Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 09:30 PM EST

PDB ID	:	7KZV
EMDB ID	:	EMD-23090
Title	:	Structure of the human fanconi anaemia Core-UBE2T-ID-DNA complex in closed state
Authors	:	Wang, S.L.; Pavletich, N.P.
Deposited on	:	2020-12-10
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

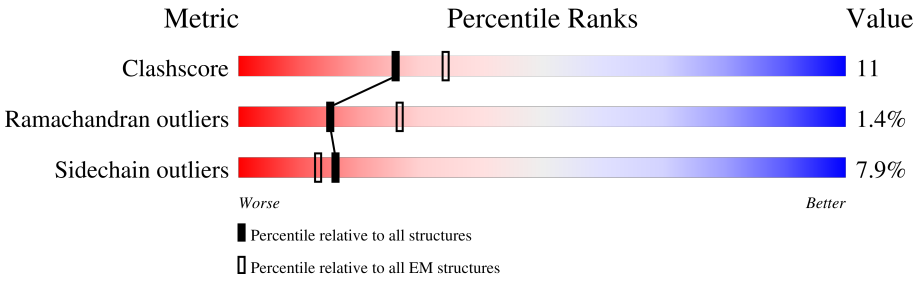
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1477	12% 55% 23% • 20%
1	S	1477	6% 61% 21% • 15%
2	B	884	• 46% 26% 6% • 21%
2	O	884	• 56% 20% • 21%
3	C	583	• 69% 22% • 6%
4	E	555	5% 43% 28% • 25%
5	F	399	• 62% 20% • 15%
6	G	641	• 57% 29% • 10%

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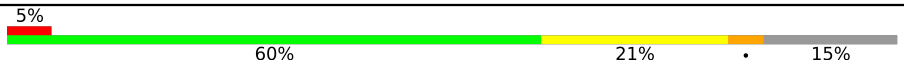
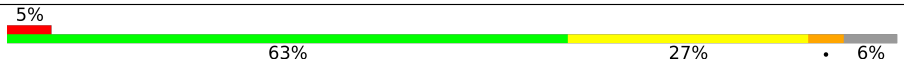
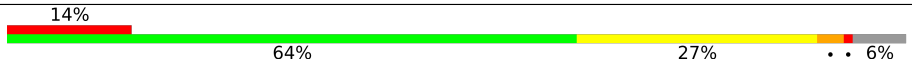
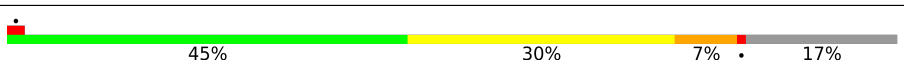
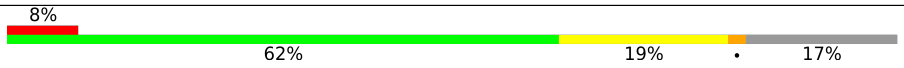
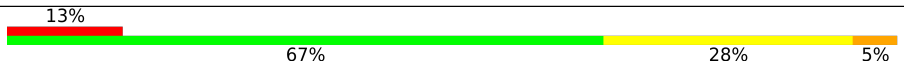
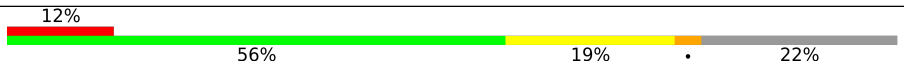
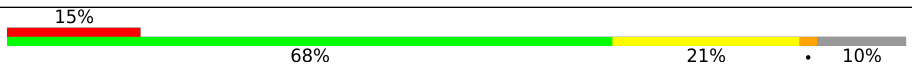
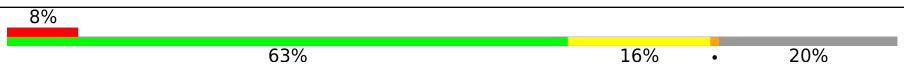
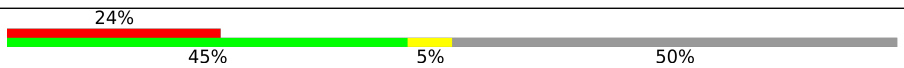
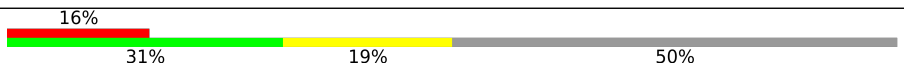
Mol	Chain	Length	Quality of chain
6	H	641	
7	L	394	
7	M	394	
8	P	906	
8	Q	906	
9	W	39	
10	X	197	
11	U	1328	
12	V	1451	
13	Y	58	
14	Z	58	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 177592 atoms, of which 89365 are hydrogens and 0 are deuteriums.

In the tables below, 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 Fanconi anemia group A protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1186	Total	C	H	N	O	S	0	0
			18889	6001	9487	1650	1692	59		
1	S	1250	Total	C	H	N	O	S	0	0
			19961	6345	10028	1747	1780	61		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1456	ALA	-	expression tag	UNP O15360
A	1457	ALA	-	expression tag	UNP O15360
A	1458	ALA	-	expression tag	UNP O15360
A	1459	LYS	-	expression tag	UNP O15360
A	1460	LEU	-	expression tag	UNP O15360
A	1461	VAL	-	expression tag	UNP O15360
A	1462	ASP	-	expression tag	UNP O15360
A	1463	GLU	-	expression tag	UNP O15360
A	1464	ASP	-	expression tag	UNP O15360
A	1465	LEU	-	expression tag	UNP O15360
A	1466	TYR	-	expression tag	UNP O15360
A	1467	PHE	-	expression tag	UNP O15360
A	1468	GLN	-	expression tag	UNP O15360
A	1469	SER	-	expression tag	UNP O15360
A	1470	ASP	-	expression tag	UNP O15360
A	1471	TYR	-	expression tag	UNP O15360
A	1472	LYS	-	expression tag	UNP O15360
A	1473	ASP	-	expression tag	UNP O15360
A	1474	ASP	-	expression tag	UNP O15360
A	1475	ASP	-	expression tag	UNP O15360
A	1476	ASP	-	expression tag	UNP O15360
A	1477	LYS	-	expression tag	UNP O15360
S	1456	ALA	-	expression tag	UNP O15360
S	1457	ALA	-	expression tag	UNP O15360
S	1458	ALA	-	expression tag	UNP O15360
S	1459	LYS	-	expression tag	UNP O15360

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1460	LEU	-	expression tag	UNP O15360
S	1461	VAL	-	expression tag	UNP O15360
S	1462	ASP	-	expression tag	UNP O15360
S	1463	GLU	-	expression tag	UNP O15360
S	1464	ASP	-	expression tag	UNP O15360
S	1465	LEU	-	expression tag	UNP O15360
S	1466	TYR	-	expression tag	UNP O15360
S	1467	PHE	-	expression tag	UNP O15360
S	1468	GLN	-	expression tag	UNP O15360
S	1469	SER	-	expression tag	UNP O15360
S	1470	ASP	-	expression tag	UNP O15360
S	1471	TYR	-	expression tag	UNP O15360
S	1472	LYS	-	expression tag	UNP O15360
S	1473	ASP	-	expression tag	UNP O15360
S	1474	ASP	-	expression tag	UNP O15360
S	1475	ASP	-	expression tag	UNP O15360
S	1476	ASP	-	expression tag	UNP O15360
S	1477	LYS	-	expression tag	UNP O15360

- Molecule 2 is a protein called Fanconi anemia group B protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	701	Total	C	H	N	O	S	0	0
			11395	3619	5790	934	1013	39		
2	O	699	Total	C	H	N	O	S	0	0
			11353	3622	5759	926	1010	36		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	initiating methionine	UNP Q8NB91
B	-23	ASP	-	expression tag	UNP Q8NB91
B	-22	TYR	-	expression tag	UNP Q8NB91
B	-21	LYS	-	expression tag	UNP Q8NB91
B	-20	ASP	-	expression tag	UNP Q8NB91
B	-19	ASP	-	expression tag	UNP Q8NB91
B	-18	ASP	-	expression tag	UNP Q8NB91
B	-17	ASP	-	expression tag	UNP Q8NB91
B	-16	LYS	-	expression tag	UNP Q8NB91
B	-15	GLU	-	expression tag	UNP Q8NB91
B	-14	ASN	-	expression tag	UNP Q8NB91
B	-13	LEU	-	expression tag	UNP Q8NB91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	TYR	-	expression tag	UNP Q8NB91
B	-11	PHE	-	expression tag	UNP Q8NB91
B	-10	GLN	-	expression tag	UNP Q8NB91
B	-9	GLY	-	expression tag	UNP Q8NB91
B	-8	GLY	-	expression tag	UNP Q8NB91
B	-7	GLY	-	expression tag	UNP Q8NB91
B	-6	ARG	-	expression tag	UNP Q8NB91
B	-5	LYS	-	expression tag	UNP Q8NB91
B	-4	LEU	-	expression tag	UNP Q8NB91
B	-3	GLY	-	expression tag	UNP Q8NB91
B	-2	THR	-	expression tag	UNP Q8NB91
B	-1	GLY	-	expression tag	UNP Q8NB91
B	0	SER	-	expression tag	UNP Q8NB91
O	-24	MET	-	initiating methionine	UNP Q8NB91
O	-23	ASP	-	expression tag	UNP Q8NB91
O	-22	TYR	-	expression tag	UNP Q8NB91
O	-21	LYS	-	expression tag	UNP Q8NB91
O	-20	ASP	-	expression tag	UNP Q8NB91
O	-19	ASP	-	expression tag	UNP Q8NB91
O	-18	ASP	-	expression tag	UNP Q8NB91
O	-17	ASP	-	expression tag	UNP Q8NB91
O	-16	LYS	-	expression tag	UNP Q8NB91
O	-15	GLU	-	expression tag	UNP Q8NB91
O	-14	ASN	-	expression tag	UNP Q8NB91
O	-13	LEU	-	expression tag	UNP Q8NB91
O	-12	TYR	-	expression tag	UNP Q8NB91
O	-11	PHE	-	expression tag	UNP Q8NB91
O	-10	GLN	-	expression tag	UNP Q8NB91
O	-9	GLY	-	expression tag	UNP Q8NB91
O	-8	GLY	-	expression tag	UNP Q8NB91
O	-7	GLY	-	expression tag	UNP Q8NB91
O	-6	ARG	-	expression tag	UNP Q8NB91
O	-5	LYS	-	expression tag	UNP Q8NB91
O	-4	LEU	-	expression tag	UNP Q8NB91
O	-3	GLY	-	expression tag	UNP Q8NB91
O	-2	THR	-	expression tag	UNP Q8NB91
O	-1	GLY	-	expression tag	UNP Q8NB91
O	0	SER	-	expression tag	UNP Q8NB91

- Molecule 3 is a protein called Fanconi anemia group C protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	550	Total	C	H	N	O	S	0	0
			8838	2826	4442	749	791	30		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	MET	-	initiating methionine	UNP Q00597
C	-23	ASP	-	expression tag	UNP Q00597
C	-22	TYR	-	expression tag	UNP Q00597
C	-21	LYS	-	expression tag	UNP Q00597
C	-20	ASP	-	expression tag	UNP Q00597
C	-19	ASP	-	expression tag	UNP Q00597
C	-18	ASP	-	expression tag	UNP Q00597
C	-17	ASP	-	expression tag	UNP Q00597
C	-16	LYS	-	expression tag	UNP Q00597
C	-15	GLU	-	expression tag	UNP Q00597
C	-14	ASN	-	expression tag	UNP Q00597
C	-13	LEU	-	expression tag	UNP Q00597
C	-12	TYR	-	expression tag	UNP Q00597
C	-11	PHE	-	expression tag	UNP Q00597
C	-10	GLN	-	expression tag	UNP Q00597
C	-9	GLY	-	expression tag	UNP Q00597
C	-8	GLY	-	expression tag	UNP Q00597
C	-7	GLY	-	expression tag	UNP Q00597
C	-6	ARG	-	expression tag	UNP Q00597
C	-5	LYS	-	expression tag	UNP Q00597
C	-4	LEU	-	expression tag	UNP Q00597
C	-3	GLY	-	expression tag	UNP Q00597
C	-2	THR	-	expression tag	UNP Q00597
C	-1	GLY	-	expression tag	UNP Q00597
C	0	SER	-	expression tag	UNP Q00597

- Molecule 4 is a protein called Fanconi anemia group E protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	419	Total	C	H	N	O	S	0	0
			6614	2048	3390	560	592	24		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	MET	-	initiating methionine	UNP Q9HB96
E	-17	ASP	-	expression tag	UNP Q9HB96

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	TYR	-	expression tag	UNP Q9HB96
E	-15	LYS	-	expression tag	UNP Q9HB96
E	-14	ASP	-	expression tag	UNP Q9HB96
E	-13	ASP	-	expression tag	UNP Q9HB96
E	-12	ASP	-	expression tag	UNP Q9HB96
E	-11	ASP	-	expression tag	UNP Q9HB96
E	-10	LYS	-	expression tag	UNP Q9HB96
E	-9	GLU	-	expression tag	UNP Q9HB96
E	-8	ASN	-	expression tag	UNP Q9HB96
E	-7	LEU	-	expression tag	UNP Q9HB96
E	-6	TYR	-	expression tag	UNP Q9HB96
E	-5	PHE	-	expression tag	UNP Q9HB96
E	-4	GLN	-	expression tag	UNP Q9HB96
E	-3	GLY	-	expression tag	UNP Q9HB96
E	-2	GLY	-	expression tag	UNP Q9HB96
E	-1	GLY	-	expression tag	UNP Q9HB96
E	0	ARG	-	expression tag	UNP Q9HB96

- Molecule 5 is a protein called Fanconi anemia group F protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	340	5466	1730	2740	506	483	7	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-24	MET	-	initiating methionine	UNP Q9NPI8
F	-23	ASP	-	expression tag	UNP Q9NPI8
F	-22	TYR	-	expression tag	UNP Q9NPI8
F	-21	LYS	-	expression tag	UNP Q9NPI8
F	-20	ASP	-	expression tag	UNP Q9NPI8
F	-19	ASP	-	expression tag	UNP Q9NPI8
F	-18	ASP	-	expression tag	UNP Q9NPI8
F	-17	ASP	-	expression tag	UNP Q9NPI8
F	-16	LYS	-	expression tag	UNP Q9NPI8
F	-15	GLU	-	expression tag	UNP Q9NPI8
F	-14	ASN	-	expression tag	UNP Q9NPI8
F	-13	LEU	-	expression tag	UNP Q9NPI8
F	-12	TYR	-	expression tag	UNP Q9NPI8
F	-11	PHE	-	expression tag	UNP Q9NPI8
F	-10	GLN	-	expression tag	UNP Q9NPI8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLY	-	expression tag	UNP Q9NPI8
F	-8	GLY	-	expression tag	UNP Q9NPI8
F	-7	GLY	-	expression tag	UNP Q9NPI8
F	-6	ARG	-	expression tag	UNP Q9NPI8
F	-5	LYS	-	expression tag	UNP Q9NPI8
F	-4	LEU	-	expression tag	UNP Q9NPI8
F	-3	GLY	-	expression tag	UNP Q9NPI8
F	-2	THR	-	expression tag	UNP Q9NPI8
F	-1	GLY	-	expression tag	UNP Q9NPI8
F	0	SER	-	expression tag	UNP Q9NPI8

- Molecule 6 is a protein called Fanconi anemia group G protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	577	Total	C	H	N	O	S	0	0
			9020	2843	4537	778	844	18		
6	H	544	Total	C	H	N	O	S	0	0
			8504	2676	4288	734	790	16		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	MET	-	initiating methionine	UNP O15287
G	-17	ASP	-	expression tag	UNP O15287
G	-16	TYR	-	expression tag	UNP O15287
G	-15	LYS	-	expression tag	UNP O15287
G	-14	ASP	-	expression tag	UNP O15287
G	-13	ASP	-	expression tag	UNP O15287
G	-12	ASP	-	expression tag	UNP O15287
G	-11	ASP	-	expression tag	UNP O15287
G	-10	LYS	-	expression tag	UNP O15287
G	-9	GLU	-	expression tag	UNP O15287
G	-8	ASN	-	expression tag	UNP O15287
G	-7	LEU	-	expression tag	UNP O15287
G	-6	TYR	-	expression tag	UNP O15287
G	-5	PHE	-	expression tag	UNP O15287
G	-4	GLN	-	expression tag	UNP O15287
G	-3	GLY	-	expression tag	UNP O15287
G	-2	GLY	-	expression tag	UNP O15287
G	-1	GLY	-	expression tag	UNP O15287
G	0	ARG	-	expression tag	UNP O15287
H	-18	MET	-	initiating methionine	UNP O15287

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	ASP	-	expression tag	UNP O15287
H	-16	TYR	-	expression tag	UNP O15287
H	-15	LYS	-	expression tag	UNP O15287
H	-14	ASP	-	expression tag	UNP O15287
H	-13	ASP	-	expression tag	UNP O15287
H	-12	ASP	-	expression tag	UNP O15287
H	-11	ASP	-	expression tag	UNP O15287
H	-10	LYS	-	expression tag	UNP O15287
H	-9	GLU	-	expression tag	UNP O15287
H	-8	ASN	-	expression tag	UNP O15287
H	-7	LEU	-	expression tag	UNP O15287
H	-6	TYR	-	expression tag	UNP O15287
H	-5	PHE	-	expression tag	UNP O15287
H	-4	GLN	-	expression tag	UNP O15287
H	-3	GLY	-	expression tag	UNP O15287
H	-2	GLY	-	expression tag	UNP O15287
H	-1	GLY	-	expression tag	UNP O15287
H	0	ARG	-	expression tag	UNP O15287

- Molecule 7 is a protein called E3 ubiquitin-protein ligase FANCL.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	370	Total	C	H	N	O	S	0	0
			5951	1914	2977	496	542	22		
7	M	370	Total	C	H	N	O	S	0	0
			5951	1914	2977	496	542	22		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-18	MET	-	initiating methionine	UNP Q9NW38
L	-17	ASP	-	expression tag	UNP Q9NW38
L	-16	TYR	-	expression tag	UNP Q9NW38
L	-15	LYS	-	expression tag	UNP Q9NW38
L	-14	ASP	-	expression tag	UNP Q9NW38
L	-13	ASP	-	expression tag	UNP Q9NW38
L	-12	ASP	-	expression tag	UNP Q9NW38
L	-11	ASP	-	expression tag	UNP Q9NW38
L	-10	LYS	-	expression tag	UNP Q9NW38
L	-9	GLU	-	expression tag	UNP Q9NW38
L	-8	ASN	-	expression tag	UNP Q9NW38
L	-7	LEU	-	expression tag	UNP Q9NW38

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	TYR	-	expression tag	UNP Q9NW38
L	-5	PHE	-	expression tag	UNP Q9NW38
L	-4	GLN	-	expression tag	UNP Q9NW38
L	-3	GLY	-	expression tag	UNP Q9NW38
L	-2	GLY	-	expression tag	UNP Q9NW38
L	-1	GLY	-	expression tag	UNP Q9NW38
L	0	ARG	-	expression tag	UNP Q9NW38
M	-18	MET	-	initiating methionine	UNP Q9NW38
M	-17	ASP	-	expression tag	UNP Q9NW38
M	-16	TYR	-	expression tag	UNP Q9NW38
M	-15	LYS	-	expression tag	UNP Q9NW38
M	-14	ASP	-	expression tag	UNP Q9NW38
M	-13	ASP	-	expression tag	UNP Q9NW38
M	-12	ASP	-	expression tag	UNP Q9NW38
M	-11	ASP	-	expression tag	UNP Q9NW38
M	-10	LYS	-	expression tag	UNP Q9NW38
M	-9	GLU	-	expression tag	UNP Q9NW38
M	-8	ASN	-	expression tag	UNP Q9NW38
M	-7	LEU	-	expression tag	UNP Q9NW38
M	-6	TYR	-	expression tag	UNP Q9NW38
M	-5	PHE	-	expression tag	UNP Q9NW38
M	-4	GLN	-	expression tag	UNP Q9NW38
M	-3	GLY	-	expression tag	UNP Q9NW38
M	-2	GLY	-	expression tag	UNP Q9NW38
M	-1	GLY	-	expression tag	UNP Q9NW38
M	0	ARG	-	expression tag	UNP Q9NW38

- Molecule 8 is a protein called Fanconi anemia core complex-associated protein 100.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	748	Total	C	H	N	O	S	0	0
			11279	3520	5681	972	1058	48		
8	Q	754	Total	C	H	N	O	S	0	0
			11355	3548	5724	978	1058	47		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-24	MET	-	initiating methionine	UNP Q0VG06
P	-23	ASP	-	expression tag	UNP Q0VG06
P	-22	TYR	-	expression tag	UNP Q0VG06
P	-21	LYS	-	expression tag	UNP Q0VG06

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-20	ASP	-	expression tag	UNP Q0VG06
P	-19	HIS	-	expression tag	UNP Q0VG06
P	-18	ASP	-	expression tag	UNP Q0VG06
P	-17	GLY	-	expression tag	UNP Q0VG06
P	-16	ASP	-	expression tag	UNP Q0VG06
P	-15	TYR	-	expression tag	UNP Q0VG06
P	-14	LYS	-	expression tag	UNP Q0VG06
P	-13	ASP	-	expression tag	UNP Q0VG06
P	-12	HIS	-	expression tag	UNP Q0VG06
P	-11	ASP	-	expression tag	UNP Q0VG06
P	-10	ILE	-	expression tag	UNP Q0VG06
P	-9	ASP	-	expression tag	UNP Q0VG06
P	-8	TYR	-	expression tag	UNP Q0VG06
P	-7	LYS	-	expression tag	UNP Q0VG06
P	-6	ASP	-	expression tag	UNP Q0VG06
P	-5	ASP	-	expression tag	UNP Q0VG06
P	-4	ASP	-	expression tag	UNP Q0VG06
P	-3	ASP	-	expression tag	UNP Q0VG06
P	-2	LYS	-	expression tag	UNP Q0VG06
P	-1	GLY	-	expression tag	UNP Q0VG06
P	0	SER	-	expression tag	UNP Q0VG06
Q	-24	MET	-	initiating methionine	UNP Q0VG06
Q	-23	ASP	-	expression tag	UNP Q0VG06
Q	-22	TYR	-	expression tag	UNP Q0VG06
Q	-21	LYS	-	expression tag	UNP Q0VG06
Q	-20	ASP	-	expression tag	UNP Q0VG06
Q	-19	HIS	-	expression tag	UNP Q0VG06
Q	-18	ASP	-	expression tag	UNP Q0VG06
Q	-17	GLY	-	expression tag	UNP Q0VG06
Q	-16	ASP	-	expression tag	UNP Q0VG06
Q	-15	TYR	-	expression tag	UNP Q0VG06
Q	-14	LYS	-	expression tag	UNP Q0VG06
Q	-13	ASP	-	expression tag	UNP Q0VG06
Q	-12	HIS	-	expression tag	UNP Q0VG06
Q	-11	ASP	-	expression tag	UNP Q0VG06
Q	-10	ILE	-	expression tag	UNP Q0VG06
Q	-9	ASP	-	expression tag	UNP Q0VG06
Q	-8	TYR	-	expression tag	UNP Q0VG06
Q	-7	LYS	-	expression tag	UNP Q0VG06
Q	-6	ASP	-	expression tag	UNP Q0VG06
Q	-5	ASP	-	expression tag	UNP Q0VG06
Q	-4	ASP	-	expression tag	UNP Q0VG06

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-3	ASP	-	expression tag	UNP Q0VG06
Q	-2	LYS	-	expression tag	UNP Q0VG06
Q	-1	GLY	-	expression tag	UNP Q0VG06
Q	0	SER	-	expression tag	UNP Q0VG06

- Molecule 9 is a protein called Fanconi anemia core complex-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	39	Total	C	H	N	O	0	0
			513	179	242	42	50		

- Molecule 10 is a protein called Ubiquitin-conjugating enzyme E2 T.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	X	153	Total	C	H	N	O	S	0	0
			2484	789	1251	216	221	7		

- Molecule 11 is a protein called Fanconi anemia, complementation group I.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	U	1198	Total	C	H	N	O	S	0	0
			19367	6076	9883	1592	1760	56		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	877	LEU	ILE	conflict	UNP B7ZMF2
U	1235	VAL	ALA	conflict	UNP B7ZMF2
U	1274	SER	ASN	conflict	UNP B7ZMF2

- Molecule 12 is a protein called Fanconi anemia group D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	V	1155	Total	C	H	N	O	S	0	0
			18807	5993	9518	1537	1706	53		

- Molecule 13 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Y	29	Total	C	H	N	O	P	0	0
			923	282	326	111	175	29		

- Molecule 14 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Z	29	Total	C	H	N	O	P	0	0
			917	280	325	110	173	29		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

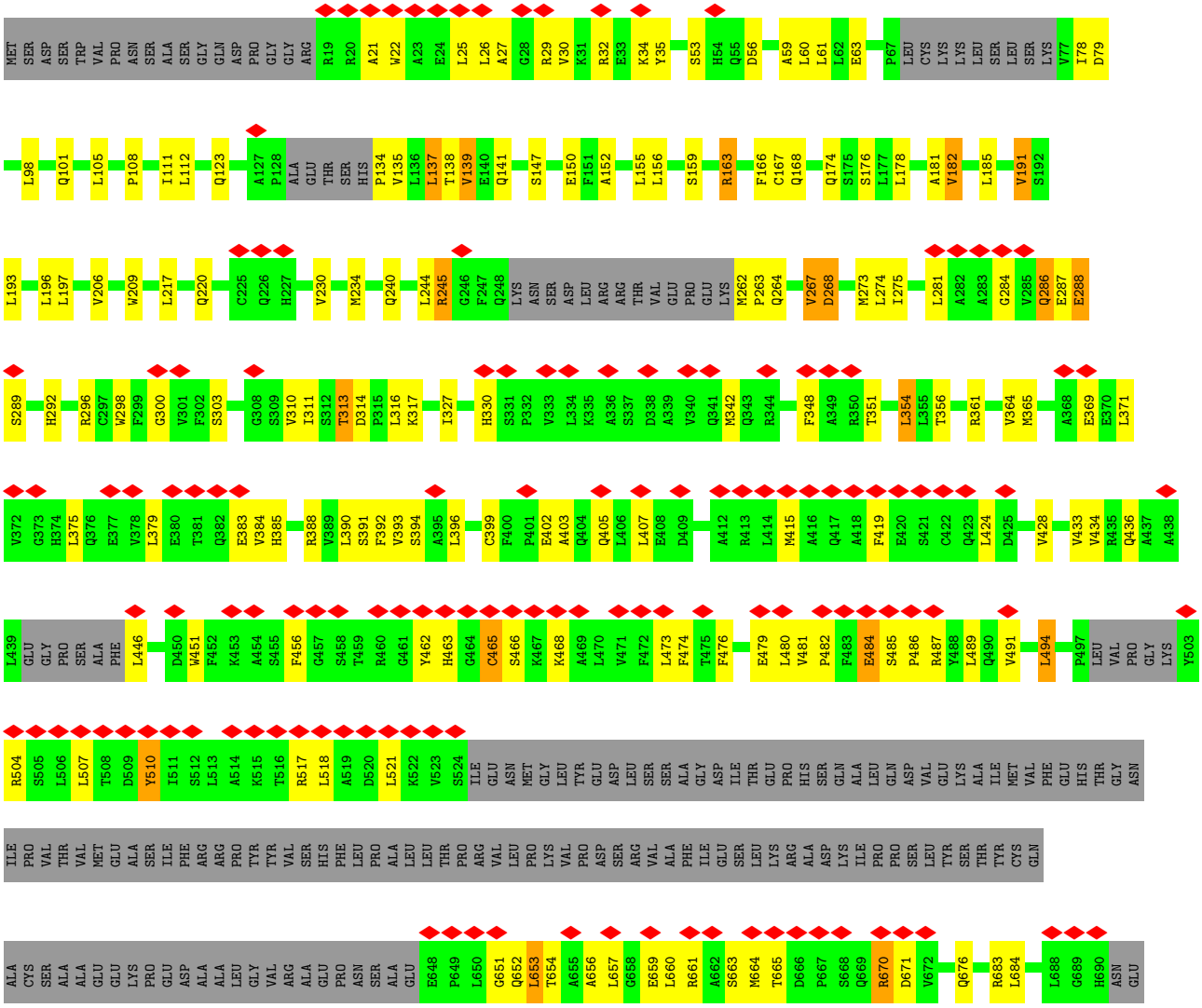
Mol	Chain	Residues	Atoms		AltConf
15	G	1	Total	Zn	0
			1	1	
15	L	2	Total	Zn	0
			2	2	
15	M	2	Total	Zn	0
			2	2	

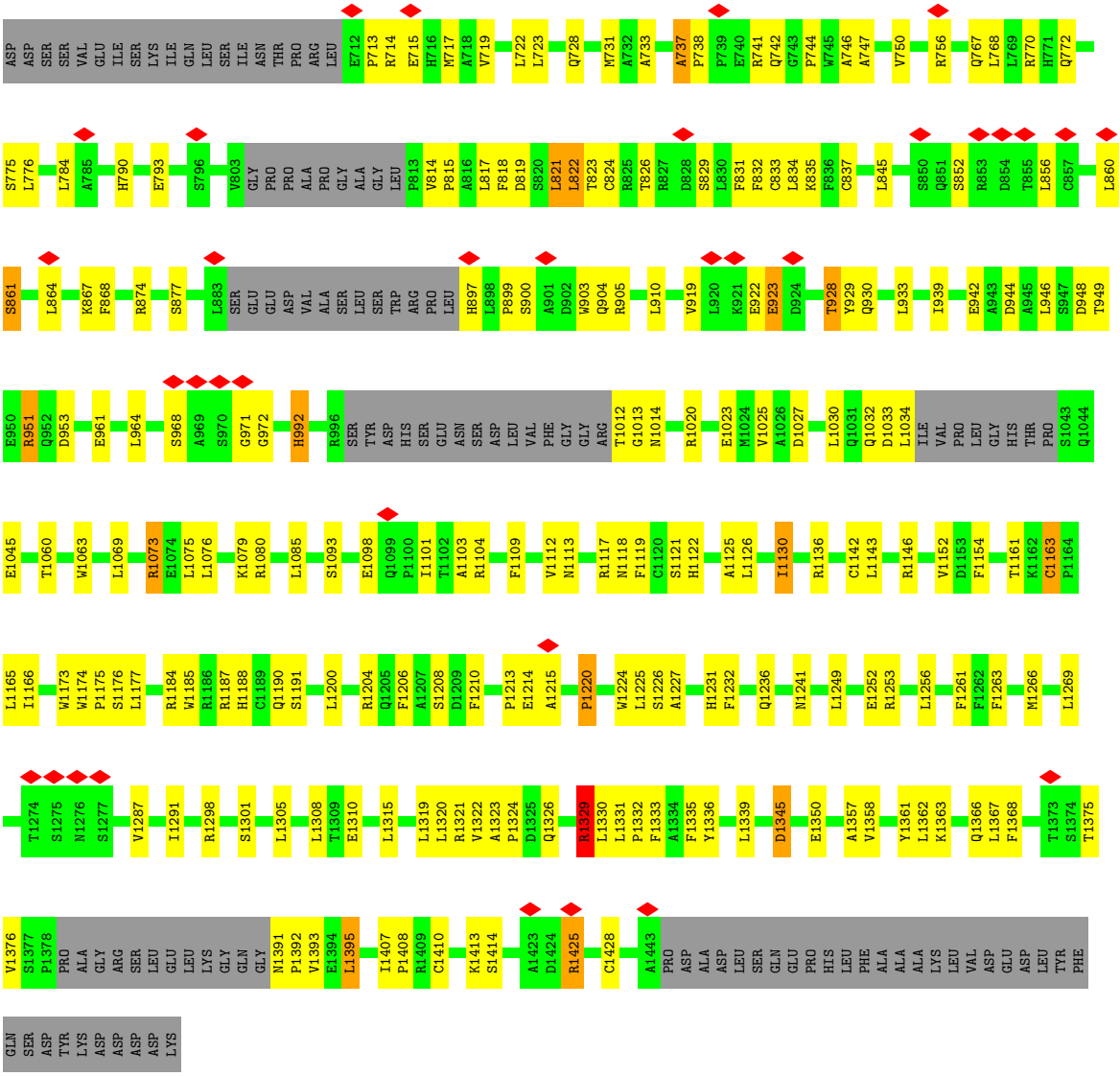
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Fanconi anemia group A protein

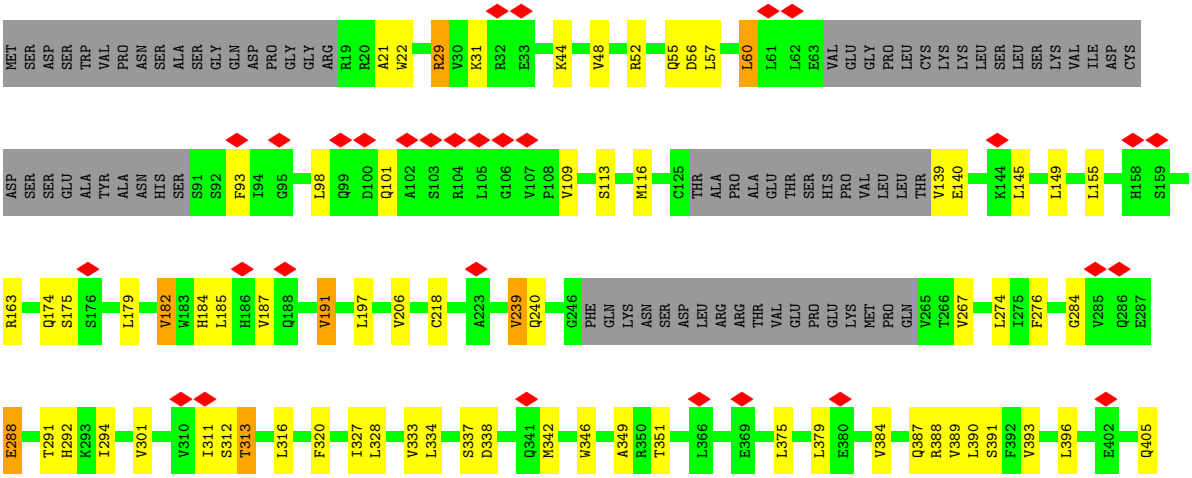
Chain A:

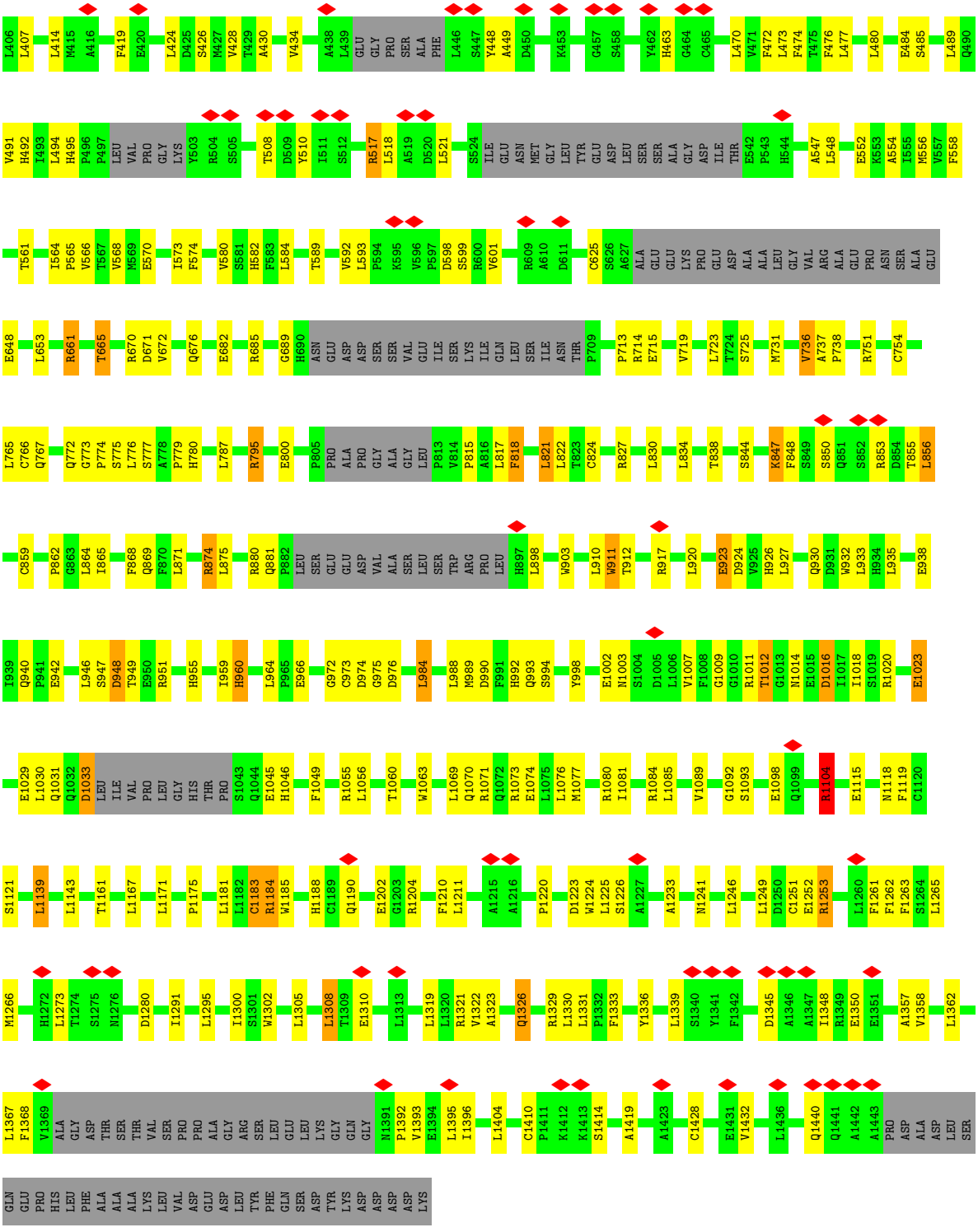




• Molecule 1: Fanconi anemia group A protein

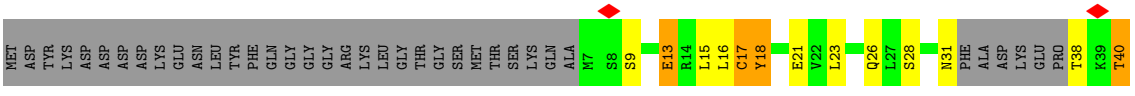
Chain S:

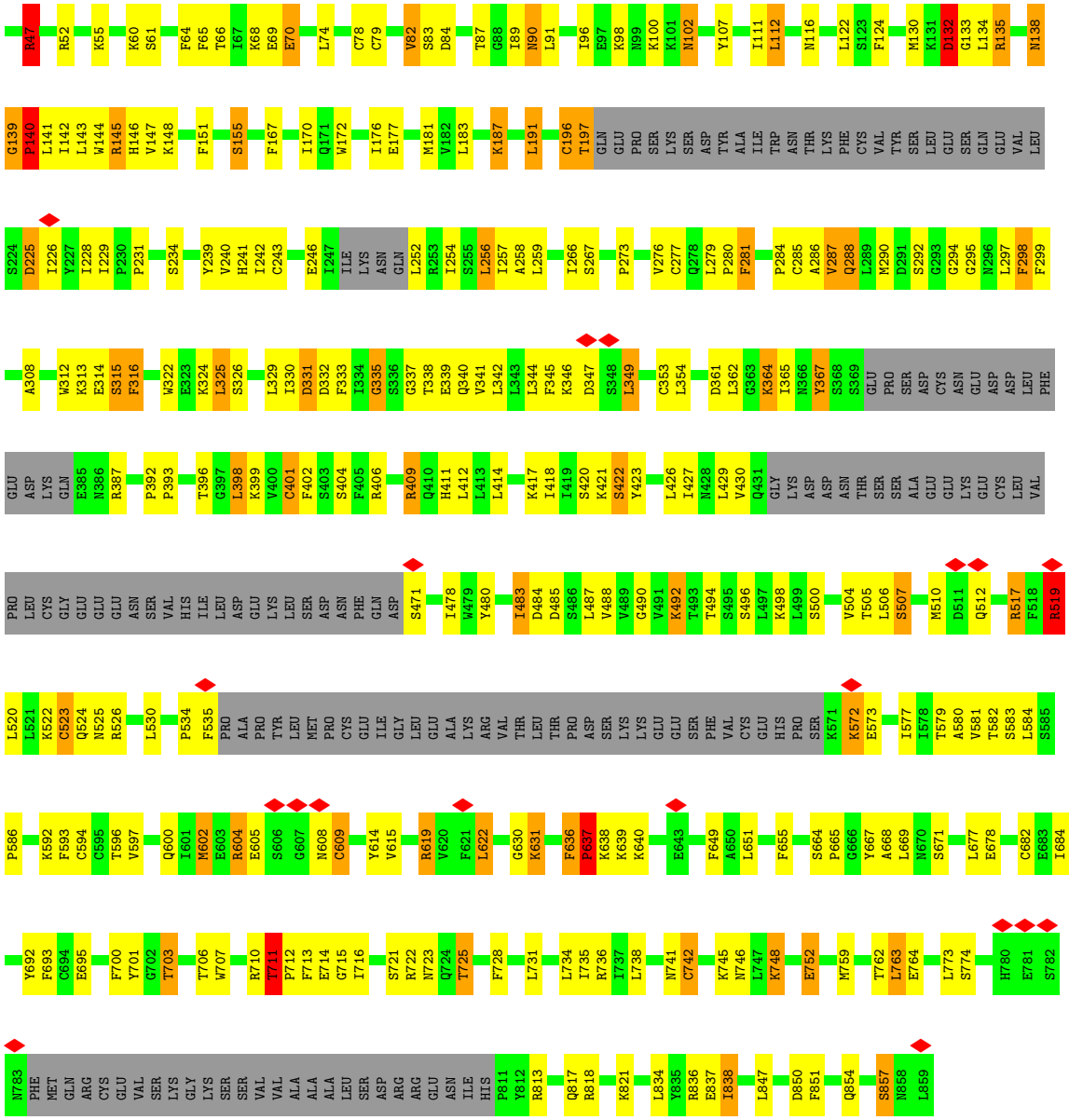




• Molecule 2: Fanconi anemia group B protein

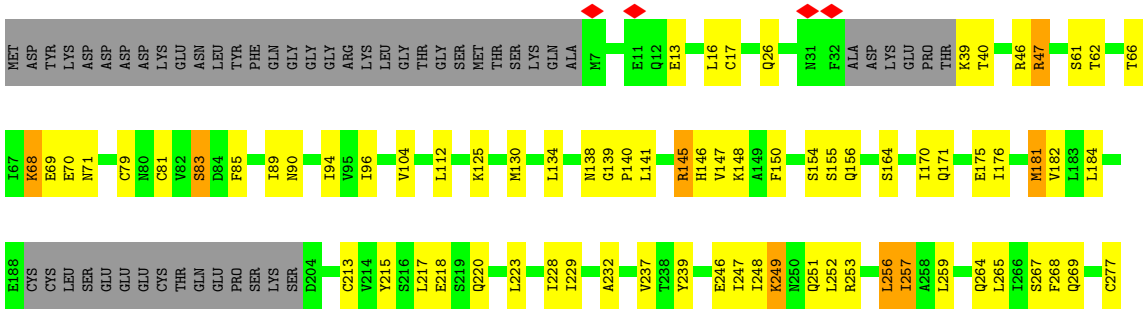
Chain B:

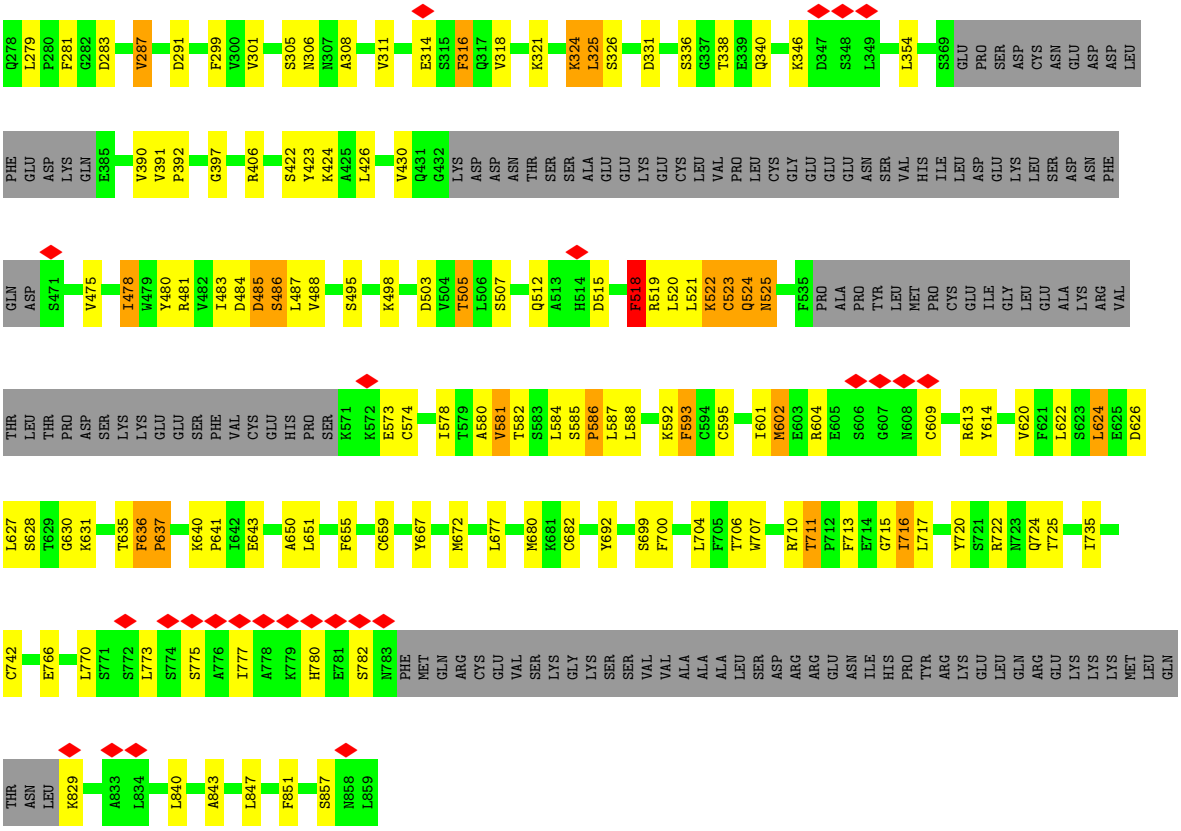




• Molecule 2: Fanconi anemia group B protein

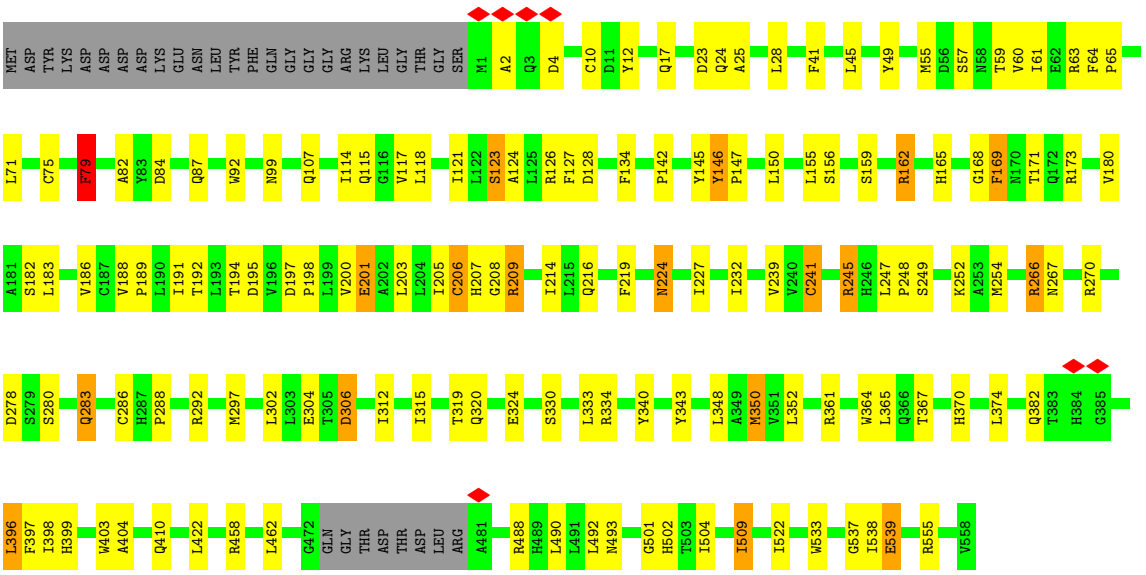
Chain O:





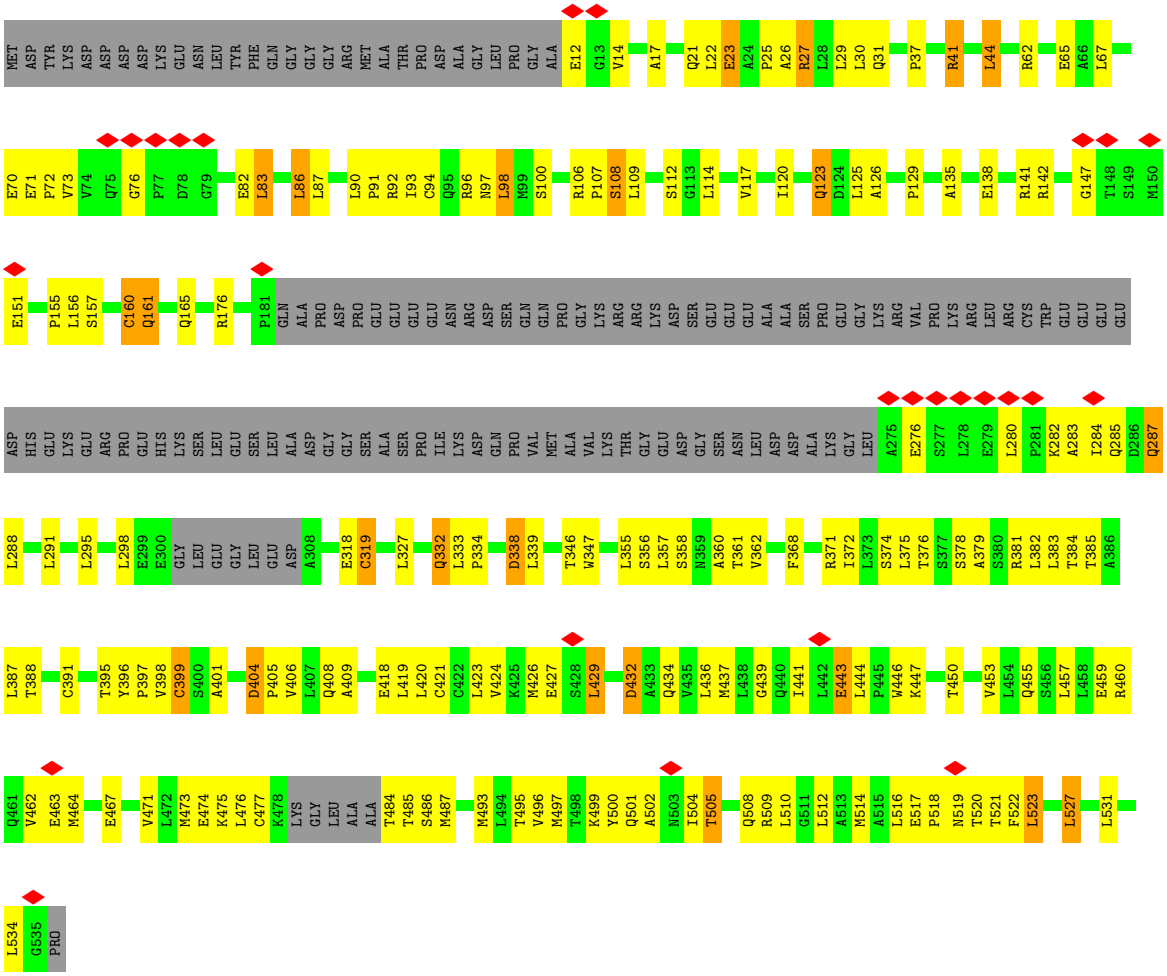
• Molecule 3: Fanconi anemia group C protein

Chain C:



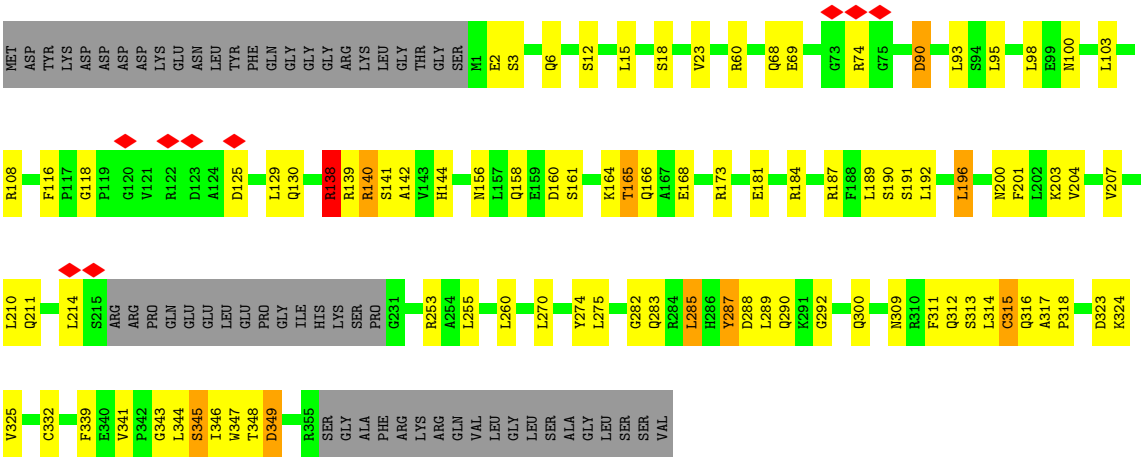
• Molecule 4: Fanconi anemia group E protein

Chain E:



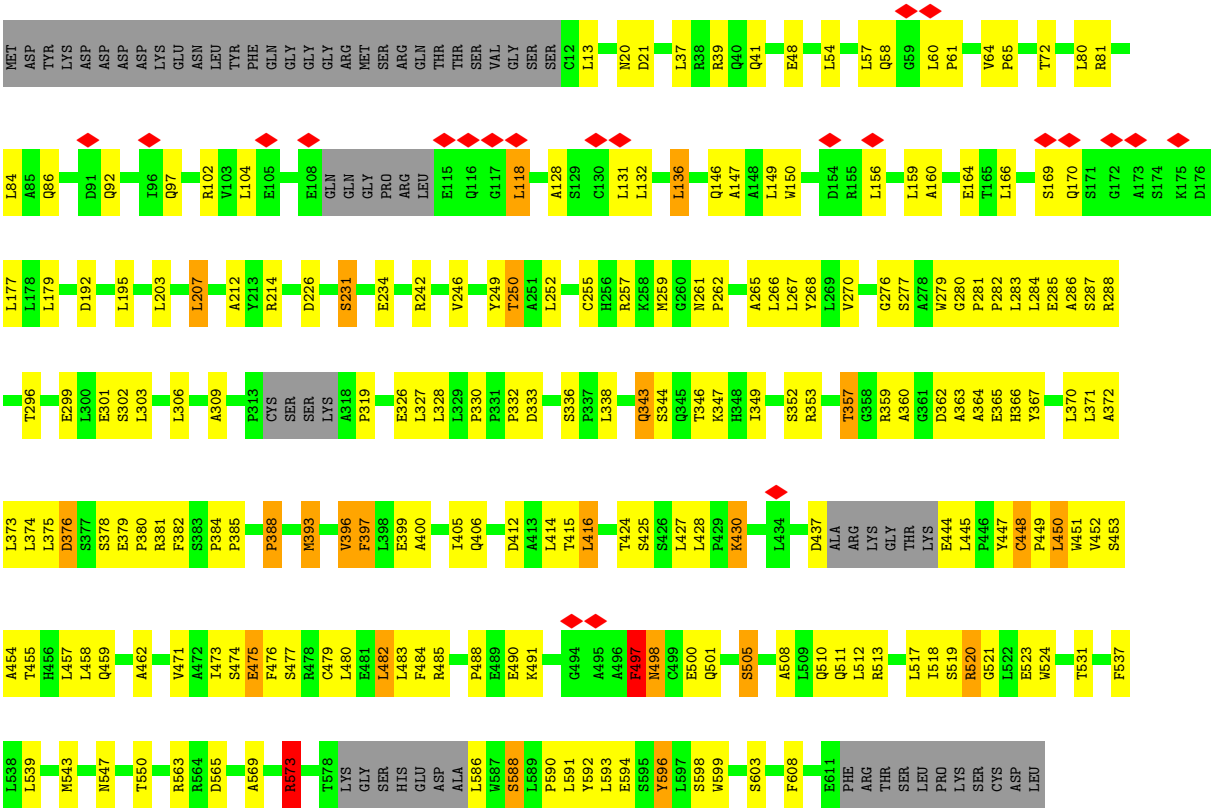
• Molecule 5: Fanconi anemia group F protein

Chain F:



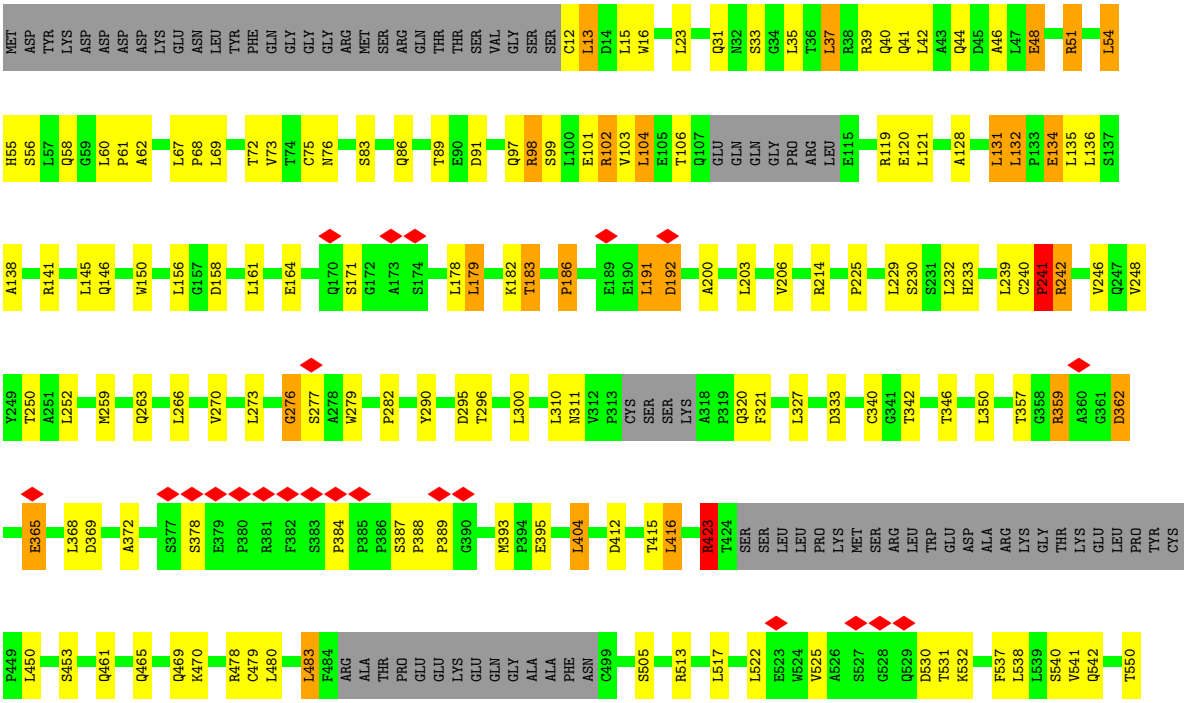
• Molecule 6: Fanconi anemia group G protein

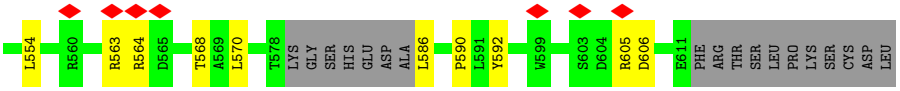
Chain G:



• Molecule 6: Fanconi anemia group G protein

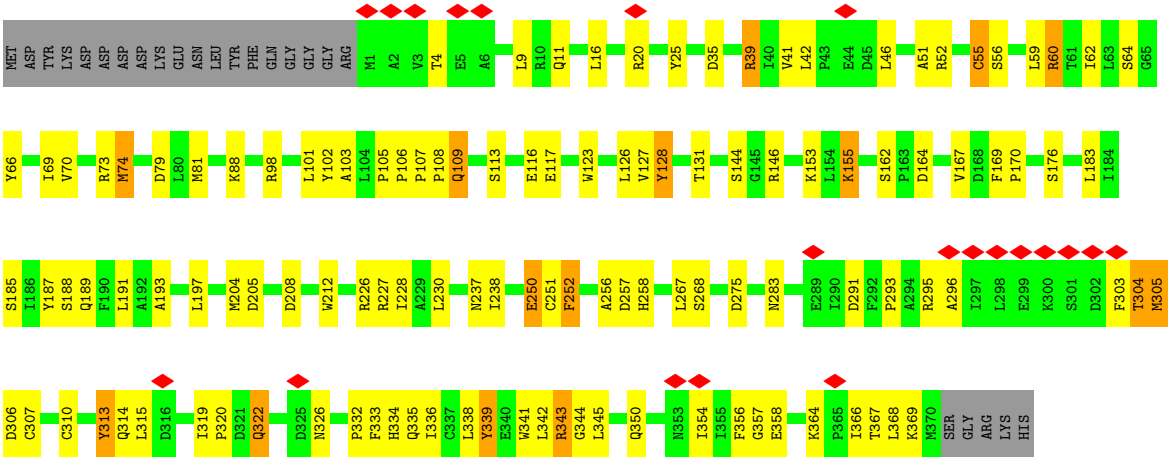
Chain H:





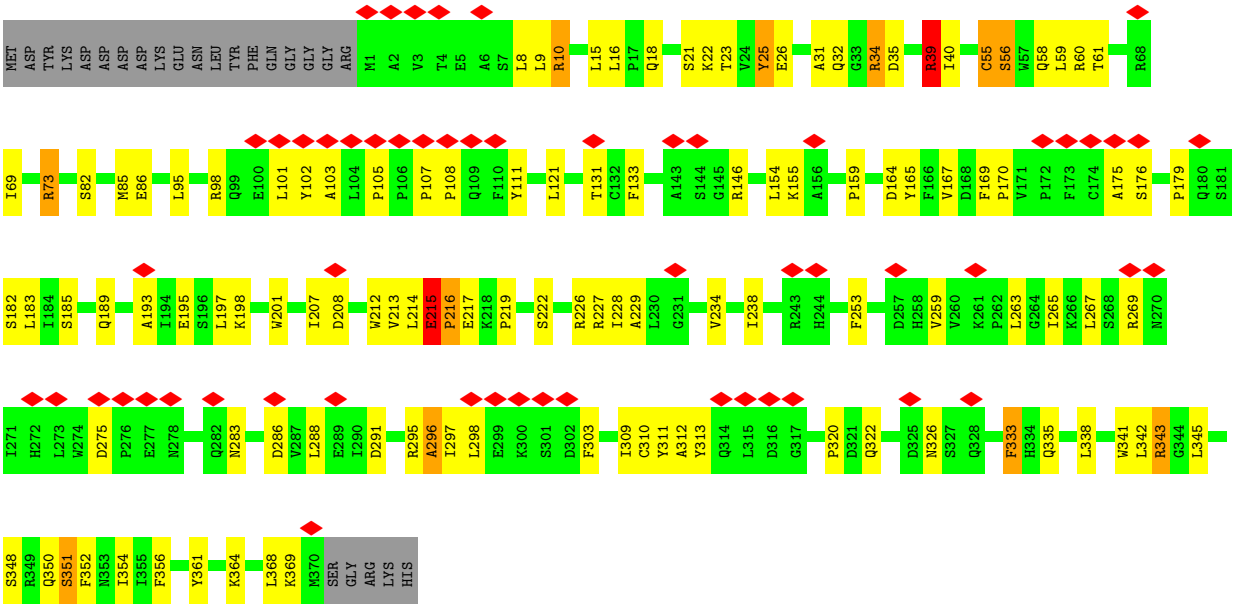
• Molecule 7: E3 ubiquitin-protein ligase FANCL

Chain L:



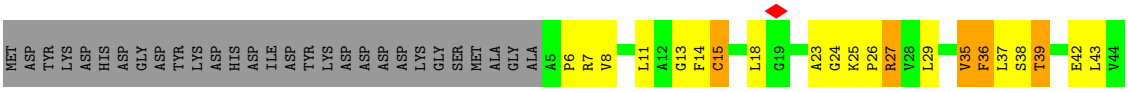
• Molecule 7: E3 ubiquitin-protein ligase FANCL

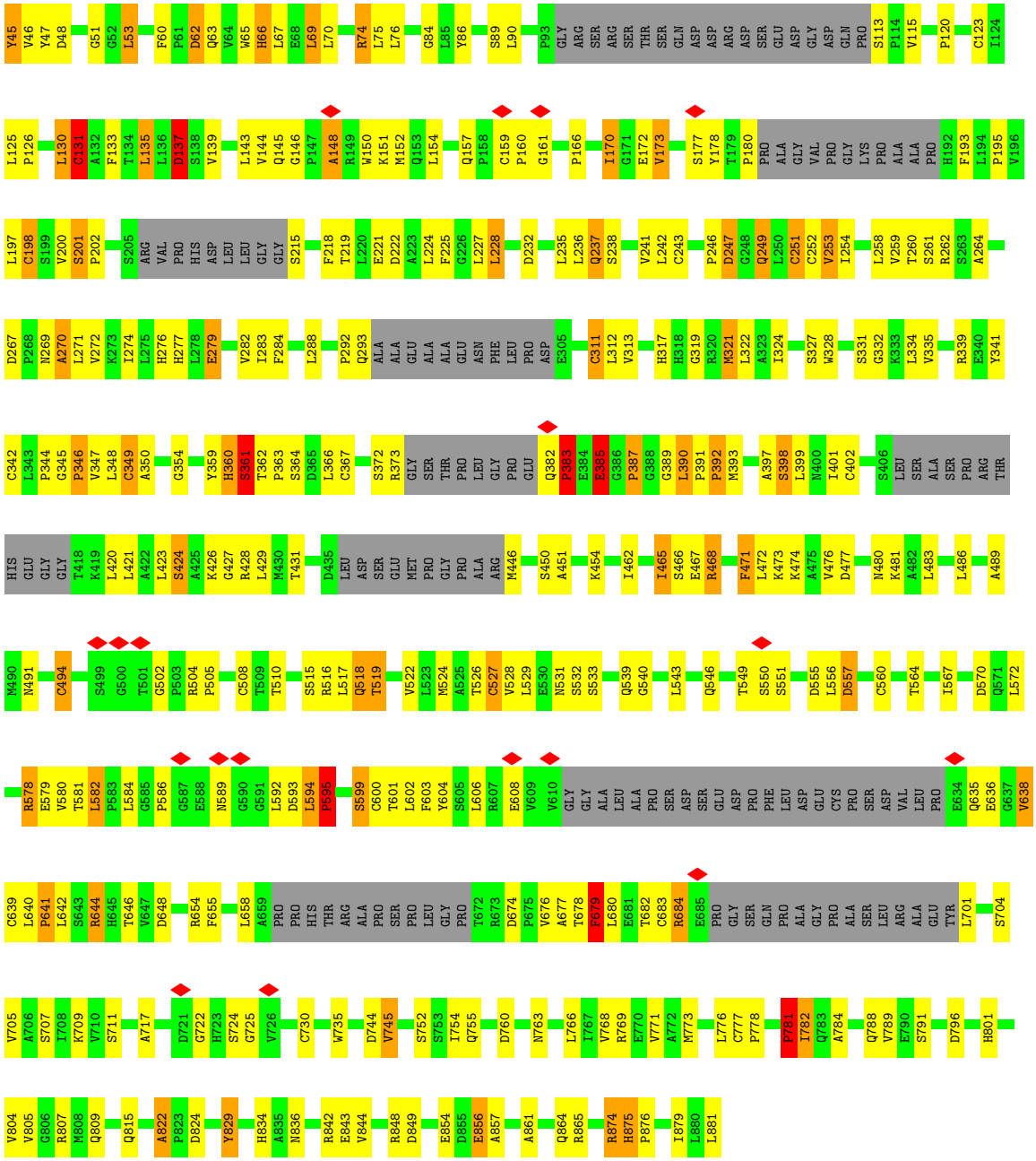
Chain M:



• Molecule 8: Fanconi anemia core complex-associated protein 100

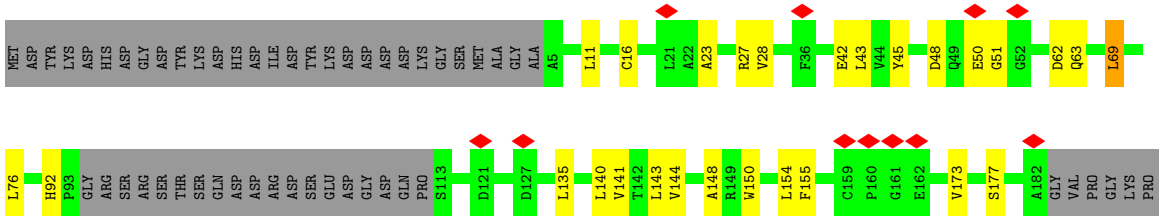
Chain P:

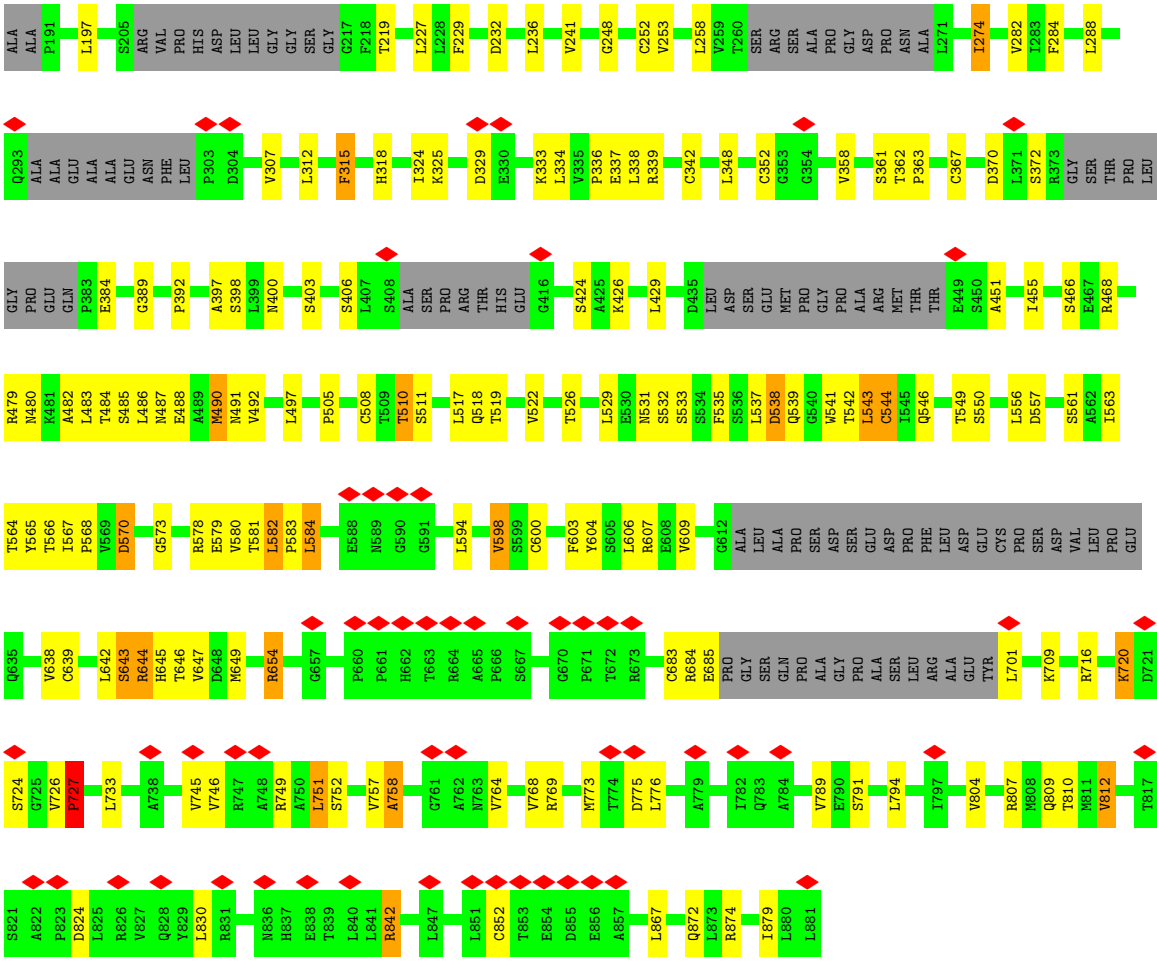




• Molecule 8: Fanconi anemia core complex-associated protein 100

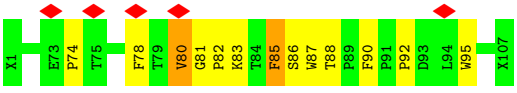
Chain Q:





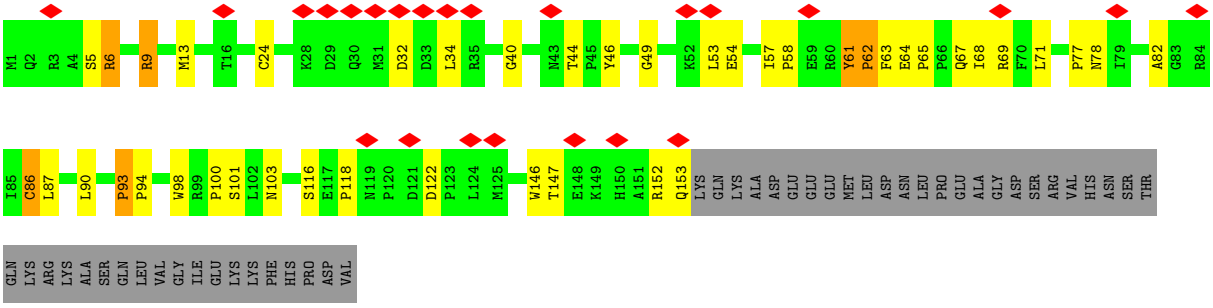
• Molecule 9: Fanconi anemia core complex-associated protein 20

Chain W:



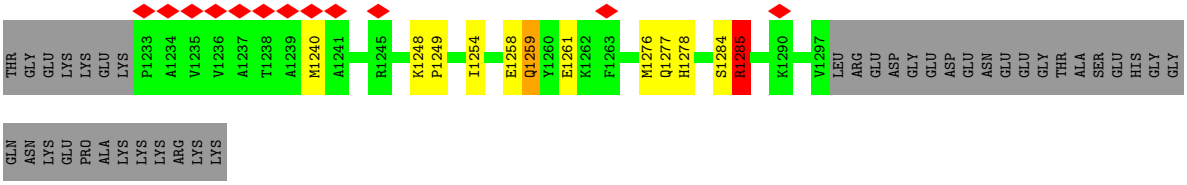
• Molecule 10: Ubiquitin-conjugating enzyme E2 T

Chain X:



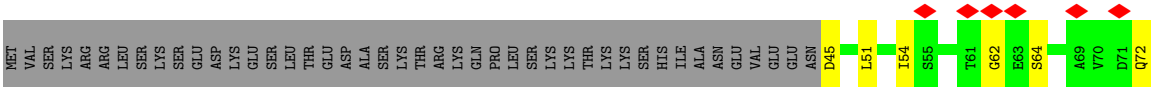
• Molecule 11: Fanconi anemia, complementation group I

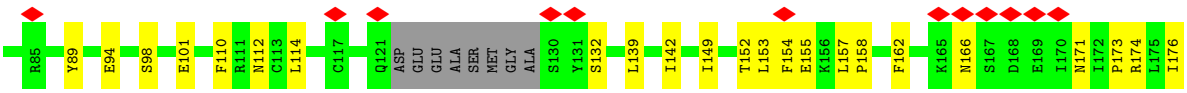
Chain U:

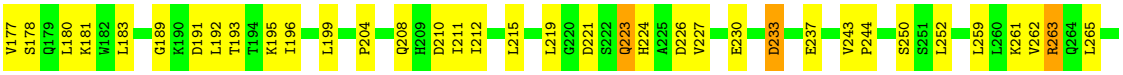


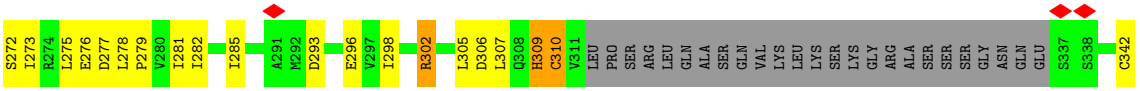
• Molecule 12: Fanconi anemia group D2 protein

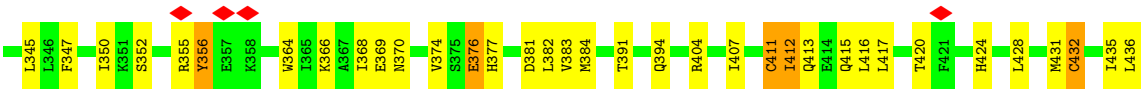
Chain V:

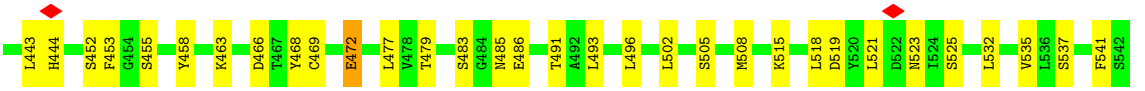


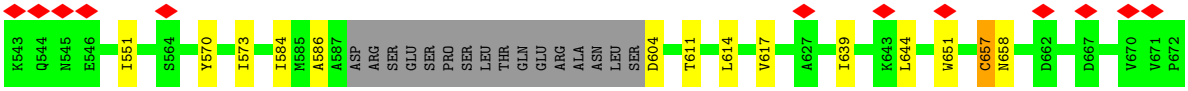


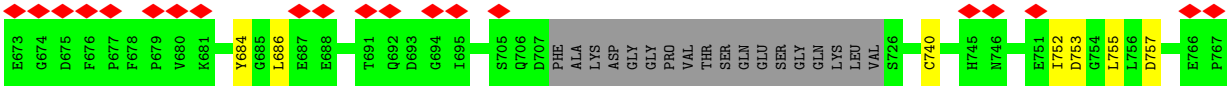


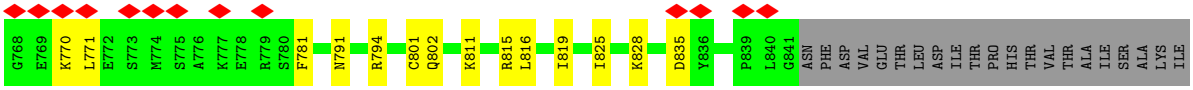


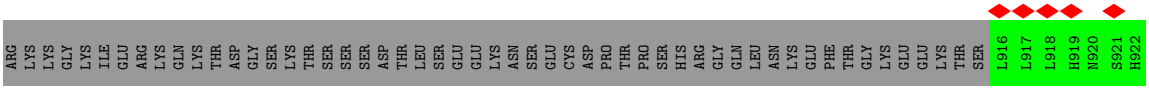


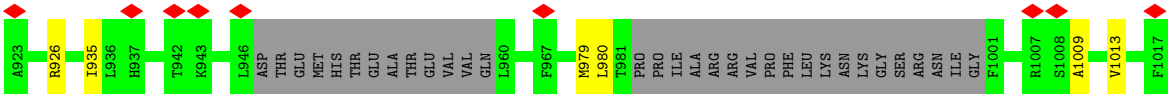


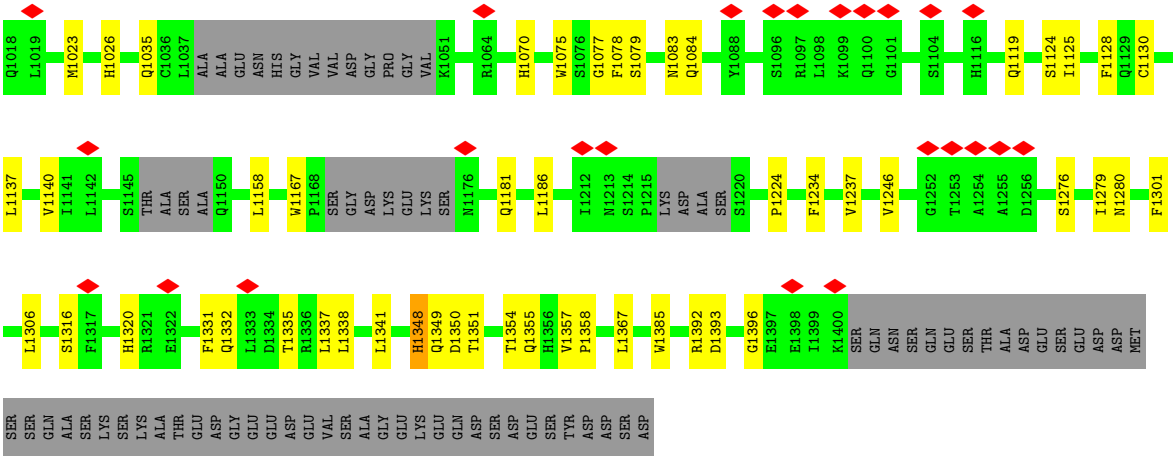




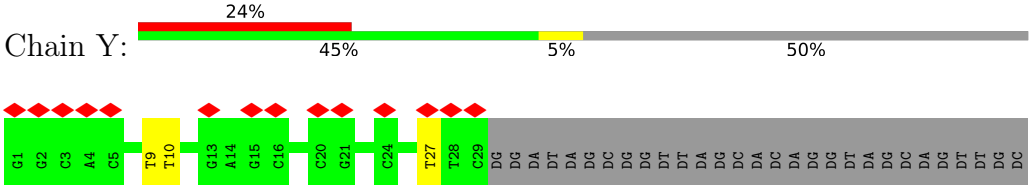




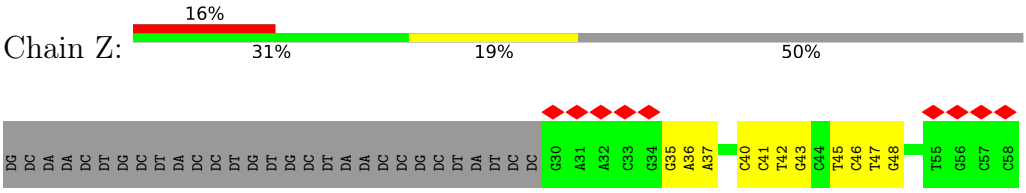




- Molecule 13: DNA (29-MER)



- Molecule 14: DNA (29-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74481	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	473.088, 473.088, 473.088	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.76	0/9605	1.05	16/13008 (0.1%)
1	S	0.76	0/10153	1.06	16/13749 (0.1%)
2	B	0.86	2/5707 (0.0%)	1.32	23/7686 (0.3%)
2	O	0.78	0/5701	1.11	6/7686 (0.1%)
3	C	0.82	1/4497 (0.0%)	1.19	12/6103 (0.2%)
4	E	0.86	1/3274 (0.0%)	1.25	8/4438 (0.2%)
5	F	0.81	0/2791	1.18	6/3790 (0.2%)
6	G	0.83	1/4568 (0.0%)	1.18	11/6215 (0.2%)
6	H	0.76	0/4293	1.12	12/5840 (0.2%)
7	L	0.82	5/3050 (0.2%)	1.16	11/4143 (0.3%)
7	M	0.79	0/3050	1.11	13/4143 (0.3%)
8	P	0.90	1/5697 (0.0%)	1.36	25/7752 (0.3%)
8	Q	0.78	0/5737	1.12	9/7810 (0.1%)
9	W	0.69	0/202	1.03	0/281
10	X	0.82	0/1267	1.15	2/1722 (0.1%)
11	U	0.81	0/9629	1.09	5/12982 (0.0%)
12	V	0.78	0/9464	1.03	3/12798 (0.0%)
13	Y	0.48	0/669	0.96	1/1031 (0.1%)
14	Z	0.49	0/663	0.95	0/1020
All	All	0.80	11/90017 (0.0%)	1.14	179/122197 (0.1%)

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	13
1	S	0	12
2	B	0	18
2	O	0	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	4
4	E	0	7
5	F	0	1
6	G	0	8
6	H	0	6
7	L	0	4
7	M	0	3
8	P	0	38
8	Q	0	10
10	X	0	5
11	U	0	5
12	V	0	5
All	All	0	152

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	332	PRO	C-N	-8.27	1.15	1.34
2	B	721	SER	CA-CB	-7.36	1.42	1.52
7	L	339	TYR	C-N	-7.29	1.17	1.34
7	L	305	MET	C-N	6.90	1.50	1.34
7	L	322	GLN	C-N	6.70	1.49	1.34
8	P	361	SER	CA-CB	6.22	1.62	1.52
2	B	315	SER	CA-CB	-5.87	1.44	1.52
3	C	201	GLU	CD-OE1	5.67	1.31	1.25
4	E	96	ARG	NE-CZ	5.44	1.40	1.33
7	L	313	TYR	C-N	5.34	1.46	1.34
6	G	344	SER	CA-CB	-5.13	1.45	1.52

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	39	ARG	CG-CD-NE	10.36	133.55	111.80
2	B	703	THR	CA-CB-OG1	-9.23	89.61	109.00
7	L	313	TYR	O-C-N	9.18	137.39	122.70
7	L	305	MET	O-C-N	9.04	137.16	122.70
8	P	27	ARG	NE-CZ-NH1	8.40	124.50	120.30
5	F	138	ARG	NE-CZ-NH1	8.23	124.42	120.30
6	H	214	ARG	CG-CD-NE	8.11	128.84	111.80
1	S	517	ARG	CG-CD-NE	8.06	128.73	111.80
7	M	333	PHE	C-N-CA	7.98	141.66	121.70
7	M	333	PHE	O-C-N	-7.79	110.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	138	ARG	NE-CZ-NH2	-7.50	116.55	120.30
6	G	397	PHE	CB-CA-C	-7.36	95.68	110.40
7	L	305	MET	CA-C-N	-7.34	101.05	117.20
1	S	874	ARG	CG-CD-NE	-7.25	96.56	111.80
8	Q	727	PRO	N-CD-CG	-7.07	92.59	103.20
6	G	594	GLU	CB-CA-C	-7.04	96.33	110.40
4	E	96	ARG	CB-CA-C	6.99	124.38	110.40
2	O	667	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	S	1104	ARG	CG-CD-NE	6.78	126.03	111.80
8	P	349	CYS	CA-CB-SG	-6.77	101.82	114.00
6	G	353	ARG	CB-CA-C	6.76	123.93	110.40
8	P	392	PRO	CB-CA-C	-6.76	95.09	112.00
10	X	6	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	S	661	ARG	CG-CD-NE	6.64	125.75	111.80
6	H	51	ARG	CG-CD-NE	-6.62	97.89	111.80
2	B	752	GLU	CB-CA-C	6.61	123.62	110.40
8	P	157	GLN	CB-CA-C	6.61	123.62	110.40
1	A	245	ARG	NE-CZ-NH1	6.60	123.60	120.30
8	P	874	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	670	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	O	481	ARG	CG-CD-NE	-6.50	98.15	111.80
8	Q	842	ARG	NE-CZ-NH2	6.49	123.55	120.30
7	M	343	ARG	NE-CZ-NH2	6.47	123.53	120.30
2	B	90	ASN	CB-CA-C	6.44	123.27	110.40
8	P	684	ARG	NE-CZ-NH2	6.41	123.50	120.30
4	E	92	ARG	NE-CZ-NH1	6.37	123.48	120.30
3	C	127	PHE	CB-CA-C	6.37	123.13	110.40
3	C	79	PHE	CA-CB-CG	-6.36	98.63	113.90
1	A	951	ARG	NE-CZ-NH2	6.32	123.46	120.30
2	B	196	CYS	C-N-CA	6.28	137.41	121.70
6	G	573	ARG	NE-CZ-NH1	6.27	123.43	120.30
2	B	519	ARG	CB-CA-C	6.26	122.92	110.40
2	B	287	VAL	CA-CB-CG2	6.25	120.27	110.90
6	H	241	PRO	N-CA-C	6.16	128.13	112.10
1	S	29	ARG	NE-CZ-NH2	-6.16	117.22	120.30
7	M	73	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	C	266	ARG	NE-CZ-NH1	6.05	123.33	120.30
7	M	60	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	B	21	GLU	CB-CA-C	6.02	122.44	110.40
2	O	586	PRO	N-CA-CB	-6.02	95.98	102.60
6	H	120	GLU	CB-CA-C	-6.00	98.39	110.40
7	L	313	TYR	CA-C-N	-6.00	103.99	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Q	468	ARG	CG-CD-NE	6.00	124.39	111.80
4	E	399	CYS	CB-CA-C	5.98	122.36	110.40
2	O	525	ASN	CB-CA-C	5.97	122.34	110.40
2	B	725	THR	CA-CB-OG1	5.96	121.52	109.00
4	E	142	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	S	517	ARG	CB-CG-CD	5.95	127.08	111.60
1	A	1184	ARG	NE-CZ-NH2	5.95	123.27	120.30
8	P	654	ARG	NE-CZ-NH2	-5.94	117.33	120.30
8	Q	654	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	1425	ARG	NE-CZ-NH1	5.93	123.27	120.30
6	H	102	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	B	135	ARG	CG-CD-NE	5.91	124.20	111.80
2	B	517	ARG	NE-CZ-NH2	5.90	123.25	120.30
2	B	519	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	O	667	TYR	CB-CG-CD1	5.86	124.52	121.00
10	X	94	PRO	N-CA-C	5.86	127.34	112.10
8	P	595	PRO	N-CD-CG	-5.85	94.43	103.20
8	P	222	ASP	CB-CA-C	5.82	122.04	110.40
6	G	396	VAL	CA-CB-CG1	5.82	119.62	110.90
1	A	286	GLN	CB-CA-C	5.79	121.98	110.40
6	G	520	ARG	NE-CZ-NH1	5.78	123.19	120.30
8	P	249	GLN	N-CA-CB	5.75	120.96	110.60
3	C	283	GLN	CB-CA-C	5.75	121.90	110.40
7	M	310	CYS	O-C-N	-5.75	113.51	122.70
1	A	714	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	B	409	ARG	NE-CZ-NH2	-5.73	117.43	120.30
7	M	333	PHE	CA-C-N	5.72	129.78	117.20
6	H	233	HIS	CB-CA-C	5.71	121.82	110.40
1	A	670	ARG	NE-CZ-NH1	5.68	123.14	120.30
8	P	385	GLU	CB-CG-CD	-5.68	98.88	114.20
7	M	34	ARG	NE-CZ-NH2	5.68	123.14	120.30
11	U	1285	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	1329	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	S	1080	ARG	NE-CZ-NH1	-5.63	117.48	120.30
8	P	39	THR	CA-CB-OG1	-5.63	97.17	109.00
6	H	120	GLU	N-CA-CB	5.62	120.72	110.60
8	Q	468	ARG	CB-CG-CD	-5.62	96.99	111.60
5	F	287	TYR	CB-CG-CD1	5.61	124.36	121.00
6	G	497	PHE	CB-CG-CD1	5.61	124.72	120.80
1	S	1184	ARG	CG-CD-NE	-5.61	100.03	111.80
7	M	39	ARG	CG-CD-NE	5.61	123.58	111.80
8	P	829	TYR	CB-CG-CD1	-5.61	117.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	1080	ARG	NE-CZ-NH2	5.61	123.10	120.30
7	M	10	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	47	ARG	CB-CA-C	5.59	121.58	110.40
7	M	310	CYS	C-N-CA	5.58	135.65	121.70
7	L	343	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	S	1049	PHE	CB-CA-C	5.55	121.51	110.40
1	A	288	GLU	CB-CA-C	5.54	121.47	110.40
8	P	684	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	A	163	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	S	1012	THR	CB-CA-C	5.51	126.47	111.60
2	B	181	MET	CA-CB-CG	5.50	122.65	113.30
8	Q	654	ARG	NE-CZ-NH2	5.49	123.04	120.30
8	Q	544	CYS	CA-CB-SG	-5.48	104.13	114.00
3	C	127	PHE	C-N-CA	5.48	135.39	121.70
3	C	343	TYR	CB-CA-C	5.48	121.35	110.40
7	L	237	ASN	CB-CA-C	5.48	121.35	110.40
2	B	18	TYR	CB-CG-CD1	-5.47	117.72	121.00
6	H	369	ASP	CB-CA-C	-5.47	99.46	110.40
1	S	29	ARG	NE-CZ-NH1	5.45	123.03	120.30
5	F	339	PHE	CB-CA-C	5.45	121.30	110.40
6	G	381	ARG	NE-CZ-NH1	5.42	123.01	120.30
12	V	302	ARG	NE-CZ-NH1	5.42	123.01	120.30
4	E	90	LEU	CB-CA-C	5.42	120.50	110.20
8	P	654	ARG	NE-CZ-NH1	5.41	123.01	120.30
11	U	226	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	714	ARG	NE-CZ-NH1	-5.38	117.61	120.30
8	P	551	SER	CB-CA-C	5.37	120.30	110.10
7	L	60	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	C	206	CYS	CB-CA-C	5.34	121.07	110.40
8	P	178	TYR	CA-CB-CG	-5.33	103.27	113.40
1	A	756	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	167	PHE	CB-CG-CD1	5.30	124.51	120.80
8	Q	490	MET	N-CA-CB	5.30	120.14	110.60
2	B	735	ILE	C-N-CA	5.30	134.94	121.70
7	M	60	ARG	CB-CG-CD	5.28	125.33	111.60
3	C	245	ARG	CB-CA-C	5.28	120.95	110.40
2	B	196	CYS	CB-CA-C	5.27	120.95	110.40
8	P	221	GLU	N-CA-CB	5.27	120.08	110.60
11	U	461	ASP	CB-CA-C	5.26	120.92	110.40
6	G	366	HIS	CB-CA-C	5.26	120.92	110.40
7	M	35	ASP	CB-CA-C	5.25	120.91	110.40
1	S	670	ARG	CB-CA-C	5.25	120.89	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	492	LYS	CB-CA-C	5.24	120.88	110.40
7	L	343	ARG	NE-CZ-NH2	-5.23	117.68	120.30
8	P	346	PRO	N-CA-C	-5.23	98.50	112.10
4	E	62	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	S	1033	ASP	CB-CG-OD2	5.22	122.99	118.30
12	V	276	GLU	CB-CA-C	5.22	120.83	110.40
6	H	423	ARG	NE-CZ-NH1	5.21	122.91	120.30
8	P	237	GLN	CB-CG-CD	5.20	125.12	111.60
2	B	135	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	C	209	ARG	CG-CD-NE	5.20	122.71	111.80
4	E	27	ARG	NE-CZ-NH2	5.20	122.90	120.30
8	P	282	VAL	CA-CB-CG2	5.20	118.69	110.90
6	G	475	GLU	CB-CA-C	5.19	120.78	110.40
1	A	1136	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	S	903	TRP	CA-CB-CG	-5.19	103.84	113.70
1	A	1146	ARG	NE-CZ-NH1	5.18	122.89	120.30
6	G	590	PRO	N-CD-CG	-5.18	95.43	103.20
8	P	467	GLU	CB-CA-C	-5.18	100.05	110.40
8	Q	583	PRO	CB-CA-C	-5.17	99.06	112.00
6	H	102	ARG	NE-CZ-NH1	5.17	122.88	120.30
13	Y	27	DT	N1-C1'-C2'	5.16	122.41	112.60
5	F	140	ARG	CG-CD-NE	-5.16	100.97	111.80
2	B	396	THR	CA-CB-OG1	-5.14	98.21	109.00
8	P	385	GLU	CB-CA-C	-5.11	100.17	110.40
12	V	263	ARG	NE-CZ-NH1	5.11	122.85	120.30
3	C	79	PHE	CB-CG-CD2	-5.11	117.23	120.80
2	O	518	PHE	CB-CA-C	5.10	120.60	110.40
6	H	75	CYS	CA-CB-SG	-5.09	104.83	114.00
11	U	1042	PRO	N-CA-CB	-5.09	97.00	102.60
3	C	324	GLU	CB-CA-C	5.07	120.55	110.40
3	C	292	ARG	CG-CD-NE	-5.06	101.18	111.80
8	P	293	GLN	CB-CA-C	5.05	120.50	110.40
7	L	305	MET	C-N-CA	-5.03	109.12	121.70
1	S	824	CYS	CB-CA-C	5.03	120.46	110.40
11	U	437	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	B	736	ARG	NE-CZ-NH1	5.02	122.81	120.30
8	P	679	PHE	CB-CG-CD1	-5.02	117.29	120.80
2	B	298	PHE	CB-CG-CD1	5.02	124.31	120.80
4	E	65	GLU	CB-CA-C	-5.02	100.37	110.40
1	A	510	TYR	CB-CA-C	-5.01	100.39	110.40
5	F	165	THR	CA-CB-OG1	-5.01	98.48	109.00
7	L	128	TYR	CB-CA-C	5.00	120.41	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	321	PHE	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (152) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	GLY	Peptide
1	A	1121	SER	Peptide
1	A	1220	PRO	Peptide
1	A	1350	GLU	Peptide
1	A	1375	THR	Peptide
1	A	138	THR	Peptide
1	A	1428	CYS	Peptide
1	A	284	GLY	Peptide
1	A	484	GLU	Peptide
1	A	824	CYS	Peptide
1	A	897	HIS	Peptide
1	A	922	GLU	Peptide
1	A	923	GLU	Peptide
2	B	132	ASP	Peptide
2	B	139	GLY	Peptide
2	B	140	PRO	Peptide
2	B	145	ARG	Peptide
2	B	191	LEU	Peptide
2	B	225	ASP	Peptide
2	B	258	ALA	Peptide
2	B	324	LYS	Peptide
2	B	335	GLY	Peptide
2	B	345	PHE	Peptide
2	B	367	TYR	Sidechain
2	B	608	ASN	Peptide
2	B	636	PHE	Peptide
2	B	637	PRO	Peptide
2	B	668	ALA	Peptide
2	B	711	THR	Peptide
2	B	748	LYS	Peptide
2	B	857	SER	Peptide
3	C	208	GLY	Peptide
3	C	278	ASP	Peptide
3	C	539	GLU	Peptide
3	C	79	PHE	Sidechain
4	E	108	SER	Peptide

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Mol	Chain	Res	Type	Group
4	E	126	ALA	Peptide
4	E	147	GLY	Peptide
4	E	151	GLU	Peptide
4	E	464	MET	Peptide
4	E	500	TYR	Peptide
4	E	76	GLY	Peptide
5	F	285	LEU	Peptide
6	G	132	LEU	Peptide
6	G	276	GLY	Peptide
6	G	388	PRO	Peptide
6	G	427	LEU	Peptide
6	G	430	LYS	Peptide
6	G	500	GLU	Peptide
6	G	563	ARG	Peptide
6	G	61	PRO	Peptide
6	H	132	LEU	Peptide
6	H	186	PRO	Peptide
6	H	276	GLY	Peptide
6	H	279	TRP	Peptide
6	H	33	SER	Peptide
6	H	563	ARG	Peptide
7	L	103	ALA	Peptide
7	L	109	GLN	Peptide
7	L	252	PHE	Peptide
7	L	55	CYS	Peptide
7	M	215	GLU	Peptide
7	M	350	GLN	Peptide
7	M	55	CYS	Peptide
2	O	154	SER	Peptide
2	O	247	ILE	Peptide
2	O	316	PHE	Peptide
2	O	483	ILE	Peptide
2	O	485	ASP	Peptide
2	O	525	ASN	Peptide
2	O	578	ILE	Peptide
2	O	581	VAL	Peptide
2	O	593	PHE	Peptide
2	O	635	THR	Peptide
2	O	636	PHE	Peptide
2	O	637	PRO	Peptide
2	O	857	SER	Peptide
8	P	131	CYS	Peptide

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Mol	Chain	Res	Type	Group
8	P	146	GLY	Peptide
8	P	170	ILE	Peptide
8	P	23	ALA	Peptide
8	P	24	GLY	Peptide
8	P	270	ALA	Peptide
8	P	283	ILE	Peptide
8	P	292	PRO	Peptide
8	P	319	GLY	Peptide
8	P	331	SER	Peptide
8	P	344	PRO	Peptide
8	P	345	GLY	Peptide
8	P	36	PHE	Peptide
8	P	361	SER	Peptide
8	P	382	GLN	Peptide
8	P	383	PRO	Peptide
8	P	389	GLY	Peptide
8	P	391	PRO	Peptide
8	P	397	ALA	Peptide
8	P	398	SER	Peptide
8	P	450	SER	Peptide
8	P	519	THR	Peptide
8	P	556	LEU	Peptide
8	P	582	LEU	Peptide
8	P	584	LEU	Peptide
8	P	589	ASN	Peptide
8	P	594	LEU	Mainchain,Peptide
8	P	62	ASP	Peptide
8	P	635	GLN	Peptide
8	P	636	GLU	Peptide
8	P	679	PHE	Sidechain
8	P	722	GLY	Peptide
8	P	724	SER	Peptide
8	P	725	GLY	Peptide
8	P	755	GLN	Peptide
8	P	781	PRO	Peptide
8	P	856	GLU	Peptide
8	Q	315	PHE	Peptide
8	Q	338	LEU	Peptide
8	Q	389	GLY	Peptide
8	Q	538	ASP	Peptide
8	Q	549	THR	Peptide
8	Q	584	LEU	Peptide

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Mol	Chain	Res	Type	Group
8	Q	594	LEU	Peptide
8	Q	647	VAL	Peptide
8	Q	720	LYS	Peptide
8	Q	724	SER	Peptide
1	S	1121	SER	Peptide
1	S	1350	GLU	Peptide
1	S	284	GLY	Peptide
1	S	31	LYS	Peptide
1	S	484	GLU	Peptide
1	S	495	HIS	Peptide
1	S	561	THR	Peptide
1	S	736	VAL	Peptide
1	S	822	LEU	Peptide
1	S	898	LEU	Peptide
1	S	923	GLU	Peptide
1	S	960	HIS	Peptide
11	U	1154	PRO	Peptide
11	U	415	ASN	Peptide
11	U	547	PHE	Peptide
11	U	640	ASP	Peptide
11	U	933	ALA	Peptide
12	V	1224	PRO	Peptide
12	V	204	PRO	Peptide
12	V	377	HIS	Peptide
12	V	411	CYS	Peptide
12	V	541	PHE	Peptide
10	X	152	ARG	Peptide
10	X	61	TYR	Mainchain,Peptide
10	X	93	PRO	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9402	9487	9431	237	0
1	S	9933	10028	9969	182	0
2	B	5605	5790	5768	200	0
2	O	5594	5759	5740	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4396	4442	4427	105	0
4	E	3224	3390	3384	113	0
5	F	2726	2740	2729	61	0
6	G	4483	4537	4523	141	0
6	H	4216	4288	4273	97	0
7	L	2974	2977	2970	90	0
7	M	2974	2977	2972	111	0
8	P	5598	5681	5652	238	0
8	Q	5631	5724	5694	108	0
9	W	271	242	195	8	0
10	X	1233	1251	1248	54	0
11	U	9484	9883	9852	182	0
12	V	9289	9518	9465	142	0
13	Y	597	326	326	2	0
14	Z	592	325	325	6	0
15	G	1	0	0	0	0
15	L	2	0	0	0	0
15	M	2	0	0	0	0
All	All	88227	89365	88943	1993	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1993) 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)
7:M:311:TYR:CD2	10:X:6:ARG:HD2	1.47	1.49
7:M:311:TYR:CD2	10:X:6:ARG:CD	2.05	1.38
7:M:361:TYR:CE1	10:X:101:SER:HA	1.69	1.26
7:M:311:TYR:HD2	10:X:6:ARG:CD	1.43	1.13
1:A:30:VAL:HG21	6:H:372:ALA:HB1	1.26	1.09
5:F:311:PHE:O	5:F:315:CYS:SG	2.09	1.09
7:M:311:TYR:CE2	10:X:6:ARG:CD	2.36	1.09
7:M:311:TYR:CD2	10:X:6:ARG:HD3	1.89	1.05
7:M:312:ALA:HB2	10:X:5:SER:HB2	1.36	1.04
7:M:215:GLU:OE1	7:M:313:TYR:OH	1.74	1.02
7:M:361:TYR:CD1	10:X:101:SER:HB3	1.95	1.02
7:M:311:TYR:HE2	10:X:6:ARG:NH1	1.59	1.00
4:E:391:CYS:SG	4:E:398:VAL:HG11	2.02	0.99
7:M:311:TYR:CE2	10:X:6:ARG:HD3	1.98	0.98
3:C:286:CYS:O	3:C:340:TYR:OH	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:393:MET:HG2	8:P:236:LEU:HD21	1.47	0.95
3:C:224:ASN:ND2	3:C:249:SER:HB3	1.80	0.94
7:M:361:TYR:CE1	10:X:101:SER:CA	2.49	0.94
7:M:312:ALA:HB2	10:X:5:SER:CB	1.99	0.92
8:P:154:LEU:HD22	8:P:258:LEU:HD23	1.49	0.91
10:X:44:THR:HG21	10:X:116:SER:HA	1.53	0.91
1:A:30:VAL:HG21	6:H:372:ALA:CB	1.99	0.91
4:E:391:CYS:SG	4:E:423:LEU:HD21	2.11	0.90
12:V:263:ARG:NH2	12:V:293:ASP:OD2	2.05	0.90
3:C:224:ASN:HD21	3:C:249:SER:HB3	1.38	0.89
6:G:214:ARG:NH1	6:G:328:LEU:O	2.05	0.88
7:L:313:TYR:CE1	7:L:319:ILE:HG23	2.07	0.88
7:L:354:ILE:CG1	7:L:369:LYS:HG2	2.03	0.88
3:C:241:CYS:SG	4:E:37:PRO:HD3	2.13	0.88
1:A:78:ILE:HG23	1:A:123:GLN:HE22	1.38	0.88
12:V:352:SER:O	12:V:356:TYR:HB2	1.75	0.87
7:L:354:ILE:HG12	7:L:369:LYS:HG2	1.56	0.87
1:S:494:LEU:HD11	1:S:518:LEU:HD11	1.57	0.87
1:A:30:VAL:CG2	6:H:372:ALA:HB1	2.04	0.86
7:M:73:ARG:HD3	7:M:86:GLU:OE1	1.75	0.86
1:A:300:GLY:O	1:A:303:SER:OG	1.94	0.85
5:F:289:LEU:HD12	6:G:539:LEU:HD21	1.57	0.85
5:F:289:LEU:HD12	6:G:539:LEU:CD2	2.07	0.85
7:M:311:TYR:HD2	10:X:6:ARG:HD2	0.91	0.85
7:L:357:GLY:O	7:L:366:ILE:HG22	1.77	0.84
8:P:679:PHE:C	8:P:679:PHE:CD2	2.50	0.84
1:S:288:GLU:HB3	1:S:292:HIS:HB2	1.59	0.84
7:M:311:TYR:HE2	10:X:6:ARG:CZ	1.89	0.84
3:C:224:ASN:ND2	3:C:249:SER:CB	2.39	0.84
1:A:30:VAL:CG2	6:H:372:ALA:CB	2.54	0.84
7:M:311:TYR:CE2	10:X:6:ARG:NH1	2.47	0.82
7:L:339:TYR:OH	7:L:343:ARG:NH1	2.11	0.81
1:S:868:PHE:CZ	1:S:910:LEU:HD22	2.16	0.81
2:B:138:ASN:ND2	8:P:15:CYS:SG	2.54	0.80
11:U:511:MET:SD	11:U:514:ARG:NH1	2.55	0.80
8:P:402:CYS:SG	8:P:421:LEU:HB2	2.22	0.80
7:M:361:TYR:CD1	10:X:101:SER:CB	2.64	0.80
8:P:198:CYS:N	8:P:242:LEU:O	2.14	0.79
11:U:525:MET:SD	11:U:594:CYS:SG	2.80	0.79
7:L:356:PHE:CD1	7:L:367:THR:HG23	2.18	0.79
6:G:303:LEU:O	6:G:306:LEU:HB3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:197:LEU:HD13	7:M:201:TRP:CZ2	2.19	0.78
12:V:586:ALA:HB1	12:V:644:LEU:HD13	1.64	0.78
1:A:919:VAL:O	1:A:923:GLU:OE2	2.01	0.78
6:G:333:ASP:OD1	6:G:336:SER:N	2.17	0.78
7:L:313:TYR:CD2	7:L:314:GLN:HG2	2.19	0.78
8:Q:531:ASN:ND2	8:Q:573:GLY:O	2.16	0.78
7:M:311:TYR:HE2	10:X:6:ARG:HH11	1.28	0.78
2:B:259:LEU:HD12	2:B:284:PRO:HB2	1.66	0.78
8:Q:510:THR:OG1	8:Q:645:HIS:ND1	2.17	0.77
6:G:547:ASN:HD22	6:G:550:THR:HG23	1.49	0.77
2:O:480:TYR:HE2	2:O:622:LEU:HD13	1.49	0.77
11:U:606:TYR:OH	11:U:662:GLU:OE2	2.02	0.77
7:M:338:LEU:HD23	7:M:368:LEU:HD13	1.66	0.77
11:U:1149:VAL:O	11:U:1212:PHE:HD2	1.68	0.77
2:O:257:ILE:HD12	2:O:299:PHE:CE2	2.21	0.76
4:E:455:GLN:NE2	4:E:459:GLU:OE1	2.18	0.76
2:O:155:SER:O	2:O:156:GLN:HB3	1.84	0.76
1:S:1033:ASP:OD2	1:S:1093:SER:HB2	1.85	0.76
5:F:18:SER:O	5:F:100:ASN:ND2	2.19	0.75
6:G:60:LEU:O	6:G:102:ARG:NH1	2.20	0.75
6:H:103:VAL:O	6:H:106:THR:OG1	2.04	0.75
1:S:974:ASP:O	1:S:976:ASP:N	2.20	0.75
1:S:288:GLU:CB	1:S:292:HIS:HB2	2.15	0.75
1:A:1113:ASN:O	1:A:1117:ARG:NE	2.20	0.74
7:M:197:LEU:CD1	7:M:201:TRP:CZ2	2.69	0.74
5:F:255:LEU:HD12	5:F:260:LEU:HD21	1.70	0.74
8:P:366:LEU:HD22	8:P:393:MET:SD	2.27	0.74
7:M:311:TYR:CE2	10:X:6:ARG:CZ	2.70	0.74
3:C:55:MET:SD	3:C:60:VAL:HG21	2.27	0.74
6:G:406:GLN:HE21	6:G:599:TRP:HB2	1.52	0.74
8:P:11:LEU:HD13	8:P:429:LEU:HD23	1.67	0.74
11:U:322:PHE:O	11:U:326:VAL:HG23	1.87	0.73
1:S:1045:GLU:OE2	1:S:1104:ARG:N	2.21	0.73
2:B:242:ILE:O	2:B:243:CYS:SG	2.46	0.73
5:F:289:LEU:O	6:G:485:ARG:NH1	2.14	0.73
7:L:342:LEU:HD21	7:L:358:GLU:O	1.87	0.73
8:Q:11:LEU:HD11	8:Q:429:LEU:HD22	1.69	0.73
1:A:286:GLN:C	1:A:288:GLU:H	1.92	0.73
1:A:944:ASP:OD1	1:A:951:ARG:NH1	2.21	0.72
8:P:527:CYS:SG	8:P:580:VAL:HB	2.29	0.72
1:A:35:TYR:HE2	6:H:311:ASN:CB	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:11:LEU:HD22	8:P:429:LEU:HD22	1.71	0.72
8:P:674:ASP:OD2	8:P:677:ALA:N	2.22	0.72
2:O:601:ILE:HD12	2:O:613:ARG:O	1.90	0.71
8:P:362:THR:HB	8:P:363:PRO:HD2	1.72	0.71
1:S:1410:CYS:SG	1:S:1414:SER:OG	2.48	0.71
2:O:423:TYR:CE1	8:Q:606:LEU:HD12	2.23	0.71
5:F:282:GLY:HA3	5:F:347:TRP:CH2	2.25	0.71
6:G:425:SER:HA	6:G:428:LEU:HD12	1.72	0.71
8:P:65:TRP:O	8:P:66:HIS:HB2	1.91	0.71
8:P:603:PHE:HD1	8:P:639:CYS:HG	1.38	0.71
3:C:118:LEU:HA	3:C:121:ILE:HD12	1.72	0.71
7:L:315:LEU:CD2	7:L:336:ILE:HD13	2.20	0.71
3:C:397:PHE:CZ	3:C:404:ALA:HA	2.26	0.71
1:S:940:GLN:HE21	1:S:1011:ARG:HD2	1.54	0.71
1:S:993:GLN:HE22	1:S:1074:GLU:HB2	1.56	0.71
1:A:394:SER:HB2	1:A:436:GLN:HE21	1.56	0.70
11:U:711:ASN:HA	11:U:714:ILE:HD12	1.73	0.70
2:B:682:CYS:HB3	2:B:692:TYR:HB3	1.73	0.70
1:A:185:LEU:HD12	1:A:191:VAL:HG22	1.74	0.70
5:F:139:ARG:O	5:F:142:ALA:HB3	1.91	0.70
3:C:82:ALA:HB3	3:C:189:PRO:HB3	1.72	0.70
1:S:830:LEU:HD22	1:S:871:LEU:HD21	1.72	0.70
7:L:204:MET:SD	7:L:226:ARG:NH1	2.64	0.70
6:G:480:LEU:HD11	6:G:517:LEU:HD23	1.74	0.70
1:A:35:TYR:CE2	6:H:311:ASN:CB	2.75	0.69
5:F:283:GLN:NE2	5:F:332:CYS:SG	2.65	0.69
8:P:11:LEU:HD13	8:P:429:LEU:CD2	2.22	0.69
11:U:647:LEU:HD13	11:U:721:PHE:CE1	2.28	0.69
1:A:34:LYS:H	1:A:34:LYS:HE2	1.56	0.69
6:G:159:LEU:HD23	6:G:177:LEU:HD12	1.74	0.69
6:G:393:MET:HG2	8:P:236:LEU:CD2	2.23	0.69
8:P:11:LEU:HD11	8:P:431:THR:HG23	1.74	0.69
8:P:446:MET:CE	8:P:451:ALA:HB2	2.23	0.69
6:H:342:THR:HB	6:H:384:PRO:HG3	1.74	0.68
8:P:735:TRP:O	8:P:807:ARG:NH1	2.26	0.68
8:P:367:CYS:HA	8:P:392:PRO:HA	1.74	0.68
1:S:428:VAL:HG22	1:S:476:PHE:CE1	2.28	0.68
7:M:197:LEU:HD13	7:M:201:TRP:CH2	2.28	0.68
12:V:435:ILE:HG22	12:V:436:LEU:HD23	1.74	0.68
1:A:1045:GLU:OE2	1:A:1104:ARG:N	2.26	0.68
2:O:581:VAL:C	2:O:582:THR:OG1	2.32	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:347:VAL:C	8:P:348:LEU:HD12	2.14	0.68
1:A:30:VAL:CG2	6:H:372:ALA:HB3	2.24	0.68
2:B:240:VAL:CG1	2:B:256:LEU:HD11	2.24	0.68
2:O:707:TRP:CH2	2:O:715:GLY:HA3	2.29	0.68
7:M:311:TYR:CE2	10:X:6:ARG:NE	2.62	0.68
1:S:751:ARG:HA	1:S:754:CYS:SG	2.33	0.68
1:S:880:ARG:HB2	1:S:881:GLN:OE1	1.93	0.68
1:A:656:ALA:HB3	1:A:683:ARG:NH2	2.09	0.68
6:G:412:ASP:O	6:G:415:THR:N	2.28	0.67
11:U:751:GLU:CD	11:U:841:TYR:OH	2.32	0.67
2:B:15:LEU:O	2:B:79:CYS:SG	2.53	0.67
8:Q:538:ASP:O	8:Q:570:ASP:O	2.13	0.67
7:M:208:ASP:O	7:M:295:ARG:NH2	2.27	0.67
6:H:83:SER:O	6:H:86:GLN:NE2	2.27	0.67
2:B:298:PHE:CE1	2:B:312:TRP:CD1	2.82	0.67
3:C:142:PRO:HA	3:C:145:TYR:HE1	1.60	0.67
1:A:139:VAL:O	1:A:141:GLN:N	2.27	0.67
3:C:227:ILE:HD11	3:C:239:VAL:HG12	1.77	0.67
11:U:746:VAL:O	11:U:750:CYS:SG	2.53	0.67
2:B:259:LEU:CD1	2:B:284:PRO:HB2	2.24	0.67
2:B:664:SER:HB2	2:B:742:CYS:SG	2.35	0.67
5:F:160:ASP:O	5:F:164:LYS:HB2	1.95	0.67
2:B:298:PHE:CE1	2:B:312:TRP:HD1	2.13	0.67
6:G:346:THR:O	6:G:349:ILE:N	2.27	0.67
2:O:602:MET:N	2:O:602:MET:SD	2.67	0.67
1:A:1224:TRP:CZ3	1:A:1225:LEU:HD13	2.30	0.66
7:M:8:LEU:HD21	7:M:25:TYR:HE2	1.60	0.66
2:B:707:TRP:CH2	2:B:715:GLY:HA3	2.31	0.66
6:G:483:LEU:O	6:G:513:ARG:NH2	2.25	0.66
8:P:84:GLY:HA3	8:P:126:PRO:HA	1.77	0.66
8:P:510:THR:HA	8:P:526:THR:O	1.95	0.66
7:M:361:TYR:CZ	10:X:101:SER:HA	2.29	0.66
1:A:868:PHE:CZ	1:A:910:LEU:HD23	2.31	0.66
1:A:159:SER:OG	8:P:848:ARG:NH1	2.28	0.66
7:L:338:LEU:HD11	7:L:342:LEU:HD11	1.77	0.66
1:S:780:HIS:NE2	9:W:88:THR:O	2.25	0.66
1:S:1419:ALA:HB2	1:S:1440:GLN:HE22	1.59	0.66
11:U:371:SER:HA	11:U:375:TRP:CD1	2.31	0.66
4:E:495:THR:HG22	12:V:162:PHE:CZ	2.31	0.66
6:G:284:LEU:O	6:G:287:SER:OG	2.11	0.66
4:E:446:TRP:CD1	4:E:450:THR:HG21	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:354:ILE:HG12	7:L:369:LYS:CG	2.26	0.66
4:E:22:LEU:O	4:E:27:ARG:NH2	2.29	0.66
8:P:861:ALA:O	8:P:865:ARG:HB2	1.96	0.66
11:U:341:LEU:O	11:U:345:GLN:NE2	2.28	0.66
7:L:322:GLN:OE1	7:L:335:GLN:NE2	2.29	0.66
1:A:833:CYS:O	1:A:837:CYS:SG	2.50	0.66
7:L:41:VAL:HB	7:L:52:ARG:HB2	1.78	0.66
8:Q:48:ASP:O	8:Q:51:GLY:O	2.13	0.65
4:E:73:VAL:HG23	4:E:82:GLU:HG3	1.77	0.65
2:O:145:ARG:HG3	2:O:150:PHE:CE1	2.31	0.65
2:B:17:CYS:O	2:B:17:CYS:SG	2.49	0.65
2:B:723:ASN:ND2	2:O:484:ASP:OD1	2.30	0.65
8:P:399:LEU:O	8:P:423:LEU:O	2.15	0.65
2:B:484:ASP:OD1	2:B:484:ASP:N	2.29	0.65
1:S:424:LEU:HD21	1:S:472:PHE:HB3	1.79	0.65
1:A:835:LYS:HE2	1:A:903:TRP:CZ2	2.31	0.65
6:G:336:SER:OG	6:G:338:LEU:N	2.22	0.65
1:S:1330:LEU:O	1:S:1333:PHE:HB3	1.97	0.65
1:S:927:LEU:CD2	1:S:932:TRP:HB2	2.28	0.65
5:F:345:SER:O	5:F:348:THR:OG1	2.15	0.64
6:G:249:TYR:HA	6:G:252:LEU:HD12	1.78	0.64
12:V:366:LYS:O	12:V:370:ASN:ND2	2.31	0.64
3:C:142:PRO:HA	3:C:145:TYR:CE1	2.32	0.64
5:F:196:LEU:HD21	5:F:201:PHE:CD1	2.32	0.64
6:G:212:ALA:O	6:G:231:SER:OG	2.15	0.64
11:U:843:VAL:O	11:U:846:ALA:HB3	1.97	0.64
11:U:1149:VAL:O	11:U:1212:PHE:CD2	2.49	0.64
2:B:298:PHE:HE1	2:B:312:TRP:CD1	2.15	0.64
6:H:73:VAL:HA	6:H:76:ASN:HD22	1.63	0.64
8:P:602:LEU:O	8:P:640:LEU:N	2.26	0.64
1:A:818:PHE:HZ	1:A:861:SER:HB2	1.61	0.64
4:E:473:MET:CE	4:E:496:VAL:HG11	2.27	0.64
4:E:495:THR:HG22	12:V:162:PHE:HZ	1.62	0.64
5:F:189:LEU:HA	5:F:192:LEU:HD12	1.78	0.64
5:F:207:VAL:HA	5:F:210:LEU:HD12	1.80	0.64
3:C:224:ASN:HD22	3:C:249:SER:CB	2.10	0.64
11:U:777:CYS:SG	11:U:778:TYR:N	2.71	0.64
11:U:1025:CYS:SG	11:U:1074:ILE:HG23	2.38	0.64
2:O:257:ILE:HD12	2:O:299:PHE:CD2	2.33	0.64
3:C:267:ASN:O	3:C:555:ARG:NH2	2.31	0.64
8:Q:603:PHE:HA	8:Q:638:VAL:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:418:GLU:OE2	12:V:237:GLU:O	2.16	0.63
2:O:248:ILE:O	2:O:249:LYS:O	2.15	0.63
1:S:959:ILE:HG22	1:S:960:HIS:CE1	2.33	0.63
1:A:1393:VAL:HG21	6:H:570:LEU:HD21	1.80	0.63
11:U:445:LEU:HD21	11:U:463:LEU:HD13	1.79	0.63
12:V:1013:VAL:HG21	12:V:1075:TRP:CD2	2.33	0.63
8:P:655:PHE:CE2	8:P:754:ILE:HD12	2.33	0.63
7:M:198:LYS:HD3	7:M:198:LYS:C	2.19	0.63
7:M:198:LYS:HD3	7:M:198:LYS:O	1.98	0.63
1:A:27:ALA:HB3	6:H:372:ALA:CB	2.28	0.63
7:M:361:TYR:CD1	10:X:101:SER:CA	2.81	0.63
6:H:461:GLN:OE1	6:H:465:GLN:NE2	2.31	0.63
1:S:1161:THR:O	1:S:1321:ARG:NH2	2.31	0.63
1:A:818:PHE:HA	1:A:821:LEU:HB3	1.81	0.63
8:P:154:LEU:CD2	8:P:258:LEU:HD23	2.27	0.63
6:G:414:LEU:HD21	6:G:462:ALA:HB3	1.80	0.62
7:L:357:GLY:O	7:L:366:ILE:CG2	2.44	0.62
1:A:845:LEU:HD23	1:A:856:LEU:HD11	1.81	0.62
2:B:299:PHE:HZ	2:B:313:LYS:HD2	1.63	0.62
1:A:35:TYR:CE2	6:H:311:ASN:HB2	2.35	0.62
7:L:356:PHE:CE1	7:L:367:THR:CG2	2.81	0.62
3:C:60:VAL:O	3:C:64:PHE:CD2	2.53	0.62
4:E:518:PRO:HB2	4:E:521:THR:HG23	1.79	0.62
1:S:1368:PHE:CZ	1:S:1392:PRO:HB2	2.35	0.62
11:U:620:ALA:O	11:U:624:MET:HG2	2.00	0.62
7:L:275:ASP:O	7:L:283:ASN:ND2	2.32	0.62
1:S:874:ARG:O	1:S:946:LEU:HD11	2.00	0.62
11:U:1060:ILE:HD11	11:U:1212:PHE:CD2	2.33	0.62
1:S:351:THR:HG21	1:S:391:SER:HB2	1.80	0.62
1:S:1336:TYR:OH	1:S:1357:ALA:O	2.18	0.62
2:B:47:ARG:NH2	2:B:112:LEU:HD21	2.15	0.61
1:A:35:TYR:HE2	6:H:311:ASN:HB2	1.64	0.61
7:L:212:TRP:CZ3	7:L:296:ALA:HB3	2.36	0.61
11:U:1047:ARG:HG2	11:U:1051:GLN:HE21	1.64	0.61
1:A:815:PRO:HA	1:A:818:PHE:CE2	2.35	0.61
11:U:341:LEU:C	11:U:345:GLN:HE22	2.02	0.61
11:U:599:ALA:HB2	11:U:661:GLN:HA	1.82	0.61
8:P:253:VAL:HG23	8:P:272:VAL:HA	1.81	0.61
7:M:95:LEU:HD22	7:M:102:TYR:OH	2.01	0.61
1:S:182:VAL:HA	1:S:185:LEU:HG	1.83	0.61
2:B:330:ILE:HG22	2:B:339:GLU:CD	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:70:GLU:CB	4:E:83:LEU:HD22	2.31	0.61
4:E:424:VAL:HA	4:E:429:LEU:HD22	1.82	0.61
5:F:275:LEU:HD22	5:F:325:VAL:HG23	1.82	0.61
6:G:367:TYR:O	6:G:370:LEU:HB3	2.00	0.61
7:M:361:TYR:CD1	10:X:101:SER:HA	2.29	0.61
1:A:327:ILE:O	1:A:388:ARG:NH1	2.34	0.61
1:A:428:VAL:HG22	1:A:476:PHE:CE1	2.36	0.61
3:C:87:GLN:CD	3:C:87:GLN:H	2.03	0.61
7:M:309:ILE:HG12	7:M:333:PHE:HD1	1.66	0.61
2:B:851:PHE:HA	2:B:854:GLN:HE21	1.65	0.61
4:E:429:LEU:O	4:E:460:ARG:NH2	2.33	0.61
8:P:241:VAL:O	8:P:253:VAL:N	2.33	0.61
8:P:284:PHE:CG	8:P:350:ALA:HB3	2.36	0.61
12:V:479:THR:O	12:V:483:SER:OG	2.12	0.61
6:G:569:ALA:O	6:G:573:ARG:HG3	2.01	0.60
2:O:181:MET:HG3	2:O:217:LEU:HD22	1.83	0.60
7:M:322:GLN:OE1	7:M:335:GLN:NE2	2.34	0.60
1:A:474:PHE:CD2	1:A:510:TYR:CD2	2.88	0.60
11:U:474:LEU:HG	11:U:506:LEU:HD11	1.82	0.60
1:A:494:LEU:HD13	1:A:518:LEU:HD22	1.82	0.60
3:C:162:ARG:HB3	3:C:162:ARG:HH11	1.66	0.60
7:M:361:TYR:HD1	10:X:101:SER:HB3	1.62	0.60
1:A:137:LEU:HD13	1:A:141:GLN:HB3	1.84	0.60
2:B:287:VAL:HG23	2:B:288:GLN:O	2.01	0.60
6:G:397:PHE:O	6:G:400:ALA:HB3	2.00	0.60
8:P:366:LEU:CD2	8:P:393:MET:SD	2.88	0.60
1:S:927:LEU:HD21	1:S:932:TRP:HB2	1.82	0.60
4:E:391:CYS:SG	4:E:398:VAL:CG1	2.86	0.60
8:P:74:ARG:HD2	8:P:90:LEU:HB2	1.83	0.60
7:M:215:GLU:CD	7:M:313:TYR:OH	2.40	0.60
11:U:450:THR:HG21	12:V:356:TYR:CD2	2.37	0.60
4:E:156:LEU:HB2	4:E:161:GLN:HE22	1.66	0.60
8:Q:487:ASN:ND2	7:M:15:LEU:O	2.33	0.60
1:S:1045:GLU:HA	1:S:1104:ARG:HD3	1.82	0.60
2:B:667:TYR:O	2:B:713:PHE:CD1	2.55	0.60
6:H:72:THR:O	6:H:76:ASN:ND2	2.34	0.60
3:C:191:ILE:HG13	3:C:232:ILE:HD12	1.84	0.60
4:E:361:THR:HG23	4:E:401:ALA:HB2	1.84	0.60
8:P:390:LEU:HG	8:P:390:LEU:O	2.02	0.60
3:C:315:ILE:HG22	3:C:399:HIS:HA	1.83	0.60
1:S:1368:PHE:CZ	1:S:1392:PRO:CB	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:SG	1:A:196:LEU:HD23	2.42	0.60
3:C:114:ILE:O	3:C:117:VAL:HG12	2.00	0.60
4:E:284:ILE:O	4:E:288:LEU:N	2.35	0.60
6:G:147:ALA:HA	6:G:159:LEU:CD1	2.32	0.59
7:L:105:PRO:O	7:L:107:PRO:HD3	2.02	0.59
2:O:522:LYS:HG3	2:O:523:CYS:H	1.67	0.59
4:E:298:LEU:HD21	4:E:347:TRP:CZ2	2.37	0.59
6:G:147:ALA:HA	6:G:159:LEU:HD11	1.83	0.59
2:O:480:TYR:CE2	2:O:622:LEU:HD13	2.34	0.59
7:M:228:ILE:HD12	7:M:238:ILE:HD12	1.84	0.59
12:V:417:LEU:HD11	12:V:453:PHE:CE1	2.38	0.59
6:G:128:ALA:HA	6:G:131:LEU:HD12	1.84	0.59
6:G:454:ALA:O	6:G:455:THR:C	2.39	0.59
2:O:522:LYS:C	2:O:523:CYS:SG	2.80	0.59
8:P:198:CYS:O	8:P:241:VAL:HA	2.02	0.59
1:A:29:ARG:NH2	6:H:365:GLU:HG3	2.17	0.59
1:S:424:LEU:O	1:S:428:VAL:HG23	2.03	0.59
7:M:361:TYR:HA	10:X:101:SER:HB3	1.84	0.59
2:O:426:LEU:HG	8:Q:490:MET:HE2	1.85	0.59
8:P:360:HIS:CE1	8:P:367:CYS:HB2	2.38	0.59
1:A:29:ARG:HH22	6:H:365:GLU:HG3	1.67	0.59
3:C:490:LEU:HA	3:C:493:ASN:HD22	1.68	0.59
4:E:291:LEU:O	4:E:295:LEU:HG	2.03	0.59
4:E:368:PHE:HD1	4:E:383:LEU:HD11	1.67	0.59
6:G:475:GLU:OE1	6:G:475:GLU:HA	2.03	0.59
2:O:586:PRO:HB2	2:O:587:LEU:HD23	1.85	0.59
11:U:331:LYS:O	11:U:334:VAL:HB	2.02	0.59
6:H:67:LEU:HD11	6:H:106:THR:HG21	1.85	0.59
1:S:547:ALA:HB1	1:S:582:HIS:HA	1.85	0.59
11:U:548:LYS:O	11:U:616:ASN:ND2	2.36	0.59
11:U:874:LEU:HA	11:U:877:LEU:HD12	1.85	0.59
1:A:21:ALA:HA	6:H:415:THR:HB	1.85	0.58
1:A:30:VAL:HG22	6:H:372:ALA:HB3	1.85	0.58
1:A:135:VAL:HA	1:A:178:LEU:HD12	1.84	0.58
2:B:130:MET:HG3	2:B:144:TRP:CD1	2.38	0.58
7:L:79:ASP:OD1	7:L:81:MET:N	2.30	0.58
8:P:328:TRP:HB3	8:P:334:LEU:HD13	1.85	0.58
2:B:519:ARG:NH1	2:B:520:LEU:O	2.35	0.58
7:L:356:PHE:CE1	7:L:367:THR:HG23	2.37	0.58
1:S:1020:ARG:O	1:S:1023:GLU:HB2	2.02	0.58
3:C:134:PHE:CE2	5:F:166:GLN:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:202:PRO:HB3	8:P:225:PHE:CD2	2.38	0.58
8:P:349:CYS:SG	8:P:399:LEU:HA	2.43	0.58
8:Q:606:LEU:O	8:Q:609:VAL:N	2.36	0.58
1:S:554:ALA:O	1:S:565:PRO:HG2	2.03	0.58
11:U:1215:TYR:O	11:U:1219:LYS:HB2	2.03	0.58
1:A:351:THR:HG21	1:A:391:SER:CB	2.32	0.58
2:B:684:ILE:HG12	2:B:692:TYR:CD2	2.39	0.58
7:L:304:THR:HG22	7:L:306:ASP:HB2	1.85	0.58
7:M:311:TYR:O	10:X:9:ARG:NE	2.37	0.58
11:U:518:ILE:HG12	11:U:587:ILE:HD11	1.84	0.58
2:B:231:PRO:O	2:B:234:SER:OG	2.15	0.58
2:B:485:ASP:OD1	2:O:725:THR:HG23	2.03	0.58
6:G:249:TYR:O	6:G:252:LEU:HB2	2.03	0.58
2:O:523:CYS:HA	2:O:581:VAL:O	2.03	0.58
8:P:339:ARG:NH1	8:P:385:GLU:O	2.37	0.58
1:A:1410:CYS:SG	1:A:1414:SER:OG	2.61	0.58
12:V:1119:GLN:HE21	12:V:1158:LEU:HD13	1.68	0.58
2:B:122:LEU:HD21	2:B:155:SER:HA	1.86	0.58
8:Q:339:ARG:NE	7:M:101:LEU:HD21	2.19	0.58
7:M:105:PRO:O	7:M:107:PRO:HD3	2.03	0.58
5:F:309:ASN:O	5:F:312:GLN:HB3	2.03	0.58
1:A:1336:TYR:OH	1:A:1357:ALA:O	2.19	0.58
2:B:346:LYS:O	2:B:349:LEU:HD12	2.03	0.58
6:G:246:VAL:O	6:G:250:THR:OG1	2.22	0.58
8:Q:141:VAL:HG21	8:Q:241:VAL:HG21	1.86	0.58
8:Q:173:VAL:HG22	8:Q:258:LEU:HD13	1.86	0.58
7:M:311:TYR:HB3	10:X:9:ARG:HD3	1.86	0.58
6:G:268:TYR:CE1	1:S:93:PHE:CE2	2.91	0.57
8:P:760:ASP:OD1	8:P:796:ASP:OD2	2.22	0.57
1:S:346:TRP:CE2	1:S:387:GLN:HG2	2.38	0.57
7:M:345:LEU:HD11	10:X:93:PRO:HG2	1.84	0.57
2:B:387:ARG:NH2	7:L:123:TRP:CD1	2.72	0.57
2:B:684:ILE:HG12	2:B:692:TYR:CE2	2.39	0.57
3:C:364:TRP:HB2	3:C:410:GLN:NE2	2.19	0.57
4:E:70:GLU:HB2	4:E:83:LEU:HD22	1.86	0.57
8:Q:508:CYS:O	8:Q:643:SER:CB	2.52	0.57
6:G:416:LEU:HD22	1:S:22:TRP:HZ3	1.68	0.57
1:S:52:ARG:HA	1:S:55:GLN:HB2	1.86	0.57
12:V:275:LEU:HA	12:V:278:LEU:HG	1.86	0.57
2:B:402:PHE:CD2	8:P:465:ILE:HD11	2.39	0.57
2:B:512:GLN:NE2	8:P:570:ASP:OD1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:229:LEU:HD23	6:H:252:LEU:HD23	1.85	0.57
8:Q:232:ASP:O	8:Q:236:LEU:HG	2.04	0.57
12:V:1279:ILE:HG22	12:V:1337:LEU:HD23	1.87	0.57
2:B:332:ASP:OD2	2:B:337:GLY:N	2.31	0.57
8:Q:716:ARG:O	8:Q:720:LYS:HG3	2.04	0.57
11:U:668:LEU:CD1	11:U:749:VAL:HG13	2.34	0.57
1:A:53:SER:HA	1:A:168:GLN:NE2	2.19	0.57
1:A:1330:LEU:C	1:A:1332:PRO:HD2	2.24	0.57
2:B:61:SER:OG	2:B:116:ASN:ND2	2.30	0.57
10:X:53:LEU:HD23	10:X:68:ILE:HG22	1.85	0.57
1:S:818:PHE:HA	1:S:821:LEU:HB2	1.86	0.57
12:V:193:THR:O	12:V:196:ILE:HG22	2.04	0.57
6:H:97:GLN:O	6:H:101:GLU:HG3	2.05	0.57
2:B:298:PHE:HE2	2:B:362:LEU:HB2	1.70	0.57
4:E:473:MET:HE1	4:E:496:VAL:HG11	1.85	0.57
8:Q:517:LEU:O	8:Q:519:THR:N	2.38	0.57
3:C:61:ILE:HG13	3:C:65:PRO:HD3	1.87	0.57
3:C:114:ILE:HA	3:C:117:VAL:HG12	1.87	0.57
11:U:297:GLN:OE1	11:U:1104:THR:O	2.22	0.57
4:E:444:LEU:O	4:E:475:LYS:NZ	2.37	0.56
6:G:252:LEU:HD13	6:G:268:TYR:CE1	2.40	0.56
2:O:522:LYS:HG3	2:O:523:CYS:N	2.19	0.56
8:P:676:VAL:O	8:P:679:PHE:HB3	2.05	0.56
7:M:98:ARG:HD2	7:M:101:LEU:HD11	1.86	0.56
11:U:171:GLN:NE2	11:U:172:GLN:OE1	2.38	0.56
2:B:393:PRO:HA	7:L:131:THR:O	2.06	0.56
2:O:13:GLU:HB3	2:O:26:GLN:HG2	1.87	0.56
8:P:29:LEU:O	8:P:36:PHE:N	2.34	0.56
8:P:480:ASN:HA	8:P:483:LEU:HD12	1.87	0.56
12:V:307:LEU:HA	12:V:310:CYS:SG	2.46	0.56
1:A:715:GLU:O	1:A:719:VAL:HG12	2.05	0.56
1:A:1331:LEU:N	1:A:1332:PRO:CD	2.68	0.56
2:B:480:TYR:CE2	2:B:622:LEU:HD11	2.40	0.56
3:C:192:THR:OG1	5:F:138:ARG:NH2	2.38	0.56
6:G:510:GLN:OE1	6:G:510:GLN:HA	2.04	0.56
6:H:138:ALA:O	6:H:141:ARG:HB3	2.05	0.56
7:L:20:ARG:O	8:P:494:CYS:SG	2.64	0.56
2:O:488:VAL:HG11	2:O:650:ALA:HA	1.87	0.56
7:M:58:GLN:O	7:M:61:THR:OG1	2.17	0.56
7:M:197:LEU:HD12	7:M:201:TRP:HZ2	1.70	0.56
12:V:443:LEU:HD22	12:V:491:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:ASN:ND2	3:C:107:GLN:OE1	2.39	0.56
1:A:393:VAL:HG13	1:A:407:LEU:HD11	1.87	0.56
1:A:1425:ARG:CZ	1:A:1425:ARG:HA	2.35	0.56
6:G:406:GLN:HG2	6:G:599:TRP:CE3	2.40	0.56
2:O:256:LEU:HD23	2:O:268:PHE:HB2	1.88	0.56
7:M:212:TRP:CZ3	7:M:296:ALA:HB3	2.40	0.56
1:A:746:ALA:O	1:A:750:VAL:HG23	2.06	0.56
7:L:313:TYR:CE2	7:L:314:GLN:HG2	2.40	0.56
11:U:1277:GLN:HE21	11:U:1278:HIS:CE1	2.23	0.56
4:E:441:ILE:HD12	4:E:457:LEU:HD22	1.87	0.56
4:E:476:LEU:HD11	4:E:493:MET:HG2	1.88	0.56
8:Q:43:LEU:HB3	8:Q:45:TYR:CE1	2.39	0.56
8:Q:563:ILE:HG22	8:Q:564:THR:N	2.20	0.56
1:S:665:THR:HA	9:W:80:VAL:HG22	1.85	0.56
1:A:1176:SER:HA	1:S:964:LEU:HD13	1.87	0.56
2:B:423:TYR:CZ	8:P:606:LEU:HB3	2.40	0.56
3:C:458:ARG:HA	3:C:458:ARG:CZ	2.36	0.56
5:F:290:GLN:O	6:G:485:ARG:NH2	2.39	0.56
1:A:1326:GLN:OE1	1:A:1326:GLN:N	2.38	0.56
2:B:398:LEU:HG	2:B:399:LYS:N	2.20	0.56
6:G:491:LYS:HD3	6:G:498:ASN:HD22	1.70	0.56
8:P:711:SER:HA	8:P:782:ILE:HG21	1.88	0.56
2:B:401:CYS:O	2:B:404:SER:OG	2.19	0.55
2:B:523:CYS:HA	2:B:581:VAL:O	2.05	0.55
2:B:759:MET:O	2:B:762:THR:OG1	2.25	0.55
3:C:169:PHE:CE2	4:E:17:ALA:HB2	2.41	0.55
4:E:406:VAL:HG11	4:E:420:LEU:HD11	1.87	0.55
6:G:450:LEU:HD13	6:G:512:LEU:HD22	1.88	0.55
11:U:912:LEU:HA	11:U:915:ILE:HD12	1.88	0.55
2:B:84:ASP:HA	2:B:140:PRO:HD3	1.88	0.55
7:L:101:LEU:HB2	7:L:102:TYR:CE2	2.41	0.55
2:O:584:LEU:C	2:O:586:PRO:HD2	2.27	0.55
8:P:66:HIS:CD2	8:P:67:LEU:N	2.75	0.55
8:P:526:THR:HG22	8:P:581:THR:HG22	1.88	0.55
12:V:794:ARG:NH2	12:V:926:ARG:O	2.37	0.55
12:V:1351:THR:HA	12:V:1354:THR:HG22	1.88	0.55
1:A:29:ARG:O	1:A:29:ARG:HG3	2.06	0.55
1:A:375:LEU:HD21	1:A:392:PHE:CE1	2.40	0.55
2:O:318:VAL:HG11	2:O:321:LYS:HE2	1.89	0.55
11:U:430:PHE:O	11:U:437:ARG:NE	2.40	0.55
3:C:247:LEU:HB3	3:C:248:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:312:ILE:HG23	3:C:398:ILE:HG23	1.87	0.55
8:P:529:LEU:N	8:P:578:ARG:O	2.36	0.55
7:M:185:SER:O	7:M:189:GLN:HG3	2.06	0.55
2:B:16:LEU:HD23	2:B:17:CYS:N	2.21	0.55
2:B:339:GLU:O	2:B:340:GLN:NE2	2.40	0.55
6:G:360:ALA:O	6:G:363:ALA:HB3	2.07	0.55
2:O:505:THR:HG21	8:Q:546:GLN:HB2	1.89	0.55
2:O:585:SER:N	2:O:586:PRO:CD	2.69	0.55
1:S:737:ALA:HB1	1:S:738:PRO:HD2	1.89	0.55
11:U:441:LEU:HD13	11:U:466:ILE:HG21	1.89	0.55
11:U:832:LEU:O	11:U:835:SER:O	2.23	0.55
1:A:1335:PHE:CE1	1:A:1339:LEU:HD12	2.41	0.55
8:Q:511:SER:OG	8:Q:526:THR:OG1	2.24	0.55
11:U:951:VAL:HG11	11:U:995:LEU:HD11	1.87	0.55
1:A:351:THR:HG21	1:A:391:SER:HB2	1.89	0.55
3:C:306:ASP:O	4:E:176:ARG:HB2	2.07	0.55
6:G:447:TYR:CD1	6:G:490:GLU:HB2	2.42	0.55
6:H:229:LEU:HD23	6:H:252:LEU:CD2	2.37	0.55
7:L:356:PHE:CD1	7:L:367:THR:CG2	2.89	0.55
2:O:503:ASP:OD1	2:O:604:ARG:NH2	2.37	0.55
8:P:546:GLN:HB3	8:P:564:THR:HG22	1.88	0.55
8:Q:28:VAL:HG23	8:Q:400:ASN:HD21	1.71	0.55
8:Q:505:PRO:HB3	8:Q:533:SER:HB3	1.88	0.55
7:M:265:ILE:HG23	7:M:269:ARG:HH12	1.71	0.55
11:U:341:LEU:HG	11:U:345:GLN:HE22	1.72	0.55
11:U:595:LEU:O	11:U:630:GLN:NE2	2.40	0.55
12:V:364:TRP:CE2	12:V:384:MET:HG2	2.41	0.55
2:B:299:PHE:CZ	2:B:313:LYS:HD2	2.41	0.55
1:S:1046:HIS:HB2	1:S:1104:ARG:HD2	1.89	0.55
12:V:193:THR:HA	12:V:196:ILE:HG22	1.88	0.55
2:B:483:ILE:HG13	2:B:488:VAL:HG21	1.88	0.55
2:B:773:LEU:HA	2:B:838:ILE:HG21	1.89	0.55
2:O:710:ARG:HD2	2:O:711:THR:HG23	1.89	0.55
8:P:65:TRP:O	8:P:66:HIS:CB	2.55	0.55
1:S:1081:ILE:O	1:S:1085:LEU:HG	2.06	0.55
11:U:867:PRO:HA	11:U:870:ILE:HD12	1.89	0.55
2:B:834:LEU:O	2:B:837:GLU:HB2	2.07	0.55
4:E:522:PHE:C	4:E:523:LEU:HG	2.27	0.55
7:L:354:ILE:HG13	7:L:369:LYS:HG2	1.86	0.55
8:P:133:PHE:CD1	8:P:133:PHE:C	2.80	0.55
12:V:221:ASP:HA	12:V:224:HIS:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:SER:HB2	8:P:15:CYS:HB2	1.89	0.54
2:B:851:PHE:O	2:B:854:GLN:HG2	2.07	0.54
3:C:124:ALA:O	5:F:140:ARG:NH1	2.40	0.54
1:S:1224:TRP:CZ3	1:S:1225:LEU:HD13	2.42	0.54
6:G:497:PHE:CD2	8:P:254:ILE:HD11	2.42	0.54
11:U:435:MET:HE3	11:U:436:ILE:HG13	1.90	0.54
11:U:668:LEU:HD12	11:U:749:VAL:HG22	1.89	0.54
1:A:385:HIS:ND1	1:A:388:ARG:CZ	2.71	0.54
2:B:700:PHE:O	2:B:703:THR:OG1	2.20	0.54
8:P:11:LEU:HD11	8:P:431:THR:CG2	2.37	0.54
8:P:25:LYS:HB2	8:P:26:PRO:HD3	1.90	0.54
8:P:36:PHE:CE1	8:P:46:VAL:HG22	2.43	0.54
1:S:715:GLU:O	1:S:719:VAL:HG13	2.06	0.54
1:S:990:ASP:O	1:S:994:SER:HB2	2.07	0.54
1:S:1368:PHE:CE2	1:S:1396:ILE:HD11	2.43	0.54
3:C:330:SER:HB2	3:C:334:ARG:HB3	1.90	0.54
6:H:179:LEU:O	6:H:183:THR:OG1	2.23	0.54
8:P:123:CYS:SG	8:P:126:PRO:HD3	2.48	0.54
1:A:942:GLU:OE1	1:A:1012:THR:HG23	2.07	0.54
2:O:682:CYS:SG	2:O:692:TYR:HB3	2.47	0.54
8:P:69:LEU:HD12	8:P:76:LEU:HD12	1.89	0.54
1:A:32:ARG:HB3	6:H:311:ASN:HD21	1.72	0.54
1:A:818:PHE:CE1	1:A:864:LEU:HG	2.41	0.54
2:B:240:VAL:HG12	2:B:241:HIS:N	2.23	0.54
2:B:308:ALA:HB3	2:B:325:LEU:CD1	2.38	0.54
4:E:420:LEU:HA	4:E:423:LEU:HD12	1.89	0.54
5:F:346:ILE:O	5:F:349:ASP:HB2	2.06	0.54
6:G:449:PRO:O	6:G:450:LEU:C	2.45	0.54
8:P:465:ILE:HG22	8:P:466:SER:N	2.23	0.54
8:P:875:HIS:HB3	8:P:876:PRO:HD3	1.90	0.54
12:V:801:CYS:SG	12:V:802:GLN:NE2	2.80	0.54
1:A:659:GLU:HG2	1:A:676:GLN:HE21	1.73	0.54
2:B:335:GLY:HA3	8:P:8:VAL:O	2.08	0.54
6:H:290:TYR:O	6:H:295:ASP:N	2.41	0.54
12:V:278:LEU:N	12:V:279:PRO:CD	2.71	0.54
12:V:404:ARG:HA	12:V:407:ILE:HG22	1.88	0.54
1:A:684:LEU:HD11	1:A:722:LEU:HD21	1.89	0.54
2:B:322:TRP:HB3	2:B:325:LEU:HD21	1.90	0.54
3:C:197:ASP:N	3:C:198:PRO:HD2	2.22	0.54
8:P:170:ILE:HG23	8:P:259:VAL:HG13	1.90	0.54
8:P:586:PRO:HD3	8:P:592:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:178:SER:HA	12:V:181:LYS:HG3	1.90	0.54
2:B:256:LEU:HG	2:B:257:ILE:N	2.23	0.54
6:G:81:ARG:HG3	6:G:92:GLN:HE21	1.71	0.54
6:G:346:THR:O	6:G:347:LYS:C	2.47	0.54
2:O:146:HIS:O	2:O:148:LYS:N	2.41	0.54
2:O:487:LEU:HB2	2:O:584:LEU:CD2	2.38	0.54
1:S:940:GLN:HE21	1:S:1011:ARG:CD	2.19	0.54
1:S:1018:ILE:HG22	1:S:1084:ARG:HD2	1.90	0.54
7:M:133:PHE:O	7:M:154:LEU:HD12	2.08	0.54
11:U:275:ILE:HD12	11:U:312:LEU:HD11	1.89	0.54
11:U:430:PHE:CD2	11:U:437:ARG:HB2	2.43	0.54
2:B:61:SER:CB	2:B:116:ASN:HD21	2.20	0.53
4:E:338:ASP:HB3	4:E:382:LEU:HD12	1.89	0.53
4:E:504:ILE:HG21	4:E:534:LEU:HD13	1.91	0.53
6:G:266:LEU:O	6:G:270:VAL:HG23	2.08	0.53
6:G:497:PHE:CE2	8:P:254:ILE:HD11	2.42	0.53
2:O:277:CYS:HB2	2:O:316:PHE:HB3	1.91	0.53
8:Q:482:ALA:O	8:Q:486:LEU:HB2	2.08	0.53
7:M:31:ALA:O	7:M:34:ARG:HB2	2.08	0.53
7:M:354:ILE:HG12	7:M:369:LYS:HG2	1.89	0.53
1:A:928:THR:HG23	1:A:971:GLY:HA3	1.89	0.53
2:B:100:LYS:HB3	2:B:102:ASN:HB2	1.90	0.53
2:B:631:LYS:O	2:B:631:LYS:HD2	2.07	0.53
6:G:483:LEU:HD12	6:G:513:ARG:HA	1.90	0.53
7:L:356:PHE:CE1	7:L:367:THR:HG21	2.42	0.53
8:P:730:CYS:SG	8:P:752:SER:N	2.82	0.53
11:U:221:SER:OG	11:U:226:ARG:HA	2.08	0.53
1:A:415:MET:HE1	1:A:419:PHE:HZ	1.73	0.53
2:B:276:VAL:HG12	2:B:277:CYS:O	2.08	0.53
2:B:731:LEU:HD13	8:P:680:LEU:HD21	1.89	0.53
3:C:71:LEU:O	3:C:75:CYS:SG	2.63	0.53
4:E:27:ARG:O	4:E:31:GLN:HB2	2.08	0.53
4:E:434:GLN:NE2	4:E:460:ARG:CZ	2.72	0.53
6:H:246:VAL:HG21	6:H:276:GLY:HA2	1.91	0.53
8:Q:491:ASN:HB3	8:Q:535:PHE:CE1	2.43	0.53
8:Q:542:THR:HG22	8:Q:603:PHE:O	2.09	0.53
8:Q:580:VAL:HG12	8:Q:582:LEU:CD2	2.38	0.53
1:S:815:PRO:HA	1:S:818:PHE:CE2	2.43	0.53
11:U:66:ARG:NH1	11:U:70:THR:OG1	2.41	0.53
11:U:751:GLU:OE2	11:U:841:TYR:OH	2.26	0.53
1:A:481:VAL:O	1:A:485:SER:OG	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:62:ALA:HA	6:H:102:ARG:HD2	1.89	0.53
8:P:249:GLN:HG2	8:P:277:HIS:CD2	2.44	0.53
11:U:221:SER:CB	11:U:229:VAL:HG21	2.37	0.53
3:C:247:LEU:N	3:C:248:PRO:CD	2.71	0.53
8:P:517:LEU:O	8:P:519:THR:N	2.42	0.53
8:P:518:GLN:N	8:Q:581:THR:O	2.42	0.53
1:A:992:HIS:O	1:A:1073:ARG:NH2	2.41	0.53
4:E:434:GLN:OE1	4:E:462:VAL:HG12	2.08	0.53
7:L:16:LEU:HD11	8:P:483:LEU:CD2	2.38	0.53
7:L:315:LEU:HB3	7:L:334:HIS:ND1	2.24	0.53
7:L:354:ILE:HA	7:L:368:LEU:O	2.08	0.53
8:P:508:CYS:HA	8:P:528:VAL:O	2.08	0.53
1:S:197:LEU:HD22	1:S:206:VAL:CG1	2.39	0.53
7:M:197:LEU:HD12	7:M:201:TRP:CZ2	2.43	0.53
1:A:1020:ARG:O	1:A:1023:GLU:HB3	2.09	0.53
6:H:40:GLN:HB3	6:H:44:GLN:HE22	1.73	0.53
7:M:311:TYR:OH	10:X:100:PRO:O	2.24	0.53
7:M:341:TRP:CH2	10:X:100:PRO:HD3	2.43	0.53
11:U:364:ILE:O	11:U:367:VAL:HB	2.09	0.53
1:A:182:VAL:O	1:A:185:LEU:HB2	2.09	0.53
4:E:391:CYS:SG	4:E:423:LEU:CD2	2.92	0.53
6:H:58:GLN:HE22	6:H:98:ARG:HG2	1.72	0.53
8:P:27:ARG:O	8:P:38:SER:N	2.35	0.53
1:S:844:SER:OG	1:S:856:LEU:HD21	2.09	0.53
7:M:155:LYS:NZ	7:M:164:ASP:OD1	2.40	0.53
13:Y:9:DT:C2'	13:Y:10:DT:H71	2.38	0.53
1:A:348:PHE:CZ	1:A:356:THR:HG23	2.43	0.53
5:F:285:LEU:HD13	5:F:346:ILE:CD1	2.39	0.53
8:P:247:ASP:OD1	8:P:247:ASP:N	2.35	0.53
8:Q:604:TYR:O	8:Q:638:VAL:HG23	2.08	0.53
6:G:262:PRO:O	6:G:265:ALA:HB3	2.09	0.53
6:H:239:LEU:CD1	6:H:241:PRO:HD3	2.39	0.53
8:P:599:SER:HB2	8:P:644:ARG:HG2	1.90	0.53
11:U:592:ARG:NH2	11:U:626:THR:OG1	2.42	0.53
1:A:27:ALA:HB3	6:H:372:ALA:HB2	1.90	0.52
2:O:164:SER:OG	2:O:215:TYR:OH	2.27	0.52
8:Q:484:THR:OG1	8:Q:485:SER:N	2.39	0.52
12:V:1186:LEU:HB3	12:V:1237:VAL:HG11	1.91	0.52
2:B:254:ILE:HG13	2:B:254:ILE:O	2.09	0.52
3:C:60:VAL:HG23	3:C:64:PHE:CZ	2.45	0.52
3:C:350:MET:SD	7:L:250:GLU:HA	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:62:ILE:HA	7:L:98:ARG:NH2	2.24	0.52
7:M:16:LEU:O	7:M:18:GLN:OE1	2.28	0.52
7:L:230:LEU:HA	7:L:293:PRO:CD	2.40	0.52
7:M:322:GLN:CD	7:M:335:GLN:NE2	2.62	0.52
12:V:979:MET:HG3	12:V:980:LEU:HD23	1.89	0.52
1:A:845:LEU:HD23	1:A:856:LEU:CD1	2.39	0.52
4:E:384:THR:O	4:E:388:THR:HG23	2.10	0.52
5:F:192:LEU:HB3	5:F:201:PHE:CZ	2.44	0.52
6:H:270:VAL:O	6:H:273:LEU:HB2	2.09	0.52
6:H:531:THR:OG1	6:H:532:LYS:N	2.42	0.52
8:P:37:LEU:CD2	8:P:39:THR:HG23	2.39	0.52
1:S:765:LEU:HD11	1:S:787:LEU:HD21	1.91	0.52
12:V:273:ILE:HG21	12:V:281:ILE:CD1	2.39	0.52
2:B:91:LEU:HD13	2:B:111:ILE:CG2	2.39	0.52
3:C:288:PRO:HA	3:C:340:TYR:CE1	2.44	0.52
10:X:44:THR:HG21	10:X:116:SER:CA	2.33	0.52
11:U:218:LEU:CD2	11:U:229:VAL:HG11	2.39	0.52
11:U:485:PHE:HD1	11:U:488:LEU:HD13	1.73	0.52
11:U:503:VAL:HG13	11:U:506:LEU:HD12	1.92	0.52
1:A:482:PRO:HD3	1:A:517:ARG:HD3	1.91	0.52
1:A:1161:THR:O	1:A:1321:ARG:NH2	2.41	0.52
2:B:191:LEU:HD23	2:B:197:THR:HG23	1.92	0.52
6:G:54:LEU:HD23	6:G:58:GLN:HG3	1.91	0.52
2:O:766:GLU:OE1	8:Q:874:ARG:NH2	2.41	0.52
1:S:1118:ASN:HB2	1:S:1119:PHE:CD1	2.44	0.52
12:V:458:TYR:CD2	12:V:477:LEU:HD21	2.45	0.52
1:A:288:GLU:HA	1:A:292:HIS:HB3	1.91	0.52
1:A:1249:LEU:HD12	1:A:1252:GLU:HB2	1.92	0.52
6:H:241:PRO:O	6:H:242:ARG:HB3	2.08	0.52
8:P:763:ASN:O	8:P:791:SER:OG	2.18	0.52
7:M:295:ARG:O	7:M:297:ILE:N	2.43	0.52
12:V:432:CYS:SG	12:V:469:CYS:SG	3.06	0.52
14:Z:42:DT:H2"	14:Z:43:DG:C8	2.45	0.52
6:G:20:ASN:HD21	6:G:72:THR:HG22	1.73	0.52
6:G:21:ASP:OD1	6:G:195:LEU:HD12	2.09	0.52
2:O:840:LEU:HD21	8:Q:812:VAL:CG1	2.39	0.52
8:Q:173:VAL:CG2	8:Q:258:LEU:HD13	2.40	0.52
7:M:354:ILE:CG1	7:M:369:LYS:HG2	2.39	0.52
12:V:518:LEU:HD23	12:V:521:LEU:HD21	1.92	0.52
1:A:240:GLN:OE1	1:A:310:VAL:HG11	2.09	0.52
1:A:874:ARG:NH1	1:A:939:ILE:HD13	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:187:ARG:O	5:F:190:SER:OG	2.23	0.52
6:G:513:ARG:HD3	6:G:543:MET:SD	2.50	0.52
6:H:225:PRO:O	6:H:259:MET:SD	2.67	0.52
1:S:448:TYR:CD2	1:S:489:LEU:HD22	2.44	0.52
12:V:586:ALA:O	12:V:644:LEU:HB2	2.09	0.52
2:B:522:LYS:C	2:B:523:CYS:SG	2.89	0.52
2:O:170:ILE:O	2:O:170:ILE:HG22	2.10	0.52
8:P:399:LEU:HD23	8:P:399:LEU:H	1.74	0.52
1:S:1183:CYS:SG	1:S:1184:ARG:N	2.82	0.52
11:U:962:PHE:CE2	11:U:992:LEU:HD11	2.45	0.52
12:V:415:GLN:N	12:V:415:GLN:OE1	2.41	0.52
3:C:183:LEU:O	3:C:186:VAL:N	2.42	0.51
6:G:483:LEU:HD13	6:G:513:ARG:HG3	1.91	0.51
1:S:558:PHE:C	1:S:558:PHE:CD2	2.83	0.51
1:A:273:MET:HB3	1:A:298:TRP:CE2	2.45	0.51
1:A:313:THR:HG22	1:A:317:LYS:HG3	1.93	0.51
1:A:874:ARG:O	1:A:946:LEU:HD11	2.10	0.51
2:B:290:MET:HA	2:B:339:GLU:OE1	2.11	0.51
4:E:391:CYS:O	4:E:395:THR:OG1	2.13	0.51
6:G:379:GLU:HB2	6:G:380:PRO:HD3	1.92	0.51
2:O:228:ILE:HG22	2:O:229:ILE:H	1.76	0.51
2:O:609:CYS:SG	8:Q:644:ARG:NH1	2.84	0.51
8:P:875:HIS:HB3	8:P:876:PRO:CD	2.40	0.51
8:Q:27:ARG:C	8:Q:400:ASN:HD21	2.12	0.51
8:Q:143:LEU:HD12	8:Q:197:LEU:HD21	1.92	0.51
1:S:736:VAL:HG12	1:S:737:ALA:HB2	1.92	0.51
11:U:1142:LEU:HD11	11:U:1205:LEU:HB2	1.92	0.51
1:A:407:LEU:HD21	1:A:433:VAL:CG1	2.41	0.51
2:B:711:THR:O	2:B:713:PHE:N	2.43	0.51
2:O:16:LEU:HD12	2:O:79:CYS:SG	2.49	0.51
8:Q:23:ALA:HB2	8:Q:348:LEU:HD23	1.91	0.51
1:S:1143:LEU:HD11	1:S:1185:TRP:HA	1.91	0.51
11:U:628:LEU:HD22	11:U:702:LEU:HD11	1.93	0.51
11:U:806:SER:O	11:U:810:VAL:HG23	2.10	0.51
1:A:296:ARG:HG2	1:A:354:LEU:HD11	1.91	0.51
1:A:474:PHE:CE2	1:A:510:TYR:CD2	2.97	0.51
7:L:66:TYR:O	7:L:69:ILE:HB	2.09	0.51
8:P:599:SER:CB	8:P:644:ARG:HG2	2.40	0.51
12:V:230:GLU:HA	12:V:233:ASP:HB3	1.93	0.51
12:V:1125:ILE:HG23	12:V:1130:CYS:HB2	1.93	0.51
1:A:465:CYS:SG	1:A:466:SER:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:ALA:HB2	1:A:1256:LEU:HD12	1.93	0.51
3:C:247:LEU:HD12	3:C:247:LEU:O	2.10	0.51
6:G:282:PRO:O	6:G:285:GLU:N	2.43	0.51
7:L:11:GLN:O	7:L:88:LYS:NZ	2.44	0.51
7:L:356:PHE:HD1	7:L:367:THR:HG1	1.58	0.51
1:S:57:LEU:HD13	1:S:116:MET:HE1	1.92	0.51
1:S:1249:LEU:HD12	1:S:1252:GLU:HB2	1.92	0.51
11:U:1076:ASN:H	11:U:1079:THR:HB	1.75	0.51
13:Y:9:DT:H2"	13:Y:10:DT:H71	1.92	0.51
1:A:34:LYS:H	1:A:34:LYS:CE	2.24	0.51
1:A:1266:MET:HE1	1:A:1323:ALA:HB1	1.91	0.51
3:C:207:HIS:CG	4:E:93:ILE:HG13	2.46	0.51
4:E:117:VAL:HA	4:E:120:ILE:HD12	1.93	0.51
5:F:317:ALA:HB1	5:F:318:PRO:CD	2.40	0.51
8:P:25:LYS:O	8:P:27:ARG:NH1	2.44	0.51
8:P:361:SER:OG	8:P:398:SER:O	2.19	0.51
1:S:1076:LEU:N	1:S:1076:LEU:HD23	2.26	0.51
7:M:275:ASP:O	7:M:283:ASN:ND2	2.43	0.51
11:U:450:THR:HG21	12:V:356:TYR:CG	2.45	0.51
11:U:466:ILE:HG22	11:U:467:VAL:N	2.25	0.51
1:A:463:HIS:NE2	1:A:473:LEU:HD22	2.26	0.51
1:A:653:LEU:O	1:A:657:LEU:HD13	2.11	0.51
1:A:1252:GLU:O	1:A:1298:ARG:NH2	2.43	0.51
2:B:593:PHE:C	2:B:593:PHE:CD1	2.84	0.51
6:G:476:PHE:CZ	6:G:519:SER:HB2	2.45	0.51
7:L:155:LYS:NZ	7:L:164:ASP:OD1	2.32	0.51
2:O:406:ARG:NH1	8:Q:318:HIS:O	2.44	0.51
8:P:341:TYR:O	8:P:342:CYS:SG	2.65	0.51
8:P:515:SER:OG	8:P:516:ARG:N	2.43	0.51
10:X:69:ARG:NH2	10:X:82:ALA:O	2.44	0.51
12:V:364:TRP:CZ2	12:V:384:MET:HG2	2.46	0.51
12:V:1246:VAL:HG11	12:V:1301:PHE:CD1	2.45	0.51
6:G:146:GLN:NE2	6:G:150:TRP:CZ2	2.79	0.51
2:O:672:MET:HG3	2:O:707:TRP:CZ2	2.46	0.51
8:Q:284:PHE:HB3	8:Q:315:PHE:HD2	1.75	0.51
1:A:929:TYR:CE1	1:A:933:LEU:HD11	2.46	0.51
2:B:308:ALA:HB3	2:B:325:LEU:HD13	1.92	0.51
3:C:60:VAL:CG2	3:C:64:PHE:CZ	2.94	0.51
2:O:281:PHE:CZ	2:O:321:LYS:HB3	2.46	0.51
8:Q:537:LEU:HD22	8:Q:541:TRP:CE2	2.46	0.51
12:V:374:VAL:HG22	12:V:376:GLU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:CYS:HB2	8:P:465:ILE:HG21	1.92	0.51
3:C:82:ALA:O	5:F:138:ARG:NH1	2.44	0.51
3:C:162:ARG:HB3	3:C:162:ARG:NH1	2.25	0.51
7:L:146:ARG:NH1	7:L:205:ASP:OD2	2.41	0.51
2:O:85:PHE:CZ	2:O:156:GLN:HB2	2.46	0.51
8:Q:563:ILE:HG21	8:Q:565:TYR:CE1	2.46	0.51
9:W:81:GLY:O	9:W:83:LYS:N	2.44	0.51
12:V:211:ILE:O	12:V:215:LEU:HG	2.11	0.51
12:V:364:TRP:CZ2	12:V:384:MET:HE2	2.46	0.51
1:A:137:LEU:HB2	1:A:141:GLN:HG3	1.92	0.50
7:L:155:LYS:NZ	7:L:162:SER:O	2.40	0.50
2:O:257:ILE:CD1	2:O:299:PHE:CE2	2.93	0.50
4:E:405:PRO:O	4:E:409:ALA:N	2.44	0.50
6:G:147:ALA:CB	6:G:159:LEU:HD11	2.42	0.50
2:O:430:VAL:HA	8:Q:497:LEU:HD11	1.93	0.50
2:O:777:ILE:HG21	8:Q:830:LEU:HD13	1.93	0.50
8:Q:367:CYS:HA	8:Q:392:PRO:HA	1.94	0.50
1:S:327:ILE:O	1:S:388:ARG:NH1	2.44	0.50
1:A:737:ALA:HB3	1:A:738:PRO:HD3	1.92	0.50
2:B:365:ILE:HG23	2:B:367:TYR:CE2	2.46	0.50
3:C:41:PHE:CE2	3:C:45:LEU:HD11	2.45	0.50
1:S:346:TRP:HE1	1:S:387:GLN:HE21	1.59	0.50
1:A:78:ILE:CG2	1:A:123:GLN:HE22	2.19	0.50
1:A:1368:PHE:HE1	1:A:1392:PRO:CG	2.24	0.50
2:B:242:ILE:CG1	2:B:243:CYS:N	2.74	0.50
2:B:520:LEU:HD12	8:P:567:ILE:HB	1.92	0.50
3:C:539:GLU:OE1	3:C:539:GLU:N	2.44	0.50
4:E:439:GLY:O	4:E:443:GLU:OE1	2.28	0.50
6:G:453:SER:OG	6:G:512:LEU:HD21	2.10	0.50
6:G:457:LEU:HD23	6:G:458:LEU:CD2	2.41	0.50
6:H:522:LEU:O	6:H:525:VAL:HB	2.12	0.50
8:Q:16:CYS:SG	8:Q:426:LYS:O	2.68	0.50
9:W:85:PHE:O	9:W:87:TRP:N	2.44	0.50
7:M:311:TYR:HB3	10:X:9:ARG:CD	2.41	0.50
1:A:78:ILE:HG23	1:A:123:GLN:NE2	2.17	0.50
1:A:163:ARG:O	1:A:166:PHE:HB3	2.12	0.50
1:A:1261:PHE:HB2	1:A:1291:ILE:HG21	1.94	0.50
2:B:277:CYS:HB2	2:B:316:PHE:HB3	1.93	0.50
2:B:299:PHE:CE2	2:B:313:LYS:HB2	2.46	0.50
3:C:168:GLY:O	7:L:344:GLY:O	2.30	0.50
4:E:284:ILE:O	4:E:288:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:139:VAL:CG1	8:P:154:LEU:HD11	2.41	0.50
2:B:636:PHE:HZ	2:B:651:LEU:HD11	1.76	0.50
3:C:92:TRP:NE1	5:F:118:GLY:HA2	2.26	0.50
4:E:333:LEU:N	4:E:334:PRO:CD	2.74	0.50
5:F:285:LEU:HD13	5:F:346:ILE:HD13	1.92	0.50
6:H:203:LEU:O	6:H:206:VAL:N	2.44	0.50
7:L:169:PHE:CZ	7:L:193:ALA:HB1	2.46	0.50
8:P:200:VAL:HA	8:P:218:PHE:O	2.11	0.50
1:S:959:ILE:HG22	1:S:960:HIS:ND1	2.27	0.50
12:V:243:VAL:HG22	12:V:244:PRO:HD3	1.93	0.50
1:A:1210:PHE:CZ	1:A:1249:LEU:HD13	2.46	0.50
2:B:423:TYR:CG	8:P:606:LEU:HD13	2.45	0.50
5:F:161:SER:O	5:F:165:THR:OG1	2.21	0.50
6:G:146:GLN:NE2	6:G:150:TRP:CE2	2.80	0.50
2:O:711:THR:O	2:O:713:PHE:N	2.45	0.50
7:M:195:GLU:HA	7:M:198:LYS:HB2	1.94	0.50
11:U:1138:LEU:HA	11:U:1141:LEU:HD23	1.92	0.50
12:V:223:GLN:O	12:V:227:VAL:HG23	2.12	0.50
12:V:282:ILE:HA	12:V:285:ILE:HD12	1.94	0.50
1:A:1075:LEU:CD1	1:A:1119:PHE:CD2	2.95	0.50
2:B:239:TYR:CD2	2:B:286:ALA:HA	2.47	0.50
5:F:253:ARG:NH2	5:F:300:GLN:O	2.45	0.50
6:G:159:LEU:HD23	6:G:177:LEU:CD1	2.42	0.50
6:G:364:ALA:O	6:G:367:TYR:N	2.45	0.50
6:G:592:TYR:CD1	6:G:593:LEU:N	2.80	0.50
8:P:197:LEU:HA	8:P:242:LEU:O	2.12	0.50
8:Q:570:ASP:OD1	8:Q:570:ASP:N	2.39	0.50
6:H:250:THR:HG22	6:H:282:PRO:HA	1.93	0.50
6:H:541:VAL:HG21	6:H:554:LEU:HD22	1.93	0.50
12:V:413:GLN:OE1	12:V:413:GLN:N	2.45	0.50
1:A:874:ARG:NH2	1:A:944:ASP:O	2.45	0.49
3:C:533:TRP:O	3:C:537:GLY:N	2.45	0.49
4:E:156:LEU:HD13	4:E:160:CYS:SG	2.52	0.49
6:G:521:GLY:HA3	6:G:537:PHE:CE1	2.47	0.49
8:Q:143:LEU:CD2	8:Q:150:TRP:HE3	2.25	0.49
7:M:216:PRO:HG2	7:M:226:ARG:HD3	1.94	0.49
11:U:218:LEU:HD21	11:U:229:VAL:HG11	1.94	0.49
11:U:647:LEU:HD12	11:U:647:LEU:N	2.26	0.49
11:U:909:LEU:HA	11:U:912:LEU:HD12	1.94	0.49
1:A:424:LEU:HD23	1:A:476:PHE:HB2	1.94	0.49
1:A:663:SER:HB3	1:A:676:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ILE:HG22	2:B:177:GLU:N	2.28	0.49
4:E:432:ASP:O	4:E:436:LEU:HG	2.12	0.49
4:E:497:MET:HG2	4:E:512:LEU:HD13	1.94	0.49
5:F:103:LEU:HD23	5:F:108:ARG:HD3	1.94	0.49
5:F:275:LEU:CD2	5:F:325:VAL:HG23	2.42	0.49
6:G:136:LEU:HD23	6:G:136:LEU:H	1.76	0.49
6:G:376:ASP:N	6:G:376:ASP:OD1	2.46	0.49
1:S:184:HIS:HA	1:S:187:VAL:HG12	1.94	0.49
1:S:548:LEU:O	1:S:552:GLU:HG3	2.11	0.49
1:S:1358:VAL:O	1:S:1362:LEU:HG	2.12	0.49
11:U:543:LEU:O	11:U:547:PHE:HB3	2.11	0.49
12:V:1013:VAL:HG21	12:V:1075:TRP:CE2	2.48	0.49
1:A:264:GLN:O	1:A:268:ASP:HB2	2.11	0.49
3:C:188:VAL:HG22	3:C:219:PHE:HA	1.94	0.49
4:E:372:ILE:HA	4:E:375:LEU:HD12	1.94	0.49
6:G:252:LEU:HA	6:G:255:CYS:SG	2.53	0.49
7:L:117:GLU:HB3	7:L:183:LEU:HD12	1.93	0.49
8:P:242:LEU:HD23	8:P:252:CYS:HB3	1.93	0.49
12:V:174:ARG:HA	12:V:177:VAL:HG12	1.94	0.49
1:A:750:VAL:HG21	1:A:790:HIS:HB3	1.94	0.49
1:A:818:PHE:CD1	1:A:864:LEU:HG	2.47	0.49
4:E:509:ARG:HD2	4:E:534:LEU:HB2	1.92	0.49
6:G:371:LEU:O	6:G:375:LEU:HD12	2.11	0.49
8:Q:505:PRO:CB	8:Q:533:SER:HB3	2.42	0.49
1:S:474:PHE:CE1	1:S:510:TYR:CE2	3.00	0.49
1:S:1115:GLU:O	1:S:1118:ASN:HB2	2.12	0.49
11:U:386:GLY:HA2	11:U:425:ILE:HD12	1.93	0.49
12:V:424:HIS:O	12:V:428:LEU:HG	2.12	0.49
1:A:818:PHE:HZ	1:A:861:SER:CB	2.23	0.49
1:A:1263:PHE:CZ	1:A:1322:VAL:HG11	2.47	0.49
2:B:636:PHE:HB3	2:B:637:PRO:HD3	1.94	0.49
6:G:280:GLY:N	6:G:281:PRO:CD	2.76	0.49
2:O:519:ARG:HG3	2:O:520:LEU:O	2.13	0.49
8:P:11:LEU:HD22	8:P:429:LEU:CD2	2.40	0.49
8:P:473:LYS:O	8:P:476:VAL:HB	2.12	0.49
8:Q:486:LEU:HD23	8:Q:490:MET:HE3	1.95	0.49
11:U:770:ASP:O	11:U:774:LEU:HD13	2.12	0.49
1:A:379:LEU:HD23	1:A:384:VAL:HG21	1.94	0.49
2:B:487:LEU:O	2:B:581:VAL:HA	2.12	0.49
2:B:763:LEU:O	2:B:764:GLU:C	2.50	0.49
6:G:336:SER:HG	6:G:338:LEU:H	1.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:139:GLY:O	2:O:141:LEU:N	2.45	0.49
8:P:7:ARG:HG3	8:P:8:VAL:HG23	1.93	0.49
8:Q:492:VAL:HG22	8:Q:535:PHE:CD2	2.48	0.49
12:V:979:MET:CE	12:V:1009:ALA:HB2	2.42	0.49
12:V:1392:ARG:HD3	12:V:1396:GLY:HA2	1.95	0.49
1:A:822:LEU:HD23	1:A:823:THR:N	2.27	0.49
2:B:254:ILE:O	2:B:254:ILE:CG1	2.60	0.49
2:B:364:LYS:HB2	2:B:365:ILE:HD12	1.95	0.49
2:B:524:GLN:O	2:B:580:ALA:HA	2.12	0.49
4:E:505:THR:HG23	4:E:508:GLN:HG3	1.95	0.49
6:H:296:THR:HG21	6:H:357:THR:CG2	2.42	0.49
7:L:315:LEU:HB3	7:L:334:HIS:CE1	2.48	0.49
2:O:585:SER:N	2:O:586:PRO:HD2	2.27	0.49
1:S:313:THR:HA	1:S:316:LEU:HB3	1.94	0.49
11:U:807:MET:O	11:U:810:VAL:HB	2.12	0.49
12:V:64:SER:O	12:V:112:ASN:ND2	2.38	0.49
1:A:286:GLN:C	1:A:288:GLU:N	2.63	0.49
2:B:723:ASN:HD22	2:O:484:ASP:CG	2.16	0.49
3:C:82:ALA:HB3	3:C:189:PRO:CB	2.40	0.49
3:C:169:PHE:CD2	4:E:17:ALA:HB2	2.48	0.49
5:F:287:TYR:CE2	5:F:343:GLY:HA2	2.48	0.49
6:G:471:VAL:O	6:G:474:SER:HB2	2.12	0.49
8:Q:505:PRO:O	8:Q:532:SER:N	2.43	0.49
1:S:288:GLU:HB2	1:S:292:HIS:HB2	1.93	0.49
1:S:1368:PHE:CZ	1:S:1392:PRO:HB3	2.48	0.49
11:U:648:GLU:HA	11:U:651:ILE:HD12	1.95	0.49
6:G:491:LYS:HD3	6:G:498:ASN:ND2	2.27	0.49
7:L:176:SER:N	7:L:189:GLN:HE22	2.11	0.49
8:P:603:PHE:HB2	8:P:639:CYS:SG	2.53	0.49
8:Q:604:TYR:HB3	8:Q:638:VAL:CG2	2.43	0.49
11:U:302:ASN:HD21	11:U:357:ARG:HB2	1.78	0.49
11:U:910:GLU:O	11:U:913:GLN:HB3	2.13	0.49
12:V:110:PHE:CZ	12:V:114:LEU:HD11	2.48	0.49
1:A:22:TRP:CZ2	6:H:423:ARG:NH2	2.81	0.49
2:B:423:TYR:CD1	8:P:606:LEU:HD22	2.48	0.49
8:P:267:ASP:OD1	8:P:269:ASN:N	2.40	0.49
8:P:279:GLU:OE1	8:P:279:GLU:HA	2.13	0.49
8:P:502:GLY:O	8:P:504:ARG:N	2.44	0.49
1:S:593:LEU:HD11	1:S:625:CYS:SG	2.53	0.49
1:S:923:GLU:HG2	1:S:926:HIS:HB2	1.94	0.49
1:A:831:PHE:CE1	1:A:899:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:SER:OG	2:B:361:ASP:OD1	2.31	0.48
2:B:423:TYR:O	2:B:427:ILE:N	2.44	0.48
5:F:95:LEU:HA	5:F:98:LEU:HD12	1.95	0.48
8:P:224:LEU:O	8:P:227:LEU:N	2.46	0.48
8:P:471:PHE:CD1	8:P:471:PHE:C	2.86	0.48
8:Q:248:GLY:HA2	8:Q:282:VAL:HG23	1.94	0.48
1:S:795:ARG:HD2	1:S:815:PRO:HD3	1.94	0.48
7:M:169:PHE:CZ	7:M:193:ALA:HB1	2.48	0.48
7:M:216:PRO:HB2	7:M:219:PRO:HB3	1.94	0.48
4:E:67:LEU:HA	4:E:86:LEU:HB3	1.95	0.48
6:G:399:GLU:CD	6:G:591:LEU:HB2	2.33	0.48
6:H:13:LEU:HA	6:H:16:TRP:CE3	2.48	0.48
2:O:580:ALA:C	2:O:581:VAL:HG23	2.33	0.48
8:P:66:HIS:CD2	8:P:66:HIS:C	2.87	0.48
8:P:527:CYS:O	8:P:580:VAL:N	2.45	0.48
8:P:705:VAL:HG13	8:P:788:GLN:HE21	1.79	0.48
1:S:1063:TRP:CZ3	1:S:1329:ARG:NH2	2.81	0.48
10:X:6:ARG:NH2	10:X:103:ASN:HA	2.28	0.48
12:V:149:ILE:HA	12:V:152:THR:HG22	1.95	0.48
1:A:245:ARG:NH2	1:A:263:PRO:HD3	2.29	0.48
6:G:476:PHE:HD2	6:G:520:ARG:HA	1.79	0.48
2:O:716:ILE:HD13	8:Q:556:LEU:HD21	1.95	0.48
8:P:359:TYR:O	8:P:401:ILE:HD13	2.13	0.48
11:U:506:LEU:HD22	11:U:513:MET:HE1	1.95	0.48
4:E:473:MET:O	4:E:477:CYS:SG	2.70	0.48
8:Q:23:ALA:HB2	8:Q:348:LEU:CD2	2.44	0.48
10:X:65:PRO:HB3	10:X:98:TRP:HB2	1.96	0.48
12:V:157:LEU:HD13	12:V:176:ILE:HG21	1.94	0.48
12:V:171:ASN:HD21	12:V:173:PRO:HB2	1.78	0.48
12:V:816:LEU:HA	12:V:819:ILE:HD12	1.95	0.48
1:A:35:TYR:HE2	6:H:311:ASN:CG	2.16	0.48
1:A:286:GLN:HB3	1:A:288:GLU:HG3	1.94	0.48
2:B:40:THR:HG21	2:B:69:GLU:O	2.13	0.48
2:B:308:ALA:N	2:B:325:LEU:HD12	2.29	0.48
2:B:430:VAL:HG21	8:P:638:VAL:CG1	2.43	0.48
6:G:451:TRP:CZ3	6:G:452:VAL:HG22	2.48	0.48
6:H:48:GLU:O	6:H:51:ARG:HB2	2.14	0.48
2:O:829:LYS:N	8:Q:824:ASP:O	2.47	0.48
8:P:527:CYS:N	8:P:580:VAL:O	2.40	0.48
8:Q:709:LYS:HB2	8:Q:879:ILE:HG22	1.95	0.48
11:U:528:ASN:HD22	12:V:250:SER:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:543:LEU:O	11:U:547:PHE:CB	2.61	0.48
12:V:259:LEU:HA	12:V:262:VAL:HG12	1.95	0.48
2:B:710:ARG:O	2:B:711:THR:OG1	2.31	0.48
3:C:146:TYR:N	3:C:147:PRO:CD	2.76	0.48
3:C:334:ARG:HD3	7:L:252:PHE:CE1	2.48	0.48
3:C:352:LEU:HD12	3:C:396:LEU:HD23	1.96	0.48
5:F:3:SER:HA	5:F:6:GLN:NE2	2.29	0.48
5:F:312:GLN:O	5:F:315:CYS:SG	2.71	0.48
6:H:480:LEU:O	6:H:483:LEU:HB3	2.14	0.48
2:O:268:PHE:O	2:O:269:GLN:HG2	2.13	0.48
1:S:139:VAL:HG12	1:S:140:GLU:N	2.29	0.48
1:S:830:LEU:HD22	1:S:871:LEU:CD2	2.41	0.48
12:V:180:LEU:HA	12:V:183:LEU:HD11	1.96	0.48
12:V:515:LYS:HD3	12:V:551:ILE:HG22	1.96	0.48
1:A:348:PHE:CZ	1:A:356:THR:CG2	2.97	0.48
2:B:172:TRP:CZ3	2:B:176:ILE:HD11	2.49	0.48
2:B:364:LYS:HG2	2:B:402:PHE:CE2	2.49	0.48
3:C:28:LEU:HD23	3:C:28:LEU:C	2.34	0.48
4:E:21:GLN:OE1	4:E:21:GLN:N	2.46	0.48
6:G:203:LEU:O	6:G:207:LEU:HD23	2.13	0.48
6:G:430:LYS:NZ	8:P:328:TRP:HB2	2.28	0.48
8:P:84:GLY:O	8:P:130:LEU:HD21	2.14	0.48
3:C:333:LEU:N	3:C:333:LEU:HD23	2.29	0.48
6:G:406:GLN:NE2	6:G:599:TRP:HB2	2.26	0.48
7:L:356:PHE:HE1	7:L:367:THR:HG21	1.79	0.48
1:S:556:MET:SD	1:S:998:TYR:CD1	3.06	0.48
12:V:825:ILE:O	12:V:828:LYS:HG2	2.14	0.48
1:A:22:TRP:HZ2	6:H:423:ARG:NH2	2.10	0.48
1:A:286:GLN:HB2	1:A:288:GLU:OE2	2.14	0.48
2:B:87:THR:HB	2:B:89:ILE:HD12	1.96	0.48
2:B:423:TYR:O	2:B:426:LEU:HB3	2.13	0.48
2:B:667:TYR:O	2:B:713:PHE:CE1	2.67	0.48
3:C:302:LEU:HD21	3:C:315:ILE:HD11	1.95	0.48
3:C:330:SER:OG	3:C:334:ARG:NH1	2.47	0.48
4:E:387:LEU:HD12	4:E:391:CYS:HG	1.79	0.48
7:M:146:ARG:CZ	7:M:201:TRP:HB2	2.44	0.48
7:M:207:ILE:HG23	7:M:228:ILE:HD11	1.96	0.48
1:A:230:VAL:HG12	1:A:234:MET:CE	2.44	0.48
1:A:1033:ASP:OD1	1:A:1093:SER:OG	2.31	0.48
2:B:426:LEU:O	2:B:429:LEU:HB3	2.14	0.48
5:F:69:GLU:HA	5:F:74:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:503:ASP:CG	2:O:604:ARG:HE	2.17	0.48
8:Q:69:LEU:HD12	8:Q:76:LEU:HD12	1.96	0.48
8:Q:654:ARG:NH2	8:Q:758:ALA:O	2.47	0.48
1:A:245:ARG:HH22	1:A:262:MET:HA	1.79	0.47
5:F:196:LEU:HD21	5:F:201:PHE:CE1	2.48	0.47
6:G:424:THR:O	6:G:428:LEU:HG	2.14	0.47
6:H:31:GLN:O	6:H:39:ARG:NH1	2.47	0.47
8:P:243:CYS:N	8:P:251:CYS:O	2.37	0.47
8:P:270:ALA:HB3	8:P:271:LEU:HB2	1.96	0.47
8:P:504:ARG:N	8:P:505:PRO:CD	2.77	0.47
8:P:771:VAL:O	8:P:784:ALA:O	2.32	0.47
1:S:494:LEU:CD1	1:S:518:LEU:HD11	2.38	0.47
1:S:948:ASP:O	1:S:951:ARG:HB3	2.14	0.47
12:V:639:ILE:HD13	12:V:740:CYS:SG	2.54	0.47
1:A:351:THR:HG21	1:A:391:SER:OG	2.14	0.47
4:E:398:VAL:HG12	4:E:399:CYS:SG	2.54	0.47
6:H:232:LEU:O	6:H:248:VAL:CG1	2.62	0.47
2:O:518:PHE:HB2	8:Q:568:PRO:HG2	1.96	0.47
2:O:651:LEU:HD23	2:O:655:PHE:CE1	2.49	0.47
8:P:151:LYS:HA	8:P:173:VAL:O	2.15	0.47
7:M:73:ARG:CD	7:M:86:GLU:OE1	2.54	0.47
11:U:1007:LEU:HA	11:U:1035:LEU:HD13	1.95	0.47
12:V:791:ASN:HA	12:V:794:ARG:HD3	1.95	0.47
1:A:181:ALA:O	1:A:185:LEU:HD23	2.15	0.47
1:A:1330:LEU:O	1:A:1333:PHE:HB3	2.14	0.47
2:B:478:ILE:HD11	2:B:597:VAL:HG21	1.96	0.47
3:C:123:SER:HA	5:F:140:ARG:NH2	2.29	0.47
5:F:200:ASN:O	5:F:204:VAL:HG23	2.15	0.47
6:G:296:THR:O	6:G:299:GLU:HB3	2.14	0.47
6:G:477:SER:HA	6:G:520:ARG:HH21	1.78	0.47
8:P:60:PHE:CD1	8:P:60:PHE:N	2.82	0.47
8:P:776:LEU:HD13	8:P:881:LEU:HD11	1.96	0.47
11:U:651:ILE:HD13	11:U:738:LYS:HG3	1.97	0.47
12:V:537:SER:HB2	12:V:584:ILE:HG21	1.96	0.47
2:B:298:PHE:CE2	2:B:362:LEU:HD12	2.50	0.47
2:B:584:LEU:C	2:B:586:PRO:HD2	2.35	0.47
6:G:332:PRO:HD2	8:P:262:ARG:O	2.13	0.47
6:G:457:LEU:HD23	6:G:458:LEU:HD23	1.95	0.47
6:G:511:GLN:HE22	6:G:547:ASN:HB2	1.80	0.47
8:P:572:LEU:HA	8:P:578:ARG:NH1	2.29	0.47
1:S:375:LEU:HD11	1:S:396:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:330:LEU:O	11:U:334:VAL:HG23	2.14	0.47
12:V:413:GLN:HB2	12:V:415:GLN:OE1	2.14	0.47
12:V:614:LEU:HA	12:V:617:VAL:HG12	1.96	0.47
2:B:411:HIS:O	2:B:414:LEU:HB3	2.15	0.47
8:P:27:ARG:O	8:P:37:LEU:HA	2.13	0.47
8:P:113:SER:OG	8:P:115:VAL:HG12	2.15	0.47
8:P:527:CYS:SG	8:P:527:CYS:O	2.71	0.47
10:X:78:ASN:HD22	10:X:86:CYS:HB3	1.79	0.47
12:V:243:VAL:N	12:V:244:PRO:CD	2.77	0.47
2:B:596:THR:HA	2:B:619:ARG:HG3	1.97	0.47
2:B:602:MET:N	2:B:602:MET:SD	2.88	0.47
3:C:224:ASN:HD21	3:C:249:SER:CB	2.11	0.47
4:E:395:THR:HG21	4:E:429:LEU:HD12	1.97	0.47
4:E:473:MET:HE2	4:E:473:MET:HA	1.97	0.47
6:G:37:LEU:O	6:G:41:GLN:HG3	2.15	0.47
6:G:214:ARG:NH1	6:G:330:PRO:HD3	2.29	0.47
7:L:16:LEU:HD11	8:P:483:LEU:HD22	1.94	0.47
8:P:843:GLU:OE1	8:P:844:VAL:HG23	2.14	0.47
8:Q:28:VAL:HG23	8:Q:400:ASN:ND2	2.30	0.47
1:S:989:MET:SD	1:S:1077:MET:HG2	2.54	0.47
1:A:263:PRO:O	1:A:267:VAL:HG12	2.14	0.47
1:A:818:PHE:CD1	1:A:819:ASP:N	2.83	0.47
1:A:1025:VAL:HG21	1:A:1085:LEU:HD13	1.95	0.47
1:A:1305:LEU:C	1:A:1308:LEU:HD21	2.35	0.47
3:C:79:PHE:N	3:C:79:PHE:CD1	2.79	0.47
3:C:180:VAL:HG11	3:C:214:ILE:CD1	2.45	0.47
4:E:283:ALA:O	4:E:287:GLN:HG3	2.14	0.47
6:G:480:LEU:CD1	6:G:517:LEU:HD23	2.44	0.47
2:O:338:THR:O	2:O:340:GLN:NE2	2.48	0.47
2:O:614:TYR:CG	8:Q:639:CYS:HB3	2.50	0.47
8:P:154:LEU:HD22	8:P:258:LEU:CD2	2.34	0.47
8:P:557:ASP:OD1	8:P:557:ASP:N	2.48	0.47
8:Q:398:SER:HA	8:Q:424:SER:HA	1.97	0.47
8:Q:491:ASN:HD21	7:M:9:LEU:HD21	1.78	0.47
8:Q:733:LEU:HD22	8:Q:746:VAL:HG11	1.97	0.47
1:S:379:LEU:HD23	1:S:384:VAL:HG21	1.95	0.47
1:S:827:ARG:HA	1:S:830:LEU:HD12	1.96	0.47
1:S:862:PRO:HA	1:S:865:ILE:HD12	1.97	0.47
11:U:321:ARG:HD2	12:V:444:HIS:CE1	2.49	0.47
11:U:643:PRO:HB3	11:U:721:PHE:CE1	2.50	0.47
11:U:1010:THR:HG22	11:U:1032:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:382:LEU:HD12	12:V:420:THR:OG1	2.14	0.47
2:B:242:ILE:C	2:B:243:CYS:SG	2.92	0.47
2:B:364:LYS:CG	2:B:402:PHE:CE2	2.98	0.47
3:C:227:ILE:HD11	3:C:239:VAL:CG1	2.43	0.47
5:F:164:LYS:O	5:F:168:GLU:HG2	2.15	0.47
8:P:359:TYR:CD2	8:P:420:LEU:HD23	2.50	0.47
1:S:580:VAL:O	1:S:584:LEU:HG	2.15	0.47
1:S:665:THR:CA	9:W:80:VAL:HG22	2.45	0.47
7:M:326:ASN:HD22	7:M:364:LYS:HG3	1.80	0.47
11:U:1010:THR:HG21	11:U:1031:LEU:HG	1.95	0.47
1:A:415:MET:HE2	1:A:451:TRP:CH2	2.49	0.47
4:E:423:LEU:O	4:E:429:LEU:HD13	2.14	0.47
6:G:283:LEU:O	6:G:286:ALA:HB3	2.15	0.47
1:S:414:LEU:HD12	1:S:426:SER:HB2	1.97	0.47
11:U:731:GLN:NE2	11:U:792:ALA:HB2	2.30	0.47
2:B:298:PHE:CD1	2:B:312:TRP:HD1	2.32	0.47
2:B:402:PHE:HD2	8:P:465:ILE:HD11	1.80	0.47
2:B:738:LEU:HD22	2:B:742:CYS:SG	2.55	0.47
6:G:393:MET:HE3	8:P:236:LEU:CD2	2.46	0.47
8:P:446:MET:HE1	8:P:451:ALA:HB2	1.97	0.47
8:Q:794:LEU:HD22	8:Q:867:LEU:HD22	1.97	0.47
1:A:768:LEU:O	1:A:772:GLN:C	2.54	0.46
1:A:923:GLU:OE1	1:A:923:GLU:HA	2.14	0.46
2:B:83:SER:OG	8:P:15:CYS:SG	2.64	0.46
2:B:281:PHE:N	2:B:281:PHE:CD1	2.83	0.46
4:E:388:THR:HB	4:E:426:MET:SD	2.55	0.46
8:P:201:SER:O	8:P:219:THR:HA	2.15	0.46
8:Q:733:LEU:CD2	8:Q:746:VAL:HG11	2.45	0.46
7:M:170:PRO:HB3	7:M:222:SER:O	2.15	0.46
7:M:341:TRP:CZ2	10:X:100:PRO:HD3	2.51	0.46
11:U:221:SER:HB2	11:U:229:VAL:HG21	1.97	0.46
12:V:62:GLY:HA2	12:V:112:ASN:HD22	1.80	0.46
12:V:1338:LEU:HD23	12:V:1341:LEU:HD23	1.97	0.46
1:A:25:LEU:HD11	6:H:416:LEU:HD13	1.96	0.46
1:A:1287:VAL:O	1:A:1291:ILE:HG12	2.15	0.46
3:C:169:PHE:CE1	3:C:209:ARG:HD3	2.49	0.46
4:E:395:THR:O	4:E:399:CYS:SG	2.73	0.46
6:G:306:LEU:O	6:G:309:ALA:HB3	2.14	0.46
8:P:288:LEU:HG	8:P:313:VAL:HG21	1.96	0.46
8:P:516:ARG:O	8:P:517:LEU:HD22	2.15	0.46
2:B:132:ASP:OD2	2:B:145:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:GLY:HA2	2:B:579:THR:HA	1.96	0.46
2:B:636:PHE:HB3	2:B:637:PRO:CD	2.46	0.46
3:C:304:GLU:CD	4:E:165:GLN:HG2	2.36	0.46
4:E:70:GLU:HB3	4:E:83:LEU:HD22	1.96	0.46
7:L:126:LEU:HD11	7:L:128:TYR:O	2.15	0.46
8:P:150:TRP:CZ3	8:P:195:PRO:HG3	2.50	0.46
1:S:1263:PHE:CZ	1:S:1322:VAL:HG11	2.51	0.46
11:U:286:GLY:O	11:U:289:LEU:HB3	2.15	0.46
11:U:707:GLU:O	11:U:710:THR:HB	2.15	0.46
12:V:98:SER:O	12:V:101:GLU:HG2	2.16	0.46
14:Z:40:DC:H2"	14:Z:41:DC:C6	2.51	0.46
1:A:174:GLN:NE2	1:A:209:TRP:CD1	2.84	0.46
1:A:361:ARG:HB3	1:A:365:MET:HE1	1.98	0.46
4:E:23:GLU:OE2	4:E:25:PRO:HG2	2.16	0.46
5:F:141:SER:O	5:F:144:HIS:HB3	2.16	0.46
5:F:158:GLN:HA	5:F:207:VAL:HG13	1.96	0.46
5:F:274:TYR:HE2	5:F:314:LEU:HD21	1.80	0.46
6:H:58:GLN:NE2	6:H:98:ARG:HG2	2.30	0.46
6:H:119:ARG:HD2	6:H:161:LEU:HD23	1.97	0.46
6:H:412:ASP:O	6:H:415:THR:OG1	2.28	0.46
8:P:159:CYS:SG	8:P:160:PRO:HD3	2.54	0.46
8:P:227:LEU:O	8:P:227:LEU:HD12	2.16	0.46
8:P:829:TYR:OH	8:P:879:ILE:CD1	2.64	0.46
1:S:470:LEU:O	1:S:473:LEU:HB2	2.14	0.46
1:S:672:VAL:HG12	1:S:676:GLN:HE21	1.81	0.46
12:V:980:LEU:HD22	12:V:1075:TRP:CZ3	2.50	0.46
2:B:40:THR:HG23	2:B:70:GLU:HA	1.97	0.46
3:C:57:SER:C	3:C:59:THR:H	2.17	0.46
3:C:458:ARG:HA	3:C:458:ARG:NE	2.30	0.46
6:G:365:GLU:HG3	1:S:29:ARG:HH22	1.81	0.46
6:G:592:TYR:CD1	6:G:592:TYR:C	2.88	0.46
1:S:477:LEU:HD13	1:S:510:TYR:OH	2.15	0.46
1:S:817:LEU:HD23	1:S:818:PHE:CD1	2.51	0.46
7:M:234:VAL:HG11	7:M:259:VAL:CG1	2.46	0.46
11:U:481:VAL:HG12	11:U:485:PHE:CZ	2.51	0.46
14:Z:47:DT:H2"	14:Z:48:DG:C8	2.50	0.46
1:A:134:PRO:HA	1:A:220:GLN:HE22	1.81	0.46
1:A:1252:GLU:O	1:A:1298:ARG:NH1	2.47	0.46
2:B:183:LEU:HD12	2:B:191:LEU:HD12	1.97	0.46
4:E:355:LEU:HD23	4:E:360:ALA:HA	1.96	0.46
6:H:513:ARG:O	6:H:517:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:66:THR:O	2:O:68:LYS:NZ	2.42	0.46
8:P:531:ASN:HB2	8:P:572:LEU:HD21	1.98	0.46
10:X:57:ILE:HG23	10:X:61:TYR:CD2	2.50	0.46
11:U:537:VAL:HG12	11:U:541:LEU:HD12	1.97	0.46
11:U:595:LEU:CD1	11:U:626:THR:HG22	2.46	0.46
12:V:193:THR:CA	12:V:196:ILE:HG22	2.45	0.46
1:A:1358:VAL:O	1:A:1362:LEU:HG	2.15	0.46
2:B:392:PRO:HB2	7:L:131:THR:HG22	1.98	0.46
3:C:315:ILE:CG2	3:C:399:HIS:CD2	2.99	0.46
6:G:473:ILE:HD11	6:G:523:GLU:HB3	1.97	0.46
6:H:387:SER:OG	6:H:388:PRO:HD2	2.16	0.46
2:O:47:ARG:HH21	2:O:112:LEU:HD21	1.79	0.46
2:O:851:PHE:CZ	8:Q:550:SER:HB2	2.51	0.46
8:P:373:ARG:NH1	8:P:383:PRO:O	2.48	0.46
1:S:163:ARG:CG	1:S:191:VAL:HG13	2.46	0.46
7:M:267:LEU:HD13	7:M:288:LEU:HD21	1.98	0.46
11:U:742:SER:O	11:U:746:VAL:HG23	2.16	0.46
1:A:424:LEU:O	1:A:428:VAL:HG23	2.16	0.46
2:B:507:SER:OG	2:B:600:GLN:NE2	2.49	0.46
2:B:637:PRO:HB3	2:B:701:TYR:CZ	2.51	0.46
6:H:538:LEU:O	6:H:542:GLN:NE2	2.49	0.46
8:P:311:CYS:HA	8:P:324:ILE:O	2.16	0.46
1:S:1220:PRO:O	1:S:1253:ARG:NH2	2.49	0.46
2:B:295:GLY:O	2:B:297:LEU:HD12	2.16	0.46
2:B:330:ILE:CG2	2:B:339:GLU:OE1	2.64	0.46
2:B:609:CYS:SG	8:P:644:ARG:NH2	2.89	0.46
3:C:283:GLN:O	3:C:286:CYS:SG	2.69	0.46
5:F:289:LEU:HD12	6:G:539:LEU:HD23	1.94	0.46
2:O:487:LEU:HB2	2:O:584:LEU:HD21	1.97	0.46
2:O:770:LEU:O	2:O:773:LEU:HB3	2.16	0.46
8:P:510:THR:HG22	8:P:527:CYS:HA	1.98	0.46
7:M:253:PHE:CE2	7:M:263:LEU:HB3	2.51	0.46
11:U:109:ALA:HB1	11:U:160:LEU:HD11	1.98	0.46
1:A:818:PHE:CG	1:A:864:LEU:HD11	2.51	0.46
1:A:1269:LEU:HD21	1:A:1330:LEU:HB2	1.97	0.46
2:B:711:THR:O	2:B:714:GLU:N	2.49	0.46
3:C:248:PRO:O	3:C:252:LYS:HB2	2.15	0.46
4:E:339:LEU:HD13	12:V:309:HIS:ND1	2.30	0.46
5:F:158:GLN:OE1	5:F:158:GLN:N	2.38	0.46
6:H:186:PRO:HB3	6:H:200:ALA:HB3	1.98	0.46
2:O:584:LEU:HB3	2:O:588:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:152:MET:O	8:P:172:GLU:HA	2.16	0.46
8:Q:508:CYS:O	8:Q:643:SER:HB2	2.16	0.46
8:Q:773:MET:HB3	8:Q:776:LEU:HG	1.98	0.46
7:M:197:LEU:CD1	7:M:201:TRP:HZ2	2.22	0.46
12:V:382:LEU:HD11	12:V:416:LEU:HB3	1.98	0.46
1:A:78:ILE:HG22	1:A:79:ASP:N	2.31	0.45
1:A:651:GLY:O	1:A:654:THR:OG1	2.34	0.45
2:B:139:GLY:O	2:B:141:LEU:HB2	2.16	0.45
2:B:315:SER:OG	2:B:315:SER:O	2.33	0.45
2:B:330:ILE:HG22	2:B:339:GLU:OE1	2.16	0.45
2:B:584:LEU:HD12	2:O:725:THR:HG21	1.97	0.45
7:L:326:ASN:HD22	7:L:364:LYS:HG3	1.80	0.45
8:P:150:TRP:HZ3	8:P:195:PRO:HG3	1.82	0.45
8:P:424:SER:OG	8:P:428:ARG:HB2	2.17	0.45
8:P:679:PHE:CD2	8:P:679:PHE:O	2.69	0.45
1:S:57:LEU:CD1	1:S:101:GLN:HE21	2.29	0.45
10:X:44:THR:CG2	10:X:116:SER:HA	2.37	0.45
11:U:646:LYS:HG3	11:U:649:ALA:HB3	1.98	0.45
11:U:1146:HIS:CD2	11:U:1208:LEU:HD13	2.51	0.45
1:A:286:GLN:HB3	1:A:292:HIS:HB2	1.98	0.45
1:A:375:LEU:HD11	1:A:392:PHE:CE1	2.51	0.45
1:A:661:ARG:NH2	1:A:728:GLN:HB3	2.30	0.45
2:B:331:ASP:CB	2:B:333:PHE:CE1	2.99	0.45
3:C:280:SER:O	3:C:283:GLN:HB2	2.16	0.45
4:E:429:LEU:HB3	4:E:460:ARG:HH12	1.80	0.45
4:E:516:LEU:HD21	4:E:527:LEU:HD13	1.97	0.45
6:H:342:THR:CB	6:H:384:PRO:HG3	2.43	0.45
7:L:66:TYR:HA	7:L:69:ILE:HG12	1.97	0.45
2:O:94:ILE:HG22	2:O:96:ILE:HG12	1.99	0.45
2:O:521:LEU:HD23	2:O:523:CYS:SG	2.55	0.45
8:P:137:ASP:N	8:P:137:ASP:OD1	2.49	0.45
8:P:540:GLY:HA2	8:P:608:GLU:CG	2.46	0.45
1:S:239:VAL:HG11	1:S:301:VAL:HG22	1.98	0.45
11:U:835:SER:O	11:U:835:SER:OG	2.32	0.45
11:U:962:PHE:CD2	11:U:992:LEU:HD11	2.50	0.45
12:V:1077:GLY:O	12:V:1083:ASN:ND2	2.47	0.45
1:A:1333:PHE:CD1	1:A:1333:PHE:C	2.90	0.45
2:B:836:ARG:CZ	8:P:822:ALA:HB2	2.47	0.45
3:C:87:GLN:CD	3:C:87:GLN:N	2.69	0.45
3:C:169:PHE:CZ	4:E:17:ALA:HB2	2.51	0.45
4:E:358:SER:O	4:E:362:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:361:THR:HG23	4:E:401:ALA:CB	2.45	0.45
4:E:387:LEU:O	4:E:391:CYS:SG	2.74	0.45
6:G:416:LEU:HD13	1:S:22:TRP:CH2	2.52	0.45
6:G:518:ILE:HD11	6:G:550:THR:HA	1.98	0.45
2:O:156:GLN:O	2:O:156:GLN:NE2	2.49	0.45
2:O:592:LYS:HG2	2:O:593:PHE:N	2.31	0.45
2:O:843:ALA:CB	8:Q:809:GLN:HE21	2.30	0.45
8:P:27:ARG:N	8:P:38:SER:OG	2.45	0.45
11:U:1099:VAL:HA	11:U:1102:LEU:HD12	1.96	0.45
12:V:1078:PHE:O	12:V:1084:GLN:NE2	2.40	0.45
1:A:392:PHE:CE1	1:A:396:LEU:HD13	2.51	0.45
2:B:228:ILE:HG22	2:B:229:ILE:H	1.81	0.45
2:B:695:GLU:HA	2:B:701:TYR:CE1	2.50	0.45
4:E:384:THR:OG1	4:E:385:THR:N	2.50	0.45
6:G:458:LEU:CD2	6:G:596:TYR:CD2	2.99	0.45
6:G:596:TYR:CD1	6:G:596:TYR:C	2.89	0.45
6:H:31:GLN:NE2	6:H:320:GLN:OE1	2.50	0.45
7:L:208:ASP:O	7:L:295:ARG:NH2	2.49	0.45
2:O:641:PRO:O	2:O:643:GLU:HG3	2.17	0.45
2:O:704:LEU:HB2	2:O:720:TYR:HB2	1.99	0.45
1:A:61:LEU:HD23	1:A:105:LEU:HD21	1.97	0.45
1:A:163:ARG:N	8:P:849:ASP:OD2	2.49	0.45
1:A:1122:HIS:N	1:A:1125:ALA:O	2.44	0.45
1:A:1376:VAL:HG11	1:A:1392:PRO:HG3	1.98	0.45
2:B:31:ASN:O	2:B:38:THR:N	2.50	0.45
2:B:398:LEU:HA	8:P:462:ILE:HG12	1.98	0.45
5:F:181:GLU:HA	5:F:184:ARG:HH12	1.81	0.45
6:H:590:PRO:HB2	6:H:592:TYR:CE2	2.51	0.45
2:O:69:GLU:O	2:O:71:ASN:N	2.50	0.45
8:P:243:CYS:SG	8:P:251:CYS:O	2.72	0.45
1:S:316:LEU:HD11	1:S:320:PHE:CZ	2.52	0.45
1:S:1029:GLU:OE2	1:S:1089:VAL:N	2.49	0.45
11:U:322:PHE:N	11:U:322:PHE:CD1	2.84	0.45
11:U:420:LYS:N	11:U:420:LYS:HD3	2.31	0.45
11:U:1003:PHE:C	11:U:1003:PHE:CD2	2.89	0.45
12:V:215:LEU:O	12:V:219:LEU:HG	2.16	0.45
12:V:243:VAL:CG2	12:V:244:PRO:HD3	2.47	0.45
1:A:474:PHE:CD2	1:A:510:TYR:CE2	3.05	0.45
2:B:91:LEU:HD13	2:B:111:ILE:HG21	1.97	0.45
2:B:144:TRP:CH2	2:B:151:PHE:HB2	2.51	0.45
3:C:171:THR:HG22	4:E:14:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:117:VAL:O	4:E:120:ILE:HB	2.17	0.45
6:G:296:THR:CG2	6:G:357:THR:HG21	2.47	0.45
7:L:51:ALA:HB3	7:L:74:MET:SD	2.57	0.45
7:L:170:PRO:HD2	7:L:197:LEU:HD13	1.98	0.45
2:O:522:LYS:CG	2:O:523:CYS:N	2.79	0.45
8:P:658:LEU:CD2	8:P:745:VAL:CG1	2.95	0.45
1:S:291:THR:HA	1:S:294:ILE:HD12	1.99	0.45
1:S:449:ALA:HB2	1:S:492:HIS:ND1	2.31	0.45
1:S:1211:LEU:HD12	1:S:1233:ALA:HB1	1.99	0.45
11:U:537:VAL:HG13	11:U:605:LEU:HD23	1.98	0.45
12:V:364:TRP:CH2	12:V:384:MET:CE	3.00	0.45
12:V:532:LEU:HA	12:V:535:VAL:HG12	1.98	0.45
1:A:32:ARG:CB	6:H:311:ASN:HD21	2.30	0.45
1:A:415:MET:O	1:A:419:PHE:CD2	2.70	0.45
1:A:1173:TRP:O	1:A:1177:LEU:HG	2.16	0.45
2:B:500:SER:O	2:B:604:ARG:NH1	2.49	0.45
2:B:713:PHE:CE2	6:H:242:ARG:NH2	2.85	0.45
6:G:459:GLN:O	6:G:462:ALA:HB3	2.16	0.45
6:H:164:GLU:HG2	6:H:171:SER:O	2.16	0.45
1:S:1302:TRP:CH2	1:S:1348:ILE:HG21	2.52	0.45
12:V:110:PHE:CE2	12:V:114:LEU:HD11	2.51	0.45
1:A:286:GLN:O	1:A:288:GLU:N	2.46	0.45
1:A:1305:LEU:HA	1:A:1308:LEU:HD21	1.98	0.45
3:C:165:HIS:HB2	3:C:206:CYS:HB3	1.99	0.45
6:G:287:SER:OG	6:G:288:ARG:N	2.49	0.45
7:L:9:LEU:HD11	8:P:491:ASN:ND2	2.32	0.45
7:L:185:SER:O	7:L:188:SER:OG	2.30	0.45
2:O:17:CYS:O	2:O:81:CYS:SG	2.75	0.45
8:P:524:MET:HA	8:P:582:LEU:O	2.17	0.45
8:Q:726:VAL:HA	8:Q:727:PRO:HD2	1.67	0.45
1:S:568:VAL:HG22	1:S:1069:LEU:HD11	1.99	0.45
1:S:776:LEU:HD22	1:S:780:HIS:HB3	1.99	0.45
1:S:1139:LEU:HD21	1:S:1181:LEU:HD22	1.99	0.45
1:S:1246:LEU:HD22	1:S:1249:LEU:HD22	1.98	0.45
1:S:1266:MET:HE1	1:S:1323:ALA:HB1	1.99	0.45
10:X:62:PRO:HD2	10:X:63:PHE:CD2	2.52	0.45
10:X:87:LEU:HD23	10:X:90:LEU:HG	1.99	0.45
11:U:748:GLY:O	11:U:752:VAL:HG23	2.17	0.45
1:A:1163:CYS:HB3	1:A:1166:ILE:HD12	1.99	0.45
2:B:330:ILE:HG22	2:B:339:GLU:OE2	2.16	0.45
2:B:630:GLY:O	2:B:631:LYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:ARG:O	4:E:44:LEU:N	2.49	0.45
6:H:178:LEU:O	6:H:182:LYS:HG3	2.16	0.45
8:P:29:LEU:N	8:P:36:PHE:O	2.45	0.45
8:P:243:CYS:SG	8:P:243:CYS:O	2.75	0.45
8:P:260:THR:HB	8:P:264:ALA:O	2.16	0.45
8:Q:229:PHE:HE1	8:Q:252:CYS:SG	2.40	0.45
10:X:77:PRO:HD2	10:X:118:PRO:HB3	1.99	0.45
11:U:115:ALA:HB1	11:U:121:LEU:HD21	1.99	0.45
12:V:570:TYR:HA	12:V:573:ILE:HD12	1.99	0.45
1:A:835:LYS:HE2	1:A:903:TRP:CE2	2.51	0.45
1:A:1206:PHE:CD1	1:A:1206:PHE:C	2.89	0.45
1:A:1220:PRO:HG2	1:A:1226:SER:CB	2.47	0.45
2:B:172:TRP:HZ3	2:B:176:ILE:HD11	1.81	0.45
2:B:292:SER:OG	2:B:292:SER:O	2.35	0.45
2:B:342:LEU:HG	2:B:344:LEU:CD2	2.46	0.45
2:B:667:TYR:CE2	6:H:239:LEU:HD11	2.51	0.45
4:E:404:ASP:O	4:E:408:GLN:N	2.36	0.45
6:H:388:PRO:HD2	6:H:389:PRO:HD3	1.98	0.45
8:P:120:PRO:O	8:P:123:CYS:HB3	2.17	0.45
8:P:228:LEU:HD11	8:P:312:LEU:HD22	1.98	0.45
10:X:57:ILE:CG2	10:X:61:TYR:CD2	2.99	0.45
11:U:658:ILE:HD13	11:U:734:SER:HA	1.97	0.45
14:Z:45:DT:H2"	14:Z:46:DC:C6	2.52	0.45
2:B:850:ASP:OD2	8:P:801:HIS:ND1	2.49	0.44
3:C:145:TYR:C	3:C:147:PRO:HD2	2.37	0.44
4:E:123:GLN:OE1	4:E:129:PRO:HA	2.17	0.44
4:E:379:ALA:HB2	4:E:419:LEU:HD11	1.98	0.44
7:L:315:LEU:HD23	7:L:336:ILE:HD13	1.97	0.44
8:Q:563:ILE:HG21	8:Q:565:TYR:CZ	2.52	0.44
1:S:476:PHE:CZ	1:S:480:LEU:HD13	2.52	0.44
10:X:54:GLU:HB2	10:X:71:LEU:HD11	1.99	0.44
11:U:491:LEU:HB2	11:U:496:VAL:CG2	2.48	0.44
11:U:1019:ARG:O	11:U:1025:CYS:SG	2.75	0.44
11:U:1248:LYS:N	11:U:1249:PRO:CD	2.80	0.44
1:A:1063:TRP:NE1	1:A:1329:ARG:NH2	2.65	0.44
1:A:1345:ASP:N	1:A:1345:ASP:OD1	2.50	0.44
2:O:397:GLY:HA3	7:M:111:TYR:CE2	2.52	0.44
8:P:327:SER:OG	8:P:335:VAL:O	2.23	0.44
8:P:861:ALA:O	8:P:865:ARG:CB	2.64	0.44
8:Q:141:VAL:HG11	8:Q:241:VAL:HG11	2.00	0.44
1:S:773:GLY:N	1:S:774:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:874:ARG:O	1:S:874:ARG:CG	2.64	0.44
1:S:1033:ASP:OD2	1:S:1093:SER:CB	2.60	0.44
7:M:361:TYR:HA	10:X:101:SER:CB	2.46	0.44
11:U:230:LEU:HD11	11:U:285:LEU:HD11	1.98	0.44
11:U:806:SER:HA	11:U:862:PRO:HD2	1.99	0.44
11:U:1095:VAL:HG13	11:U:1137:GLN:NE2	2.32	0.44
11:U:1151:THR:O	11:U:1212:PHE:HE2	2.01	0.44
12:V:412:ILE:HA	12:V:416:LEU:HD12	1.98	0.44
2:B:96:ILE:O	2:B:107:TYR:HA	2.18	0.44
7:L:101:LEU:HB2	7:L:102:TYR:CD2	2.53	0.44
2:O:486:SER:HA	2:O:582:THR:O	2.18	0.44
8:P:251:CYS:SG	8:P:274:ILE:HB	2.57	0.44
8:P:516:ARG:NH1	8:Q:579:GLU:O	2.49	0.44
8:P:874:ARG:HA	8:P:874:ARG:HE	1.82	0.44
1:S:240:GLN:HA	1:S:311:ILE:HD11	1.99	0.44
1:S:1167:LEU:O	1:S:1171:LEU:HG	2.17	0.44
7:M:39:ARG:NH1	7:M:55:CYS:O	2.51	0.44
1:A:108:PRO:HG2	1:A:111:ILE:HD12	1.99	0.44
1:A:1101:ILE:HD13	1:A:1154:PHE:CE2	2.52	0.44
3:C:216:GLN:O	3:C:219:PHE:HB3	2.17	0.44
4:E:97:ASN:O	4:E:98:LEU:C	2.56	0.44
5:F:203:LYS:O	5:F:207:VAL:HG23	2.18	0.44
6:G:371:LEU:O	6:G:372:ALA:C	2.56	0.44
1:S:599:SER:CB	1:S:1009:GLY:HA3	2.47	0.44
1:S:911:TRP:CE3	1:S:917:ARG:NH1	2.85	0.44
1:S:1175:PRO:HD3	1:S:1204:ARG:NH1	2.32	0.44
12:V:154:PHE:CD2	12:V:195:LYS:HB3	2.53	0.44
12:V:463:LYS:HE2	12:V:502:LEU:HD11	1.99	0.44
1:A:403:ALA:O	1:A:407:LEU:HB2	2.18	0.44
2:B:266:ILE:HG22	2:B:267:SER:O	2.18	0.44
4:E:106:ARG:N	4:E:107:PRO:CD	2.81	0.44
4:E:282:LYS:CD	4:E:282:LYS:N	2.81	0.44
6:H:99:SER:O	6:H:103:VAL:HG23	2.18	0.44
6:H:146:GLN:NE2	6:H:150:TRP:CE2	2.86	0.44
7:L:126:LEU:HD12	7:L:127:VAL:N	2.32	0.44
2:O:265:LEU:HD22	2:O:311:VAL:HG21	1.98	0.44
2:O:624:LEU:HD12	2:O:624:LEU:HA	1.78	0.44
8:Q:466:SER:HB2	7:M:108:PRO:HD3	1.98	0.44
1:S:992:HIS:CD2	1:S:1073:ARG:NH2	2.85	0.44
12:V:383:VAL:CG2	12:V:420:THR:HG23	2.47	0.44
12:V:686:LEU:HD12	12:V:757:ASP:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:ARG:O	1:A:1324:PRO:HB3	2.17	0.44
2:B:651:LEU:HD23	2:B:655:PHE:CE1	2.52	0.44
3:C:55:MET:CE	3:C:60:VAL:HG21	2.48	0.44
3:C:319:THR:O	3:C:320:GLN:C	2.55	0.44
3:C:490:LEU:O	3:C:493:ASN:HB2	2.17	0.44
4:E:368:PHE:O	4:E:371:ARG:N	2.50	0.44
4:E:501:GLN:CG	4:E:502:ALA:N	2.80	0.44
5:F:292:GLY:HA3	6:G:485:ARG:HD2	2.00	0.44
6:G:147:ALA:CA	6:G:159:LEU:HD11	2.47	0.44
6:H:23:LEU:HD22	6:H:46:ALA:HA	1.99	0.44
7:L:69:ILE:O	7:L:73:ARG:HG2	2.18	0.44
8:P:604:TYR:HB3	8:P:638:VAL:HG23	1.99	0.44
1:S:847:LYS:HG2	1:S:848:PHE:CD2	2.53	0.44
7:M:214:LEU:HD12	7:M:229:ALA:HB2	1.99	0.44
10:X:9:ARG:O	10:X:13:MET:HB2	2.18	0.44
11:U:439:GLU:HG2	11:U:440:ILE:N	2.32	0.44
11:U:485:PHE:HA	11:U:488:LEU:HB2	1.99	0.44
11:U:731:GLN:NE2	11:U:792:ALA:CB	2.81	0.44
11:U:1033:PHE:CE2	11:U:1087:LEU:HD22	2.53	0.44
12:V:208:GLN:O	12:V:212:ILE:HG12	2.17	0.44
12:V:278:LEU:N	12:V:279:PRO:HD3	2.33	0.44
12:V:1348:HIS:O	12:V:1350:ASP:N	2.49	0.44
1:A:32:ARG:HB3	6:H:311:ASN:ND2	2.32	0.44
3:C:12:TYR:CE2	3:C:63:ARG:HB3	2.53	0.44
4:E:108:SER:O	4:E:109:LEU:HD23	2.18	0.44
4:E:467:GLU:O	4:E:471:VAL:HG23	2.18	0.44
6:G:505:SER:HB3	6:G:508:ALA:H	1.83	0.44
6:H:104:LEU:HD13	6:H:121:LEU:HD23	1.99	0.44
7:L:4:THR:HB	7:L:81:MET:HB2	1.98	0.44
7:L:338:LEU:HD11	7:L:342:LEU:CD1	2.46	0.44
8:P:778:PRO:HD3	8:P:824:ASP:O	2.18	0.44
1:S:430:ALA:O	1:S:434:VAL:HG23	2.16	0.44
1:S:818:PHE:CD2	1:S:864:LEU:HD11	2.52	0.44
10:X:49:GLY:HA3	10:X:147:THR:HG23	1.99	0.44
11:U:506:LEU:HD13	11:U:513:MET:SD	2.58	0.44
11:U:643:PRO:CB	11:U:721:PHE:CE1	3.01	0.44
12:V:189:GLY:O	12:V:192:LEU:HB3	2.17	0.44
2:B:146:HIS:O	2:B:148:LYS:N	2.51	0.44
2:B:430:VAL:HG21	8:P:638:VAL:HG12	1.99	0.44
2:B:480:TYR:CD1	2:B:480:TYR:N	2.86	0.44
2:B:817:GLN:HE21	2:B:821:LYS:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:313:SER:O	5:F:316:GLN:N	2.50	0.44
6:G:267:LEU:HD21	1:S:60:LEU:HD11	1.99	0.44
6:G:393:MET:CE	8:P:236:LEU:HD21	2.48	0.44
6:H:368:LEU:HD11	6:H:404:LEU:HD11	2.00	0.44
8:P:67:LEU:HD22	8:P:76:LEU:HD21	1.99	0.44
1:S:342:MET:HB3	1:S:346:TRP:CZ2	2.52	0.44
11:U:295:VAL:HA	11:U:301:SER:HB3	1.99	0.44
12:V:368:ILE:HD13	12:V:381:ASP:HB3	2.00	0.44
2:B:745:LYS:HG2	2:B:746:ASN:N	2.32	0.44
3:C:254:MET:HB3	3:C:297:MET:CE	2.48	0.44
5:F:168:GLU:OE2	5:F:211:GLN:HG3	2.18	0.44
7:L:354:ILE:HG23	7:L:367:THR:CG2	2.47	0.44
2:O:17:CYS:SG	2:O:331:ASP:HB2	2.58	0.44
2:O:287:VAL:HB	2:O:301:VAL:HG22	1.99	0.44
8:P:269:ASN:N	8:P:269:ASN:HD22	2.16	0.44
1:S:566:VAL:CG1	1:S:1273:LEU:HD21	2.48	0.44
7:M:69:ILE:O	7:M:73:ARG:HG2	2.18	0.44
11:U:324:ASP:N	11:U:324:ASP:OD1	2.50	0.44
11:U:372:VAL:C	11:U:374:SER:N	2.71	0.44
11:U:1081:ALA:HB3	11:U:1082:PRO:HD3	2.00	0.44
11:U:1146:HIS:ND1	11:U:1204:HIS:HB3	2.33	0.44
12:V:298:ILE:O	12:V:302:ARG:HB2	2.17	0.44
12:V:801:CYS:SG	12:V:802:GLN:N	2.91	0.44
12:V:1306:LEU:HG	12:V:1367:LEU:HD13	1.99	0.44
12:V:1355:GLN:HE22	14:Z:35:DG:H5”	1.82	0.44
12:V:1357:VAL:HB	12:V:1358:PRO:HD3	2.00	0.44
1:A:197:LEU:HD22	1:A:206:VAL:HG13	1.99	0.43
2:B:665:PRO:HD2	2:B:741:ASN:HB2	1.99	0.43
4:E:71:GLU:HB3	4:E:72:PRO:CD	2.48	0.43
5:F:346:ILE:HG23	5:F:347:TRP:CD2	2.53	0.43
6:G:447:TYR:CD1	6:G:488:PRO:O	2.71	0.43
2:O:423:TYR:CD1	8:Q:606:LEU:HD12	2.51	0.43
8:P:423:LEU:HA	8:P:428:ARG:O	2.17	0.43
8:P:704:SER:N	8:P:791:SER:O	2.51	0.43
1:S:218:CYS:HB3	1:S:294:ILE:HA	1.99	0.43
1:S:731:MET:SD	1:S:779:PRO:HB3	2.58	0.43
7:M:21:SER:O	7:M:23:THR:N	2.51	0.43
7:M:165:TYR:CE1	7:M:175:ALA:HB3	2.53	0.43
11:U:448:VAL:O	11:U:456:ILE:CD1	2.66	0.43
11:U:473:VAL:HG13	11:U:474:LEU:N	2.33	0.43
11:U:504:GLN:HE22	11:U:543:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:PRO:HB2	1:A:747:ALA:HB3	2.00	0.43
2:B:534:PRO:HA	2:B:572:LYS:NZ	2.32	0.43
4:E:381:ARG:N	12:V:272:SER:HA	2.32	0.43
8:P:170:ILE:CG2	8:P:259:VAL:HG22	2.47	0.43
8:P:773:MET:C	8:P:781:PRO:HB3	2.38	0.43
8:Q:42:GLU:OE1	8:Q:62:ASP:N	2.50	0.43
8:Q:543:LEU:C	8:Q:544:CYS:SG	2.97	0.43
1:S:393:VAL:HA	1:S:396:LEU:HD12	2.00	0.43
11:U:86:VAL:HA	11:U:89:ILE:HG22	2.00	0.43
11:U:499:LEU:HG	11:U:500:LEU:HD23	2.00	0.43
1:A:313:THR:HA	1:A:316:LEU:HB3	2.01	0.43
1:A:1232:PHE:O	1:A:1236:GLN:OE1	2.36	0.43
2:B:669:LEU:HB3	2:B:712:PRO:O	2.19	0.43
3:C:492:LEU:HD13	3:C:522:ILE:HG23	1.99	0.43
4:E:517:GLU:HB2	4:E:518:PRO:HD3	2.01	0.43
7:L:109:GLN:NE2	7:L:113:SER:OG	2.51	0.43
8:P:276:HIS:ND1	8:P:277:HIS:N	2.66	0.43
8:Q:284:PHE:HB3	8:Q:315:PHE:CD2	2.54	0.43
7:M:198:LYS:C	7:M:198:LYS:CD	2.86	0.43
7:M:343:ARG:NH1	12:V:472:GLU:OE1	2.51	0.43
11:U:2:ASP:HB2	11:U:35:ASN:HD21	1.84	0.43
11:U:422:GLY:HA2	11:U:425:ILE:HD12	1.99	0.43
12:V:342:CYS:HA	12:V:345:LEU:HD12	2.00	0.43
1:A:1034:LEU:CD2	1:S:1188:HIS:CD2	3.02	0.43
1:A:1331:LEU:HB3	1:A:1332:PRO:HD3	2.01	0.43
1:A:1368:PHE:CZ	1:A:1393:VAL:HG22	2.54	0.43
2:B:725:THR:CG2	2:O:485:ASP:HA	2.49	0.43
3:C:315:ILE:CG2	3:C:399:HIS:HA	2.46	0.43
3:C:365:LEU:CD1	3:C:422:LEU:HD11	2.48	0.43
5:F:116:PHE:HD1	5:F:130:GLN:HG3	1.82	0.43
6:G:367:TYR:HD1	6:G:370:LEU:HD23	1.83	0.43
6:H:450:LEU:O	6:H:453:SER:OG	2.34	0.43
2:O:170:ILE:O	2:O:171:GLN:C	2.56	0.43
2:O:519:ARG:HG3	2:O:520:LEU:N	2.33	0.43
8:P:13:GLY:C	8:P:14:PHE:CD1	2.92	0.43
8:P:35:VAL:HG12	8:P:47:TYR:HB2	1.99	0.43
8:P:253:VAL:HG23	8:P:272:VAL:CA	2.48	0.43
8:P:321:MET:HG2	8:P:322:LEU:N	2.33	0.43
11:U:1254:ILE:O	11:U:1258:GLU:HG2	2.19	0.43
12:V:752:ILE:O	12:V:755:LEU:N	2.45	0.43
12:V:1013:VAL:HG21	12:V:1075:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:MET:HE1	1:A:419:PHE:CZ	2.51	0.43
3:C:207:HIS:CD2	4:E:93:ILE:HG13	2.53	0.43
7:L:66:TYR:O	7:L:70:VAL:HG23	2.18	0.43
8:P:474:LYS:O	8:P:477:ASP:HB2	2.18	0.43
10:X:40:GLY:HA3	10:X:46:TYR:O	2.19	0.43
12:V:686:LEU:HD13	12:V:811:LYS:HG2	2.01	0.43
2:B:240:VAL:HG13	2:B:256:LEU:HD11	1.99	0.43
2:B:742:CYS:O	8:P:684:ARG:HD2	2.18	0.43
3:C:188:VAL:CG2	3:C:219:PHE:HA	2.48	0.43
2:O:83:SER:HA	2:O:89:ILE:O	2.18	0.43
8:P:143:LEU:HB2	8:P:197:LEU:HD11	2.01	0.43
8:P:361:SER:CB	8:P:398:SER:O	2.66	0.43
8:Q:348:LEU:HD11	8:Q:363:PRO:HD3	2.00	0.43
1:S:328:LEU:HD22	1:S:389:VAL:CG2	2.48	0.43
1:S:772:GLN:NE2	9:W:95:TRP:CZ2	2.87	0.43
1:S:1262:PHE:CD2	1:S:1319:LEU:HD22	2.54	0.43
7:M:121:LEU:HD11	7:M:183:LEU:HB3	2.01	0.43
11:U:537:VAL:CG1	11:U:541:LEU:HD12	2.49	0.43
11:U:854:LYS:HD2	11:U:914:LYS:HB3	2.01	0.43
12:V:1186:LEU:HD21	12:V:1234:PHE:CE2	2.54	0.43
1:A:59:ALA:O	1:A:63:GLU:HG3	2.19	0.43
1:A:327:ILE:HG23	1:A:388:ARG:HD3	2.01	0.43
1:A:1266:MET:HE2	1:A:1266:MET:HA	2.00	0.43
2:B:242:ILE:HG12	2:B:243:CYS:N	2.34	0.43
2:B:480:TYR:HE2	2:B:622:LEU:HD11	1.82	0.43
3:C:501:GLY:O	3:C:502:HIS:ND1	2.52	0.43
6:G:458:LEU:HD22	6:G:596:TYR:CD2	2.53	0.43
6:H:128:ALA:HA	6:H:131:LEU:HD12	2.00	0.43
6:H:362:ASP:OD1	6:H:362:ASP:N	2.52	0.43
8:Q:764:VAL:HG23	8:Q:791:SER:HB2	1.99	0.43
1:S:598:ASP:O	1:S:601:VAL:HB	2.19	0.43
1:S:661:ARG:HD2	9:W:78:PHE:CE1	2.53	0.43
11:U:283:TYR:CE1	12:V:483:SER:HB2	2.54	0.43
11:U:1045:LEU:HG	11:U:1072:PHE:CZ	2.54	0.43
11:U:1155:SER:HA	11:U:1159:VAL:CG1	2.48	0.43
12:V:463:LYS:CE	12:V:502:LEU:HD11	2.49	0.43
1:A:101:GLN:CG	1:A:112:LEU:HD13	2.49	0.43
1:A:152:ALA:HA	1:A:155:LEU:HD12	2.00	0.43
1:A:286:GLN:CB	1:A:288:GLU:HG3	2.48	0.43
6:H:300:LEU:HD13	6:H:359:ARG:HD2	2.00	0.43
7:L:144:SER:OG	7:L:146:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:148:ALA:O	8:P:180:PRO:HD2	2.19	0.43
8:Q:141:VAL:HG22	8:Q:154:LEU:CD1	2.48	0.43
8:Q:339:ARG:HE	7:M:101:LEU:HD21	1.84	0.43
1:S:113:SER:HB2	1:S:155:LEU:HD13	2.01	0.43
7:M:215:GLU:CB	7:M:227:ARG:HB3	2.49	0.43
11:U:466:ILE:HG22	11:U:467:VAL:HG23	2.01	0.43
11:U:668:LEU:HD11	11:U:749:VAL:HG13	2.00	0.43
11:U:1050:SER:HB3	11:U:1144:PHE:CD1	2.53	0.43
12:V:94:GLU:OE1	12:V:94:GLU:N	2.49	0.43
12:V:1128:PHE:CE2	12:V:1181:GLN:HB3	2.52	0.43
1:A:262:MET:HB3	1:A:264:GLN:HE21	1.84	0.43
1:A:1079:LYS:HG3	1:A:1130:ILE:HD13	2.01	0.43
2:B:13:GLU:HG2	2:B:26:GLN:HG3	2.01	0.43
5:F:289:LEU:HD13	6:G:484:PHE:CE2	2.54	0.43
6:H:54:LEU:O	6:H:58:GLN:HG2	2.19	0.43
2:O:79:CYS:CB	2:O:94:ILE:HD13	2.49	0.43
2:O:580:ALA:C	2:O:581:VAL:CG2	2.86	0.43
2:O:706:THR:O	2:O:717:LEU:HD12	2.19	0.43
8:Q:325:LYS:HE2	8:Q:384:GLU:HB3	2.01	0.43
1:S:935:LEU:O	1:S:938:GLU:HB2	2.19	0.43
1:S:1056:LEU:O	1:S:1071:ARG:NH2	2.51	0.43
7:M:311:TYR:HE2	10:X:6:ARG:HD3	1.65	0.43
11:U:430:PHE:CE2	11:U:466:ILE:HG23	2.54	0.43
11:U:665:ASP:OD1	11:U:665:ASP:N	2.52	0.43
12:V:611:THR:HG23	12:V:651:TRP:CZ2	2.54	0.43
1:A:504:ARG:HE	1:A:504:ARG:N	2.16	0.43
1:A:1075:LEU:HD12	1:A:1119:PHE:CD2	2.54	0.43
2:B:298:PHE:CD2	2:B:362:LEU:HD12	2.54	0.43
2:B:682:CYS:HA	2:B:693:PHE:O	2.19	0.43
3:C:348:LEU:HD23	3:C:396:LEU:HD22	2.00	0.43
6:G:257:ARG:NE	6:G:285:GLU:OE2	2.44	0.43
6:G:382:PHE:CE2	8:P:139:VAL:HG21	2.54	0.43
2:O:218:GLU:HB2	2:O:220:GLN:HE21	1.83	0.43
8:Q:563:ILE:CG2	8:Q:564:THR:N	2.82	0.43
7:M:212:TRP:HA	7:M:295:ARG:HD3	2.01	0.43
7:M:295:ARG:C	7:M:297:ILE:N	2.71	0.43
11:U:746:VAL:HG11	11:U:781:LEU:HD11	2.00	0.43
11:U:962:PHE:CD1	11:U:988:VAL:HG11	2.54	0.43
1:A:364:VAL:N	2:B:817:GLN:HE22	2.17	0.42
3:C:24:GLN:O	3:C:25:ALA:C	2.57	0.42
3:C:64:PHE:N	3:C:65:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:387:LEU:HD12	4:E:391:CYS:SG	2.59	0.42
7:L:320:PRO:HA	7:L:333:PHE:O	2.19	0.42
2:O:184:LEU:HD23	2:O:184:LEU:HA	1.85	0.42
8:Q:488:GLU:HA	8:Q:491:ASN:HD22	1.83	0.42
1:S:1368:PHE:CD2	1:S:1396:ILE:HD11	2.54	0.42
11:U:134:LEU:HD21	11:U:160:LEU:HD23	2.01	0.42
11:U:530:LEU:CD1	11:U:598:GLN:HE21	2.31	0.42
11:U:758:PHE:N	11:U:771:ILE:HD11	2.34	0.42
1:A:108:PRO:CG	1:A:111:ILE:HD12	2.49	0.42
1:A:327:ILE:O	1:A:388:ARG:HD2	2.19	0.42
2:B:418:ILE:O	2:B:422:SER:OG	2.29	0.42
4:E:457:LEU:O	4:E:462:VAL:HG13	2.19	0.42
6:G:280:GLY:N	6:G:281:PRO:HD2	2.34	0.42
7:L:55:CYS:HB3	7:L:59:LEU:HB3	1.99	0.42
7:L:226:ARG:HA	7:L:226:ARG:HD3	1.90	0.42
8:P:288:LEU:N	8:P:311:CYS:O	2.49	0.42
8:Q:140:LEU:HD23	8:Q:155:PHE:HB2	2.01	0.42
8:Q:312:LEU:HD23	8:Q:324:ILE:HD12	2.02	0.42
1:S:485:SER:OG	1:S:521:LEU:HD13	2.20	0.42
12:V:505:SER:O	12:V:508:MET:HB2	2.18	0.42
1:A:476:PHE:CZ	1:A:480:LEU:HD11	2.54	0.42
1:A:1407:ILE:N	1:A:1408:PRO:HD2	2.35	0.42
2:B:592:LYS:HG2	2:B:593:PHE:N	2.34	0.42
3:C:159:SER:O	3:C:162:ARG:HB2	2.19	0.42
4:E:510:LEU:O	4:E:514:MET:HG2	2.19	0.42
4:E:516:LEU:HD21	4:E:527:LEU:HD22	2.01	0.42
6:G:384:PRO:HB2	6:G:385:PRO:HD2	2.01	0.42
6:H:69:LEU:O	6:H:72:THR:HB	2.19	0.42
2:O:422:SER:HA	7:M:18:GLN:NE2	2.35	0.42
8:P:424:SER:HB3	8:P:428:ARG:HB2	2.02	0.42
8:Q:227:LEU:HD11	8:Q:336:PRO:HD3	2.01	0.42
1:S:589:THR:O	1:S:625:CYS:SG	2.76	0.42
1:A:1063:TRP:CE2	1:A:1329:ARG:CZ	3.02	0.42
1:A:1143:LEU:HD21	1:A:1185:TRP:CE3	2.53	0.42
3:C:61:ILE:HA	3:C:64:PHE:HB2	2.01	0.42
4:E:26:ALA:O	4:E:29:LEU:N	2.53	0.42
6:G:416:LEU:HD22	1:S:22:TRP:CZ3	2.52	0.42
7:L:307:CYS:CB	7:L:310:CYS:SG	3.06	0.42
2:O:239:TYR:HD2	2:O:259:LEU:HD21	1.84	0.42
2:O:627:LEU:O	2:O:630:GLY:N	2.53	0.42
2:O:680:MET:SD	2:O:700:PHE:CD2	3.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:777:ILE:HG21	8:Q:830:LEU:CD1	2.48	0.42
8:P:75:LEU:C	8:P:90:LEU:HD21	2.40	0.42
8:P:451:ALA:O	8:P:454:LYS:HB3	2.19	0.42
1:S:57:LEU:HD12	1:S:101:GLN:HE21	1.84	0.42
1:S:834:LEU:O	1:S:838:THR:OG1	2.35	0.42
1:S:1220:PRO:HG2	1:S:1226:SER:CB	2.50	0.42
7:M:320:PRO:HA	7:M:333:PHE:O	2.19	0.42
11:U:638:LYS:O	11:U:712:ARG:CZ	2.66	0.42
11:U:1042:PRO:O	11:U:1046:LEU:HG	2.19	0.42
11:U:1060:ILE:HG23	11:U:1215:TYR:CD1	2.54	0.42
11:U:1213:ILE:HG21	11:U:1285:ARG:HH22	1.84	0.42
12:V:1035:GLN:HB2	12:V:1124:SER:HB2	2.00	0.42
1:A:832:PHE:O	1:A:835:LYS:HB3	2.20	0.42
1:A:1034:LEU:HD22	1:S:1188:HIS:CG	2.55	0.42
1:A:1118:ASN:HA	1:A:1324:PRO:HB3	2.00	0.42
1:A:1331:LEU:N	1:A:1332:PRO:HD2	2.34	0.42
4:E:429:LEU:HD21	4:E:437:MET:HG3	2.01	0.42
4:E:516:LEU:HD12	4:E:531:LEU:HD22	2.01	0.42
6:G:374:LEU:HD13	6:G:393:MET:HE1	2.01	0.42
6:G:521:GLY:HA3	6:G:537:PHE:CZ	2.54	0.42
6:H:134:GLU:OE1	6:H:134:GLU:HA	2.20	0.42
6:H:537:PHE:O	6:H:540:SER:OG	2.30	0.42
2:O:308:ALA:N	2:O:325:LEU:HD12	2.34	0.42
8:P:317:HIS:O	8:P:346:PRO:HA	2.18	0.42
8:P:402:CYS:O	8:P:420:LEU:HB2	2.19	0.42
1:S:276:PHE:HE2	1:S:294:ILE:HG21	1.84	0.42
1:S:346:TRP:CD2	1:S:387:GLN:HA	2.53	0.42
1:S:869:GLN:CD	1:S:920:LEU:HD21	2.40	0.42
7:M:8:LEU:CD2	7:M:25:TYR:HE2	2.30	0.42
7:M:159:PRO:O	7:M:179:PRO:HA	2.18	0.42
11:U:959:ILE:HG13	11:U:992:LEU:HD22	2.01	0.42
11:U:1014:CYS:HA	11:U:1074:ILE:HD12	2.02	0.42
12:V:657:CYS:SG	12:V:658:ASN:N	2.91	0.42
1:A:818:PHE:HE2	1:A:861:SER:HG	1.60	0.42
1:A:821:LEU:HD23	1:A:821:LEU:C	2.40	0.42
1:A:823:THR:HG21	1:A:829:SER:HB2	2.02	0.42
1:A:1142:CYS:SG	1:A:1152:VAL:HG22	2.60	0.42
1:A:1200:LEU:O	1:A:1204:ARG:HG2	2.19	0.42
2:B:18:TYR:HB3	2:B:23:LEU:HD11	2.02	0.42
3:C:49:TYR:CE1	3:C:92:TRP:HB3	2.54	0.42
3:C:367:THR:HG21	3:C:403:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:296:THR:HG21	6:H:357:THR:HG23	2.01	0.42
2:O:423:TYR:CD1	8:Q:606:LEU:CD1	3.02	0.42
2:O:478:ILE:HG23	2:O:478:ILE:O	2.20	0.42
8:Q:135:LEU:HD12	8:Q:140:LEU:HD12	2.01	0.42
8:Q:485:SER:O	8:Q:486:LEU:C	2.56	0.42
1:S:767:GLN:HA	1:S:767:GLN:NE2	2.34	0.42
1:S:1305:LEU:O	1:S:1308:LEU:HG	2.19	0.42
11:U:94:MET:HE2	11:U:94:MET:HA	2.02	0.42
11:U:169:TRP:HH2	11:U:194:VAL:HG23	1.84	0.42
1:A:776:LEU:HD13	1:A:784:LEU:CD1	2.49	0.42
1:A:1305:LEU:C	1:A:1308:LEU:CD2	2.88	0.42
3:C:462:LEU:O	3:C:504:ILE:HD13	2.19	0.42
7:L:126:LEU:HD12	7:L:127:VAL:H	1.85	0.42
7:L:187:TYR:CE2	7:L:191:LEU:HD21	2.55	0.42
2:O:592:LYS:HG3	2:O:622:LEU:O	2.19	0.42
8:P:37:LEU:HD12	8:P:429:LEU:HD12	2.01	0.42
8:Q:479:ARG:HA	8:Q:479:ARG:HD3	1.73	0.42
7:M:361:TYR:CE1	10:X:101:SER:N	2.87	0.42
11:U:660:LEU:HD13	11:U:745:LEU:HD11	2.02	0.42
12:V:420:THR:HG22	12:V:428:LEU:HD11	2.00	0.42
1:A:1112:VAL:HG12	1:A:1165:LEU:HD12	2.02	0.42
2:B:187:LYS:HG2	2:B:229:ILE:CG1	2.49	0.42
6:G:81:ARG:CG	6:G:92:GLN:HE21	2.32	0.42
6:G:160:ALA:O	6:G:164:GLU:HB2	2.20	0.42
6:G:588:SER:O	6:G:588:SER:OG	2.34	0.42
1:S:1404:LEU:HD21	1:S:1432:VAL:HG22	2.02	0.42
7:M:309:ILE:HG12	7:M:333:PHE:CD1	2.49	0.42
11:U:653:THR:HG23	11:U:658:ILE:HG13	2.01	0.42
12:V:1316:SER:HB2	12:V:1320:HIS:ND1	2.34	0.42
1:A:156:LEU:HD22	1:A:163:ARG:HH22	1.85	0.42
1:A:1363:LYS:HA	1:A:1366:GLN:OE1	2.20	0.42
2:B:534:PRO:HA	2:B:572:LYS:CE	2.50	0.42
2:B:774:SER:HB2	8:P:834:HIS:ND1	2.35	0.42
5:F:289:LEU:HD13	6:G:484:PHE:HE2	1.85	0.42
7:L:313:TYR:CD1	7:L:320:PRO:HD2	2.55	0.42
8:Q:746:VAL:HG13	8:Q:751:LEU:HB3	2.02	0.42
1:S:145:LEU:HG	1:S:149:LEU:CD1	2.50	0.42
11:U:430:PHE:CZ	11:U:466:ILE:HG23	2.55	0.42
11:U:836:ASN:O	11:U:839:MET:HB2	2.19	0.42
12:V:149:ILE:O	12:V:152:THR:HG22	2.19	0.42
12:V:468:TYR:CD2	12:V:469:CYS:SG	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:36:DA:C2	14:Z:37:DA:C5	3.08	0.42
2:B:667:TYR:HE2	6:H:239:LEU:HD11	1.85	0.42
5:F:2:GLU:O	5:F:6:GLN:OE1	2.38	0.42
5:F:341:VAL:HG13	5:F:344:LEU:HD12	2.01	0.42
6:H:240:CYS:O	6:H:242:ARG:N	2.53	0.42
7:L:42:LEU:HD12	7:L:46:LEU:HD23	2.02	0.42
7:L:228:ILE:HD12	7:L:238:ILE:HD12	2.02	0.42
8:P:74:ARG:HA	8:P:74:ARG:HD3	1.80	0.42
8:P:601:THR:HG22	8:P:641:PRO:HA	2.01	0.42
1:S:346:TRP:CZ3	1:S:390:LEU:HD22	2.55	0.42
1:S:998:TYR:HB3	1:S:1007:VAL:HG22	2.00	0.42
1:S:1210:PHE:HE1	1:S:1246:LEU:HD23	1.85	0.42
1:S:1261:PHE:HB2	1:S:1291:ILE:HG21	2.01	0.42
11:U:507:LEU:CD1	11:U:517:LEU:HD22	2.50	0.42
12:V:1332:GLN:O	12:V:1335:THR:HB	2.20	0.42
2:B:52:ARG:O	2:B:55:LYS:NZ	2.32	0.41
2:B:365:ILE:HG23	2:B:367:TYR:CD2	2.54	0.41
2:B:423:TYR:CE2	8:P:606:LEU:HB3	2.55	0.41
4:E:501:GLN:HG3	4:E:502:ALA:N	2.35	0.41
5:F:90:ASP:O	5:F:93:LEU:HB3	2.20	0.41
6:G:296:THR:HG21	6:G:357:THR:HG21	2.01	0.41
7:L:81:MET:HE3	7:L:81:MET:O	2.20	0.41
7:L:170:PRO:HD2	7:L:197:LEU:CD1	2.50	0.41
8:P:37:LEU:CD1	8:P:429:LEU:HD12	2.50	0.41
1:S:44:LYS:O	1:S:48:VAL:HG23	2.20	0.41
1:S:1266:MET:CE	1:S:1323:ALA:HB1	2.50	0.41
7:M:15:LEU:HD23	7:M:15:LEU:HA	1.89	0.41
7:M:342:LEU:O	7:M:348:SER:CB	2.68	0.41
11:U:113:ILE:O	11:U:117:ARG:HG2	2.20	0.41
12:V:355:ARG:HA	12:V:391:THR:HG21	2.02	0.41
1:A:814:VAL:HB	1:A:815:PRO:HD3	2.01	0.41
2:B:525:ASN:HD22	2:B:525:ASN:N	2.17	0.41
2:B:614:TYR:O	2:B:615:VAL:HG23	2.20	0.41
6:G:306:LEU:CD2	6:G:346:THR:HG21	2.51	0.41
6:H:69:LEU:O	6:H:73:VAL:HG23	2.20	0.41
6:H:250:THR:HG22	6:H:282:PRO:CA	2.49	0.41
6:H:388:PRO:N	6:H:389:PRO:CD	2.84	0.41
2:O:306:ASN:O	2:O:324:LYS:N	2.52	0.41
8:Q:580:VAL:HG12	8:Q:582:LEU:HD23	2.01	0.41
1:S:573:ILE:HG22	1:S:574:PHE:CE1	2.56	0.41
1:S:1014:ASN:ND2	1:S:1016:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:356:PHE:CE2	11:U:376:ASP:OD2	2.73	0.41
11:U:676:ALA:O	11:U:680:ASN:ND2	2.53	0.41
12:V:157:LEU:N	12:V:158:PRO:CD	2.83	0.41
12:V:684:TYR:O	12:V:815:ARG:NH1	2.53	0.41
1:A:818:PHE:CZ	1:A:861:SER:HB2	2.50	0.41
2:B:134:LEU:CD1	2:B:142:ILE:HG23	2.51	0.41
2:B:494:THR:OG1	2:B:496:SER:OG	2.34	0.41
6:G:97:GLN:HB2	6:G:118:LEU:HD21	2.03	0.41
6:H:60:LEU:HD21	2:O:232:ALA:HB1	2.01	0.41
8:P:133:PHE:HE1	8:P:135:LEU:HD12	1.85	0.41
8:P:472:LEU:O	8:P:476:VAL:HG23	2.19	0.41
8:Q:288:LEU:HD11	8:Q:358:VAL:HG23	2.03	0.41
1:S:1295:LEU:HD23	1:S:1300:ILE:HD12	2.02	0.41
11:U:391:ASP:HB3	12:V:394:GLN:HE22	1.86	0.41
11:U:757:ASN:ND2	11:U:770:ASP:OD2	2.53	0.41
12:V:1137:LEU:O	12:V:1140:VAL:HG12	2.20	0.41
2:B:83:SER:HB2	8:P:15:CYS:CB	2.50	0.41
3:C:361:ARG:HD2	3:C:538:ILE:HD12	2.02	0.41
4:E:109:LEU:HD12	4:E:114:LEU:HD21	2.02	0.41
4:E:319:CYS:SG	4:E:327:LEU:HD22	2.60	0.41
6:G:447:TYR:CE1	6:G:488:PRO:O	2.72	0.41
8:P:13:GLY:HA2	8:P:427:GLY:O	2.20	0.41
8:P:249:GLN:HG2	8:P:277:HIS:NE2	2.35	0.41
8:P:678:THR:OG1	8:P:679:PHE:N	2.54	0.41
11:U:986:VAL:O	11:U:990:THR:OG1	2.31	0.41
1:A:652:GLN:O	1:A:683:ARG:NH1	2.53	0.41
1:A:728:GLN:O	1:A:731:MET:HB2	2.20	0.41
2:B:418:ILE:HA	2:B:421:LYS:HB3	2.03	0.41
4:E:135:ALA:O	4:E:138:GLU:HB2	2.21	0.41
6:H:55:HIS:O	2:O:264:GLN:NE2	2.54	0.41
2:O:176:ILE:HD12	2:O:182:VAL:HG21	2.01	0.41
8:P:366:LEU:HD23	8:P:366:LEU:C	2.41	0.41
8:Q:177:SER:HB2	8:Q:274:ILE:HD13	2.02	0.41
1:S:955:HIS:HB3	1:S:1020:ARG:HE	1.86	0.41
12:V:452:SER:O	12:V:455:SER:OG	2.28	0.41
1:A:1174:TRP:HB3	1:A:1204:ARG:NH1	2.36	0.41
4:E:418:GLU:O	4:E:421:CYS:HB2	2.20	0.41
5:F:323:ASP:OD1	5:F:324:LYS:N	2.54	0.41
8:P:284:PHE:CD1	8:P:350:ALA:HB3	2.56	0.41
1:S:568:VAL:CG2	1:S:1069:LEU:HD11	2.50	0.41
1:S:570:GLU:OE1	1:S:574:PHE:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:772:GLN:HE22	9:W:95:TRP:HH2	1.65	0.41
1:S:989:MET:HG3	1:S:1055:ARG:HD3	2.02	0.41
1:S:1139:LEU:CD2	1:S:1181:LEU:HD22	2.50	0.41
12:V:139:LEU:HA	12:V:142:ILE:HD12	2.02	0.41
1:A:60:LEU:HG	6:H:263:GLN:HB3	2.03	0.41
1:A:1109:PHE:HA	1:A:1163:CYS:SG	2.60	0.41
1:A:1336:TYR:HB3	1:A:1395:LEU:HD23	2.02	0.41
2:B:40:THR:HG23	2:B:70:GLU:CD	2.41	0.41
2:B:583:SER:OG	2:B:584:LEU:N	2.54	0.41
2:B:723:ASN:ND2	2:B:725:THR:HG23	2.36	0.41
3:C:188:VAL:HB	3:C:189:PRO:HD3	2.03	0.41
3:C:200:VAL:HA	3:C:203:LEU:HD12	2.03	0.41
3:C:370:HIS:NE2	3:C:374:LEU:HD11	2.35	0.41
6:G:64:VAL:N	6:G:65:PRO:HD2	2.36	0.41
6:G:415:THR:HG21	1:S:21:ALA:HB1	2.03	0.41
6:G:479:CYS:O	6:G:482:LEU:N	2.53	0.41
7:L:307:CYS:HB3	7:L:310:CYS:SG	2.59	0.41
2:O:777:ILE:HD13	8:Q:830:LEU:HD13	2.03	0.41
8:P:131:CYS:SG	8:P:145:GLN:HB2	2.61	0.41
7:M:297:ILE:HG22	7:M:298:LEU:HD22	2.02	0.41
7:M:352:PHE:CD1	11:U:439:GLU:OE1	2.73	0.41
11:U:137:LEU:HD11	11:U:156:CYS:HB3	2.03	0.41
11:U:865:GLN:O	11:U:867:PRO:HD3	2.21	0.41
12:V:51:LEU:HA	12:V:54:ILE:HD12	2.02	0.41
1:A:240:GLN:HA	1:A:311:ILE:HD11	2.01	0.41
1:A:275:ILE:HG12	1:A:330:HIS:CE1	2.56	0.41
1:A:1075:LEU:CD1	1:A:1119:PHE:HD2	2.33	0.41
2:B:170:ILE:HG23	2:B:170:ILE:O	2.21	0.41
2:B:294:GLY:C	2:B:409:ARG:HH22	2.24	0.41
3:C:509:ILE:HD13	3:C:509:ILE:N	2.36	0.41
4:E:31:GLN:HB3	7:L:341:TRP:CH2	2.56	0.41
5:F:156:ASN:C	5:F:158:GLN:OE1	2.59	0.41
8:P:465:ILE:CG2	8:P:466:SER:N	2.82	0.41
8:P:801:HIS:O	8:P:805:VAL:HG23	2.21	0.41
1:S:419:PHE:CE2	1:S:463:HIS:ND1	2.89	0.41
1:S:1056:LEU:HD13	1:S:1115:GLU:HG3	2.02	0.41
1:S:1326:GLN:HA	1:S:1329:ARG:HH21	1.86	0.41
11:U:670:CYS:O	11:U:674:CYS:SG	2.76	0.41
11:U:1052:ASP:OD1	11:U:1071:HIS:HB2	2.21	0.41
12:V:199:LEU:HD23	12:V:199:LEU:C	2.41	0.41
1:A:517:ARG:O	1:A:521:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:PRO:O	1:A:717:MET:HG2	2.21	0.41
1:A:1103:ALA:O	1:A:1104:ARG:HB2	2.20	0.41
2:B:74:LEU:CD2	2:B:98:LYS:HD3	2.51	0.41
2:B:82:VAL:O	2:B:83:SER:OG	2.36	0.41
2:B:124:PHE:O	2:B:124:PHE:CD1	2.74	0.41
2:B:487:LEU:HB2	2:B:584:LEU:HD23	2.02	0.41
2:B:522:LYS:O	2:B:582:THR:OG1	2.28	0.41
2:B:530:LEU:HD12	2:B:649:PHE:CE1	2.56	0.41
2:B:725:THR:O	2:B:728:PHE:N	2.54	0.41
4:E:396:TYR:HB3	4:E:397:PRO:HD3	2.03	0.41
4:E:485:THR:OG1	4:E:520:THR:HG21	2.21	0.41
6:G:299:GLU:O	6:G:302:SER:OG	2.37	0.41
6:G:372:ALA:O	6:G:373:LEU:C	2.58	0.41
6:G:448:CYS:O	6:G:448:CYS:SG	2.79	0.41
6:G:483:LEU:HD21	6:G:512:LEU:HD23	2.03	0.41
6:H:67:LEU:O	6:H:68:PRO:C	2.58	0.41
6:H:266:LEU:O	6:H:270:VAL:HG23	2.20	0.41
7:L:107:PRO:N	7:L:108:PRO:CD	2.84	0.41
7:L:113:SER:O	7:L:116:GLU:HB3	2.20	0.41
7:L:169:PHE:CZ	7:L:193:ALA:CB	3.04	0.41
7:L:256:ALA:HB1	7:L:258:HIS:CE1	2.56	0.41
7:L:313:TYR:CZ	7:L:319:ILE:HG23	2.52	0.41
2:O:170:ILE:O	2:O:170:ILE:CG2	2.69	0.41
2:O:524:GLN:HE21	2:O:524:GLN:HB3	1.48	0.41
8:P:51:GLY:O	8:P:53:LEU:N	2.54	0.41
8:P:143:LEU:C	8:P:143:LEU:HD23	2.41	0.41
8:P:471:PHE:C	8:P:471:PHE:HD1	2.24	0.41
8:P:486:LEU:O	8:P:489:ALA:HB3	2.21	0.41
8:P:593:ASP:O	8:P:594:LEU:HD23	2.20	0.41
8:P:709:LYS:HB2	8:P:879:ILE:HG22	2.03	0.41
8:P:717:ALA:HB3	8:P:815:GLN:NE2	2.36	0.41
8:Q:337:GLU:OE2	8:Q:339:ARG:NH1	2.54	0.41
1:S:346:TRP:CZ2	1:S:387:GLN:HG2	2.55	0.41
1:S:874:ARG:O	1:S:875:LEU:HD23	2.21	0.41
7:M:55:CYS:HB3	7:M:59:LEU:HB3	2.02	0.41
11:U:286:GLY:O	11:U:290:VAL:HG23	2.21	0.41
11:U:867:PRO:O	11:U:923:TYR:OH	2.33	0.41
12:V:305:LEU:HD22	12:V:307:LEU:HD21	2.03	0.41
12:V:611:THR:HG23	12:V:651:TRP:CH2	2.56	0.41
12:V:1276:SER:O	12:V:1280:ASN:ND2	2.53	0.41
1:A:281:LEU:HA	1:A:286:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:HA	2:B:280:PRO:HD3	1.87	0.41
2:B:338:THR:O	2:B:340:GLN:NE2	2.53	0.41
2:B:773:LEU:CA	2:B:838:ILE:HG21	2.50	0.41
2:B:818:ARG:NH1	2:B:821:LYS:HD3	2.36	0.41
3:C:200:VAL:O	3:C:201:GLU:C	2.58	0.41
4:E:374:SER:O	4:E:376:THR:HG23	2.21	0.41
6:G:360:ALA:HB1	6:G:406:GLN:HB2	2.02	0.41
6:H:191:LEU:HD12	6:H:192:ASP:N	2.36	0.41
2:O:61:SER:OG	2:O:62:THR:N	2.53	0.41
2:O:391:VAL:HB	2:O:392:PRO:HD3	2.03	0.41
2:O:478:ILE:HD11	2:O:620:VAL:HG13	2.02	0.41
8:P:341:TYR:C	8:P:342:CYS:SG	2.98	0.41
8:P:504:ARG:O	8:P:532:SER:OG	2.32	0.41
8:P:679:PHE:O	8:P:682:THR:OG1	2.38	0.41
8:Q:510:THR:HG21	8:Q:598:VAL:CG2	2.50	0.41
8:Q:733:LEU:HD13	8:Q:751:LEU:O	2.21	0.41
1:S:1033:ASP:CG	1:S:1093:SER:HB2	2.42	0.41
7:M:32:GLN:O	7:M:34:ARG:HG3	2.21	0.41
7:M:295:ARG:C	7:M:297:ILE:H	2.25	0.41
11:U:281:LEU:O	12:V:523:ASN:ND2	2.54	0.41
11:U:924:GLN:N	11:U:925:PRO:CD	2.84	0.41
12:V:364:TRP:CH2	12:V:384:MET:HE2	2.55	0.41
1:A:486:PRO:HG2	1:A:489:LEU:HD12	2.03	0.40
1:A:770:ARG:HD3	1:A:821:LEU:HA	2.03	0.40
2:B:332:ASP:OD1	2:B:335:GLY:N	2.53	0.40
6:H:37:LEU:O	6:H:41:GLN:HG3	2.21	0.40
6:H:310:LEU:HD11	6:H:340:CYS:SG	2.60	0.40
7:L:313:TYR:CE1	7:L:319:ILE:CG2	2.92	0.40
2:O:130:MET:CE	2:O:134:LEU:HD22	2.51	0.40
8:P:43:LEU:HB3	8:P:45:TYR:CE1	2.56	0.40
8:Q:451:ALA:O	8:Q:455:ILE:HG12	2.21	0.40
1:S:349:ALA:HB2	1:S:682:GLU:HG3	2.03	0.40
10:X:58:PRO:HD3	10:X:67:GLN:NE2	2.36	0.40
11:U:651:ILE:HD13	11:U:738:LYS:CG	2.51	0.40
11:U:668:LEU:HB3	11:U:752:VAL:HG11	2.02	0.40
11:U:843:VAL:O	11:U:846:ALA:N	2.54	0.40
12:V:72:GLN:NE2	12:V:132:SER:OG	2.55	0.40
12:V:816:LEU:HD11	12:V:935:ILE:HD13	2.02	0.40
1:A:1224:TRP:CH2	1:A:1225:LEU:HD13	2.56	0.40
4:E:408:GLN:HE21	4:E:444:LEU:HD13	1.86	0.40
6:G:279:TRP:C	6:G:282:PRO:HD2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:303:PHE:O	7:L:305:MET:N	2.54	0.40
2:O:592:LYS:CG	2:O:593:PHE:N	2.84	0.40
2:O:843:ALA:HB3	8:Q:809:GLN:HE21	1.86	0.40
8:P:311:CYS:SG	8:P:324:ILE:O	2.77	0.40
1:S:933:LEU:HD21	1:S:984:LEU:HD12	2.03	0.40
1:S:1092:GLY:HA2	1:S:1104:ARG:HH21	1.86	0.40
7:M:56:SER:HG	7:M:59:LEU:H	1.70	0.40
11:U:308:PHE:O	11:U:311:ALA:HB3	2.21	0.40
11:U:970:LEU:O	11:U:1019:ARG:NH2	2.54	0.40
12:V:252:LEU:HD23	12:V:252:LEU:HA	1.99	0.40
2:B:362:LEU:O	8:P:468:ARG:NH2	2.54	0.40
4:E:280:LEU:O	4:E:285:GLN:NE2	2.54	0.40
6:G:39:ARG:NH2	6:G:319:PRO:O	2.54	0.40
6:G:414:LEU:HD21	6:G:459:GLN:O	2.21	0.40
2:O:426:LEU:HG	8:Q:490:MET:CE	2.50	0.40
8:P:429:LEU:HD23	8:P:429:LEU:C	2.42	0.40
8:P:505:PRO:HA	8:P:533:SER:HB3	2.03	0.40
8:P:640:LEU:HA	8:P:641:PRO:HD3	1.81	0.40
10:X:24:CYS:SG	10:X:34:LEU:HB3	2.62	0.40
11:U:504:GLN:HE22	11:U:543:LEU:HD23	1.86	0.40
11:U:1206:THR:O	11:U:1209:CYS:HB2	2.21	0.40
1:A:733:ALA:HB1	1:A:742:GLN:CD	2.42	0.40
1:A:822:LEU:HD12	1:A:867:LYS:CE	2.52	0.40
4:E:424:VAL:HG12	4:E:437:MET:CE	2.52	0.40
5:F:116:PHE:CD1	5:F:130:GLN:HG3	2.57	0.40
7:L:98:ARG:HD2	7:L:101:LEU:HD11	2.03	0.40
8:P:48:ASP:HB3	8:P:53:LEU:HD23	2.03	0.40
8:P:86:TYR:CD1	8:P:86:TYR:N	2.89	0.40
8:Q:508:CYS:SG	8:Q:600:CYS:SG	3.17	0.40
1:S:765:LEU:HD21	1:S:787:LEU:CD2	2.51	0.40
10:X:57:ILE:HG23	10:X:61:TYR:CG	2.57	0.40
11:U:385:LEU:HA	11:U:388:ILE:HD12	2.03	0.40
11:U:434:GLU:HG3	11:U:437:ARG:NH2	2.37	0.40
11:U:1259:GLN:HE21	12:V:1358:PRO:HG2	1.86	0.40
12:V:347:PHE:HA	12:V:350:ILE:HD12	2.03	0.40
12:V:479:THR:O	12:V:483:SER:CB	2.68	0.40
1:A:1027:ASP:OD2	1:S:1184:ARG:NH2	2.43	0.40
1:A:1174:TRP:N	1:A:1175:PRO:CD	2.85	0.40
1:A:1213:PRO:O	1:A:1215:ALA:N	2.54	0.40
1:A:1315:LEU:O	1:A:1319:LEU:HD12	2.22	0.40
1:A:1361:TYR:CD1	1:A:1361:TYR:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:332:GLN:HA	4:E:334:PRO:HD2	2.03	0.40
6:G:84:LEU:O	6:G:86:GLN:HG2	2.22	0.40
2:O:520:LEU:HD22	8:P:518:GLN:O	2.22	0.40
8:P:11:LEU:HD13	8:P:429:LEU:HD22	2.02	0.40
8:P:193:PHE:HD1	8:P:193:PHE:HA	1.76	0.40
8:P:424:SER:CB	8:P:428:ARG:HB2	2.51	0.40
8:P:528:VAL:HA	8:P:579:GLU:HA	2.03	0.40
7:M:8:LEU:HD21	7:M:25:TYR:CE2	2.48	0.40
11:U:90:ILE:HD13	11:U:93:LEU:HD12	2.02	0.40
12:V:261:LYS:O	12:V:265:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1160/1477 (78%)	1060 (91%)	92 (8%)	8 (1%)	22 62
1	S	1224/1477 (83%)	1101 (90%)	110 (9%)	13 (1%)	14 52
2	B	685/884 (78%)	572 (84%)	100 (15%)	13 (2%)	8 41
2	O	685/884 (78%)	587 (86%)	81 (12%)	17 (2%)	5 35
3	C	546/583 (94%)	472 (86%)	66 (12%)	8 (2%)	10 46
4	E	411/555 (74%)	366 (89%)	45 (11%)	0	100 100
5	F	336/399 (84%)	295 (88%)	40 (12%)	1 (0%)	41 76
6	G	567/641 (88%)	497 (88%)	65 (12%)	5 (1%)	17 56
6	H	532/641 (83%)	473 (89%)	55 (10%)	4 (1%)	19 60
7	L	368/394 (93%)	328 (89%)	37 (10%)	3 (1%)	19 60
7	M	368/394 (93%)	328 (89%)	33 (9%)	7 (2%)	8 41
8	P	726/906 (80%)	608 (84%)	90 (12%)	28 (4%)	3 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	Q	732/906 (81%)	624 (85%)	94 (13%)	14 (2%)	8 41
9	W	21/39 (54%)	12 (57%)	3 (14%)	6 (29%)	0 0
10	X	151/197 (77%)	140 (93%)	10 (7%)	1 (1%)	22 62
11	U	1180/1328 (89%)	1051 (89%)	116 (10%)	13 (1%)	14 52
12	V	1131/1451 (78%)	1042 (92%)	80 (7%)	9 (1%)	19 60
All	All	10823/13156 (82%)	9556 (88%)	1117 (10%)	150 (1%)	15 47

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLU
1	A	737	ALA
2	B	132	ASP
2	B	133	GLY
2	B	138	ASN
2	B	147	VAL
3	C	4	ASP
3	C	84	ASP
6	H	192	ASP
6	H	241	PRO
6	H	242	ARG
2	O	70	GLU
2	O	83	SER
2	O	147	VAL
2	O	249	LYS
2	O	354	LEU
8	P	857	ALA
8	Q	50	GLU
8	Q	539	GLN
8	Q	557	ASP
8	Q	649	MET
1	S	288	GLU
1	S	972	GLY
1	S	975	GLY
9	W	80	VAL
11	U	451	ARG
11	U	548	LYS
11	U	598	GLN
1	A	972	GLY
1	A	1214	GLU

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Mol	Chain	Res	Type
2	B	196	CYS
6	G	192	ASP
2	O	251	GLN
2	O	314	GLU
2	O	324	LYS
2	O	631	LYS
2	O	636	PHE
2	O	637	PRO
8	P	137	ASP
8	P	383	PRO
8	P	518	GLN
8	P	595	PRO
8	P	781	PRO
8	Q	63	GLN
8	Q	397	ALA
8	Q	643	SER
1	S	592	VAL
1	S	689	GLY
1	S	947	SER
1	S	1003	ASN
9	W	86	SER
7	M	176	SER
7	M	296	ALA
11	U	374	SER
11	U	456	ILE
11	U	724	ASP
1	A	26	LEU
1	A	670	ARG
2	B	140	PRO
2	B	314	GLU
2	B	316	PHE
2	B	325	LEU
2	B	637	PRO
3	C	2	ALA
3	C	128	ASP
3	C	173	ARG
7	L	304	THR
2	O	138	ASN
8	P	62	ASP
8	P	63	GLN
8	P	148	ALA
8	P	426	LYS

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Mol	Chain	Res	Type
8	P	550	SER
8	P	557	ASP
8	P	642	LEU
8	P	782	ILE
8	Q	518	GLN
9	W	85	PHE
7	M	103	ALA
7	M	351	SER
11	U	1042	PRO
12	V	412	ILE
12	V	1348	HIS
1	A	484	GLU
6	G	445	LEU
7	L	227	ARG
2	O	223	LEU
2	O	325	LEU
2	O	495	SER
8	P	15	CYS
8	P	161	GLY
8	P	332	GLY
8	P	354	GLY
8	P	385	GLU
8	P	387	PRO
8	P	549	THR
8	P	875	HIS
8	Q	607	ARG
8	Q	757	VAL
1	S	1104	ARG
7	M	22	LYS
11	U	361	SER
11	U	975	GLU
12	V	166	ASN
2	B	82	VAL
2	B	273	PRO
6	G	343	GLN
6	H	61	PRO
2	O	140	PRO
2	O	711	THR
8	P	66	HIS
8	P	166	PRO
8	P	372	SER
8	P	822	ALA

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Mol	Chain	Res	Type
1	S	338	ASP
1	S	1023	GLU
10	X	62	PRO
11	U	449	VAL
11	U	1019	ARG
12	V	296	GLU
12	V	411	CYS
12	V	466	ASP
12	V	753	ASP
12	V	1167	TRP
12	V	1349	GLN
1	A	314	ASP
2	B	711	THR
3	C	23	ASP
3	C	169	PHE
3	C	382	GLN
6	G	261	ASN
8	P	641	PRO
8	Q	92	HIS
8	Q	148	ALA
8	Q	758	ALA
1	S	564	ILE
1	S	1002	GLU
9	W	82	PRO
7	M	215	GLU
11	U	341	LEU
11	U	729	PHE
5	F	23	VAL
8	Q	727	PRO
1	S	1331	LEU
8	P	6	PRO
7	M	216	PRO
9	W	74	PRO
9	W	92	PRO
6	G	242	ARG
7	L	106	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1034/1282 (81%)	937 (91%)	97 (9%)	8 30
1	S	1092/1282 (85%)	1011 (93%)	81 (7%)	13 40
2	B	644/810 (80%)	556 (86%)	88 (14%)	3 20
2	O	641/810 (79%)	580 (90%)	61 (10%)	8 30
3	C	480/507 (95%)	456 (95%)	24 (5%)	24 51
4	E	358/467 (77%)	311 (87%)	47 (13%)	4 21
5	F	288/336 (86%)	271 (94%)	17 (6%)	19 47
6	G	483/538 (90%)	429 (89%)	54 (11%)	6 25
6	H	454/538 (84%)	401 (88%)	53 (12%)	5 23
7	L	334/354 (94%)	316 (95%)	18 (5%)	22 50
7	M	334/354 (94%)	317 (95%)	17 (5%)	24 51
8	P	627/749 (84%)	553 (88%)	74 (12%)	5 23
8	Q	630/749 (84%)	577 (92%)	53 (8%)	11 37
9	W	22/22 (100%)	21 (96%)	1 (4%)	27 54
10	X	136/175 (78%)	129 (95%)	7 (5%)	24 51
11	U	1092/1204 (91%)	1052 (96%)	40 (4%)	34 59
12	V	1067/1324 (81%)	1029 (96%)	38 (4%)	35 60
All	All	9716/11501 (84%)	8946 (92%)	770 (8%)	16 39

All (770) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	98	LEU
1	A	137	LEU
1	A	139	VAL
1	A	147	SER
1	A	150	GLU
1	A	176	SER
1	A	182	VAL
1	A	191	VAL
1	A	193	LEU
1	A	217	LEU
1	A	244	LEU

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Mol	Chain	Res	Type
1	A	267	VAL
1	A	268	ASP
1	A	274	LEU
1	A	289	SER
1	A	313	THR
1	A	342	MET
1	A	354	LEU
1	A	369	GLU
1	A	371	LEU
1	A	383	GLU
1	A	390	LEU
1	A	399	CYS
1	A	402	GLU
1	A	405	GLN
1	A	434	VAL
1	A	446	LEU
1	A	456	PHE
1	A	462	TYR
1	A	465	CYS
1	A	468	LYS
1	A	479	GLU
1	A	487	ARG
1	A	491	VAL
1	A	494	LEU
1	A	507	LEU
1	A	653	LEU
1	A	660	LEU
1	A	664	MET
1	A	665	THR
1	A	671	ASP
1	A	723	LEU
1	A	741	ARG
1	A	767	GLN
1	A	775	SER
1	A	793	GLU
1	A	817	LEU
1	A	821	LEU
1	A	822	LEU
1	A	826	THR
1	A	834	LEU
1	A	852	SER
1	A	860	LEU

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Mol	Chain	Res	Type
1	A	861	SER
1	A	877	SER
1	A	900	SER
1	A	904	GLN
1	A	905	ARG
1	A	928	THR
1	A	930	GLN
1	A	948	ASP
1	A	949	THR
1	A	953	ASP
1	A	961	GLU
1	A	964	LEU
1	A	968	SER
1	A	992	HIS
1	A	1014	ASN
1	A	1030	LEU
1	A	1032	GLN
1	A	1060	THR
1	A	1069	LEU
1	A	1073	ARG
1	A	1076	LEU
1	A	1080	ARG
1	A	1098	GLU
1	A	1126	LEU
1	A	1130	ILE
1	A	1163	CYS
1	A	1187	ARG
1	A	1188	HIS
1	A	1190	GLN
1	A	1191	SER
1	A	1208	SER
1	A	1231	HIS
1	A	1241	ASN
1	A	1253	ARG
1	A	1301	SER
1	A	1310	GLU
1	A	1320	LEU
1	A	1329	ARG
1	A	1345	ASP
1	A	1367	LEU
1	A	1391	ASN
1	A	1395	LEU

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Mol	Chain	Res	Type
1	A	1413	LYS
2	B	9	SER
2	B	13	GLU
2	B	17	CYS
2	B	28	SER
2	B	40	THR
2	B	47	ARG
2	B	60	LYS
2	B	64	PHE
2	B	65	PHE
2	B	66	THR
2	B	68	LYS
2	B	70	GLU
2	B	78	CYS
2	B	90	ASN
2	B	102	ASN
2	B	112	LEU
2	B	135	ARG
2	B	143	LEU
2	B	155	SER
2	B	187	LYS
2	B	197	THR
2	B	225	ASP
2	B	226	ILE
2	B	246	GLU
2	B	252	LEU
2	B	256	LEU
2	B	281	PHE
2	B	285	CYS
2	B	288	GLN
2	B	326	SER
2	B	329	LEU
2	B	331	ASP
2	B	341	VAL
2	B	347	ASP
2	B	349	LEU
2	B	353	CYS
2	B	354	LEU
2	B	364	LYS
2	B	398	LEU
2	B	401	CYS
2	B	406	ARG

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Mol	Chain	Res	Type
2	B	412	LEU
2	B	417	LYS
2	B	420	SER
2	B	422	SER
2	B	471	SER
2	B	483	ILE
2	B	492	LYS
2	B	498	LYS
2	B	504	VAL
2	B	505	THR
2	B	506	LEU
2	B	507	SER
2	B	510	MET
2	B	517	ARG
2	B	519	ARG
2	B	523	CYS
2	B	526	ARG
2	B	535	PHE
2	B	572	LYS
2	B	573	GLU
2	B	577	ILE
2	B	594	CYS
2	B	602	MET
2	B	604	ARG
2	B	605	GLU
2	B	609	CYS
2	B	619	ARG
2	B	622	LEU
2	B	631	LYS
2	B	638	LYS
2	B	639	LYS
2	B	640	LYS
2	B	671	SER
2	B	677	LEU
2	B	678	GLU
2	B	706	THR
2	B	716	ILE
2	B	722	ARG
2	B	734	LEU
2	B	742	CYS
2	B	748	LYS
2	B	752	GLU

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Mol	Chain	Res	Type
2	B	763	LEU
2	B	813	ARG
2	B	838	ILE
2	B	847	LEU
2	B	857	SER
3	C	10	CYS
3	C	17	GLN
3	C	115	GLN
3	C	123	SER
3	C	126	ARG
3	C	146	TYR
3	C	150	LEU
3	C	155	LEU
3	C	156	SER
3	C	162	ARG
3	C	182	SER
3	C	194	THR
3	C	195	ASP
3	C	205	ILE
3	C	224	ASN
3	C	241	CYS
3	C	245	ARG
3	C	266	ARG
3	C	270	ARG
3	C	306	ASP
3	C	350	MET
3	C	396	LEU
3	C	488	ARG
3	C	509	ILE
4	E	12	GLU
4	E	23	GLU
4	E	30	LEU
4	E	41	ARG
4	E	44	LEU
4	E	83	LEU
4	E	86	LEU
4	E	87	LEU
4	E	91	PRO
4	E	94	CYS
4	E	98	LEU
4	E	100	SER
4	E	112	SER

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Mol	Chain	Res	Type
4	E	123	GLN
4	E	125	LEU
4	E	141	ARG
4	E	155	PRO
4	E	157	SER
4	E	160	CYS
4	E	161	GLN
4	E	276	GLU
4	E	287	GLN
4	E	318	GLU
4	E	319	CYS
4	E	332	GLN
4	E	338	ASP
4	E	346	THR
4	E	356	SER
4	E	357	LEU
4	E	378	SER
4	E	404	ASP
4	E	427	GLU
4	E	429	LEU
4	E	432	ASP
4	E	443	GLU
4	E	447	LYS
4	E	453	VAL
4	E	463	GLU
4	E	474	GLU
4	E	484	THR
4	E	486	SER
4	E	487	MET
4	E	499	LYS
4	E	505	THR
4	E	519	ASN
4	E	523	LEU
4	E	527	LEU
5	F	12	SER
5	F	15	LEU
5	F	60	ARG
5	F	68	GLN
5	F	90	ASP
5	F	125	ASP
5	F	129	LEU
5	F	138	ARG

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Mol	Chain	Res	Type
5	F	173	ARG
5	F	191	SER
5	F	196	LEU
5	F	214	LEU
5	F	270	LEU
5	F	288	ASP
5	F	315	CYS
5	F	345	SER
5	F	349	ASP
6	G	13	LEU
6	G	48	GLU
6	G	57	LEU
6	G	80	LEU
6	G	104	LEU
6	G	118	LEU
6	G	136	LEU
6	G	149	LEU
6	G	156	LEU
6	G	166	LEU
6	G	169	SER
6	G	170	GLN
6	G	179	LEU
6	G	207	LEU
6	G	226	ASP
6	G	231	SER
6	G	234	GLU
6	G	250	THR
6	G	259	MET
6	G	277	SER
6	G	301	GLU
6	G	326	GLU
6	G	327	LEU
6	G	343	GLN
6	G	352	SER
6	G	357	THR
6	G	359	ARG
6	G	362	ASP
6	G	376	ASP
6	G	378	SER
6	G	388	PRO
6	G	393	MET
6	G	396	VAL

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Mol	Chain	Res	Type
6	G	405	ILE
6	G	416	LEU
6	G	437	ASP
6	G	444	GLU
6	G	448	CYS
6	G	450	LEU
6	G	482	LEU
6	G	497	PHE
6	G	498	ASN
6	G	501	GLN
6	G	505	SER
6	G	524	TRP
6	G	531	THR
6	G	565	ASP
6	G	573	ARG
6	G	586	LEU
6	G	588	SER
6	G	596	TYR
6	G	598	SER
6	G	603	SER
6	G	608	PHE
6	H	12	CYS
6	H	13	LEU
6	H	15	LEU
6	H	35	LEU
6	H	37	LEU
6	H	42	LEU
6	H	48	GLU
6	H	54	LEU
6	H	56	SER
6	H	89	THR
6	H	91	ASP
6	H	98	ARG
6	H	104	LEU
6	H	131	LEU
6	H	132	LEU
6	H	134	GLU
6	H	135	LEU
6	H	136	LEU
6	H	145	LEU
6	H	156	LEU
6	H	158	ASP

Continued on next page...

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Mol	Chain	Res	Type
6	H	179	LEU
6	H	183	THR
6	H	191	LEU
6	H	230	SER
6	H	241	PRO
6	H	277	SER
6	H	327	LEU
6	H	333	ASP
6	H	346	THR
6	H	350	LEU
6	H	359	ARG
6	H	362	ASP
6	H	365	GLU
6	H	378	SER
6	H	393	MET
6	H	395	GLU
6	H	404	LEU
6	H	416	LEU
6	H	423	ARG
6	H	469	GLN
6	H	470	LYS
6	H	478	ARG
6	H	479	CYS
6	H	483	LEU
6	H	505	SER
6	H	530	ASP
6	H	550	THR
6	H	564	ARG
6	H	568	THR
6	H	586	LEU
6	H	605	ARG
6	H	606	ASP
7	L	25	TYR
7	L	35	ASP
7	L	39	ARG
7	L	56	SER
7	L	60	ARG
7	L	64	SER
7	L	74	MET
7	L	153	LYS
7	L	155	LYS
7	L	167	VAL

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Mol	Chain	Res	Type
7	L	250	GLU
7	L	251	CYS
7	L	257	ASP
7	L	267	LEU
7	L	268	SER
7	L	291	ASP
7	L	345	LEU
7	L	350	GLN
2	O	39	LYS
2	O	40	THR
2	O	46	ARG
2	O	47	ARG
2	O	68	LYS
2	O	90	ASN
2	O	104	VAL
2	O	125	LYS
2	O	145	ARG
2	O	175	GLU
2	O	181	MET
2	O	213	CYS
2	O	237	VAL
2	O	246	GLU
2	O	252	LEU
2	O	253	ARG
2	O	256	LEU
2	O	257	ILE
2	O	267	SER
2	O	279	LEU
2	O	283	ASP
2	O	287	VAL
2	O	291	ASP
2	O	305	SER
2	O	326	SER
2	O	336	SER
2	O	346	LYS
2	O	390	VAL
2	O	424	LYS
2	O	475	VAL
2	O	478	ILE
2	O	486	SER
2	O	498	LYS
2	O	505	THR

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Mol	Chain	Res	Type
2	O	507	SER
2	O	512	GLN
2	O	515	ASP
2	O	518	PHE
2	O	522	LYS
2	O	523	CYS
2	O	524	GLN
2	O	573	GLU
2	O	574	CYS
2	O	595	CYS
2	O	602	MET
2	O	624	LEU
2	O	626	ASP
2	O	628	SER
2	O	640	LYS
2	O	659	CYS
2	O	677	LEU
2	O	699	SER
2	O	716	ILE
2	O	722	ARG
2	O	724	GLN
2	O	735	ILE
2	O	742	CYS
2	O	775	SER
2	O	780	HIS
2	O	782	SER
2	O	847	LEU
8	P	18	LEU
8	P	35	VAL
8	P	42	GLU
8	P	45	TYR
8	P	53	LEU
8	P	69	LEU
8	P	70	LEU
8	P	74	ARG
8	P	89	SER
8	P	125	LEU
8	P	130	LEU
8	P	131	CYS
8	P	135	LEU
8	P	137	ASP
8	P	144	VAL

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Mol	Chain	Res	Type
8	P	173	VAL
8	P	177	SER
8	P	198	CYS
8	P	201	SER
8	P	215	SER
8	P	228	LEU
8	P	232	ASP
8	P	235	LEU
8	P	237	GLN
8	P	238	SER
8	P	246	PRO
8	P	247	ASP
8	P	251	CYS
8	P	253	VAL
8	P	261	SER
8	P	279	GLU
8	P	311	CYS
8	P	321	MET
8	P	360	HIS
8	P	364	SER
8	P	387	PRO
8	P	390	LEU
8	P	424	SER
8	P	465	ILE
8	P	468	ARG
8	P	471	PHE
8	P	481	LYS
8	P	494	CYS
8	P	522	VAL
8	P	527	CYS
8	P	539	GLN
8	P	543	LEU
8	P	555	ASP
8	P	560	CYS
8	P	578	ARG
8	P	595	PRO
8	P	599	SER
8	P	600	CYS
8	P	638	VAL
8	P	644	ARG
8	P	646	THR
8	P	648	ASP

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Mol	Chain	Res	Type
8	P	683	CYS
8	P	701	LEU
8	P	707	SER
8	P	744	ASP
8	P	745	VAL
8	P	766	LEU
8	P	768	VAL
8	P	769	ARG
8	P	777	CYS
8	P	789	VAL
8	P	804	VAL
8	P	809	GLN
8	P	836	ASN
8	P	842	ARG
8	P	854	GLU
8	P	856	GLU
8	P	864	GLN
8	Q	69	LEU
8	Q	144	VAL
8	Q	219	THR
8	Q	253	VAL
8	Q	274	ILE
8	Q	307	VAL
8	Q	329	ASP
8	Q	333	LYS
8	Q	334	LEU
8	Q	342	CYS
8	Q	352	CYS
8	Q	361	SER
8	Q	362	THR
8	Q	370	ASP
8	Q	372	SER
8	Q	403	SER
8	Q	406	SER
8	Q	480	ASN
8	Q	483	LEU
8	Q	510	THR
8	Q	522	VAL
8	Q	529	LEU
8	Q	543	LEU
8	Q	561	SER
8	Q	566	THR

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Mol	Chain	Res	Type
8	Q	567	ILE
8	Q	570	ASP
8	Q	578	ARG
8	Q	582	LEU
8	Q	584	LEU
8	Q	598	VAL
8	Q	642	LEU
8	Q	644	ARG
8	Q	646	THR
8	Q	683	CYS
8	Q	684	ARG
8	Q	685	GLU
8	Q	701	LEU
8	Q	745	VAL
8	Q	749	ARG
8	Q	751	LEU
8	Q	752	SER
8	Q	768	VAL
8	Q	769	ARG
8	Q	775	ASP
8	Q	789	VAL
8	Q	804	VAL
8	Q	807	ARG
8	Q	810	THR
8	Q	812	VAL
8	Q	842	ARG
8	Q	852	CYS
8	Q	872	GLN
1	S	56	ASP
1	S	60	LEU
1	S	98	LEU
1	S	109	VAL
1	S	174	GLN
1	S	175	SER
1	S	179	LEU
1	S	182	VAL
1	S	191	VAL
1	S	239	VAL
1	S	267	VAL
1	S	274	LEU
1	S	312	SER
1	S	313	THR

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Mol	Chain	Res	Type
1	S	333	VAL
1	S	334	LEU
1	S	337	SER
1	S	405	GLN
1	S	407	LEU
1	S	491	VAL
1	S	508	THR
1	S	517	ARG
1	S	648	GLU
1	S	653	LEU
1	S	665	THR
1	S	671	ASP
1	S	685	ARG
1	S	713	PRO
1	S	714	ARG
1	S	723	LEU
1	S	725	SER
1	S	766	CYS
1	S	775	SER
1	S	777	SER
1	S	795	ARG
1	S	800	GLU
1	S	818	PHE
1	S	821	LEU
1	S	847	LYS
1	S	850	SER
1	S	853	ARG
1	S	855	THR
1	S	856	LEU
1	S	859	CYS
1	S	911	TRP
1	S	912	THR
1	S	924	ASP
1	S	930	GLN
1	S	942	GLU
1	S	948	ASP
1	S	949	THR
1	S	966	GLU
1	S	973	CYS
1	S	984	LEU
1	S	988	LEU
1	S	1012	THR

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Mol	Chain	Res	Type
1	S	1016	ASP
1	S	1030	LEU
1	S	1031	GLN
1	S	1060	THR
1	S	1070	GLN
1	S	1098	GLU
1	S	1139	LEU
1	S	1183	CYS
1	S	1190	GLN
1	S	1202	GLU
1	S	1223	ASP
1	S	1241	ASN
1	S	1251	CYS
1	S	1253	ARG
1	S	1265	LEU
1	S	1280	ASP
1	S	1308	LEU
1	S	1310	GLU
1	S	1326	GLN
1	S	1339	LEU
1	S	1345	ASP
1	S	1367	LEU
1	S	1393	VAL
1	S	1395	LEU
1	S	1428	CYS
9	W	90	PHE
7	M	10	ARG
7	M	25	TYR
7	M	26	GLU
7	M	39	ARG
7	M	40	ILE
7	M	56	SER
7	M	82	SER
7	M	85	MET
7	M	131	THR
7	M	167	VAL
7	M	182	SER
7	M	213	VAL
7	M	217	GLU
7	M	286	ASP
7	M	291	ASP
7	M	303	PHE

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Mol	Chain	Res	Type
7	M	351	SER
10	X	9	ARG
10	X	32	ASP
10	X	64	GLU
10	X	86	CYS
10	X	122	ASP
10	X	146	TRP
10	X	153	GLN
11	U	56	CYS
11	U	265	ARG
11	U	275	ILE
11	U	284	GLU
11	U	333	SER
11	U	337	SER
11	U	375	TRP
11	U	384	GLU
11	U	413	MET
11	U	419	CYS
11	U	453	SER
11	U	466	ILE
11	U	490	PHE
11	U	505	PRO
11	U	513	MET
11	U	528	ASN
11	U	529	GLN
11	U	531	ASP
11	U	603	LEU
11	U	777	CYS
11	U	779	LYS
11	U	783	ASP
11	U	799	LYS
11	U	812	SER
11	U	835	SER
11	U	836	ASN
11	U	837	GLU
11	U	872	GLN
11	U	884	ARG
11	U	1012	LYS
11	U	1082	PRO
11	U	1141	LEU
11	U	1171	THR
11	U	1214	SER

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Mol	Chain	Res	Type
11	U	1240	MET
11	U	1259	GLN
11	U	1261	GLU
11	U	1276	MET
11	U	1284	SER
11	U	1285	ARG
12	V	45	ASP
12	V	89	TYR
12	V	153	LEU
12	V	155	GLU
12	V	191	ASP
12	V	210	ASP
12	V	223	GLN
12	V	226	ASP
12	V	233	ASP
12	V	277	ASP
12	V	306	ASP
12	V	309	HIS
12	V	310	CYS
12	V	356	TYR
12	V	369	GLU
12	V	376	GLU
12	V	431	MET
12	V	432	CYS
12	V	472	GLU
12	V	485	ASN
12	V	486	GLU
12	V	493	LEU
12	V	496	LEU
12	V	519	ASP
12	V	525	SER
12	V	604	ASP
12	V	657	CYS
12	V	770	LYS
12	V	771	LEU
12	V	781	PHE
12	V	835	ASP
12	V	1023	MET
12	V	1026	HIS
12	V	1070	HIS
12	V	1079	SER
12	V	1331	PHE

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Mol	Chain	Res	Type
12	V	1385	TRP
12	V	1393	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	168	GLN
1	A	188	GLN
1	A	220	GLN
1	A	227	HIS
1	A	264	GLN
1	A	286	GLN
1	A	330	HIS
1	A	376	GLN
1	A	417	GLN
1	A	436	GLN
1	A	676	GLN
1	A	993	GLN
1	A	1188	HIS
1	A	1327	HIS
1	A	1355	HIS
1	A	1417	HIS
2	B	90	ASN
2	B	116	ASN
2	B	171	GLN
2	B	241	HIS
2	B	270	ASN
2	B	306	ASN
2	B	366	ASN
2	B	600	GLN
2	B	670	ASN
2	B	746	ASN
2	B	817	GLN
2	B	825	GLN
2	B	854	GLN
3	C	3	GLN
3	C	13	GLN
3	C	42	GLN
3	C	152	ASN
3	C	207	HIS
3	C	216	GLN

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Mol	Chain	Res	Type
3	C	224	ASN
3	C	410	GLN
3	C	441	GLN
3	C	493	ASN
3	C	557	GLN
4	E	161	GLN
4	E	314	GLN
4	E	359	ASN
4	E	408	GLN
4	E	503	ASN
4	E	508	GLN
5	F	36	GLN
5	F	68	GLN
5	F	100	ASN
5	F	144	HIS
5	F	154	ASN
5	F	286	HIS
5	F	308	HIS
5	F	309	ASN
6	G	31	GLN
6	G	58	GLN
6	G	86	GLN
6	G	215	GLN
6	G	320	GLN
6	G	406	GLN
6	G	498	ASN
6	G	501	GLN
6	G	511	GLN
6	G	547	ASN
6	H	31	GLN
6	H	44	GLN
6	H	58	GLN
6	H	76	ASN
6	H	167	ASN
6	H	311	ASN
6	H	320	GLN
6	H	343	GLN
6	H	461	GLN
6	H	465	GLN
6	H	547	ASN
7	L	109	GLN
7	L	180	GLN

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Mol	Chain	Res	Type
7	L	189	GLN
7	L	237	ASN
7	L	258	HIS
7	L	335	GLN
2	O	102	ASN
2	O	138	ASN
2	O	156	GLN
2	O	178	ASN
2	O	220	GLN
2	O	241	HIS
2	O	270	ASN
2	O	410	GLN
2	O	753	ASN
8	P	66	HIS
8	P	269	ASN
8	P	293	GLN
8	P	645	HIS
8	P	734	GLN
8	P	788	GLN
8	P	815	GLN
8	Q	153	GLN
8	Q	400	ASN
8	Q	478	GLN
8	Q	635	GLN
8	Q	809	GLN
1	S	101	GLN
1	S	376	GLN
1	S	490	GLN
1	S	549	GLN
1	S	767	GLN
1	S	940	GLN
1	S	962	HIS
1	S	992	HIS
1	S	993	GLN
1	S	1003	ASN
1	S	1014	ASN
1	S	1113	ASN
1	S	1128	GLN
1	S	1140	ASN
1	S	1327	HIS
1	S	1366	GLN
1	S	1440	GLN

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Mol	Chain	Res	Type
7	M	32	GLN
7	M	37	HIS
7	M	109	GLN
7	M	335	GLN
10	X	67	GLN
11	U	22	GLN
11	U	82	GLN
11	U	98	HIS
11	U	171	GLN
11	U	172	GLN
11	U	244	HIS
11	U	266	HIS
11	U	297	GLN
11	U	302	ASN
11	U	345	GLN
11	U	415	ASN
11	U	416	GLN
11	U	504	GLN
11	U	580	ASN
11	U	680	ASN
11	U	731	GLN
11	U	757	ASN
11	U	1017	ASN
11	U	1030	ASN
11	U	1137	GLN
11	U	1217	GLN
11	U	1252	ASN
11	U	1259	GLN
11	U	1278	HIS
12	V	65	GLN
12	V	76	GLN
12	V	86	HIS
12	V	171	ASN
12	V	370	ASN
12	V	394	GLN
12	V	405	ASN
12	V	444	HIS
12	V	480	HIS
12	V	523	ASN
12	V	791	ASN
12	V	823	GLN
12	V	1063	GLN

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Mol	Chain	Res	Type
12	V	1119	GLN
12	V	1129	GLN
12	V	1150	GLN
12	V	1151	ASN
12	V	1355	GLN
12	V	1378	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	2
7	L	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	9:UNK	C	73:GLU	N	36.41
1	W	95:TRP	C	101:UNK	N	6.57
1	L	339:TYR	C	340:GLU	N	1.17
1	L	332:PRO	C	333:PHE	N	1.15

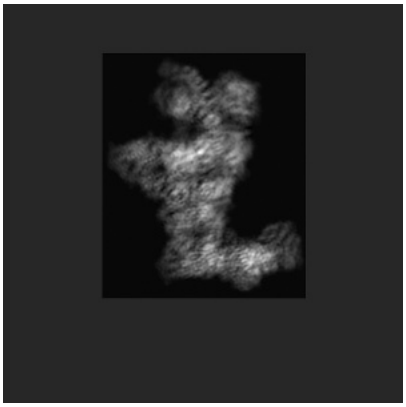
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23090. These allow visual inspection of the internal detail of the map and identification of artifacts.

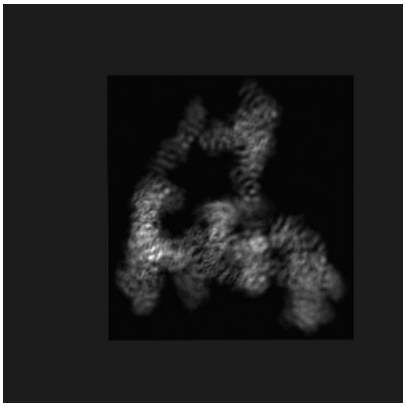
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

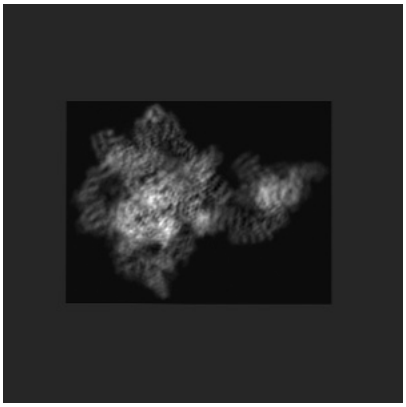
6.1.1 Primary map



X



Y



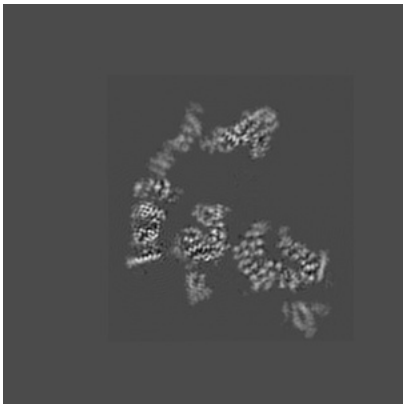
Z

The images above show the map projected in three orthogonal directions.

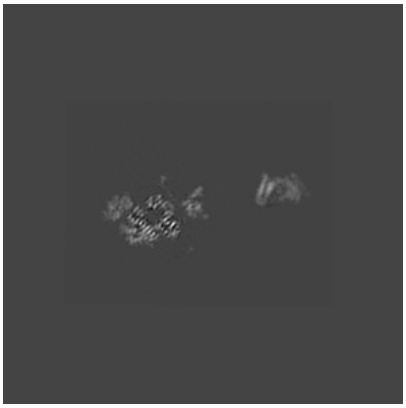
6.2 Central slices

6.2.1 Primary map

X Index: 224



Y Index: 224



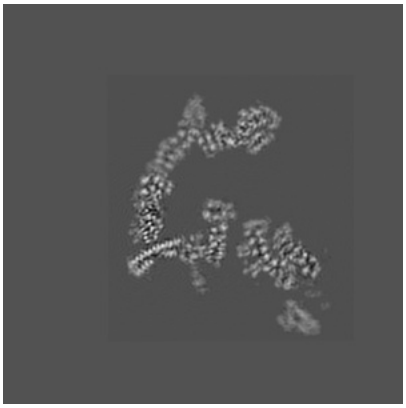
Z Index: 224

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 166



Y Index: 232

Z Index: 162

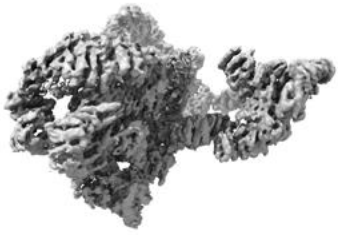
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

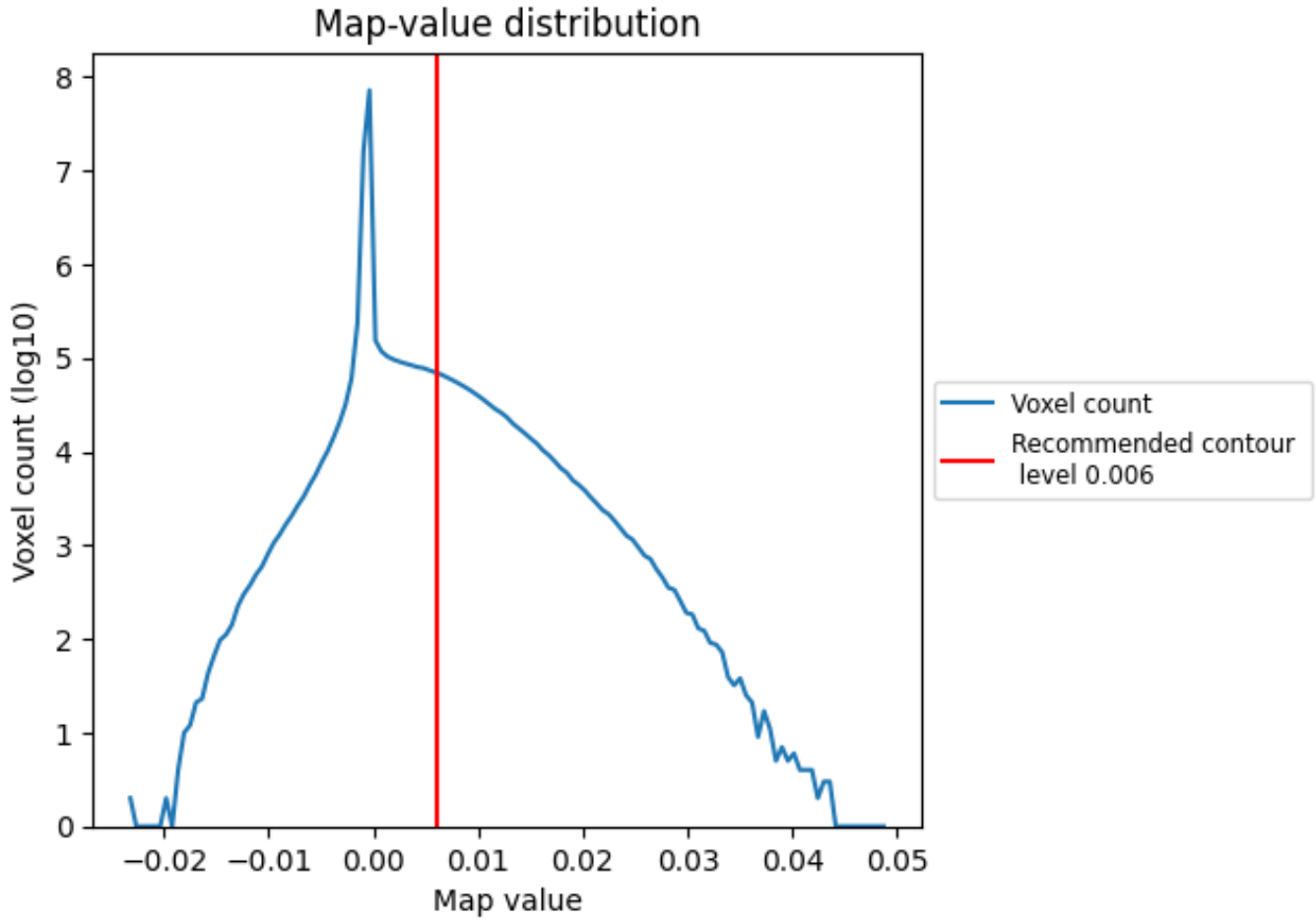
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

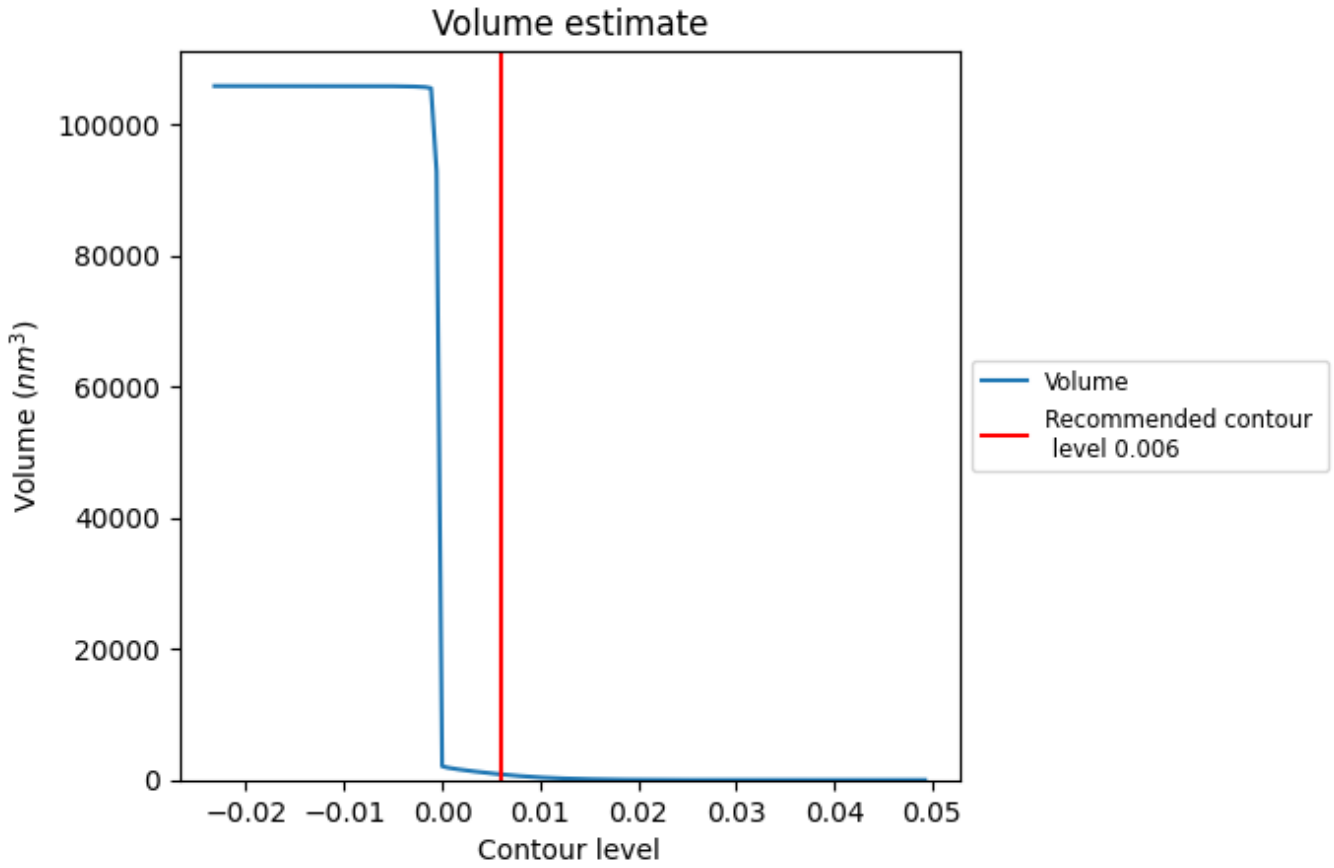
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

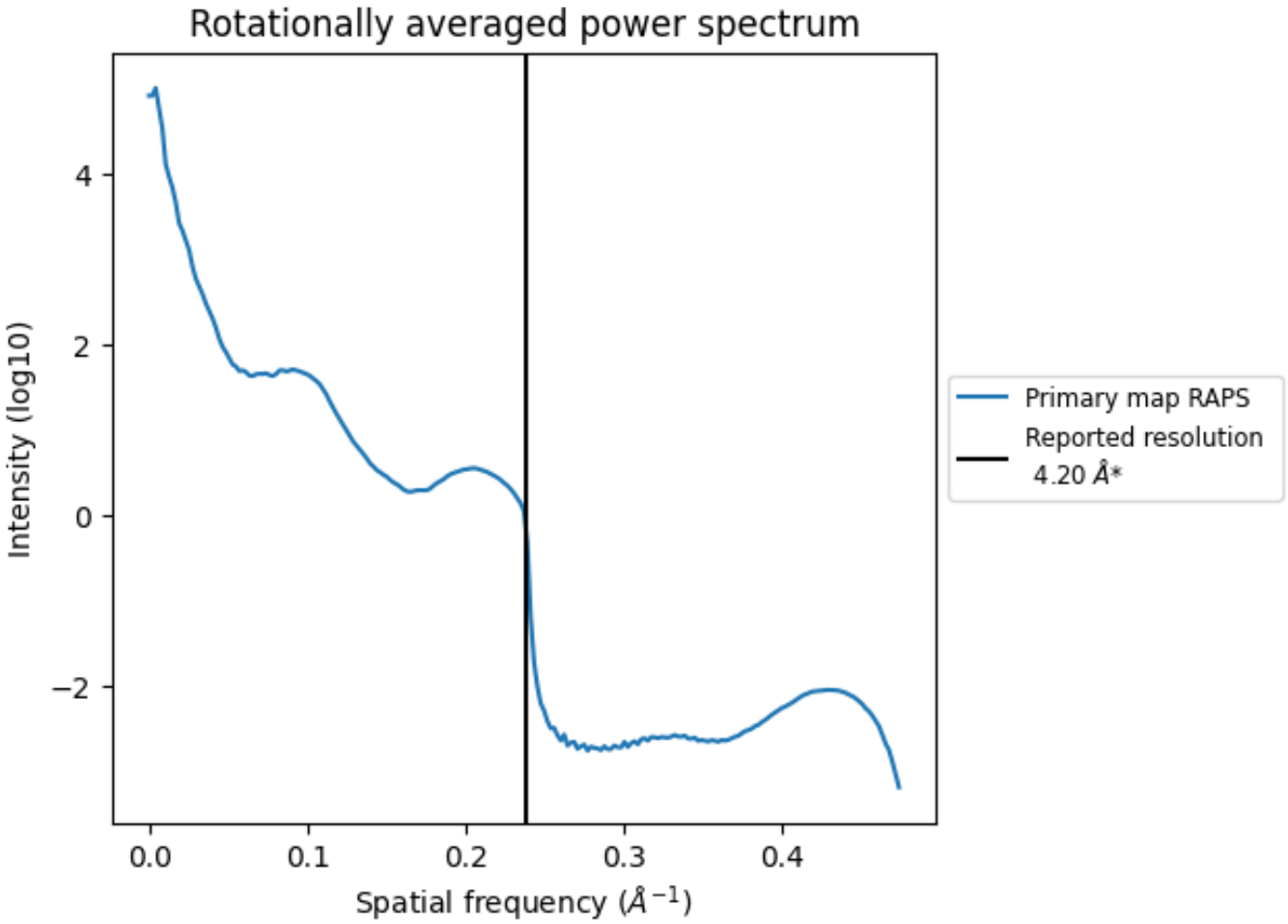
7.2 Volume estimate



The volume at the recommended contour level is 860 nm^3; this corresponds to an approximate mass of 777 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

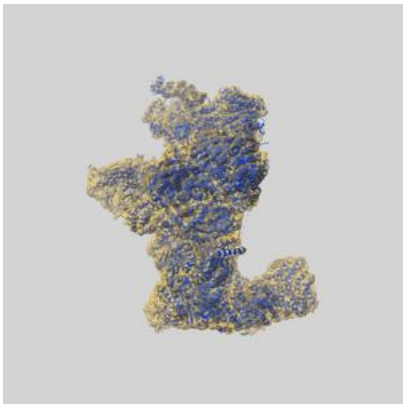
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

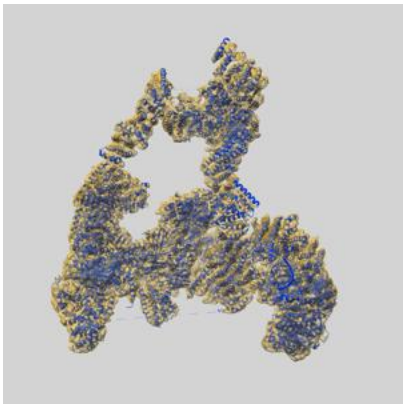
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23090 and PDB model 7KZV. Per-residue inclusion information can be found in section 3 on page 15.

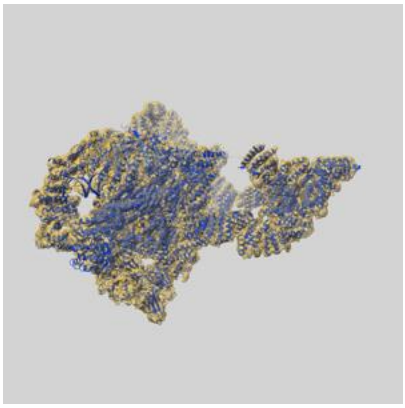
9.1 Map-model overlay



X



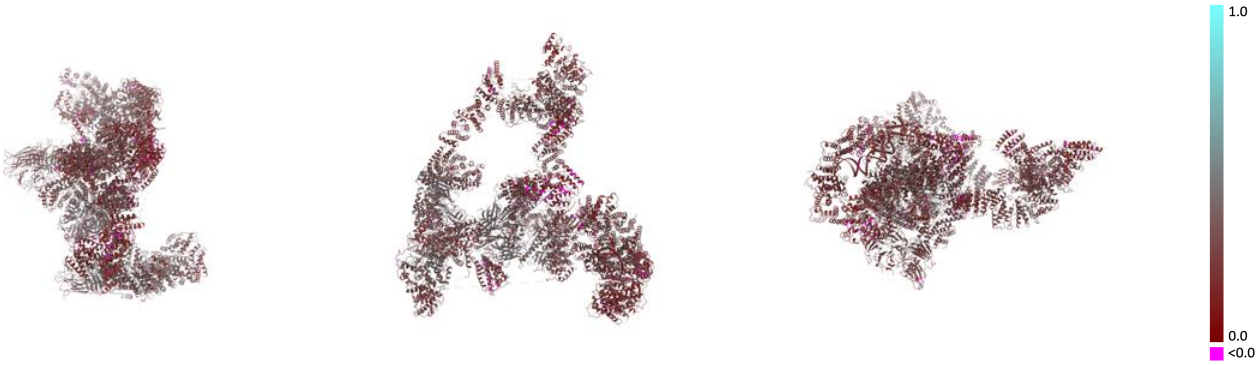
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

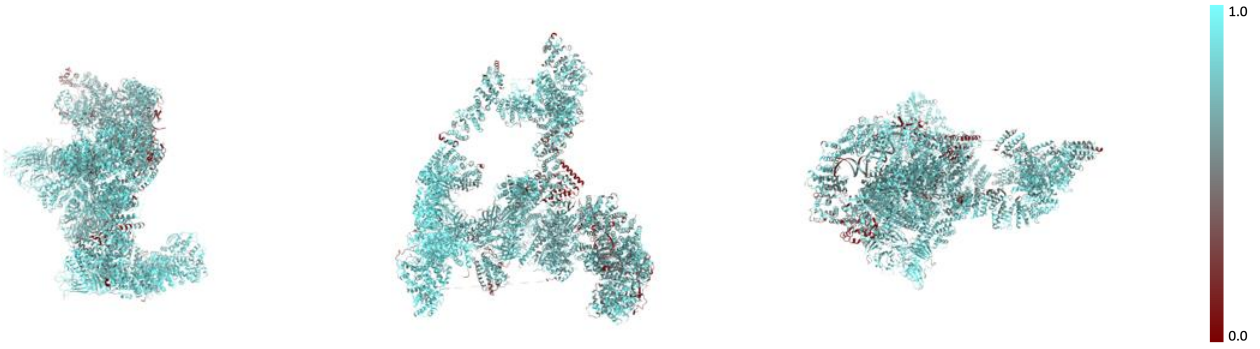
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

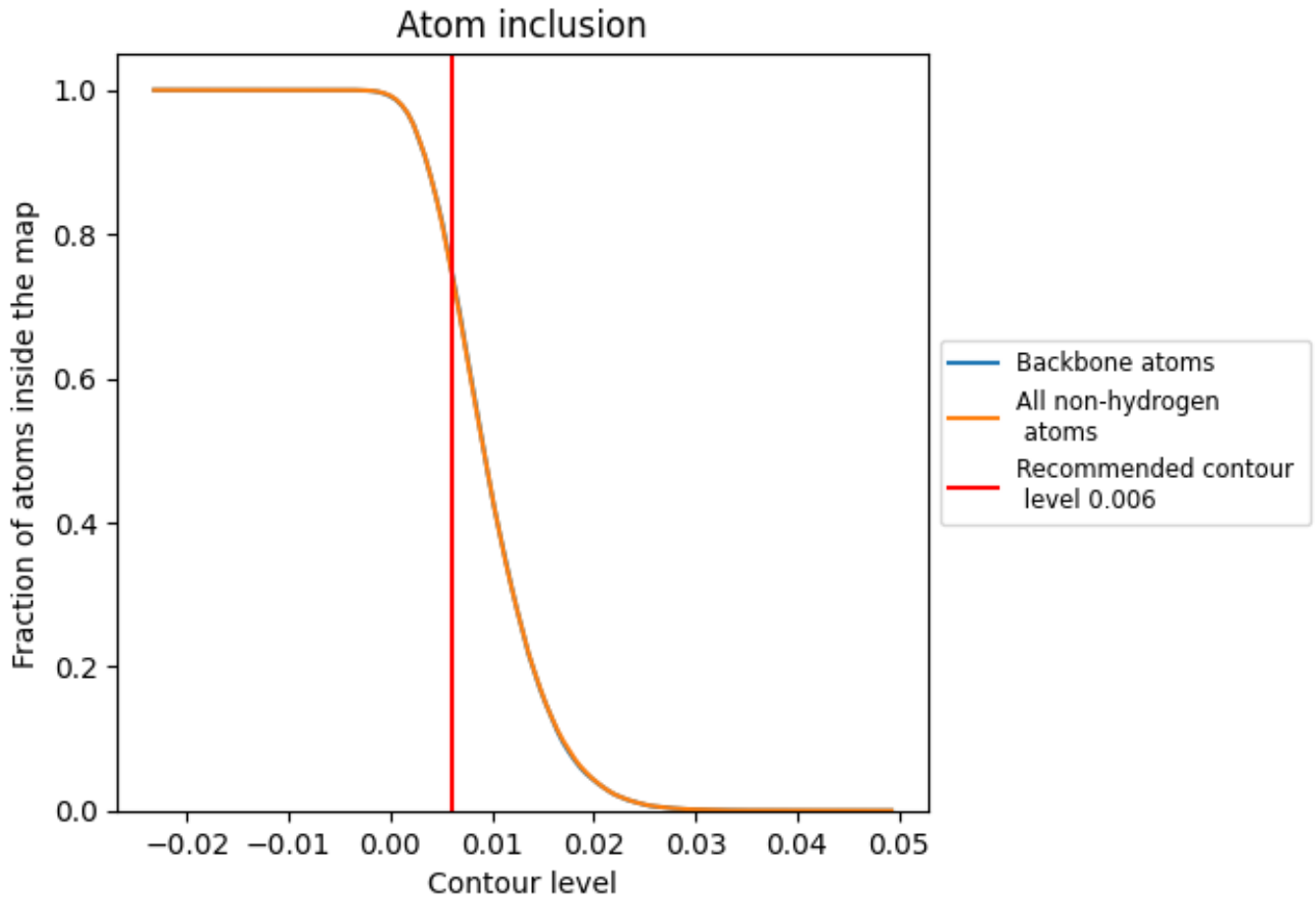
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7499	0.2930
A	0.7075	0.2510
B	0.8311	0.3630
C	0.8753	0.3400
E	0.7600	0.3100
F	0.8750	0.3400
G	0.8331	0.3180
H	0.7806	0.2750
L	0.8165	0.3350
M	0.7330	0.2580
O	0.8075	0.3070
P	0.8499	0.3840
Q	0.7641	0.3010
S	0.7554	0.2700
U	0.6528	0.2630
V	0.7072	0.2530
W	0.7286	0.3270
X	0.6708	0.2410
Y	0.3886	0.1710
Z	0.4291	0.1980