51	0.41
1:E:971:LEU:HD12	1:E:971:LEU:HA	1.68	0.41
1:E:1094:TYR:HD1	1:E:1094:TYR:N	2.18	0.41
1:F:1017:LYS:HE2	1:F:1017:LYS:HB3	1.93	0.41
1:G:512:MET:HE3	1:G:550:VAL:HG11	2.02	0.41
1:G:550:VAL:CG2	1:G:608:LEU:HD12	2.46	0.41
1:G:583:VAL:HG21	1:G:596:GLN:HE21	1.86	0.41
1:G:587:VAL:HG21	1:G:597:GLU:HA	2.03	0.41
1:G:749:HIS:HA	1:G:752:MET:SD	2.60	0.41
1:G:966:ARG:HD3	1:G:975:LEU:O	2.21	0.41
1:H:613:GLU:O	1:H:615:GLN:HG2	2.20	0.41
1:H:971:LEU:HB3	1:H:972:TYR:CE2	2.55	0.41
1:A:1023:ILE:HD13	1:A:1023:ILE:HG21	1.86	0.41
1:B:793:ILE:HD12	1:B:793:ILE:HA	1.79	0.41
1:B:923:LEU:HD13	1:B:994:ALA:O	2.21	0.41
1:B:986:THR:HG21	1:B:1114:GLU:HB3	2.03	0.41
1:B:1006:SER:HB3	1:B:1012:THR:HG22	2.03	0.41
1:D:520:GLU:HG3	1:D:544:ILE:CD1	2.51	0.41
1:D:1021:THR:HA	1:D:1024:ILE:HG12	2.03	0.41
1:E:522:HIS:HB3	1:E:540:TYR:CE2	2.56	0.41
1:E:616:THR:HB	1:E:661:TRP:CG	2.56	0.41
1:E:791:TRP:HD1	1:E:835:ILE:HD13	1.85	0.41
1:E:1025:LYS:O	1:E:1028:SER:HB3	2.20	0.41
1:E:1074:MET:HE2	1:E:1076:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:MET:SD	1:F:377:PRO:HD2	2.61	0.41
1:F:753:MET:HE3	1:F:753:MET:HB3	1.88	0.41
1:F:905:ARG:O	1:F:909:PHE:HB2	2.20	0.41
1:F:969:LYS:O	1:F:970:MET:HE2	2.20	0.41
1:F:1088:GLN:NE2	1:F:1113:LYS:HG3	2.35	0.41
1:G:404:VAL:H	1:G:600:GLN:HE22	1.69	0.41
1:G:416:PHE:CE1	1:G:425:VAL:HG21	2.56	0.41
1:G:1040:VAL:HA	1:G:1073:GLN:OE1	2.21	0.41
1:B:551:VAL:HG22	1:B:589:ALA:HB2	2.04	0.40
1:B:919:ILE:O	1:B:923:LEU:HG	2.21	0.40
1:D:646:LEU:HA	1:D:646:LEU:HD12	1.82	0.40
1:D:994:ALA:N	1:D:1001:ALA:HA	2.36	0.40
1:E:499:THR:O	1:E:501:PRO:HD3	2.21	0.40
1:E:677:PHE:O	1:E:770:GLY:HA2	2.21	0.40
1:E:829:ALA:O	1:E:833:GLN:HG3	2.20	0.40
1:E:1087:ALA:HB2	1:E:1094:TYR:CD2	2.56	0.40
1:F:1055:GLY:HA2	1:F:1128:PHE:CE1	2.53	0.40
1:H:366:PHE:CD1	1:H:385:ALA:HB1	2.56	0.40
1:H:731:VAL:HA	1:H:734:VAL:HG12	2.04	0.40
1:H:850:GLN:OE1	1:H:971:LEU:HB2	2.21	0.40
1:A:619:SER:HB3	1:A:679:ASN:HB3	2.02	0.40
1:A:1033:GLU:H	1:A:1033:GLU:CD	2.29	0.40
1:B:699:LEU:HA	1:B:699:LEU:HD23	1.84	0.40
1:C:432:MET:HE3	1:C:442:ILE:HG21	2.02	0.40
1:C:1127:LYS:HD2	1:C:1128:PHE:C	2.46	0.40
1:D:727:MET:O	1:D:730:ILE:HB	2.22	0.40
1:E:801:ARG:HG2	1:E:816:GLY:O	2.21	0.40
1:F:627:CYS:HA	1:F:630:MET:CE	2.51	0.40
1:F:650:GLN:HB3	1:F:707:VAL:CG1	2.51	0.40
1:F:1052:THR:CG2	1:F:1055:GLY:H	2.26	0.40
1:G:701:MET:HG2	1:G:714:LEU:HD21	2.02	0.40
1:H:400:ASP:HA	1:H:573:ARG:NH1	2.34	0.40
1:H:653:ILE:O	1:H:656:CYS:HB2	2.22	0.40
1:H:783:TRP:HH2	1:H:853:HIS:HB2	1.86	0.40
1:A:618:LEU:CD1	1:A:862:MET:HE1	2.45	0.40
1:A:622:ARG:NH1	1:A:765:ASP:HA	2.36	0.40
1:B:1088:GLN:HG2	1:B:1116:GLN:OE1	2.21	0.40
1:C:653:ILE:HG23	1:C:712:PRO:CD	2.46	0.40
1:C:713:SER:HA	1:C:740:PHE:CE1	2.56	0.40
1:C:791:TRP:HB2	1:C:792:PRO:HD3	2.03	0.40
1:D:536:ARG:HG2	1:D:873:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:885:HIS:CE1	1:D:966:ARG:HH22	2.40	0.40
1:D:1122:ARG:HA	3:D:1325:HOH:O	2.21	0.40
1:E:1075:GLN:OE1	1:E:1100:ARG:NH1	2.54	0.40
1:E:1094:TYR:N	1:E:1094:TYR:CD1	2.87	0.40
1:G:503:TYR:O	1:G:507:LEU:HB3	2.22	0.40
1:H:341:THR:OG1	1:H:647:GLU:HG3	2.21	0.40
1:H:739:GLY:HA2	1:H:1077:SER:HA	2.03	0.40
1:H:854:ARG:HA	1:H:877:ALA:HB1	2.02	0.40
1:A:419:ASP:OD1	1:A:419:ASP:N	2.50	0.40
1:A:742:ALA:HB1	1:A:1073:GLN:HE21	1.87	0.40
1:D:828:ASP:HA	1:D:831:VAL:HG22	2.04	0.40
1:E:513:ASN:ND2	1:E:589:ALA:HB1	2.36	0.40
1:E:861:LEU:O	1:E:862:MET:C	2.65	0.40
1:F:681:THR:CG2	1:F:768:LEU:HD23	2.52	0.40
1:F:957:ILE:HD12	1:F:957:ILE:HA	1.89	0.40
1:G:571:ALA:HA	1:G:574:ARG:CZ	2.52	0.40
1:G:655:LYS:HG3	1:G:658:GLU:OE1	2.21	0.40
1:G:835:ILE:O	1:G:839:VAL:HG23	2.20	0.40
1:H:718:ILE:HD12	1:H:743:CYS:HB3	2.03	0.40
1:A:620:LEU:HD12	1:A:680:LEU:HD12	2.03	0.40
1:B:348:ARG:O	1:B:352:LEU:HD12	2.21	0.40
1:B:418:PRO:HB2	1:B:458:TRP:CG	2.56	0.40
1:D:350:HIS:O	1:D:353:THR:OG1	2.37	0.40
1:D:687:ARG:HD2	1:D:765:ASP:OD2	2.22	0.40
1:F:419:ASP:HB3	1:F:458:TRP:CH2	2.56	0.40
1:F:963:LYS:HB2	1:F:963:LYS:HE2	1.68	0.40
1:H:380:LEU:HA	1:H:542:ALA:HB2	2.04	0.40
1:H:402:LEU:HA	1:H:580:ILE:HD11	2.03	0.40
1:H:562:ARG:HG3	1:H:581:ALA:HB1	2.04	0.40
1:H:801:ARG:HG2	1:H:801:ARG:NH1	2.27	0.40
1:H:922:ALA:HA	1:H:930:TYR:CE2	2.57	0.40
1:H:1080:ASP:HB3	1:H:1083:VAL:HG23	2.03	0.40

All (2) 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:F:912:LYS:NZ	1:G:822:ARG:NH1[1_455]	1.92	0.28
1:D:822:ARG:NH1	1:E:820:ASP:OD2[1_455]	2.02	0.18

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%)	749 (95%)	41 (5%)	0	100	100
1	B	790/1150 (69%)	750 (95%)	39 (5%)	1 (0%)	48	73
1	C	789/1150 (69%)	753 (95%)	35 (4%)	1 (0%)	48	73
1	D	790/1150 (69%)	736 (93%)	54 (7%)	0	100	100
1	E	790/1150 (69%)	741 (94%)	49 (6%)	0	100	100
1	F	790/1150 (69%)	725 (92%)	63 (8%)	2 (0%)	36	60
1	G	790/1150 (69%)	734 (93%)	55 (7%)	1 (0%)	48	73
1	H	790/1150 (69%)	716 (91%)	73 (9%)	1 (0%)	48	73
All	All	6319/9200 (69%)	5904 (93%)	409 (6%)	6 (0%)	48	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	982	ILE
1	F	982	ILE
1	F	771	CYS
1	G	819	ARG
1	H	571	ALA
1	B	982	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	668/955 (70%)	668 (100%)	0	100	100
1	B	668/955 (70%)	668 (100%)	0	100	100
1	C	667/955 (70%)	667 (100%)	0	100	100
1	D	668/955 (70%)	668 (100%)	0	100	100
1	E	668/955 (70%)	668 (100%)	0	100	100
1	F	668/955 (70%)	668 (100%)	0	100	100
1	G	668/955 (70%)	668 (100%)	0	100	100
1	H	668/955 (70%)	668 (100%)	0	100	100
All	All	5343/7640 (70%)	5343 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	ASN
1	A	572	GLN
1	A	721	GLN
1	A	811	GLN
1	A	837	HIS
1	A	853	HIS
1	A	884	ASN
1	A	1057	HIS
1	B	642	HIS
1	B	837	HIS
1	B	952	GLN
1	B	1042	ASN
1	B	1057	HIS
1	B	1075	GLN
1	C	470	GLN
1	C	560	HIS
1	C	811	GLN
1	C	1071	ASN
1	C	1073	GLN
1	C	1075	GLN
1	D	350	HIS
1	D	494	ASN
1	D	590	ASN
1	D	650	GLN
1	D	675	GLN

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Mol	Chain	Res	Type
1	D	744	HIS
1	D	884	ASN
1	D	885	HIS
1	D	926	ASN
1	D	939	ASN
1	D	1036	ASN
1	D	1075	GLN
1	D	1088	GLN
1	E	373	ASN
1	E	388	HIS
1	E	569	GLN
1	E	590	ASN
1	E	811	GLN
1	E	837	HIS
1	E	993	ASN
1	E	1031	ASN
1	E	1036	ASN
1	E	1075	GLN
1	F	350	HIS
1	F	398	GLN
1	F	492	GLN
1	F	494	ASN
1	F	569	GLN
1	F	596	GLN
1	F	675	GLN
1	F	711	GLN
1	F	749	HIS
1	F	800	ASN
1	F	837	HIS
1	F	948	ASN
1	F	952	GLN
1	F	1036	ASN
1	F	1075	GLN
1	F	1088	GLN
1	G	513	ASN
1	G	530	ASN
1	G	552	ASN
1	G	569	GLN
1	G	570	ASN
1	G	586	ASN
1	G	596	GLN
1	G	642	HIS

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Mol	Chain	Res	Type
1	G	724	GLN
1	G	749	HIS
1	G	775	GLN
1	G	790	GLN
1	G	1081	ASN
1	G	1089	GLN
1	H	494	ASN
1	H	570	ASN
1	H	642	HIS
1	H	721	GLN
1	H	790	GLN
1	H	811	GLN
1	H	884	ASN
1	H	918	GLN
1	H	1089	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	A1H9K	A	1201	-	8,9,9	3.27	2 (25%)	8,13,13	1.53	2 (25%)
2	A1H9K	B	1201	-	8,9,9	3.21	2 (25%)	8,13,13	0.74	0
2	A1H9K	G	1201	-	8,9,9	3.23	2 (25%)	8,13,13	0.85	0
2	A1H9K	D	1201	-	8,9,9	3.13	3 (37%)	8,13,13	1.62	1 (12%)
2	A1H9K	E	1201	-	8,9,9	2.93	2 (25%)	8,13,13	0.71	0
2	A1H9K	H	1201	-	8,9,9	3.23	2 (25%)	8,13,13	0.76	0
2	A1H9K	F	1201	-	8,9,9	3.32	2 (25%)	8,13,13	0.67	0
2	A1H9K	C	1201	-	8,9,9	3.30	3 (37%)	8,13,13	0.70	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	A1H9K	A	1201	-	-	2/4/12/12	0/1/1/1
2	A1H9K	B	1201	-	-	1/4/12/12	0/1/1/1
2	A1H9K	G	1201	-	-	3/4/12/12	0/1/1/1
2	A1H9K	D	1201	-	-	1/4/12/12	0/1/1/1
2	A1H9K	E	1201	-	-	4/4/12/12	0/1/1/1
2	A1H9K	H	1201	-	-	1/4/12/12	0/1/1/1
2	A1H9K	F	1201	-	-	3/4/12/12	0/1/1/1
2	A1H9K	C	1201	-	-	0/4/12/12	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1201	A1H9K	C3-N4	-8.72	1.47	1.55
2	A	1201	A1H9K	C3-N4	-8.64	1.47	1.55
2	G	1201	A1H9K	C3-N4	-8.50	1.47	1.55
2	C	1201	A1H9K	C3-N4	-8.37	1.47	1.55
2	H	1201	A1H9K	C3-N4	-8.37	1.47	1.55
2	B	1201	A1H9K	C3-N4	-8.34	1.47	1.55
2	D	1201	A1H9K	C3-N4	-7.98	1.47	1.55
2	E	1201	A1H9K	C3-N4	-7.55	1.48	1.55
2	D	1201	A1H9K	C2-C3	2.57	1.53	1.47
2	C	1201	A1H9K	C2-C3	2.49	1.53	1.47
2	C	1201	A1H9K	C1-C3	2.43	1.53	1.47
2	F	1201	A1H9K	C1-C3	2.26	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1201	A1H9K	C1-C3	2.25	1.53	1.47
2	B	1201	A1H9K	C2-C3	2.24	1.52	1.47
2	G	1201	A1H9K	C1-C3	2.20	1.52	1.47
2	A	1201	A1H9K	C1-C3	2.14	1.52	1.47
2	D	1201	A1H9K	C1-C3	2.11	1.52	1.47
2	E	1201	A1H9K	C1-C3	2.06	1.52	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	A1H9K	C9-N4-C5	-3.45	101.13	109.48
2	A	1201	A1H9K	C8-N4-C5	2.95	116.63	109.48
2	A	1201	A1H9K	C9-N4-C5	2.55	115.66	109.48

There are no chirality outliers.

All (15) torsion outliers are listed below:

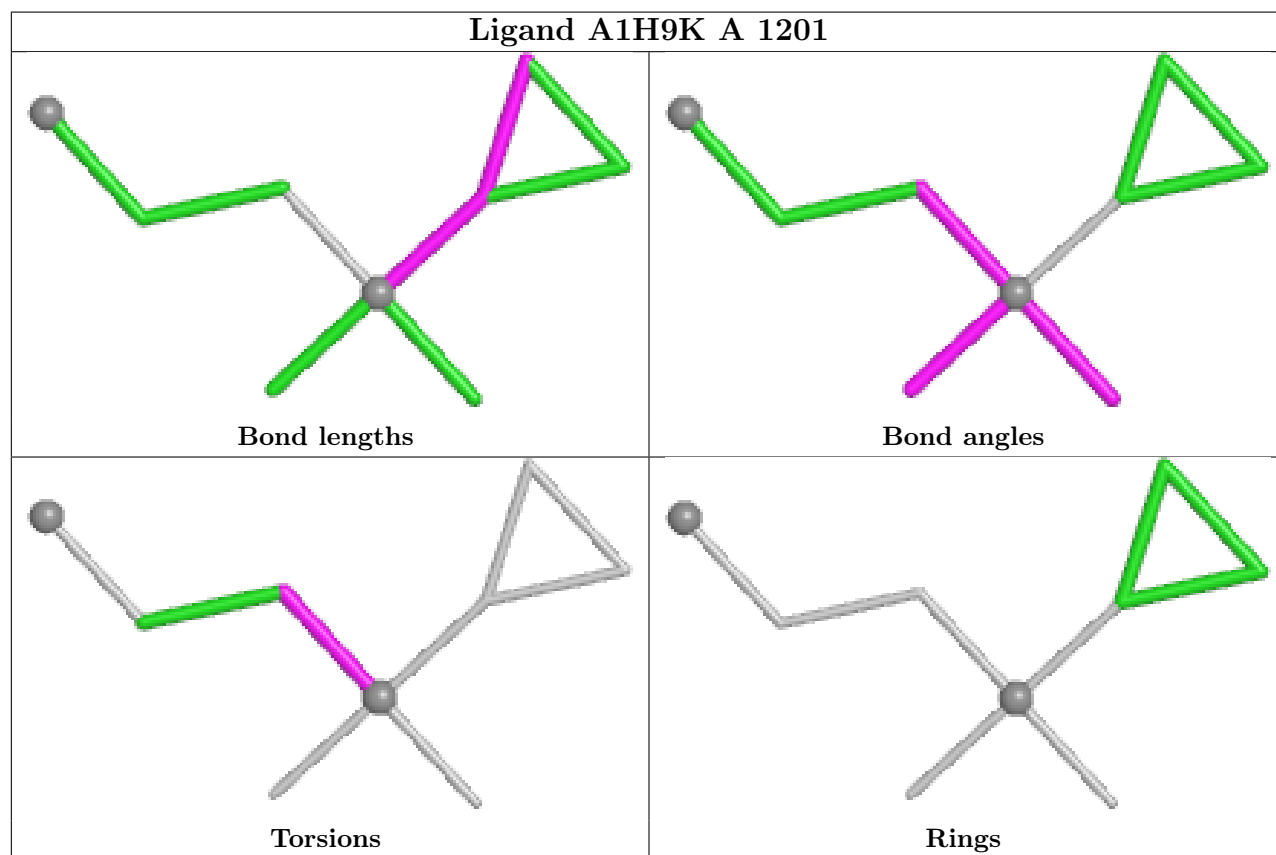
Mol	Chain	Res	Type	Atoms
2	B	1201	A1H9K	N4-C5-C6-O1
2	E	1201	A1H9K	C6-C5-N4-C9
2	E	1201	A1H9K	N4-C5-C6-O1
2	G	1201	A1H9K	N4-C5-C6-O1
2	E	1201	A1H9K	C6-C5-N4-C8
2	G	1201	A1H9K	C6-C5-N4-C8
2	G	1201	A1H9K	C6-C5-N4-C9
2	F	1201	A1H9K	C6-C5-N4-C9
2	F	1201	A1H9K	C6-C5-N4-C8
2	H	1201	A1H9K	N4-C5-C6-O1
2	F	1201	A1H9K	N4-C5-C6-O1
2	E	1201	A1H9K	C6-C5-N4-C3
2	D	1201	A1H9K	N4-C5-C6-O1
2	A	1201	A1H9K	C6-C5-N4-C8
2	A	1201	A1H9K	C6-C5-N4-C9

There are no ring outliers.

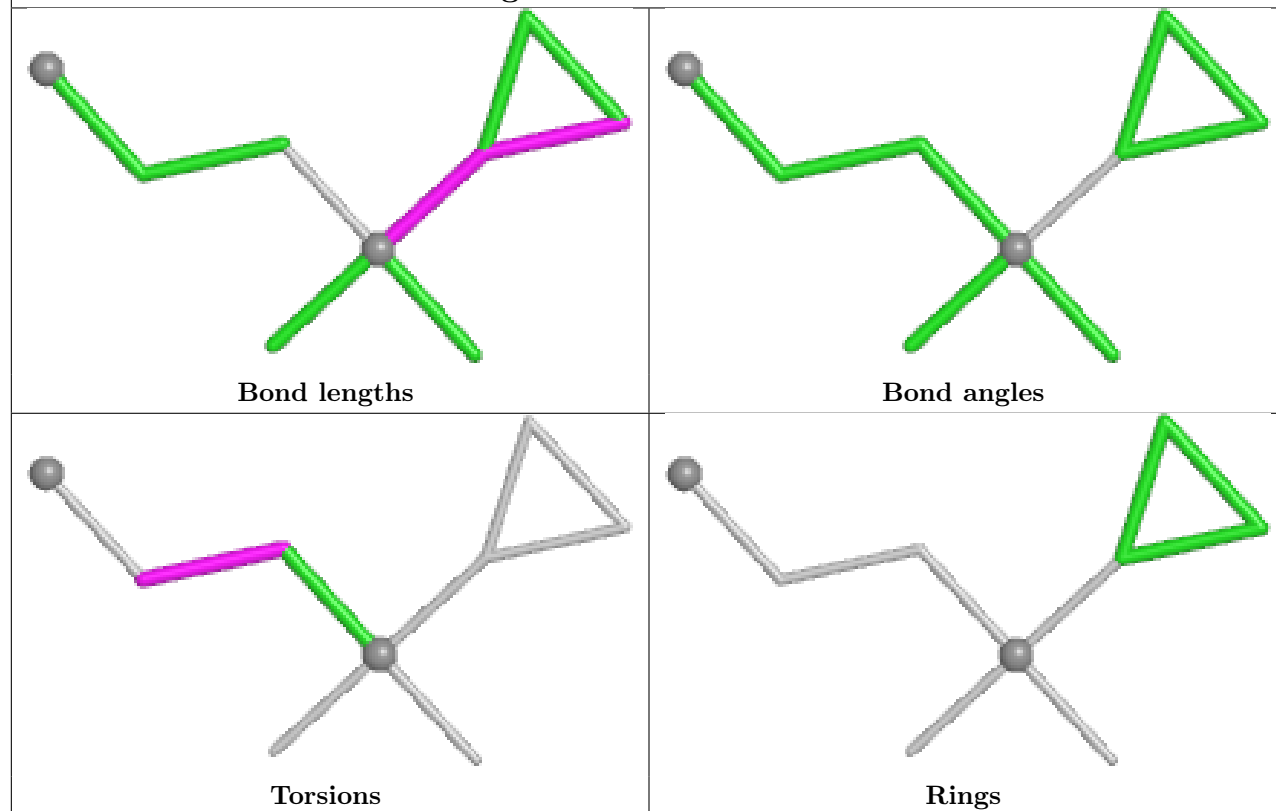
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1201	A1H9K	2	0
2	D	1201	A1H9K	1	0
2	F	1201	A1H9K	1	0

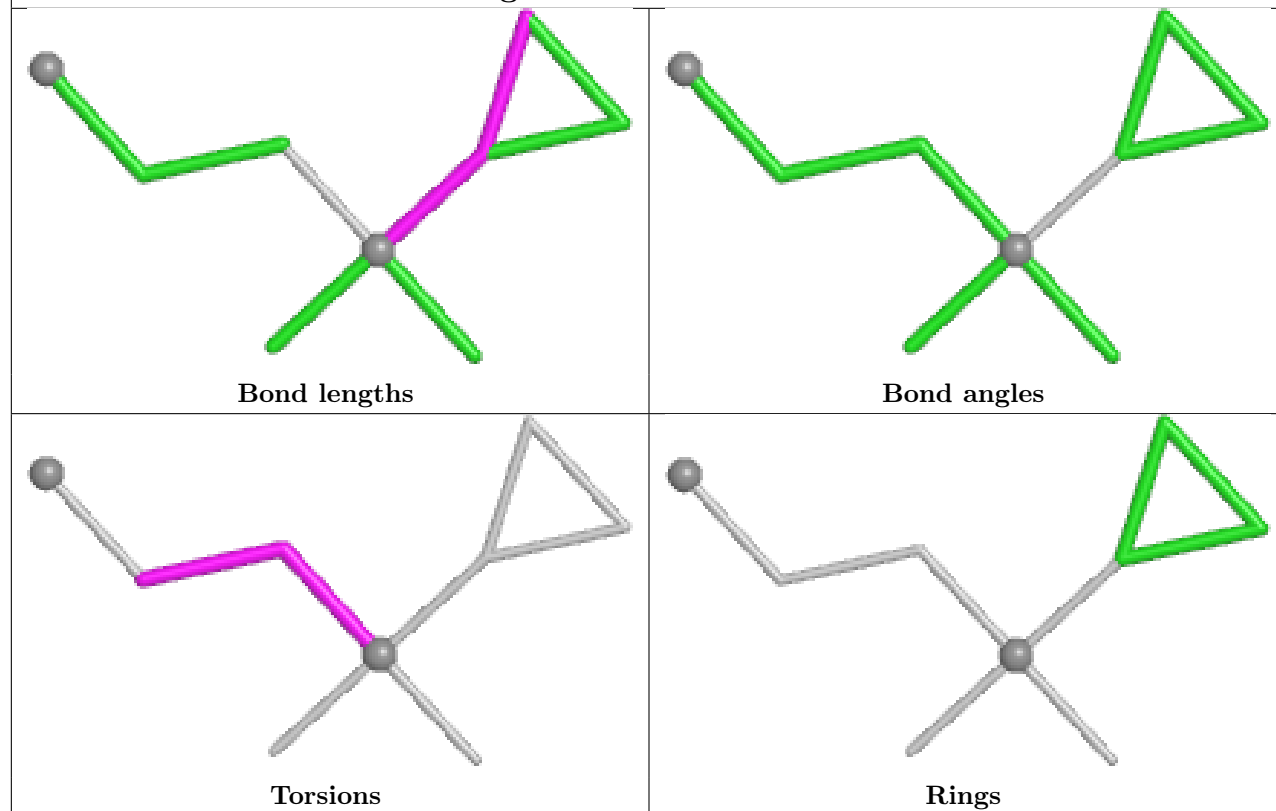
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



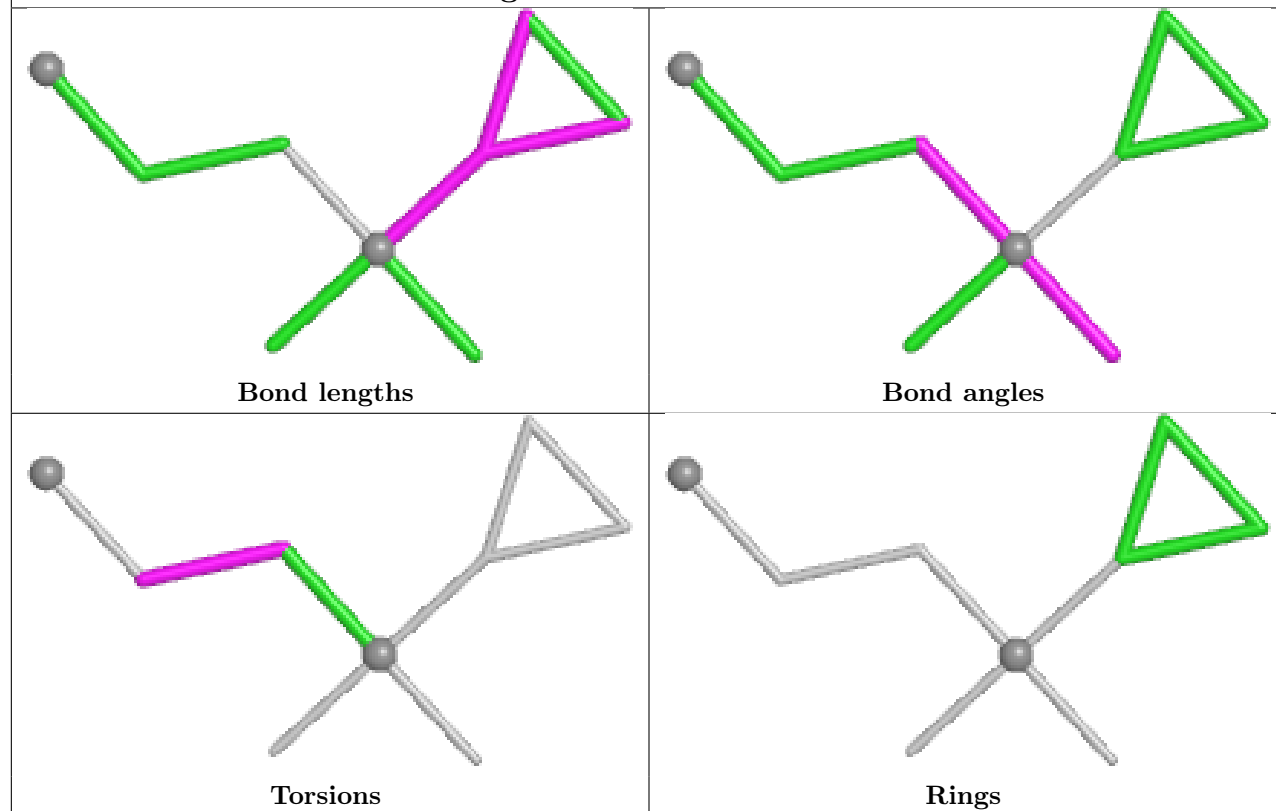
Ligand A1H9K B 1201



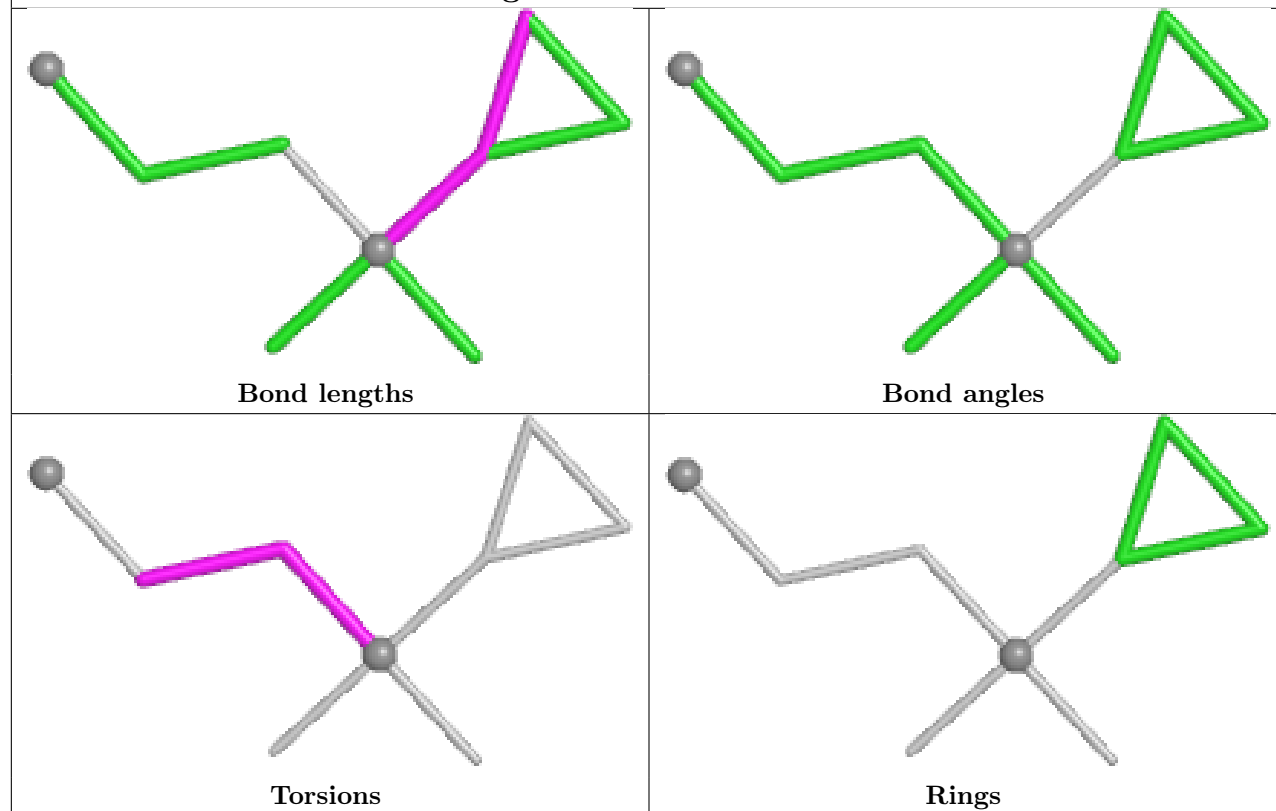
Ligand A1H9K G 1201



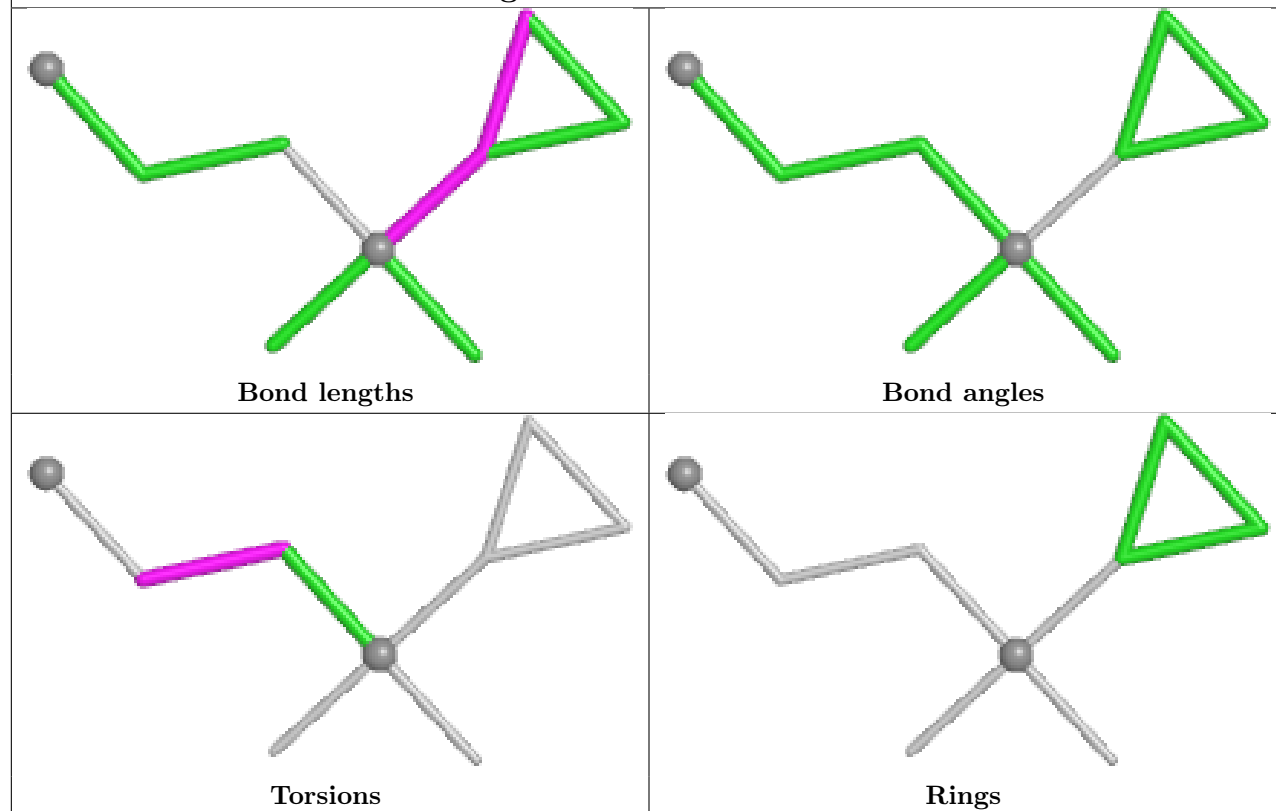
Ligand A1H9K D 1201



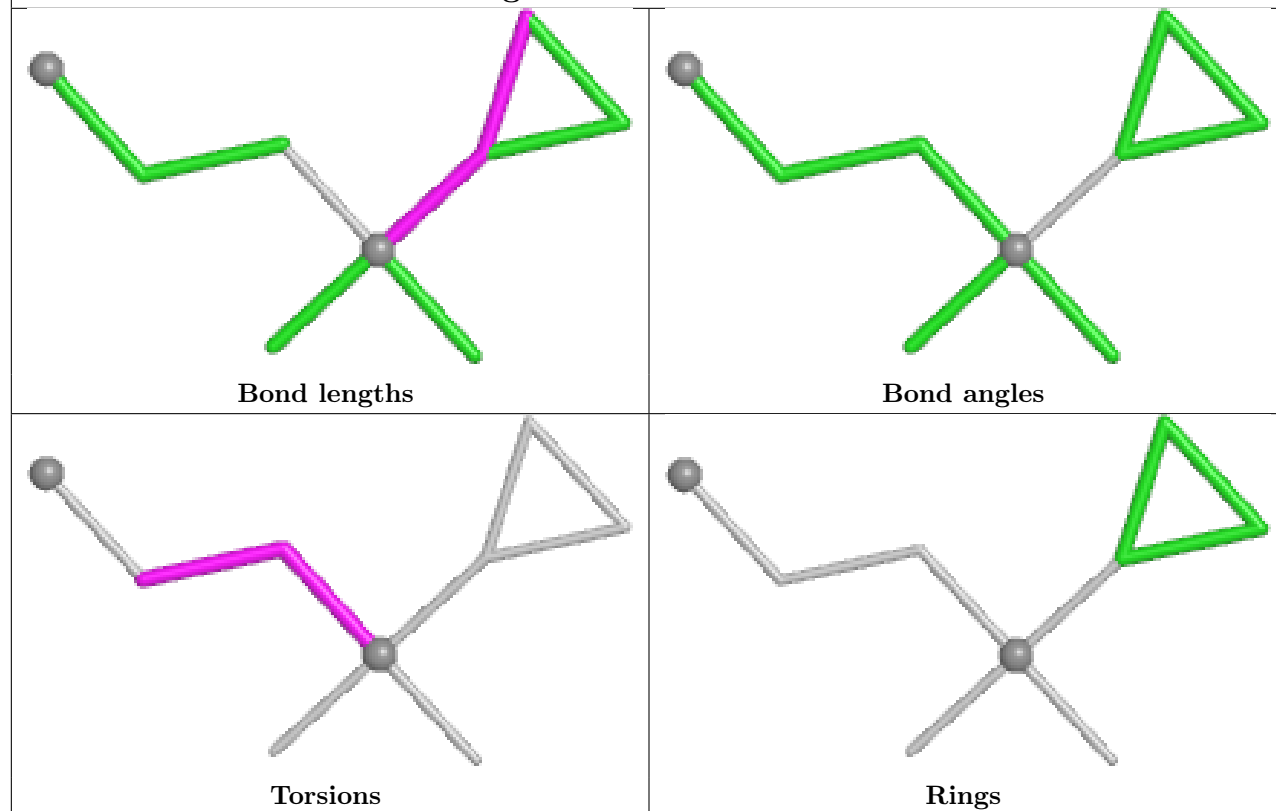
Ligand A1H9K E 1201

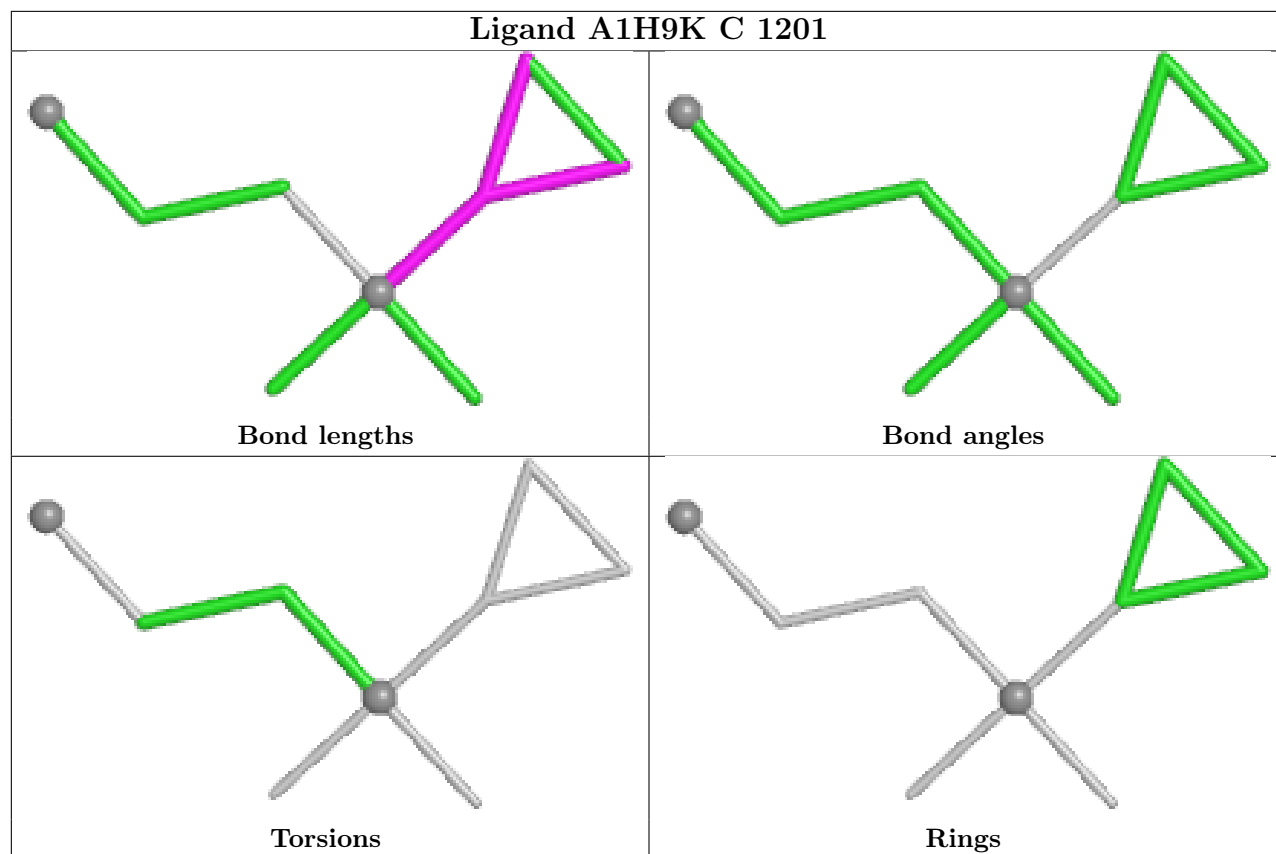


Ligand A1H9K H 1201



Ligand A1H9K 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%)	-0.41	2 (0%) 90 89	15, 26, 47, 74	0
1	B	792/1150 (68%)	-0.36	0 100 100	13, 29, 44, 71	0
1	C	791/1150 (68%)	-0.07	1 (0%) 92 91	21, 36, 53, 74	0
1	D	792/1150 (68%)	0.40	20 (2%) 58 55	19, 46, 63, 83	0
1	E	792/1150 (68%)	0.51	43 (5%) 31 27	20, 48, 77, 93	0
1	F	792/1150 (68%)	0.64	72 (9%) 15 12	23, 48, 74, 94	0
1	G	792/1150 (68%)	0.73	60 (7%) 20 17	29, 53, 79, 106	0
1	H	792/1150 (68%)	1.00	106 (13%) 7 6	35, 62, 86, 103	0
All	All	6335/9200 (68%)	0.30	304 (4%) 35 32	13, 43, 75, 106	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	651	ALA	5.8
1	E	922	ALA	4.6
1	E	821	LEU	4.6
1	H	577	LEU	4.3
1	H	564	LEU	4.3
1	H	1106	ALA	4.2
1	F	901	MET	4.2
1	F	897	TYR	4.2
1	H	396	LEU	4.0
1	E	1119	ILE	3.9
1	G	561	ALA	3.9
1	E	916	LEU	3.8
1	F	826	GLU	3.7
1	H	561	ALA	3.7
1	H	1097	LEU	3.7
1	F	907	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	710	TYR	3.6
1	H	737	GLY	3.6
1	G	709	VAL	3.6
1	H	1045	PHE	3.5
1	G	339	GLY	3.5
1	H	361	TYR	3.5
1	G	566	ALA	3.4
1	H	337	MET	3.4
1	G	739	GLY	3.3
1	H	397	ILE	3.3
1	F	943	TYR	3.3
1	E	921	ASP	3.3
1	H	1098	ILE	3.3
1	H	440	PHE	3.3
1	F	953	TYR	3.2
1	F	458	TRP	3.2
1	F	982	ILE	3.2
1	D	981	SER	3.1
1	H	578	LEU	3.1
1	E	902	ALA	3.1
1	F	890	ILE	3.1
1	H	554	ALA	3.1
1	H	579	THR	3.1
1	H	395	ILE	3.1
1	G	1076	PHE	3.1
1	D	643	ASP	3.0
1	E	895	ALA	3.0
1	F	992	THR	3.0
1	H	653	ILE	3.0
1	F	927	PHE	3.0
1	F	799	LEU	3.0
1	F	802	GLY	3.0
1	G	642	HIS	3.0
1	F	930	TYR	3.0
1	H	403	ILE	3.0
1	E	915	THR	3.0
1	H	558	ALA	3.0
1	H	565	ALA	3.0
1	F	797	PHE	3.0
1	H	1077	SER	2.9
1	G	403	ILE	2.9
1	F	903	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	736	ALA	2.9
1	G	1083	VAL	2.9
1	H	654	ILE	2.9
1	F	909	PHE	2.9
1	F	916	LEU	2.9
1	H	1076	PHE	2.9
1	F	671	PHE	2.9
1	E	1009	ILE	2.8
1	E	930	TYR	2.8
1	H	771	CYS	2.8
1	G	596	GLN	2.8
1	H	405	GLY	2.8
1	H	409	GLY	2.8
1	E	351	TYR	2.8
1	H	1046	LEU	2.8
1	G	681	THR	2.8
1	F	914	TYR	2.8
1	G	550	VAL	2.8
1	H	671	PHE	2.8
1	H	1124	VAL	2.8
1	G	337	MET	2.8
1	G	1020	PRO	2.8
1	H	640	LEU	2.8
1	H	642	HIS	2.8
1	H	566	ALA	2.8
1	H	538	TYR	2.8
1	H	342	PRO	2.7
1	F	919	ILE	2.7
1	D	1050	LEU	2.7
1	E	818	LEU	2.7
1	G	414	GLY	2.7
1	F	1108	PHE	2.7
1	G	631	PHE	2.7
1	G	682	VAL	2.7
1	F	818	LEU	2.7
1	H	1050	LEU	2.7
1	D	1058	GLY	2.7
1	F	791	TRP	2.7
1	G	981	SER	2.7
1	G	633	ALA	2.7
1	E	1046	LEU	2.7
1	G	549	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	627	CYS	2.7
1	E	1045	PHE	2.7
1	G	551	VAL	2.7
1	H	709	VAL	2.7
1	F	918	GLN	2.6
1	H	603	TRP	2.6
1	G	740	PHE	2.6
1	F	952	GLN	2.6
1	H	1107	TYR	2.6
1	H	339	GLY	2.6
1	H	673	GLY	2.6
1	H	394	PRO	2.6
1	H	418	PRO	2.6
1	H	645	ALA	2.6
1	G	698	TYR	2.6
1	G	1097	LEU	2.6
1	E	925	ALA	2.6
1	H	1105	SER	2.6
1	F	821	LEU	2.6
1	F	1019	GLY	2.6
1	H	575	ALA	2.6
1	F	900	SER	2.5
1	G	654	ILE	2.5
1	H	678	ILE	2.5
1	H	1057	HIS	2.5
1	F	1032	VAL	2.5
1	G	579	THR	2.5
1	G	577	LEU	2.5
1	H	659	LEU	2.5
1	D	893	GLY	2.5
1	H	549	GLY	2.5
1	G	592	PRO	2.5
1	E	1079	VAL	2.5
1	F	831	VAL	2.5
1	G	404	VAL	2.5
1	H	707	VAL	2.5
1	E	899	ASP	2.5
1	F	904	ILE	2.5
1	H	1044	LYS	2.5
1	H	666	LEU	2.5
1	F	994	ALA	2.5
1	E	920	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	933	LEU	2.5
1	F	988	ILE	2.5
1	H	595	LEU	2.5
1	H	649	LEU	2.5
1	H	399	ASP	2.5
1	F	932	ALA	2.5
1	F	997	ASN	2.4
1	D	897	TYR	2.4
1	F	476	VAL	2.4
1	F	669	LYS	2.4
1	G	640	LEU	2.4
1	H	381	LEU	2.4
1	G	630	MET	2.4
1	E	1091	PRO	2.4
1	H	404	VAL	2.4
1	H	1104	TYR	2.4
1	D	933	LEU	2.4
1	E	924	LEU	2.4
1	F	838	ILE	2.4
1	H	560	HIS	2.4
1	F	827	PHE	2.4
1	H	340	LEU	2.4
1	H	442	ILE	2.4
1	H	933	LEU	2.4
1	F	489	SER	2.4
1	H	357	SER	2.4
1	A	574	ARG	2.4
1	F	950	VAL	2.4
1	F	1045	PHE	2.4
1	G	565	ALA	2.4
1	H	347	LEU	2.3
1	F	974	THR	2.3
1	G	644	THR	2.3
1	F	486	SER	2.3
1	F	1086	LYS	2.3
1	E	933	LEU	2.3
1	H	402	LEU	2.3
1	H	1084	LEU	2.3
1	E	1031	ASN	2.3
1	D	830	ALA	2.3
1	F	925	ALA	2.3
1	G	714	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	1120	ILE	2.3
1	E	1012	THR	2.3
1	H	553	TYR	2.3
1	H	630	MET	2.3
1	F	803	ARG	2.3
1	F	339	GLY	2.3
1	D	1063	LEU	2.3
1	G	1046	LEU	2.3
1	H	408	CYS	2.3
1	H	1128	PHE	2.3
1	D	1121	SER	2.3
1	G	402	LEU	2.3
1	H	358	VAL	2.3
1	H	733	VAL	2.3
1	G	575	ALA	2.2
1	F	670	TYR	2.2
1	H	433	SER	2.2
1	G	683	GLY	2.2
1	H	623	VAL	2.2
1	H	1109	VAL	2.2
1	E	927	PHE	2.2
1	H	740	PHE	2.2
1	H	376	MET	2.2
1	D	644	THR	2.2
1	D	1033	GLU	2.2
1	G	401	GLU	2.2
1	G	726	TYR	2.2
1	H	1081	ASN	2.2
1	H	1053	PRO	2.2
1	H	675	GLN	2.2
1	H	722	SER	2.2
1	E	938	LEU	2.2
1	G	699	LEU	2.2
1	H	714	LEU	2.2
1	E	954	ALA	2.2
1	F	415	ALA	2.2
1	F	1102	ALA	2.2
1	E	974	THR	2.2
1	H	351	TYR	2.2
1	G	411	PRO	2.2
1	G	1050	LEU	2.2
1	G	1062	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1027	VAL	2.2
1	F	422	TRP	2.2
1	F	661	TRP	2.2
1	F	1043	PHE	2.2
1	G	909	PHE	2.2
1	G	1106	ALA	2.2
1	H	598	ALA	2.2
1	G	338	GLU	2.2
1	F	1094	TYR	2.2
1	G	1078	TYR	2.2
1	H	407	PRO	2.2
1	F	834	GLN	2.2
1	H	596	GLN	2.2
1	E	907	LEU	2.2
1	G	628	TYR	2.1
1	G	1049	LEU	2.1
1	H	1055	GLY	2.1
1	D	1109	VAL	2.1
1	E	1006	SER	2.1
1	G	1099	VAL	2.1
1	A	338	GLU	2.1
1	F	1090	GLU	2.1
1	E	1020	PRO	2.1
1	F	1093	LYS	2.1
1	H	1091	PRO	2.1
1	H	345	GLN	2.1
1	F	804	MET	2.1
1	E	897	TYR	2.1
1	H	1078	TYR	2.1
1	C	339	GLY	2.1
1	D	690	GLY	2.1
1	D	1070	GLY	2.1
1	H	587	VAL	2.1
1	H	1083	VAL	2.1
1	D	892	SER	2.1
1	E	824	PHE	2.1
1	H	706	PHE	2.1
1	E	1001	ALA	2.1
1	H	451	ARG	2.1
1	E	567	LYS	2.1
1	F	792	PRO	2.1
1	F	1049	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	659	LEU	2.1
1	E	1078	TYR	2.1
1	E	898	VAL	2.1
1	E	1098	ILE	2.1
1	E	1125	ILE	2.1
1	F	805	VAL	2.1
1	F	1083	VAL	2.1
1	F	891	PHE	2.1
1	G	713	SER	2.1
1	F	477	TRP	2.1
1	G	655	LYS	2.1
1	F	823	THR	2.1
1	D	996	PRO	2.1
1	G	738	MET	2.1
1	G	398	GLN	2.1
1	H	1049	LEU	2.1
1	H	390	CYS	2.1
1	G	1107	TYR	2.1
1	F	485	VAL	2.1
1	D	909	PHE	2.1
1	G	1102	ALA	2.0
1	F	979	THR	2.0
1	H	592	PRO	2.0
1	E	889	LEU	2.0
1	F	980	LEU	2.0
1	G	653	ILE	2.0
1	G	351	TYR	2.0
1	H	416	PHE	2.0
1	F	899	ASP	2.0
1	H	581	ALA	2.0
1	E	1003	MET	2.0
1	H	352	LEU	2.0
1	E	945	ASN	2.0
1	D	822	ARG	2.0
1	E	1124	VAL	2.0
1	H	682	VAL	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

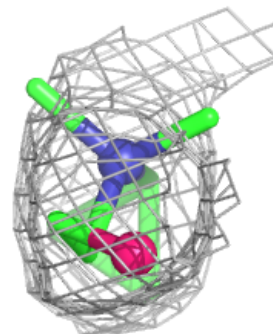
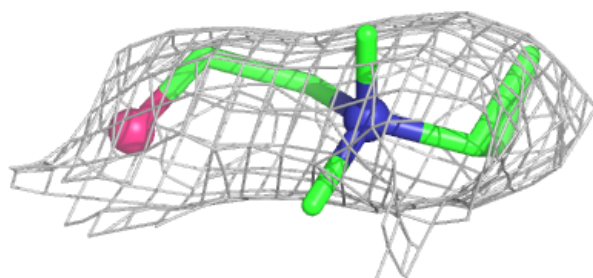
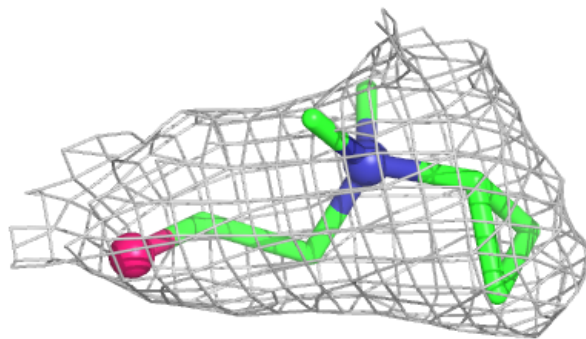
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1H9K	H	1201	9/9	0.88	0.18	55,58,61,64	0
2	A1H9K	E	1201	9/9	0.89	0.14	33,38,44,45	0
2	A1H9K	G	1201	9/9	0.90	0.13	38,42,51,51	0
2	A1H9K	C	1201	9/9	0.93	0.13	24,30,33,36	0
2	A1H9K	F	1201	9/9	0.93	0.13	41,44,49,52	0
2	A1H9K	A	1201	9/9	0.95	0.11	17,19,23,24	0
2	A1H9K	D	1201	9/9	0.95	0.09	25,34,36,41	0
2	A1H9K	B	1201	9/9	0.96	0.09	16,20,24,26	0

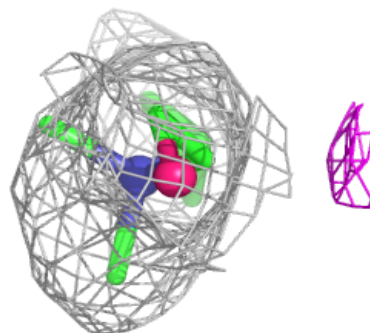
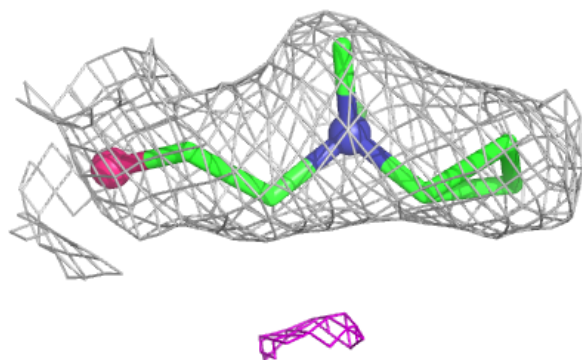
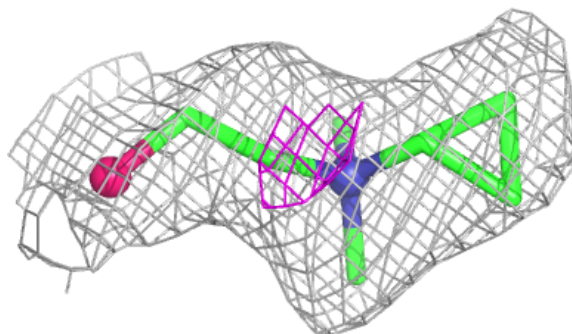
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H9K 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)

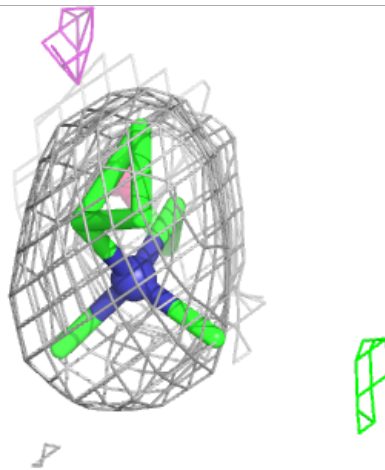
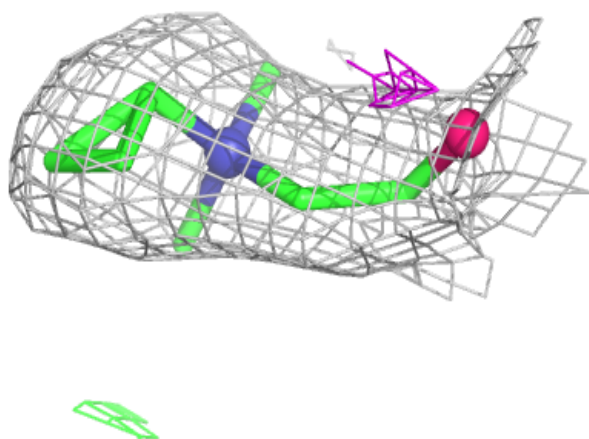
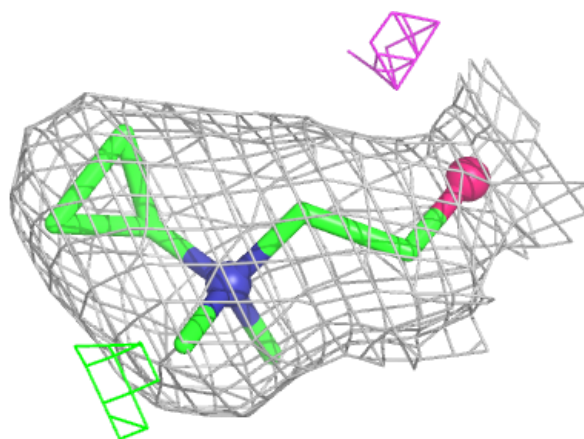
**Electron density around A1H9K E 1201:**

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



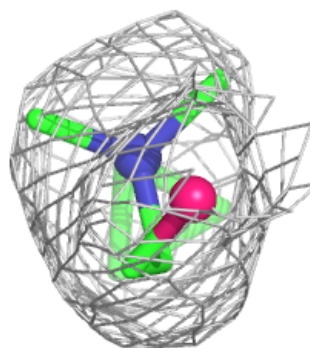
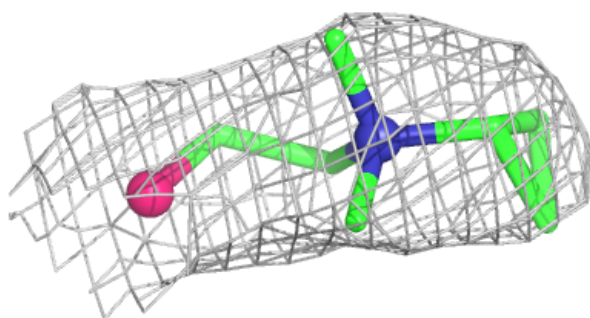
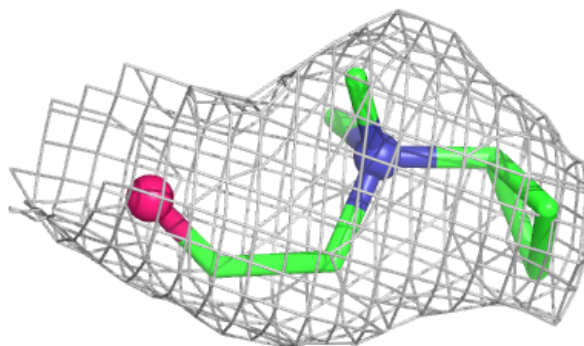
Electron density around A1H9K G 1201:

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

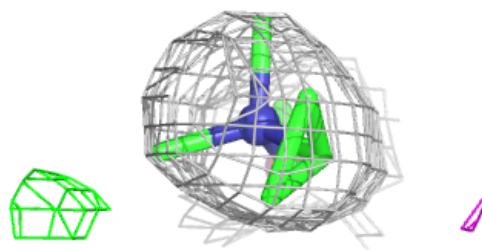
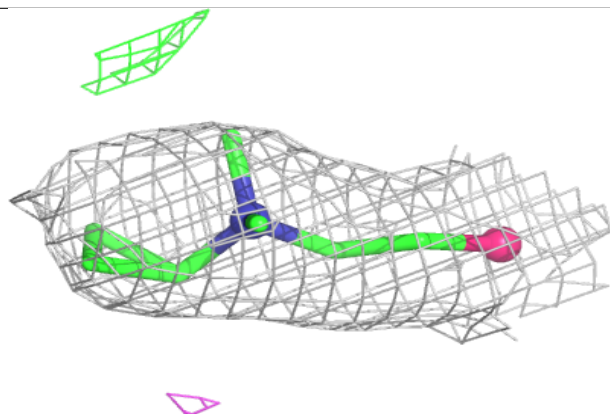
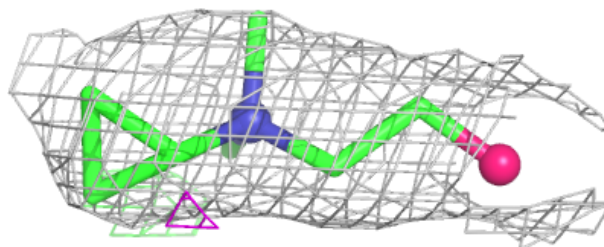


Electron density around A1H9K C 1201:

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

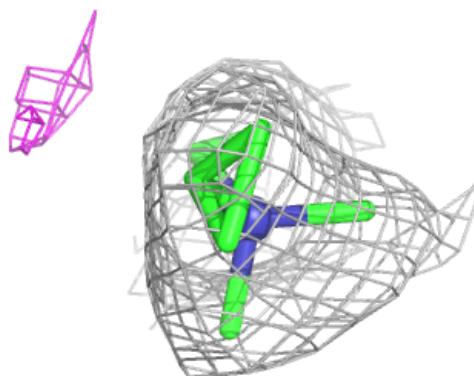
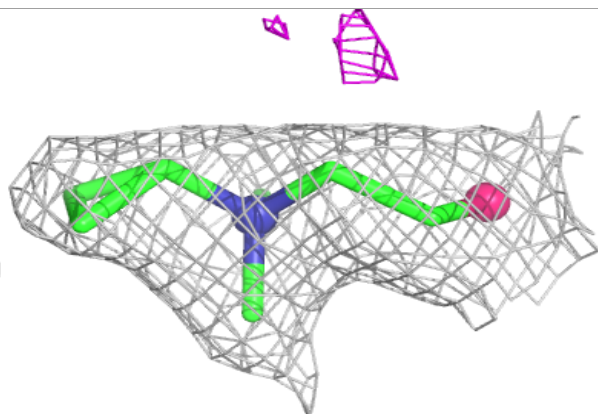
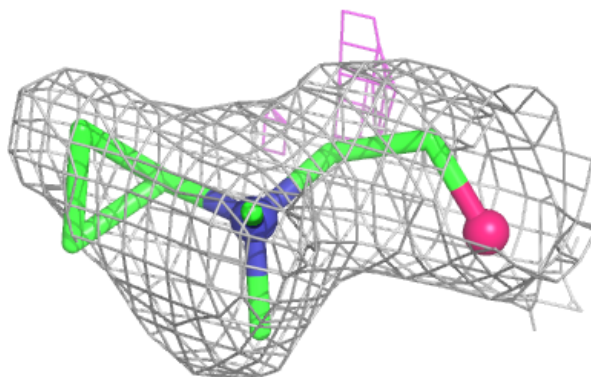
**Electron density around A1H9K F 1201:**

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

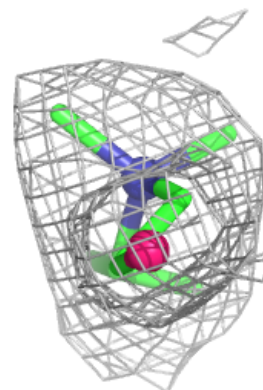
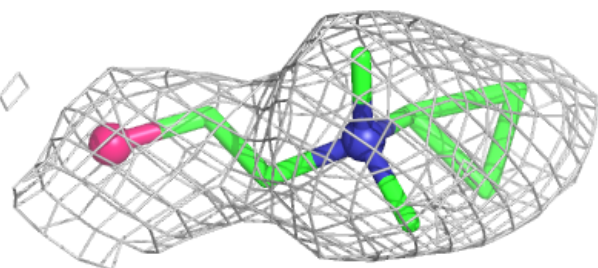
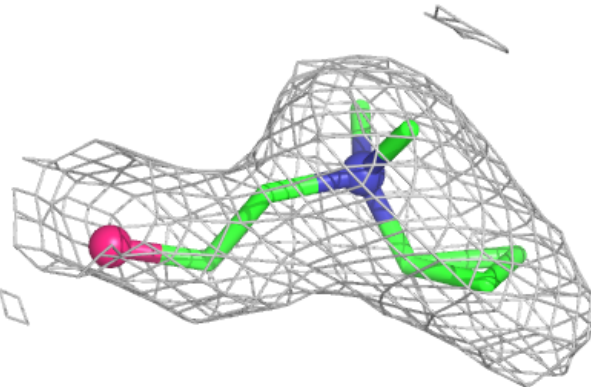


Electron density around A1H9K A 1201:

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

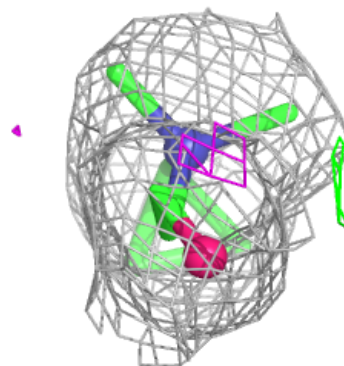
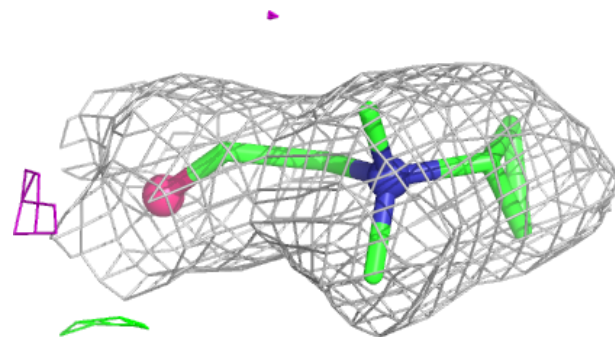
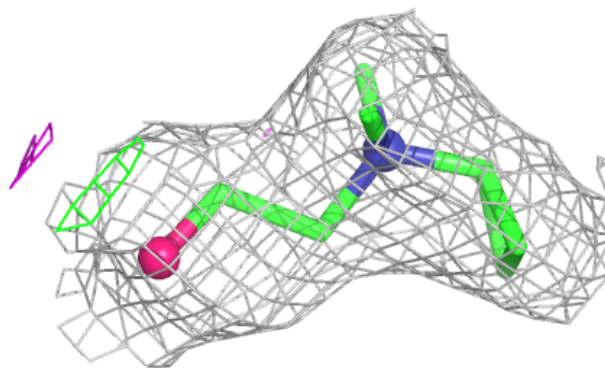
**Electron density around A1H9K D 1201:**

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



Electron density around A1H9K B 1201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.