Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 09:27 PM EST

PDB ID	:	7KZT
EMDB ID	:	EMD-23089
Title	:	Structure of the human fanconi anaemia Core-UBE2T-ID-DNA complex in intermediate 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:

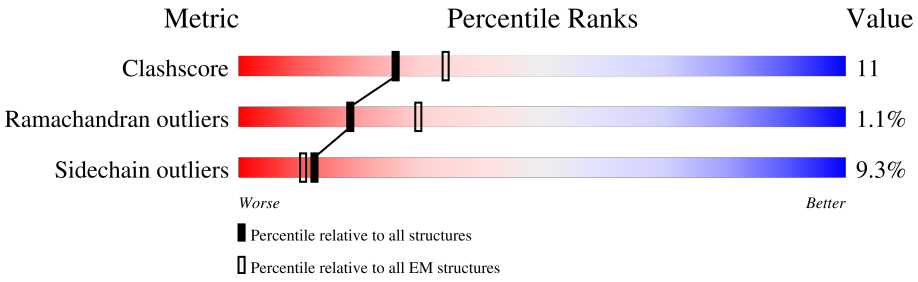
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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	9% 57% 21% • 20%
1	S	1477	• 60% 22% • 15%
2	B	884	• 49% 24% 5% 21%
2	O	884	• 57% 19% • 21%
3	C	583	• 66% 26% • 6%
4	E	555	• 44% 27% 5% 25%
5	F	399	• 64% 20% • 15%
6	G	641	• 62% 25% • 10%

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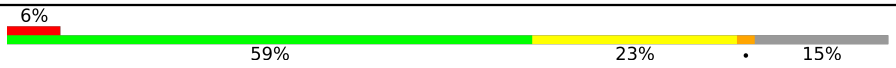
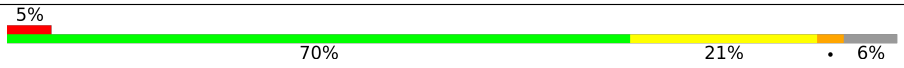
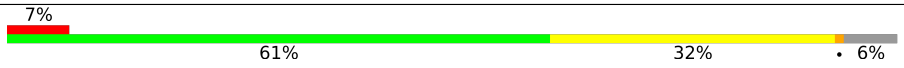
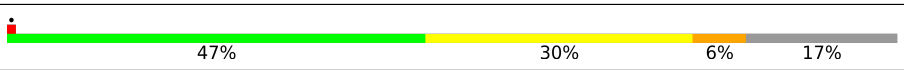
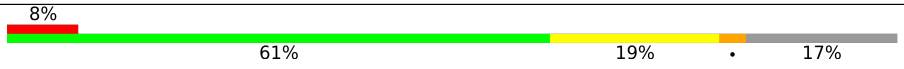
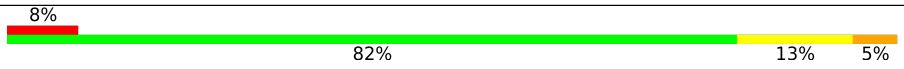
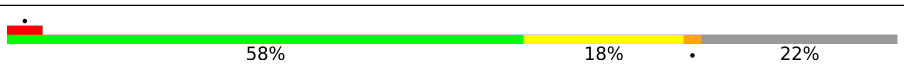
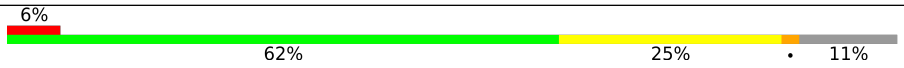
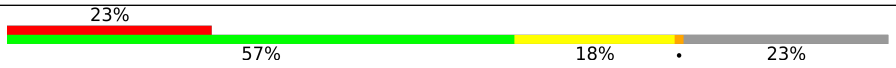
Mol	Chain	Length	Quality of chain
6	H	641	
7	L	394	
7	M	394	
8	P	906	
8	Q	906	
9	W	39	
10	X	197	
11	U	1328	
12	V	1451	
13	Y	58	
14	Z	58	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 176284 atoms, of which 88770 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	1181	Total	C	H	N	O	S	0	0
			19089	5991	9739	1569	1735	55		

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	1120	Total	C	H	N	O	S	0	0
			18221	5802	9224	1485	1657	53		

- Molecule 13 is a DNA chain called DNA (22-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Y	22	Total	C	H	N	O	P	0	0
			704	215	246	91	130	22		

- Molecule 14 is a DNA chain called DNA (22-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Z	22	Total	C	H	N	O	P	0	0
			692	211	248	77	134	22		

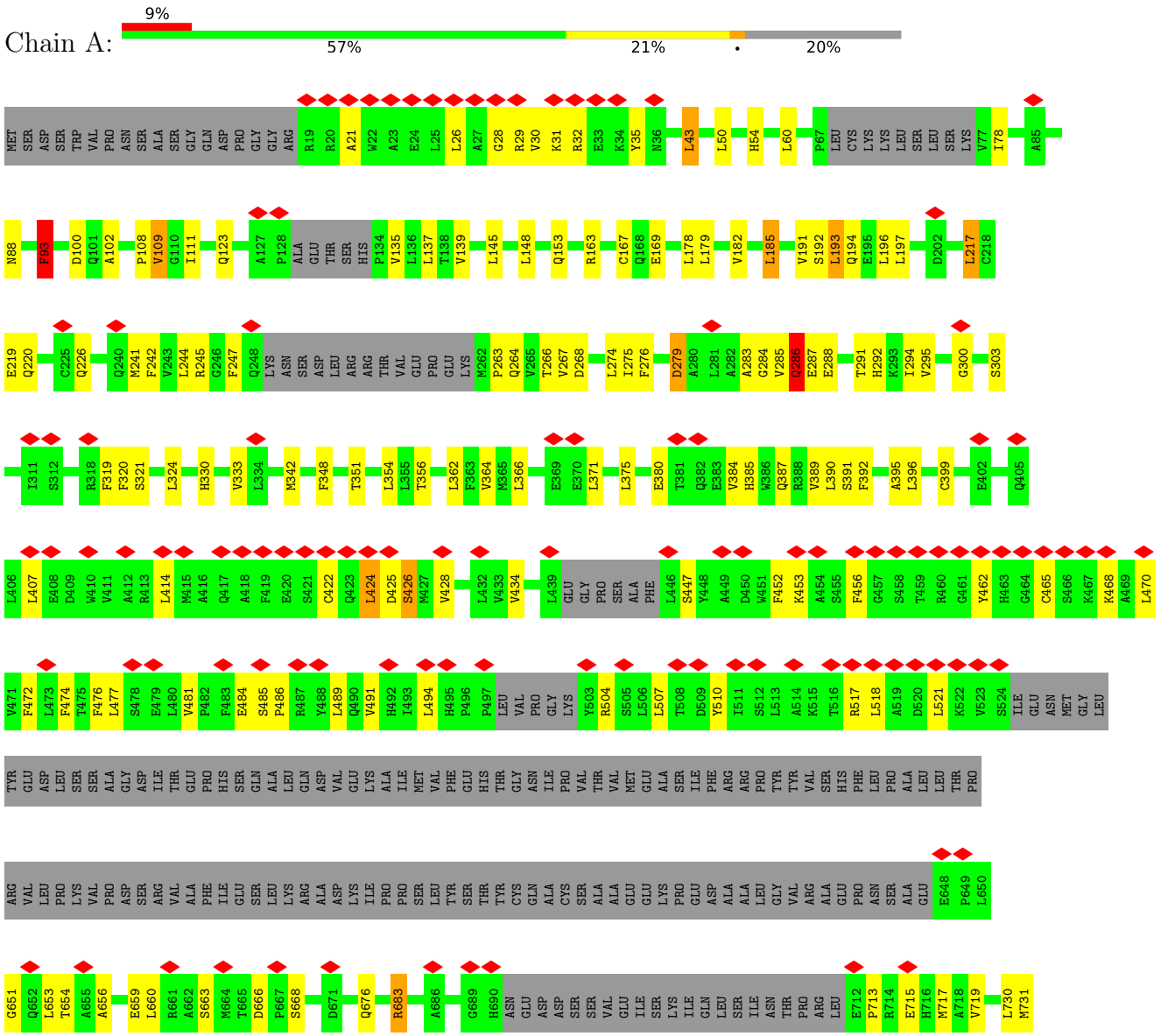
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

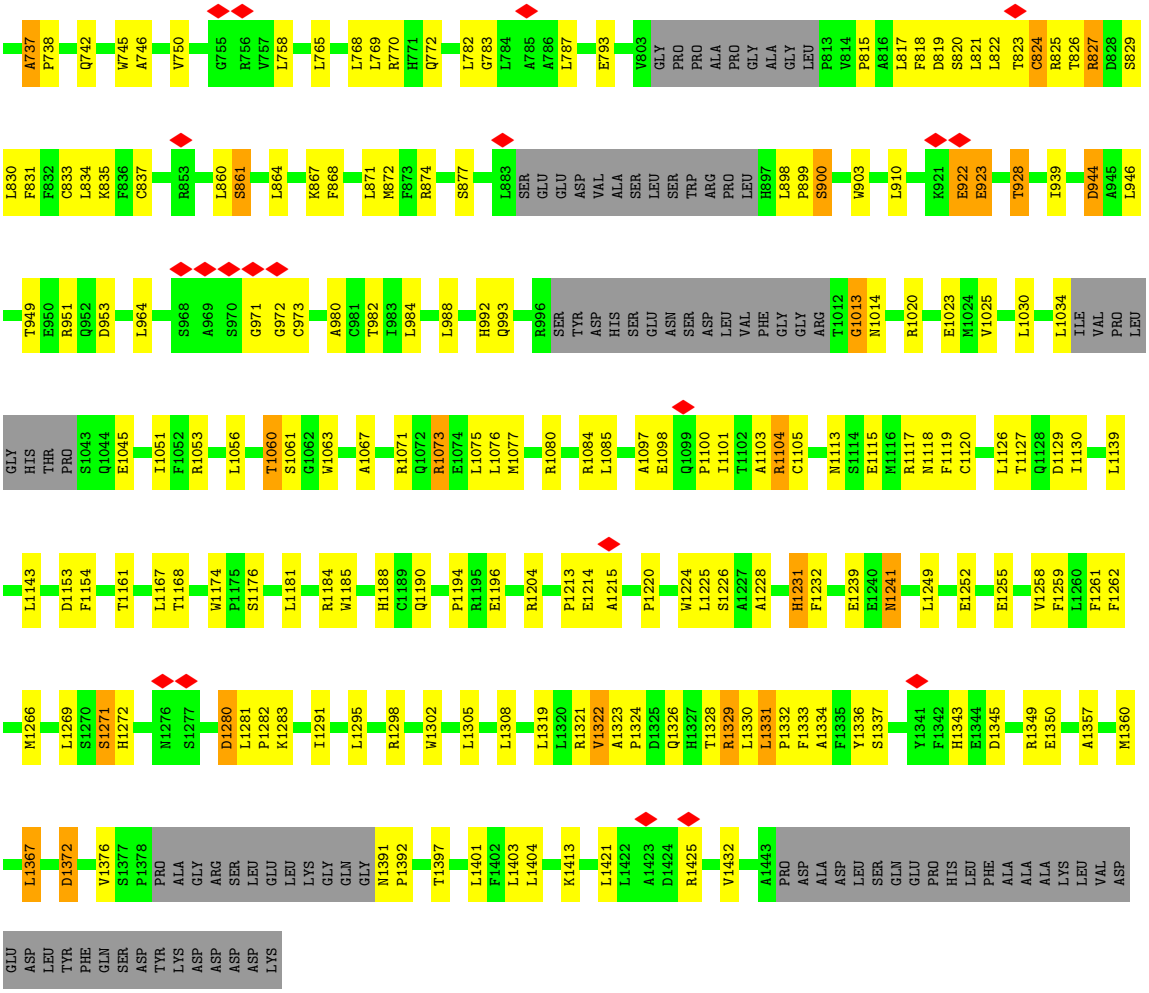
Mol	Chain	Residues	Atoms		AltConf
15	G	1	Total	Zn	0
			1	1	
15	L	2	Total	Zn	0
			2	2	
15	M	2	Total	Zn	0
			2	2	

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.

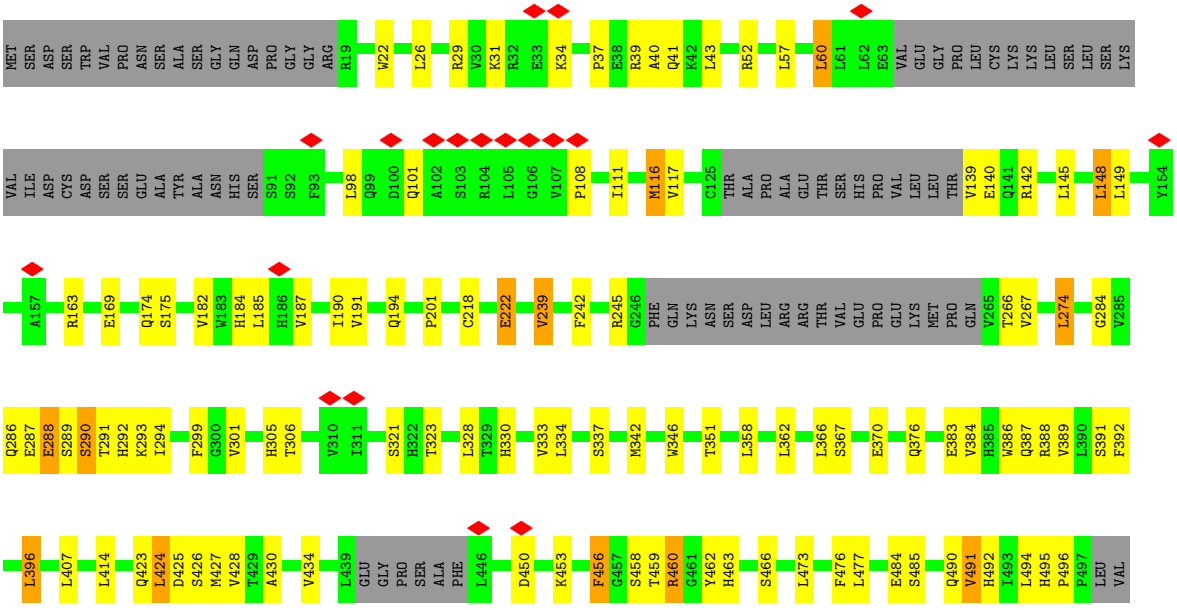
• Molecule 1: Fanconi anemia group A protein

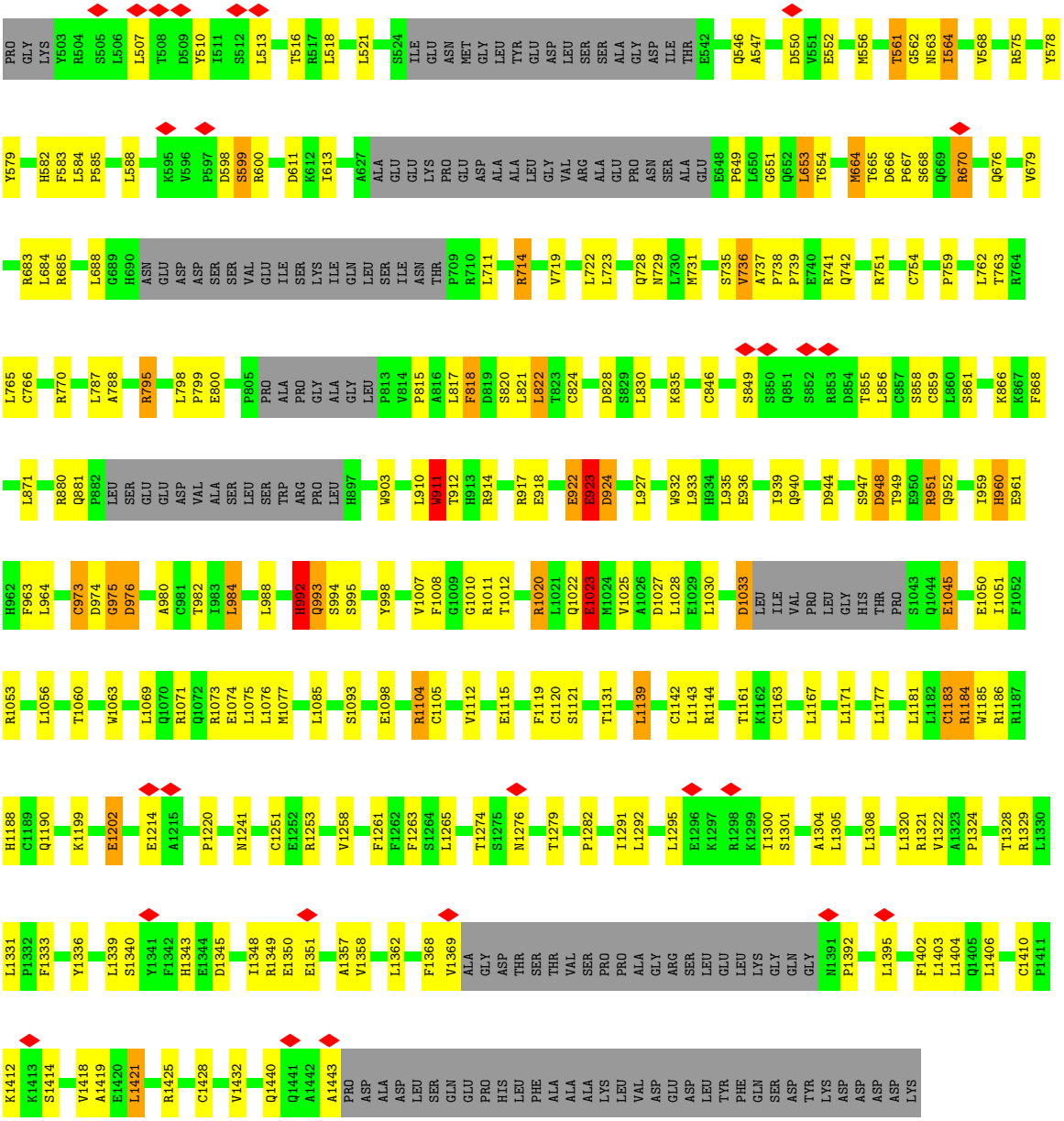




• Molecule 1: Fanconi anemia group A protein

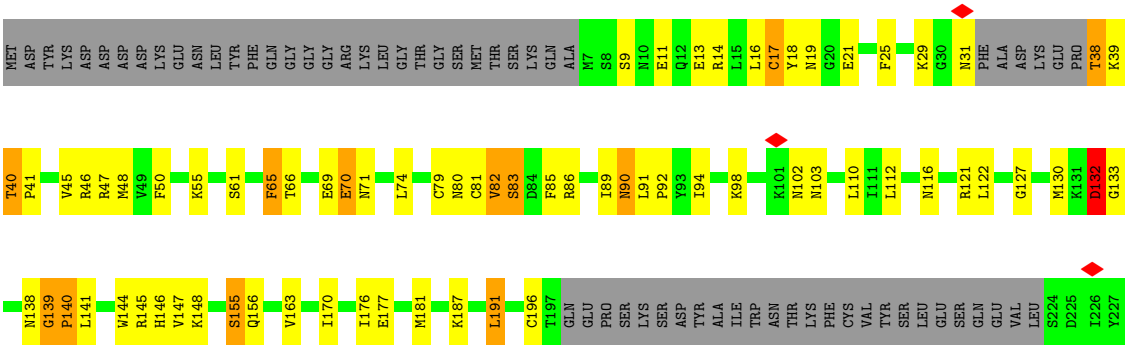
Chain S:

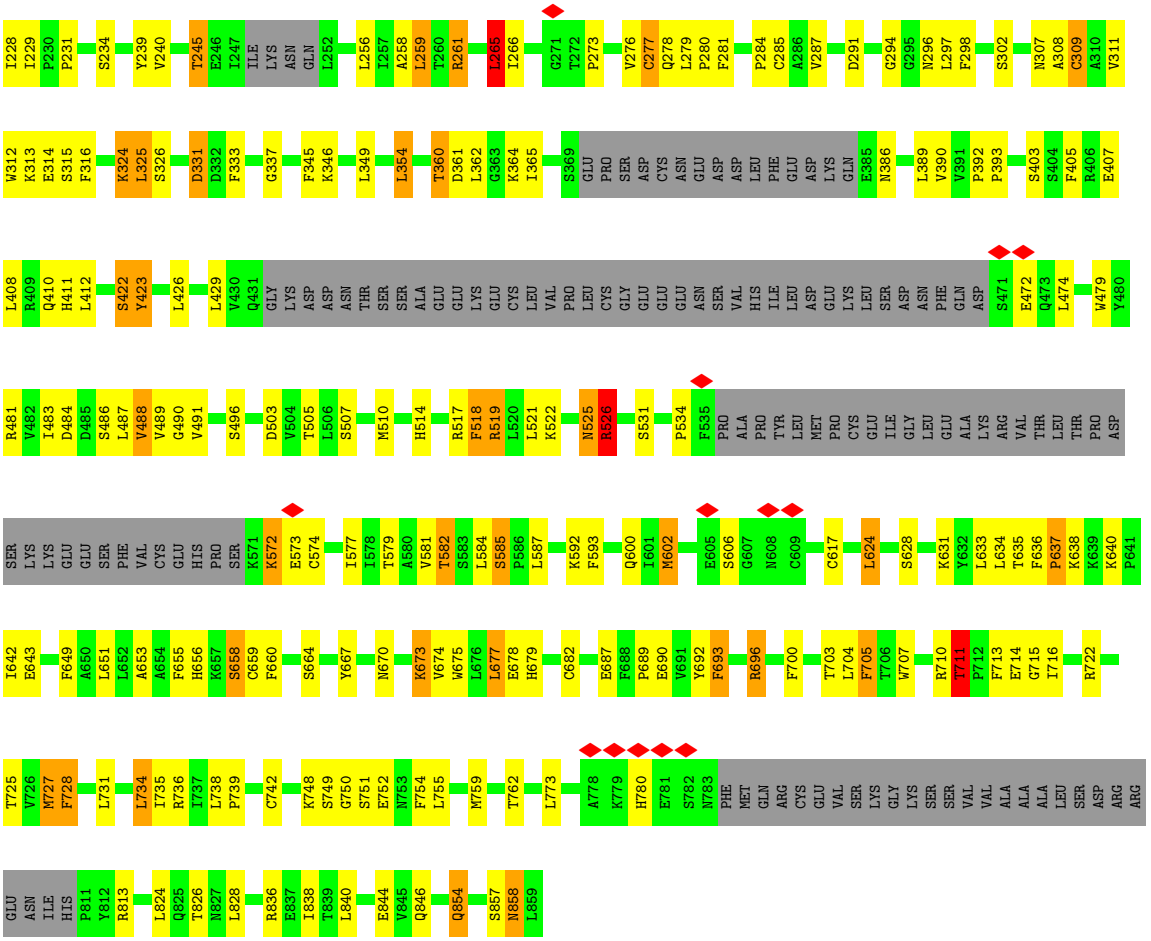




• Molecule 2: Fanconi anemia group B protein

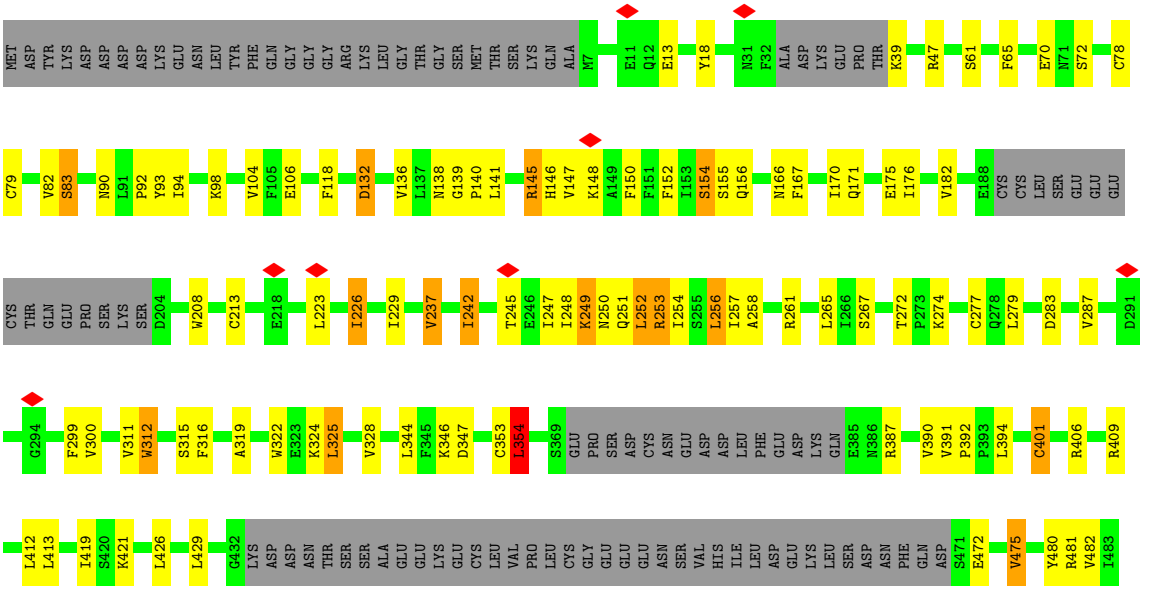
Chain B:

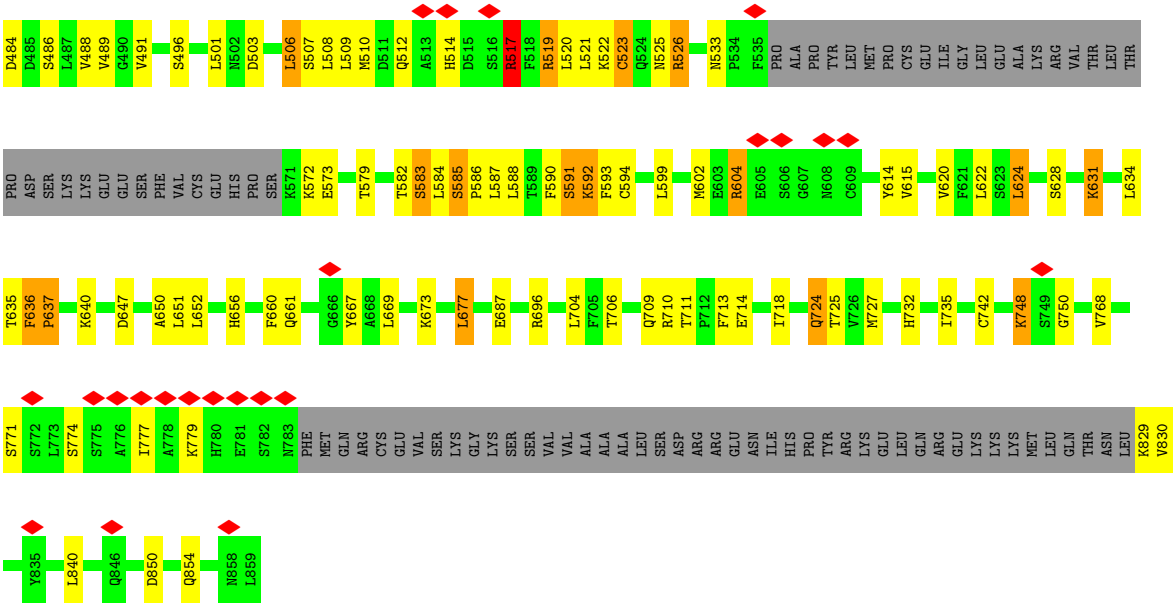




• Molecule 2: Fanconi anemia group B protein

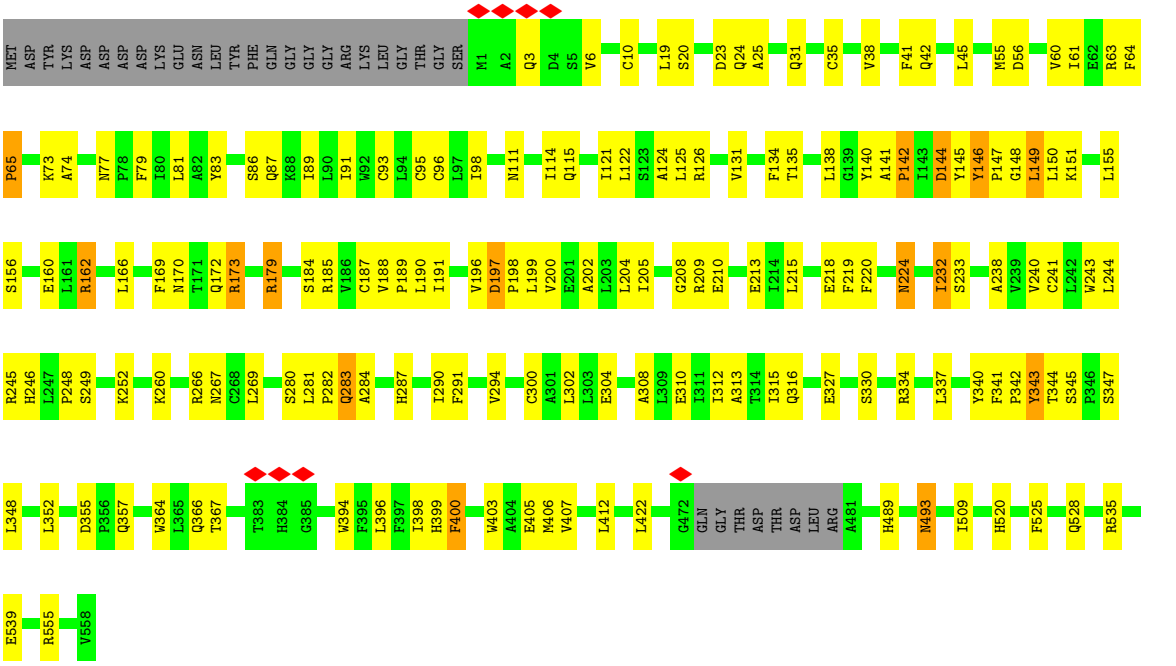
Chain O:





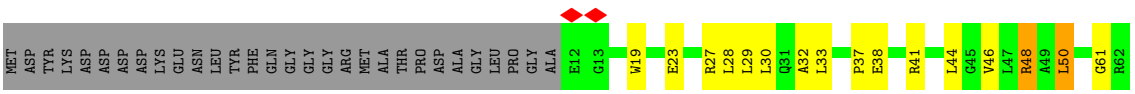
• Molecule 3: Fanconi anemia group C protein

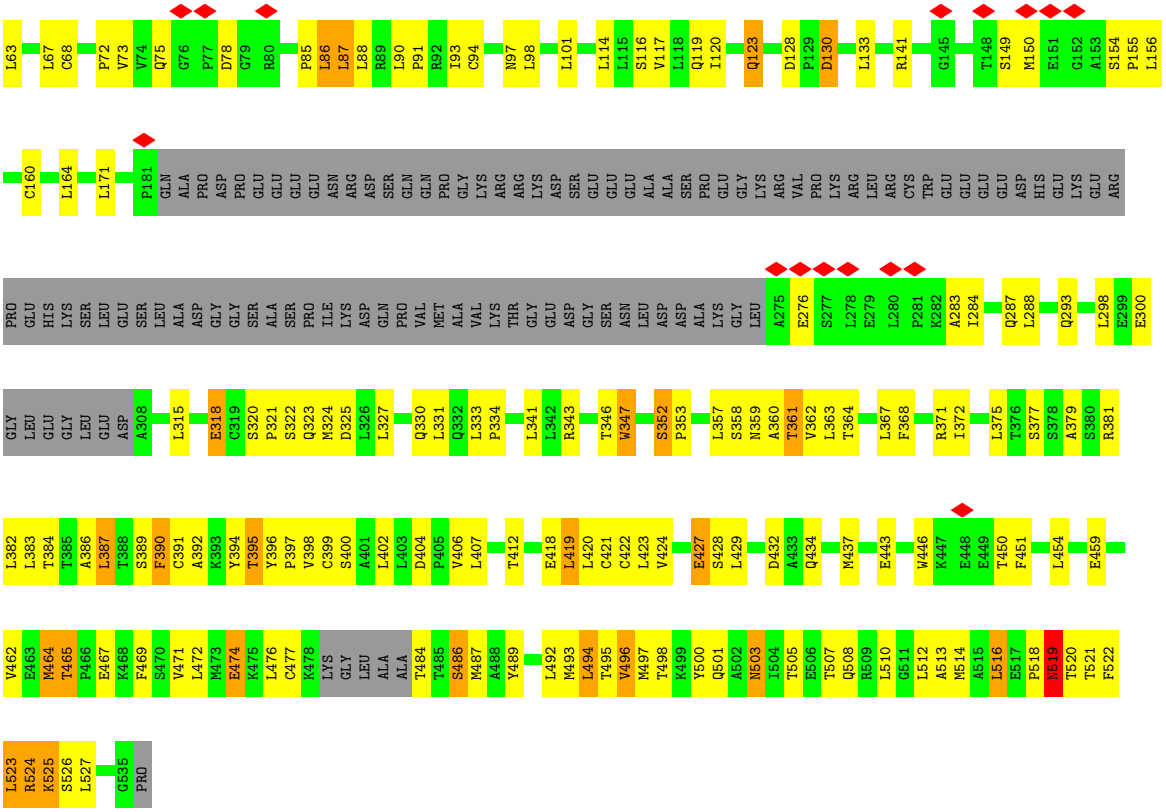
Chain C:



• Molecule 4: Fanconi anemia group E protein

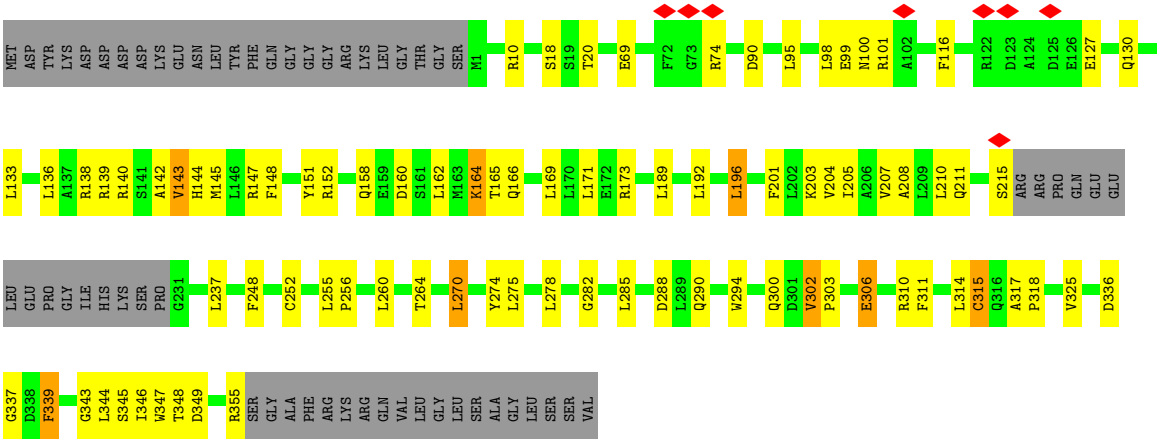
Chain E:





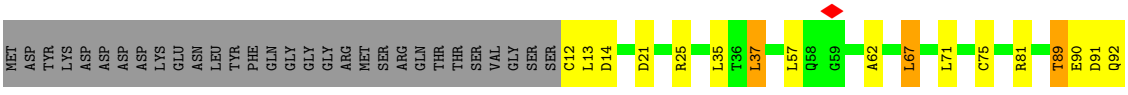
• Molecule 5: Fanconi anemia group F protein

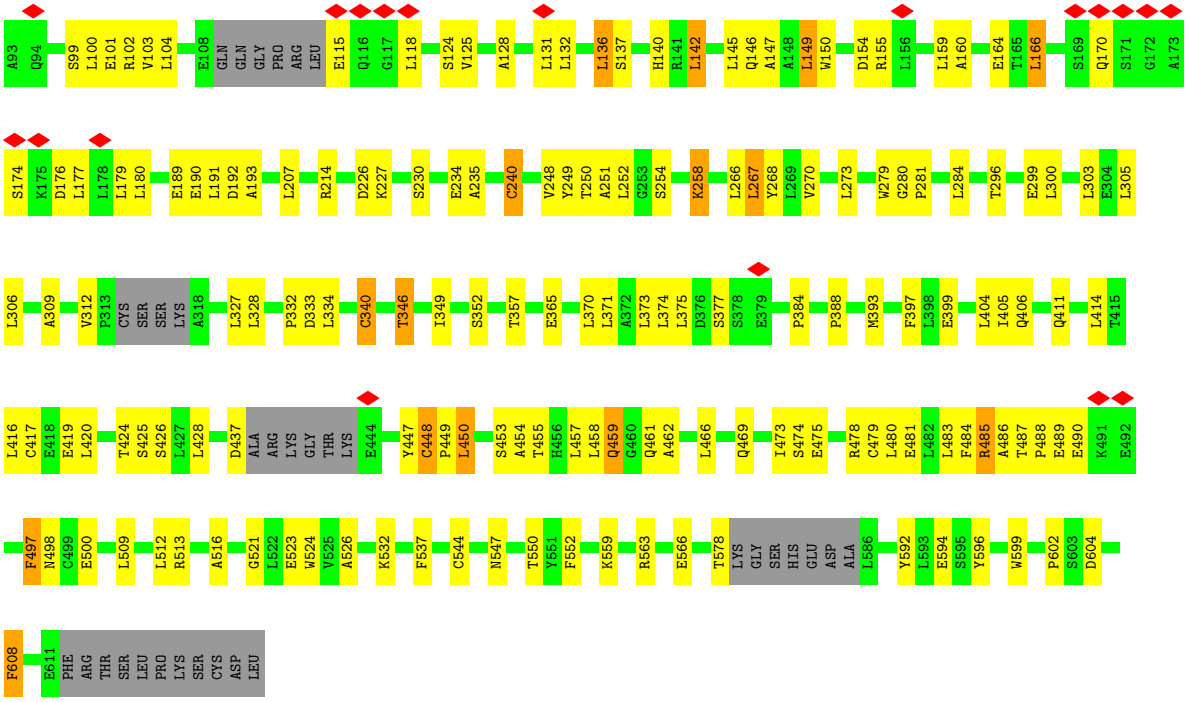
Chain F:



• Molecule 6: Fanconi anemia group G protein

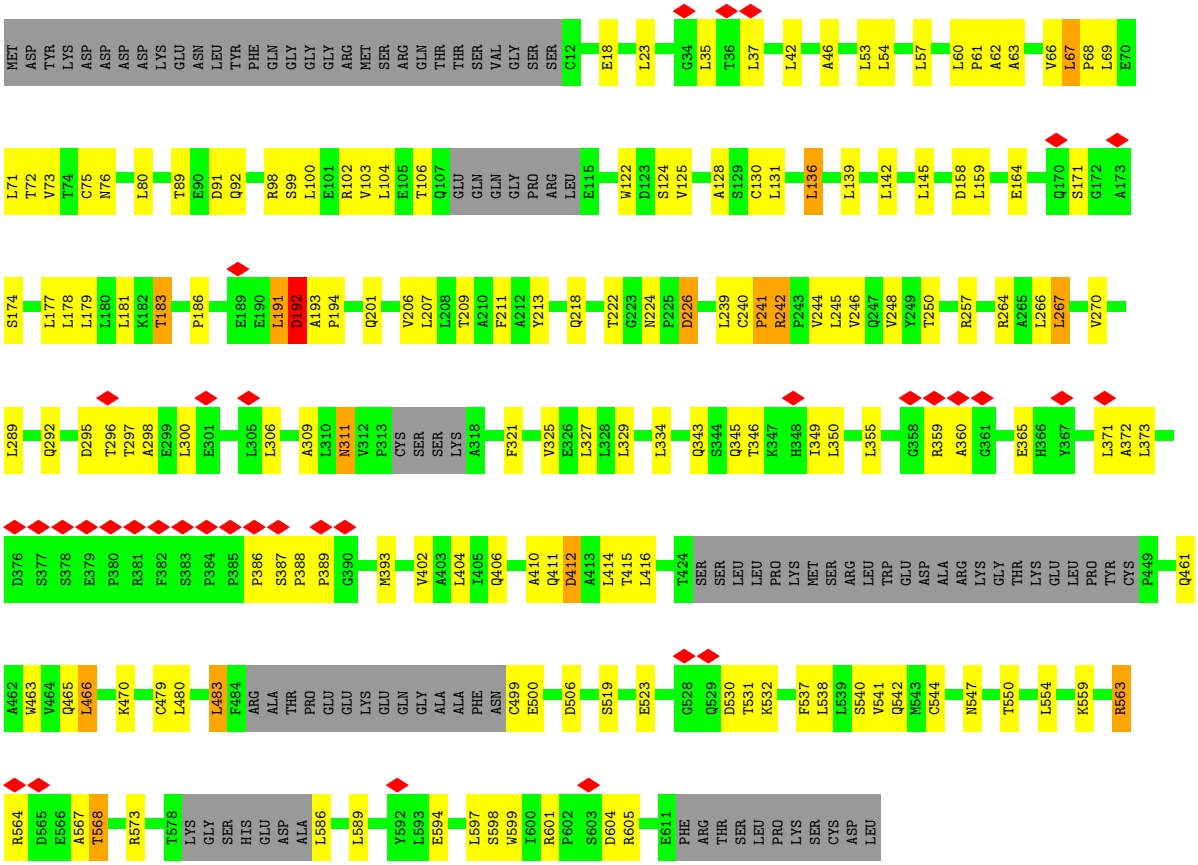
Chain G:





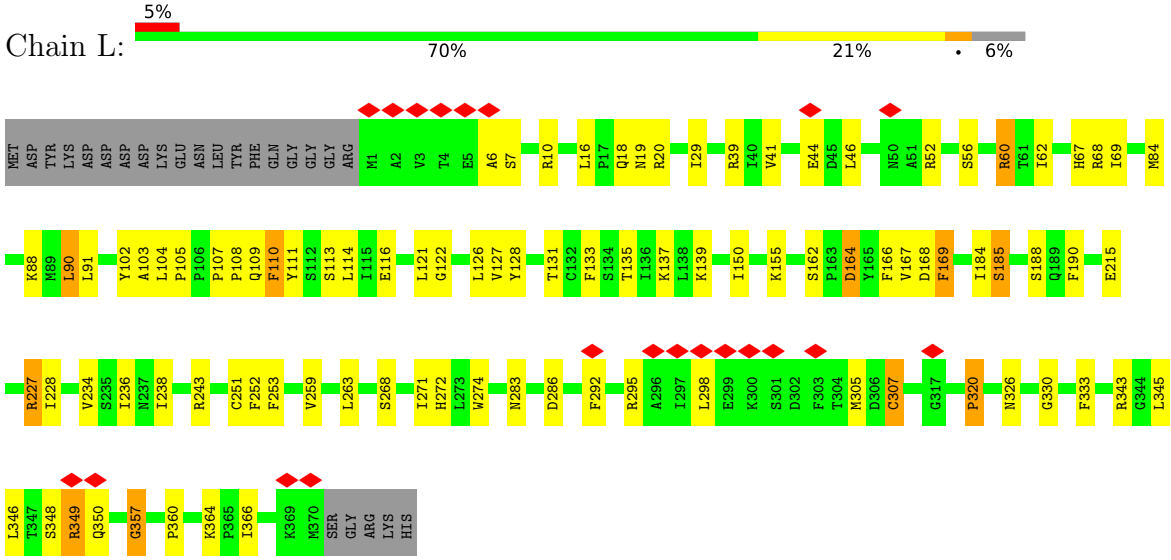
• Molecule 6: Fanconi anemia group G protein

Chain H:



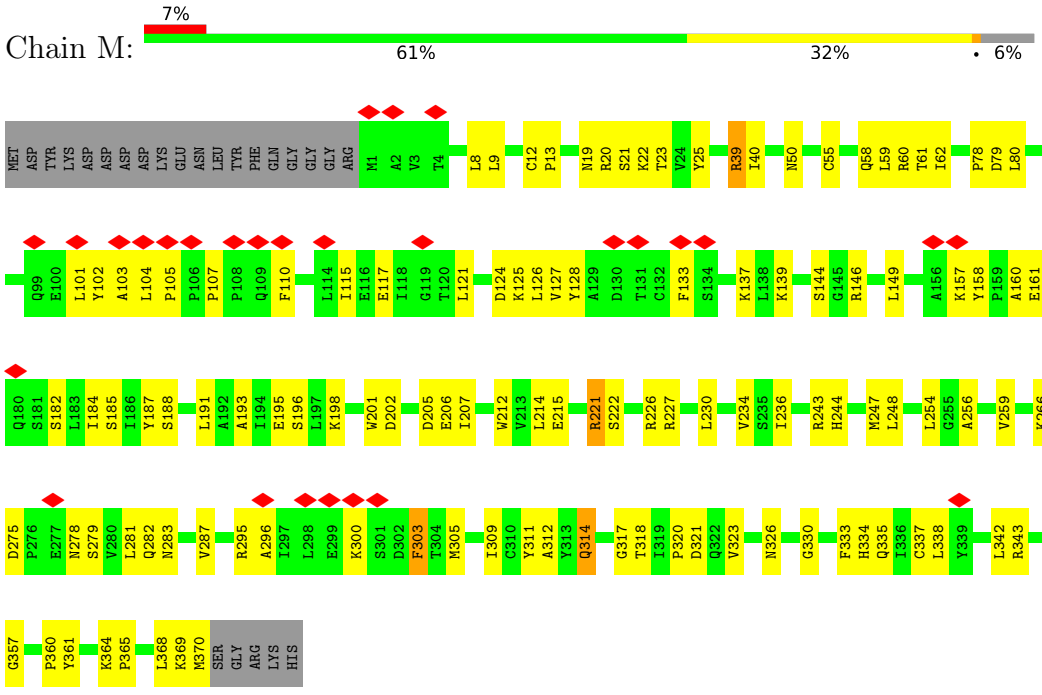
• Molecule 7: E3 ubiquitin-protein ligase FANCL

Chain L:



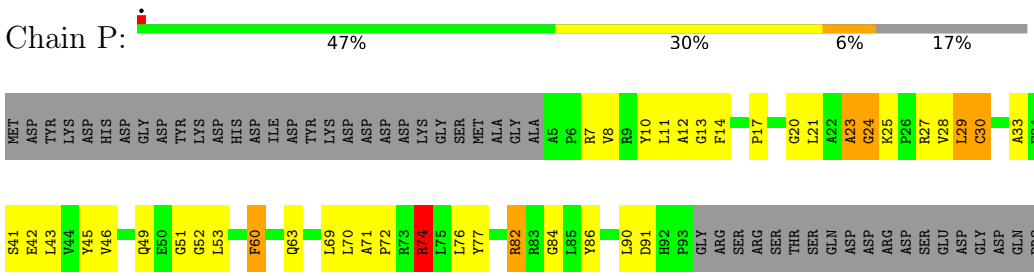
• Molecule 7: E3 ubiquitin-protein ligase FANCL

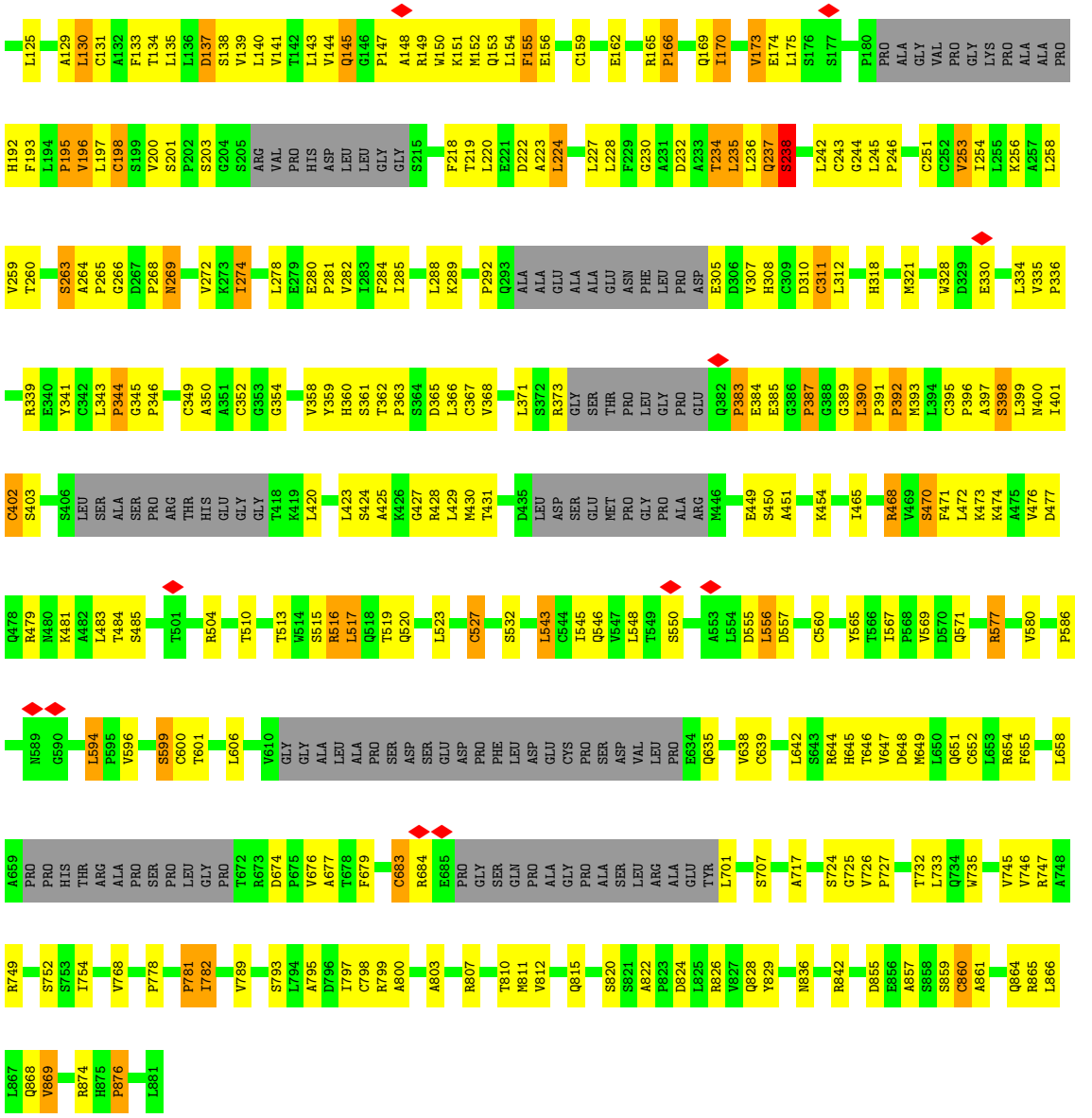
Chain M:



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

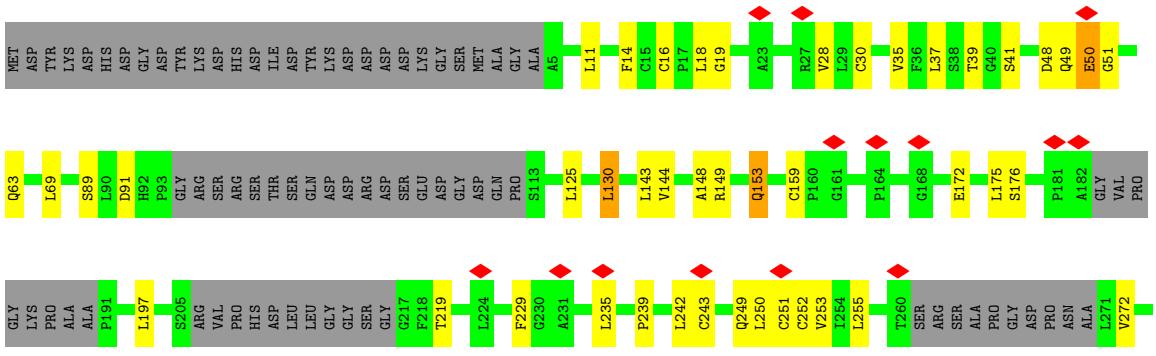
Chain P:

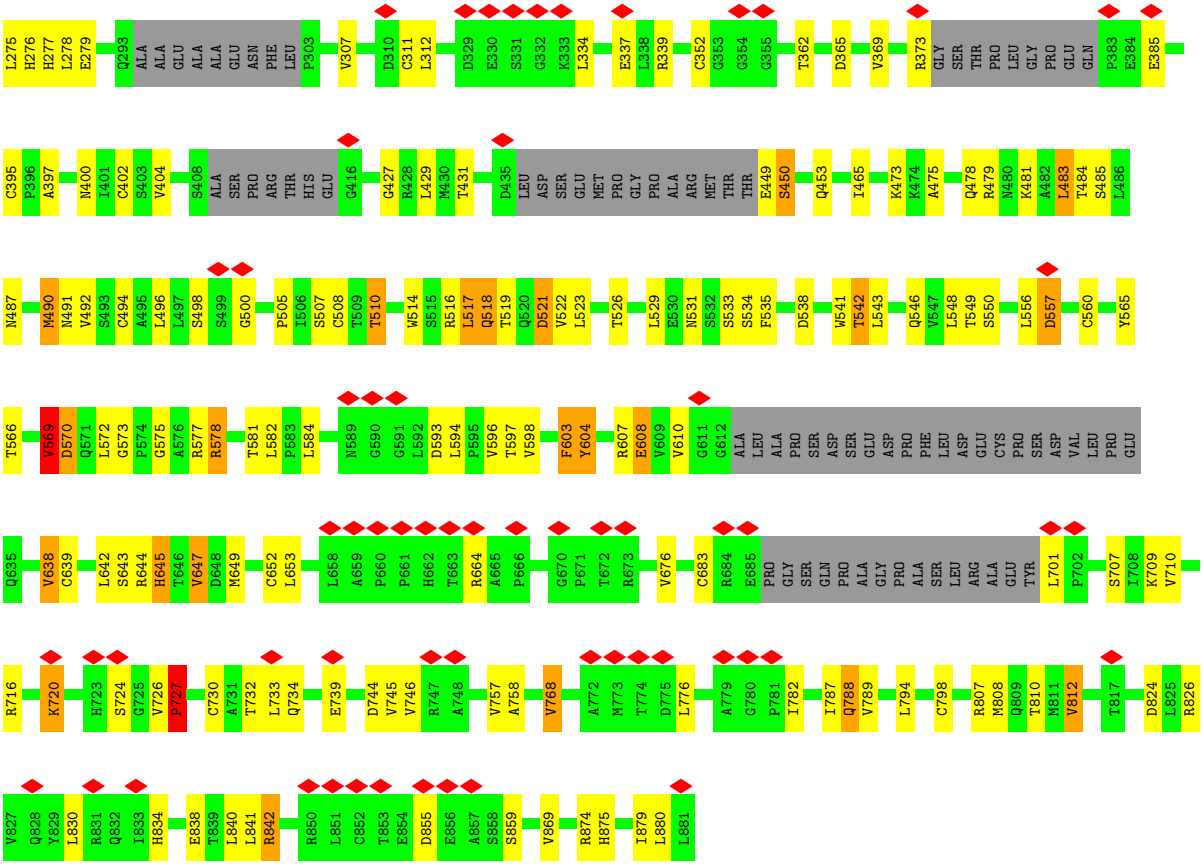




• Molecule 8: Fanconi anemia core complex-associated protein 100

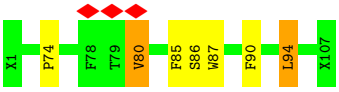
Chain Q:





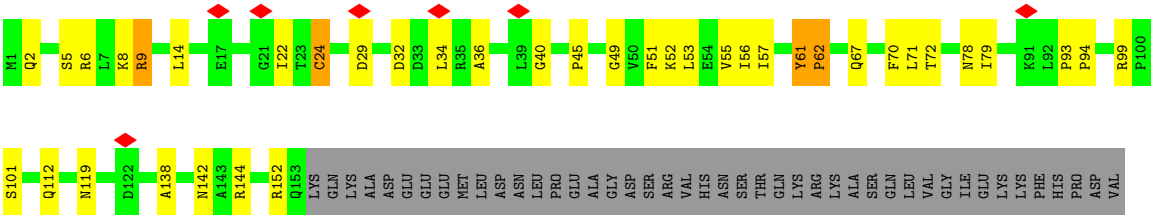
• Molecule 9: Fanconi anemia core complex-associated protein 20

Chain W:



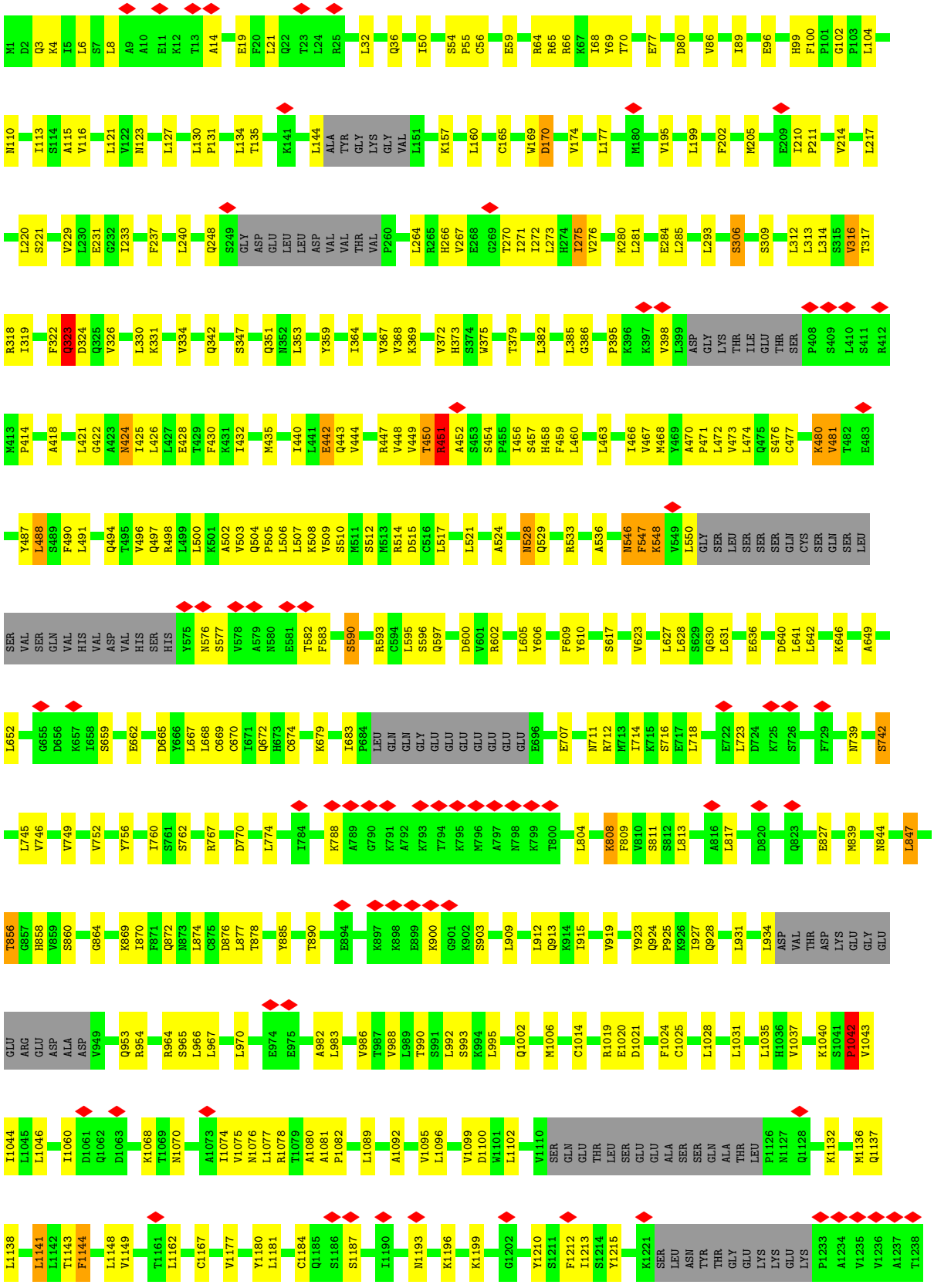
• Molecule 10: Ubiquitin-conjugating enzyme E2 T

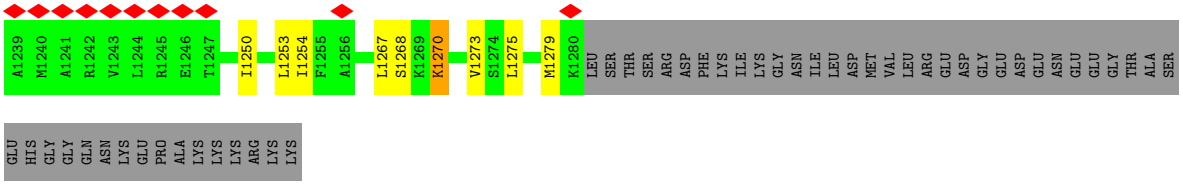
Chain X:



• Molecule 11: Fanconi anemia, complementation group I

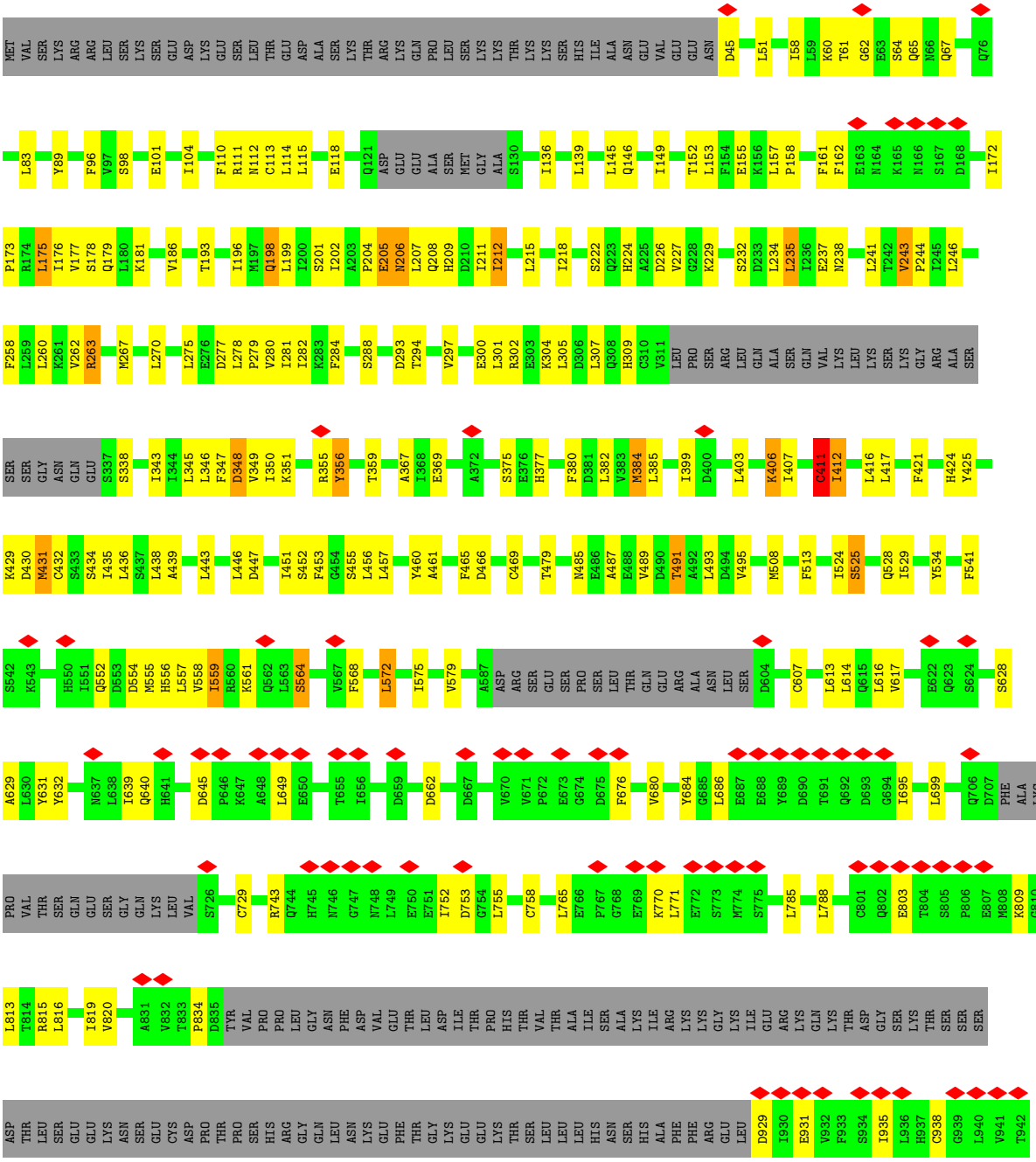
Chain U:

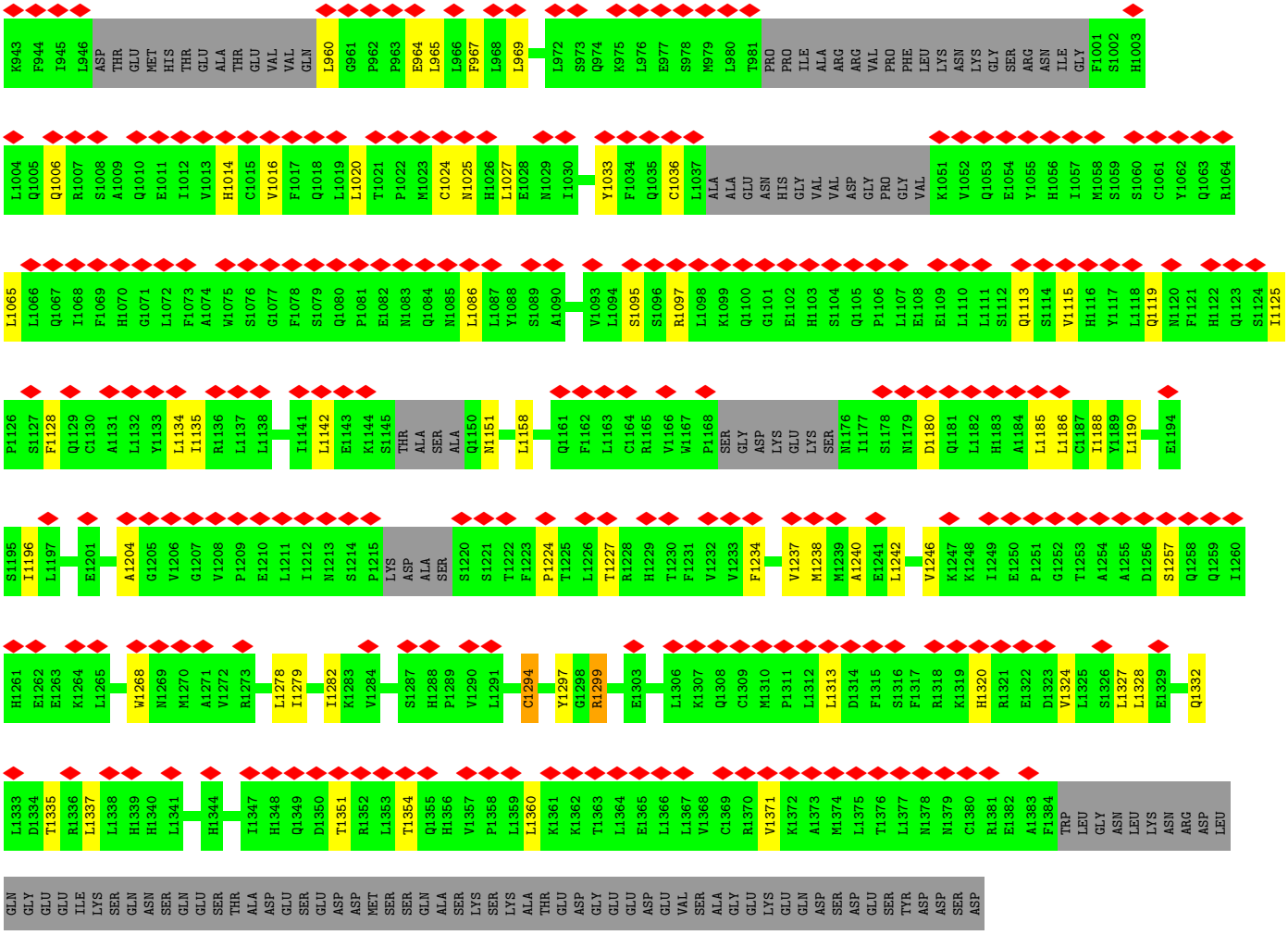




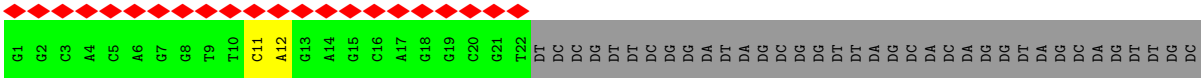
• Molecule 12: Fanconi anemia group D2 protein

Chain V:

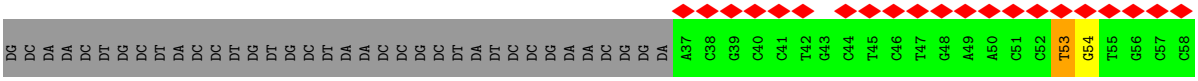




- Molecule 13: DNA (22-MER)



- Molecule 14: DNA (22-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69111	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	0.047	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0055	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	1.01	6/13008 (0.0%)
1	S	0.75	0/10153	1.05	12/13749 (0.1%)
2	B	0.79	0/5707	1.18	10/7686 (0.1%)
2	O	0.74	0/5701	1.05	6/7686 (0.1%)
3	C	0.80	0/4497	1.13	8/6103 (0.1%)
4	E	0.80	0/3274	1.21	7/4438 (0.2%)
5	F	0.79	0/2791	1.14	2/3790 (0.1%)
6	G	0.81	0/4568	1.11	2/6215 (0.0%)
6	H	0.72	0/4293	1.02	1/5840 (0.0%)
7	L	0.77	1/3050 (0.0%)	1.09	6/4143 (0.1%)
7	M	0.72	0/3050	1.05	8/4143 (0.2%)
8	P	0.84	1/5697 (0.0%)	1.26	15/7752 (0.2%)
8	Q	0.74	0/5737	1.05	3/7810 (0.0%)
9	W	0.65	0/202	0.96	0/281
10	X	0.71	0/1267	0.98	0/1722
11	U	0.79	0/9494	1.10	6/12802 (0.0%)
12	V	0.79	0/9163	1.06	5/12390 (0.0%)
13	Y	0.47	0/515	0.98	0/794
14	Z	0.48	0/495	0.98	1/760 (0.1%)
All	All	0.77	2/89259 (0.0%)	1.09	98/121112 (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	8
1	S	0	11
2	B	0	19
2	O	0	8

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	6
4	E	0	5
5	F	0	1
6	G	0	3
6	H	0	1
7	L	0	5
8	P	0	24
8	Q	0	9
10	X	0	3
11	U	0	13
12	V	0	9
All	All	0	125

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	330	GLY	C-N	-10.95	1.08	1.34
8	P	238	SER	CA-CB	-5.23	1.45	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	321	ASP	O-C-N	-9.22	107.95	122.70
7	L	357	GLY	O-C-N	-8.58	108.97	122.70
8	Q	727	PRO	N-CD-CG	-8.33	90.71	103.20
7	M	321	ASP	C-N-CA	7.69	140.92	121.70
7	M	330	GLY	O-C-N	7.69	135.00	122.70
7	L	357	GLY	CA-C-N	7.26	133.18	117.20
2	B	261	ARG	CG-CD-NE	7.19	126.91	111.80
11	U	450	THR	CA-CB-OG1	-7.14	94.00	109.00
7	M	321	ASP	CA-C-N	7.06	132.74	117.20
3	C	160	GLU	CB-CA-C	6.92	124.24	110.40
11	U	375	TRP	CA-CB-CG	6.79	126.60	113.70
7	L	357	GLY	C-N-CA	6.62	138.25	121.70
4	E	48	ARG	NE-CZ-NH2	6.57	123.59	120.30
1	S	960	HIS	CB-CA-C	6.55	123.50	110.40
4	E	72	PRO	N-CD-CG	-6.49	93.46	103.20
2	O	517	ARG	NE-CZ-NH1	6.47	123.54	120.30
3	C	179	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	S	1184	ARG	CG-CD-NE	-6.43	98.30	111.80
8	P	577	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	O	406	ARG	NE-CZ-NH2	-6.34	117.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	481	GLU	CB-CG-CD	6.30	131.22	114.20
11	U	876	ASP	CB-CA-C	6.30	123.01	110.40
11	U	498	ARG	NE-CZ-NH1	6.22	123.41	120.30
8	P	30	CYS	CB-CA-C	6.14	122.68	110.40
12	V	243	VAL	CA-CB-CG2	6.01	119.92	110.90
8	P	468	ARG	NE-CZ-NH1	5.99	123.29	120.30
7	L	343	ARG	NE-CZ-NH1	5.98	123.29	120.30
4	E	97	ASN	CB-CA-C	5.97	122.34	110.40
7	L	227	ARG	NE-CZ-NH1	5.97	123.28	120.30
8	P	74	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	S	1144	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	O	667	TYR	CB-CG-CD2	-5.80	117.52	121.00
14	Z	53	DT	N1-C1'-C2'	5.79	123.60	112.60
7	L	349	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	B	736	ARG	NE-CZ-NH1	5.73	123.17	120.30
3	C	197	ASP	CB-CA-C	5.70	121.81	110.40
8	Q	842	ARG	NE-CZ-NH2	5.70	123.15	120.30
8	P	479	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	S	960	HIS	C-N-CA	5.68	135.90	121.70
8	P	82	ARG	NE-CZ-NH2	5.65	123.13	120.30
3	C	185	ARG	NE-CZ-NH1	5.60	123.10	120.30
8	P	308	HIS	CB-CA-C	5.59	121.59	110.40
8	P	398	SER	CB-CA-C	5.58	120.71	110.10
3	C	187	CYS	CB-CA-C	-5.58	99.24	110.40
12	V	384	MET	CG-SD-CE	5.57	109.11	100.20
12	V	263	ARG	CG-CD-NE	5.55	123.45	111.80
5	F	339	PHE	CB-CG-CD1	5.54	124.68	120.80
3	C	185	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	286	GLN	CB-CA-C	5.50	121.39	110.40
2	O	667	TYR	CB-CG-CD1	5.50	124.30	121.00
3	C	357	GLN	CB-CA-C	-5.49	99.41	110.40
1	S	992	HIS	CA-CB-CG	-5.47	104.30	113.60
8	P	516	ARG	NE-CZ-NH1	5.46	123.03	120.30
8	P	237	GLN	CB-CG-CD	5.46	125.78	111.60
4	E	399	CYS	CB-CA-C	5.41	121.22	110.40
1	S	951	ARG	NE-CZ-NH1	5.41	123.01	120.30
2	B	526	ARG	CB-CG-CD	5.40	125.65	111.60
1	A	245	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	519	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	S	961	GLU	CB-CA-C	-5.40	99.60	110.40
2	B	728	PHE	CB-CA-C	5.39	121.19	110.40
8	P	654	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	U	324	ASP	CB-CA-C	5.34	121.08	110.40
6	H	321	PHE	CB-CA-C	5.34	121.07	110.40
8	P	479	ARG	NE-CZ-NH1	-5.33	117.63	120.30
6	G	384	PRO	CB-CA-C	-5.33	98.68	112.00
2	B	736	ARG	NE-CZ-NH2	-5.29	117.65	120.30
7	M	39	ARG	NE-CZ-NH1	5.26	122.93	120.30
5	F	306	GLU	CB-CA-C	5.26	120.92	110.40
2	B	386	ASN	CB-CA-C	5.24	120.89	110.40
2	O	421	LYS	CB-CA-C	5.24	120.89	110.40
4	E	465	THR	N-CA-CB	5.24	120.25	110.30
7	M	60	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	S	1033	ASP	CB-CG-OD2	5.22	123.00	118.30
4	E	427	GLU	CB-CA-C	5.21	120.82	110.40
7	M	349	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	93	PHE	CB-CG-CD1	5.19	124.43	120.80
12	V	356	TYR	CB-CG-CD1	5.19	124.11	121.00
12	V	1033	TYR	CB-CG-CD1	5.17	124.10	121.00
8	P	468	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	B	196	CYS	C-N-CA	5.16	134.59	121.70
4	E	503	ASN	CB-CA-C	5.15	120.71	110.40
8	Q	727	PRO	N-CA-CB	-5.15	96.94	102.60
3	C	245	ARG	CB-CG-CD	5.14	124.97	111.60
1	A	1080	ARG	NE-CZ-NH1	5.13	122.86	120.30
7	M	221	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	S	1023	GLU	CA-CB-CG	5.12	124.67	113.40
1	S	714	ARG	NE-CZ-NH1	5.08	122.84	120.30
11	U	318	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	1329	ARG	NE-CZ-NH1	5.06	122.83	120.30
8	P	358	VAL	CA-CB-CG2	5.05	118.48	110.90
2	B	423	TYR	CB-CA-C	-5.05	100.31	110.40
1	S	52	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	683	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	S	911	TRP	CB-CG-CD1	-5.03	120.46	127.00
8	P	155	PHE	CB-CG-CD1	5.02	124.31	120.80
2	B	725	THR	N-CA-CB	5.02	119.83	110.30
2	O	387	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	1350	GLU	Peptide
1	A	284	GLY	Peptide
1	A	286	GLN	Peptide
1	A	484	GLU	Peptide
1	A	824	CYS	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	258	ALA	Peptide
2	B	265	LEU	Peptide
2	B	287	VAL	Peptide
2	B	309	CYS	Peptide
2	B	345	PHE	Peptide
2	B	354	LEU	Peptide
2	B	361	ASP	Peptide
2	B	38	THR	Peptide
2	B	518	PHE	Peptide
2	B	636	PHE	Peptide
2	B	637	PRO	Peptide
2	B	696	ARG	Peptide
2	B	711	THR	Peptide
2	B	734	LEU	Peptide
3	C	173	ARG	Peptide
3	C	208	GLY	Peptide
3	C	24	GLN	Peptide
3	C	400	PHE	Peptide
3	C	539	GLU	Peptide
3	C	83	TYR	Peptide
4	E	352	SER	Peptide
4	E	464	MET	Peptide
4	E	50	LEU	Peptide
4	E	516	LEU	Peptide
4	E	519	ASN	Peptide
5	F	343	GLY	Peptide
6	G	388	PRO	Peptide
6	G	500	GLU	Peptide
6	G	563	ARG	Peptide
6	H	563	ARG	Peptide

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Mol	Chain	Res	Type	Group
7	L	103	ALA	Peptide
7	L	122	GLY	Peptide
7	L	135	THR	Peptide
7	L	168	ASP	Peptide
7	L	169	PHE	Peptide
2	O	154	SER	Peptide
2	O	213	CYS	Peptide
2	O	247	ILE	Peptide
2	O	312	TRP	Peptide
2	O	636	PHE	Peptide
2	O	637	PRO	Peptide
2	O	696	ARG	Peptide
2	O	748	LYS	Peptide
8	P	13	GLY	Peptide
8	P	23	ALA	Peptide
8	P	24	GLY	Peptide
8	P	263	SER	Peptide
8	P	292	PRO	Peptide
8	P	344	PRO	Peptide
8	P	345	GLY	Peptide
8	P	36	PHE	Peptide
8	P	383	PRO	Peptide
8	P	389	GLY	Peptide
8	P	392	PRO	Peptide
8	P	427	GLY	Peptide
8	P	449	GLU	Peptide
8	P	513	THR	Peptide
8	P	556	LEU	Peptide
8	P	594	LEU	Peptide,Mainchain
8	P	60	PHE	Peptide
8	P	635	GLN	Peptide
8	P	683	CYS	Peptide
8	P	724	SER	Peptide
8	P	725	GLY	Peptide
8	P	781	PRO	Peptide
8	P	820	SER	Peptide
8	Q	534	SER	Peptide
8	Q	549	THR	Peptide
8	Q	569	VAL	Peptide
8	Q	584	LEU	Peptide
8	Q	594	LEU	Peptide
8	Q	604	TYR	Peptide

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Mol	Chain	Res	Type	Group
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	561	THR	Peptide
1	S	736	VAL	Peptide
1	S	822	LEU	Peptide
1	S	922	GLU	Peptide
1	S	923	GLU	Peptide
1	S	960	HIS	Peptide
11	U	1042	PRO	Peptide
11	U	1187	SER	Peptide
11	U	1270	LYS	Peptide
11	U	306	SER	Peptide
11	U	323	GLN	Peptide
11	U	359	TYR	Peptide
11	U	373	HIS	Peptide
11	U	451	ARG	Peptide
11	U	452	ALA	Peptide
11	U	488	LEU	Peptide
11	U	547	PHE	Peptide
11	U	641	LEU	Peptide
11	U	860	SER	Peptide
12	V	1224	PRO	Peptide
12	V	204	PRO	Peptide
12	V	222	SER	Peptide
12	V	293	ASP	Peptide
12	V	377	HIS	Peptide
12	V	411	CYS	Peptide
12	V	485	ASN	Peptide
12	V	541	PHE	Peptide
12	V	564	SER	Peptide
10	X	152	ARG	Peptide
10	X	61	TYR	Peptide
10	X	93	PRO	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	200	0
1	S	9933	10028	9969	210	0
2	B	5605	5790	5768	166	0
2	O	5594	5759	5740	106	0
3	C	4396	4442	4427	115	0
4	E	3224	3390	3384	134	0
5	F	2726	2740	2729	72	0
6	G	4483	4537	4523	107	0
6	H	4216	4288	4273	108	0
7	L	2974	2977	2970	48	0
7	M	2974	2977	2972	97	0
8	P	5598	5681	5652	218	0
8	Q	5631	5724	5694	102	0
9	W	271	242	196	10	0
10	X	1233	1251	1248	24	0
11	U	9350	9739	9708	238	0
12	V	8997	9224	9173	196	0
13	Y	458	246	246	1	0
14	Z	444	248	248	1	0
15	G	1	0	0	0	0
15	L	2	0	0	0	0
15	M	2	0	0	0	0
All	All	87514	88770	88351	1979	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 (1979) 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)
4:E:391:CYS:SG	4:E:398:VAL:HG11	1.86	1.14
6:H:345:GLN:HG2	6:H:386:PRO:HB3	1.20	1.12
2:B:828:LEU:HD23	8:P:826:ARG:HA	1.33	1.10
1:A:35:TYR:CE1	6:H:311:ASN:CB	2.36	1.09
12:V:146:GLN:HE22	12:V:186:VAL:HA	1.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:CE1	6:H:311:ASN:HB3	1.92	1.04
4:E:387:LEU:HD12	4:E:391:CYS:HG	1.24	1.02
5:F:311:PHE:O	5:F:315:CYS:SG	2.16	1.02
8:P:243:CYS:SG	8:P:251:CYS:HB2	2.00	1.02
6:H:345:GLN:HG2	6:H:386:PRO:CB	1.90	1.01
12:V:965:LEU:HD11	12:V:1027:LEU:HD13	1.42	1.01
1:A:32:ARG:HD3	6:H:343:GLN:HE22	1.24	1.00
2:B:828:LEU:CD2	8:P:826:ARG:HA	1.92	0.98
4:E:387:LEU:HD12	4:E:391:CYS:SG	2.05	0.96
11:U:503:VAL:O	11:U:506:LEU:HG	1.65	0.96
2:B:522:LYS:O	2:B:582:THR:OG1	1.81	0.96
6:H:345:GLN:CG	6:H:386:PRO:HB3	1.94	0.96
1:A:35:TYR:HE1	6:H:311:ASN:CB	1.79	0.95
1:S:561:THR:HG22	1:S:562:GLY:O	1.70	0.91
1:A:35:TYR:CD1	6:H:311:ASN:HB3	2.05	0.91
1:A:32:ARG:HD3	6:H:343:GLN:NE2	1.86	0.91
2:B:667:TYR:CE2	6:H:239:LEU:HD13	2.08	0.88
8:Q:11:LEU:HD11	8:Q:429:LEU:HD22	1.56	0.88
1:S:288:GLU:HB3	1:S:292:HIS:HB2	1.57	0.86
3:C:266:ARG:NH2	3:C:310:GLU:OE2	2.08	0.85
5:F:252:CYS:O	5:F:310:ARG:NH1	2.11	0.84
7:L:16:LEU:HD11	8:P:483:LEU:HD22	1.60	0.84
8:P:402:CYS:O	8:P:402:CYS:SG	2.36	0.84
1:A:35:TYR:CE1	6:H:311:ASN:HB2	2.14	0.83
8:P:220:LEU:HD13	8:P:224:LEU:HD22	1.61	0.83
2:O:401:CYS:SG	7:M:107:PRO:HG2	2.20	0.82
2:B:828:LEU:HD23	8:P:826:ARG:CA	2.09	0.81
2:B:61:SER:OG	2:B:116:ASN:ND2	2.13	0.81
2:B:337:GLY:O	8:P:395:CYS:HA	1.79	0.81
4:E:321:PRO:HA	4:E:324:MET:HB3	1.62	0.81
6:G:306:LEU:HD21	6:G:346:THR:HG21	1.63	0.81
1:S:1033:ASP:OD2	1:S:1093:SER:HB2	1.82	0.80
12:V:816:LEU:O	12:V:820:VAL:HG13	1.81	0.80
8:P:361:SER:CB	8:P:398:SER:O	2.29	0.80
2:B:17:CYS:O	2:B:17:CYS:SG	2.40	0.79
1:S:1075:LEU:HD12	1:S:1119:PHE:HD2	1.47	0.79
2:O:526:ARG:NH2	2:O:652:LEU:O	2.14	0.79
6:G:346:THR:O	6:G:349:ILE:N	2.15	0.79
11:U:669:CYS:SG	11:U:804:LEU:O	2.41	0.79
1:A:1113:ASN:O	1:A:1117:ARG:NE	2.16	0.79
3:C:267:ASN:O	3:C:555:ARG:NH2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:391:CYS:SG	4:E:423:LEU:HD21	2.23	0.79
7:M:365:PRO:HB3	11:U:266:HIS:NE2	1.98	0.79
1:S:988:LEU:HD21	1:S:1077:MET:CE	2.13	0.78
3:C:124:ALA:O	5:F:140:ARG:NH1	2.16	0.78
1:S:868:PHE:CZ	1:S:910:LEU:HD22	2.18	0.78
11:U:474:LEU:HD22	11:U:506:LEU:HD11	1.66	0.78
6:H:410:ALA:HB3	6:H:466:LEU:HD22	1.65	0.78
6:G:406:GLN:NE2	6:G:599:TRP:HB2	2.00	0.77
11:U:1213:ILE:HD11	11:U:1253:LEU:HD23	1.65	0.77
5:F:255:LEU:HD12	5:F:260:LEU:HD21	1.67	0.76
1:A:286:GLN:C	1:A:288:GLU:H	1.88	0.76
4:E:343:ARG:O	4:E:346:THR:HB	1.86	0.76
4:E:382:LEU:O	4:E:386:ALA:N	2.19	0.76
2:B:16:LEU:HD23	2:B:17:CYS:N	1.99	0.75
7:M:234:VAL:HG11	7:M:259:VAL:HG11	1.66	0.75
1:S:1075:LEU:HD11	1:S:1115:GLU:HB3	1.67	0.75
11:U:69:TYR:OH	11:U:96:GLU:O	2.03	0.75
12:V:205:GLU:HA	12:V:208:GLN:HG2	1.69	0.75
8:P:154:LEU:HD22	8:P:258:LEU:HD23	1.67	0.75
6:G:214:ARG:NH1	6:G:328:LEU:O	2.19	0.74
11:U:711:ASN:HA	11:U:714:ILE:HD12	1.69	0.74
4:E:446:TRP:CZ2	4:E:454:LEU:HD22	2.23	0.74
7:L:155:LYS:NZ	7:L:162:SER:O	2.21	0.74
6:G:137:SER:OG	6:G:190:GLU:OE1	2.03	0.74
4:E:372:ILE:HA	4:E:375:LEU:HD12	1.68	0.74
11:U:808:LYS:O	11:U:811:SER:OG	2.06	0.74
1:A:900:SER:OG	1:A:903:TRP:CD1	2.39	0.74
3:C:134:PHE:CE2	5:F:166:GLN:HB3	2.23	0.73
7:M:342:LEU:CD2	7:M:357:GLY:HA3	2.18	0.73
8:P:133:PHE:CG	8:P:133:PHE:O	2.39	0.73
8:P:359:TYR:O	8:P:401:ILE:HD13	1.89	0.73
1:S:737:ALA:HB1	1:S:738:PRO:HD2	1.70	0.73
8:Q:516:ARG:NH2	8:Q:521:ASP:OD1	2.22	0.73
8:P:260:THR:HB	8:P:264:ALA:O	1.88	0.73
2:B:89:ILE:O	2:B:91:LEU:HG	1.88	0.73
1:S:988:LEU:HD21	1:S:1077:MET:HE2	1.69	0.73
1:S:1263:PHE:CZ	1:S:1322:VAL:HG11	2.24	0.73
1:S:414:LEU:HD12	1:S:426:SER:HB3	1.71	0.73
4:E:298:LEU:HD11	4:E:347:TRP:CZ3	2.24	0.72
7:M:342:LEU:HD21	7:M:357:GLY:HA3	1.70	0.72
7:M:361:TYR:CE1	10:X:101:SER:HA	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:62:ALA:HB2	6:G:102:ARG:HD2	1.70	0.72
2:B:703:THR:HG22	2:B:705:PHE:HE1	1.54	0.72
5:F:201:PHE:CE2	5:F:205:ILE:HD11	2.24	0.72
11:U:316:VAL:HG12	11:U:326:VAL:HG21	1.72	0.72
3:C:316:GLN:NE2	3:C:405:GLU:OE2	2.21	0.72
11:U:426:LEU:HD23	11:U:440:ILE:HG23	1.72	0.71
1:S:974:ASP:O	1:S:976:ASP:N	2.24	0.71
6:H:68:PRO:O	6:H:72:THR:OG1	2.08	0.71
7:M:365:PRO:HG3	11:U:266:HIS:CE1	2.24	0.71
6:G:393:MET:SD	8:P:236:LEU:HD21	2.30	0.71
6:H:388:PRO:HD2	6:H:389:PRO:HD3	1.72	0.71
7:M:79:ASP:OD1	7:M:80:LEU:N	2.23	0.71
3:C:134:PHE:HD2	5:F:166:GLN:HE21	1.36	0.71
6:H:239:LEU:HD12	6:H:240:CYS:N	2.06	0.71
1:A:1076:LEU:HD23	1:A:1120:CYS:SG	2.30	0.71
4:E:320:SER:O	4:E:324:MET:N	2.17	0.71
1:S:1075:LEU:HD12	1:S:1119:PHE:CD2	2.24	0.70
1:A:1075:LEU:HD12	1:A:1119:PHE:CD2	2.25	0.70
12:V:302:ARG:NE	12:V:367:ALA:O	2.24	0.70
8:P:230:GLY:O	8:P:234:THR:OG1	2.10	0.70
12:V:114:LEU:O	12:V:179:GLN:NE2	2.25	0.70
2:O:519:ARG:HG3	2:O:520:LEU:O	1.92	0.69
1:A:830:LEU:HD22	1:A:871:LEU:HD21	1.74	0.69
3:C:315:ILE:CG2	3:C:399:HIS:HA	2.22	0.69
2:O:588:LEU:O	2:O:591:SER:N	2.23	0.69
6:G:377:SER:O	8:P:256:LYS:NZ	2.26	0.69
7:L:155:LYS:NZ	7:L:164:ASP:OD1	2.25	0.69
11:U:450:THR:HG21	12:V:356:TYR:O	1.91	0.69
6:G:235:ALA:O	6:G:240:CYS:SG	2.51	0.69
1:S:751:ARG:HA	1:S:754:CYS:SG	2.32	0.69
7:M:193:ALA:O	7:M:196:SER:OG	2.09	0.69
7:M:333:PHE:CZ	7:M:360:PRO:HD2	2.28	0.69
1:A:295:VAL:HG12	1:A:354:LEU:HD12	1.75	0.69
5:F:205:ILE:O	5:F:208:ALA:HB3	1.93	0.69
6:G:81:ARG:HG2	6:G:92:GLN:HE21	1.56	0.69
8:P:25:LYS:NZ	8:P:192:HIS:O	2.25	0.69
7:M:95:LEU:HD22	7:M:102:TYR:OH	1.92	0.69
7:M:354:ILE:CG1	7:M:369:LYS:HG2	2.22	0.69
1:A:656:ALA:HB3	1:A:683:ARG:NH2	2.08	0.69
7:M:58:GLN:O	7:M:61:THR:OG1	2.11	0.69
11:U:1268:SER:HA	11:U:1273:VAL:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:432:CYS:HA	12:V:465:PHE:HE2	1.57	0.69
6:G:414:LEU:HD21	6:G:462:ALA:HB3	1.74	0.68
1:S:770:ARG:NH1	1:S:820:SER:O	2.26	0.68
2:O:155:SER:O	2:O:156:GLN:HB3	1.92	0.68
1:A:822:LEU:HD12	1:A:867:LYS:HD3	1.75	0.68
2:B:703:THR:CG2	2:B:705:PHE:HE1	2.06	0.68
1:S:1161:THR:O	1:S:1321:ARG:NH2	2.27	0.68
11:U:668:LEU:C	11:U:752:VAL:HG11	2.14	0.68
8:P:151:LYS:HB2	8:P:173:VAL:O	1.94	0.68
8:Q:604:TYR:HB3	8:Q:638:VAL:HG23	1.74	0.68
5:F:203:LYS:O	5:F:207:VAL:HG23	1.94	0.68
1:S:1336:TYR:OH	1:S:1357:ALA:O	2.11	0.68
8:Q:716:ARG:O	8:Q:720:LYS:HG3	1.92	0.68
11:U:293:LEU:HD12	11:U:313:LEU:HD21	1.75	0.68
2:O:176:ILE:HG23	2:O:245:THR:HG21	1.75	0.68
1:S:477:LEU:HD13	1:S:510:TYR:OH	1.93	0.68
6:G:406:GLN:HE21	6:G:599:TRP:HB2	1.59	0.67
8:P:200:VAL:HG21	8:P:242:LEU:HD12	1.76	0.67
3:C:240:VAL:HG22	3:C:284:ALA:HA	1.76	0.67
11:U:66:ARG:NH1	11:U:70:THR:OG1	2.28	0.67
11:U:473:VAL:HG13	11:U:474:LEU:HD12	1.75	0.67
1:A:474:PHE:HD1	1:A:477:LEU:HD12	1.59	0.67
6:G:136:LEU:HD23	6:G:136:LEU:H	1.60	0.67
2:O:482:VAL:HG13	2:O:584:LEU:HD11	1.77	0.67
1:A:1336:TYR:OH	1:A:1357:ALA:O	2.11	0.67
6:G:521:GLY:HA3	6:G:537:PHE:CE1	2.29	0.67
7:L:109:GLN:O	7:L:113:SER:OG	2.07	0.67
8:P:363:PRO:HA	8:P:397:ALA:HB2	1.77	0.67
8:Q:570:ASP:OD1	8:Q:570:ASP:N	2.25	0.67
2:B:526:ARG:NH2	2:B:653:ALA:O	2.29	0.67
6:H:103:VAL:O	6:H:106:THR:OG1	2.12	0.66
8:P:368:VAL:O	8:P:390:LEU:HB2	1.95	0.66
1:S:818:PHE:HA	1:S:821:LEU:HB2	1.77	0.66
11:U:1095:VAL:HG13	11:U:1137:GLN:NE2	2.11	0.66
8:Q:494:CYS:SG	7:M:20:ARG:O	2.54	0.66
11:U:521:LEU:HD22	11:U:536:ALA:HA	1.77	0.66
6:G:306:LEU:O	6:G:309:ALA:HB3	1.96	0.66
8:P:371:LEU:O	8:P:385:GLU:OE2	2.14	0.66
4:E:522:PHE:C	4:E:523:LEU:HG	2.16	0.65
6:G:453:SER:HB2	6:G:483:LEU:HD23	1.78	0.65
11:U:442:GLU:OE2	11:U:480:LYS:NZ	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:HB3	1:A:288:GLU:HG3	1.78	0.65
12:V:938:CYS:HG	12:V:960:LEU:N	1.95	0.65
4:E:497:MET:O	4:E:501:GLN:CG	2.44	0.65
5:F:274:TYR:HE2	5:F:314:LEU:HD21	1.59	0.65
4:E:476:LEU:HD13	4:E:492:LEU:HD23	1.78	0.65
8:Q:37:LEU:CD1	8:Q:429:LEU:HD12	2.25	0.65
7:M:8:LEU:HD21	7:M:25:TYR:HE2	1.62	0.65
12:V:208:GLN:O	12:V:212:ILE:HG12	1.96	0.65
11:U:440:ILE:O	11:U:444:VAL:HG23	1.97	0.65
1:A:769:LEU:HD13	1:A:821:LEU:HD11	1.78	0.65
4:E:518:PRO:HB2	4:E:520:THR:HG22	1.79	0.65
4:E:522:PHE:HA	4:E:524:ARG:CZ	2.27	0.65
6:G:475:GLU:OE2	6:G:478:ARG:NH2	2.30	0.65
8:P:196:VAL:O	8:P:243:CYS:HA	1.95	0.65
1:S:485:SER:OG	1:S:490:GLN:NE2	2.29	0.65
1:S:1075:LEU:HD11	1:S:1115:GLU:CB	2.27	0.65
11:U:874:LEU:O	11:U:878:THR:OG1	2.12	0.65
12:V:110:PHE:CZ	12:V:114:LEU:HD11	2.33	0.65
1:S:351:THR:HG21	1:S:391:SER:HB2	1.79	0.64
11:U:424:ASN:O	11:U:428:GLU:HG2	1.97	0.64
5:F:317:ALA:HB1	5:F:318:PRO:CD	2.27	0.64
6:H:23:LEU:HD22	6:H:46:ALA:HA	1.78	0.64
1:S:288:GLU:CB	1:S:292:HIS:HB2	2.25	0.64
12:V:452:SER:O	12:V:455:SER:OG	2.14	0.64
3:C:142:PRO:HA	3:C:145:TYR:CE1	2.32	0.64
8:Q:229:PHE:HE1	8:Q:252:CYS:HG	1.42	0.64
5:F:116:PHE:HA	5:F:130:GLN:HE21	1.62	0.64
2:B:667:TYR:CD2	6:H:239:LEU:HD13	2.33	0.64
2:O:777:ILE:HG21	8:Q:830:LEU:HD13	1.79	0.64
4:E:383:LEU:HA	4:E:386:ALA:HB3	1.80	0.64
3:C:111:ASN:HA	3:C:114:ILE:HD12	1.80	0.64
3:C:355:ASP:OD1	3:C:535:ARG:NH1	2.30	0.64
6:H:71:LEU:O	6:H:75:CYS:SG	2.54	0.64
2:B:21:GLU:HB2	2:B:48:MET:O	1.98	0.64
11:U:202:PHE:CE1	11:U:210:ILE:HG23	2.32	0.64
1:A:833:CYS:O	1:A:837:CYS:SG	2.54	0.64
11:U:1213:ILE:HG21	11:U:1250:ILE:HG23	1.78	0.64
12:V:307:LEU:HD11	12:V:380:PHE:HD2	1.62	0.64
1:A:715:GLU:O	1:A:719:VAL:HG12	1.98	0.64
3:C:348:LEU:HD23	3:C:396:LEU:CD2	2.28	0.64
12:V:307:LEU:HD11	12:V:380:PHE:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:457:LEU:HD11	6:G:516:ALA:HA	1.80	0.63
8:P:284:PHE:CD2	8:P:350:ALA:HB3	2.32	0.63
1:S:428:VAL:HG22	1:S:476:PHE:CE1	2.33	0.63
1:S:765:LEU:HD11	1:S:787:LEU:HD21	1.80	0.63
7:L:126:LEU:HD11	7:L:128:TYR:O	1.97	0.63
2:O:850:ASP:O	8:Q:798:CYS:HB3	1.98	0.63
7:M:247:MET:SD	11:U:508:LYS:O	2.57	0.63
4:E:446:TRP:CH2	4:E:454:LEU:HD22	2.33	0.63
2:O:840:LEU:HD21	8:Q:812:VAL:CG1	2.28	0.63
1:S:37:PRO:O	1:S:41:GLN:OE1	2.17	0.63
3:C:122:LEU:O	5:F:140:ARG:NE	2.31	0.63
1:S:762:LEU:HD23	1:S:765:LEU:HD12	1.81	0.63
4:E:283:ALA:O	4:E:287:GLN:HG2	1.98	0.63
4:E:454:LEU:HD21	4:E:472:LEU:HD13	1.79	0.63
11:U:679:LYS:HA	11:U:683:ILE:HD12	1.81	0.63
3:C:266:ARG:NH2	3:C:520:HIS:HB3	2.12	0.63
7:M:320:PRO:HD3	7:M:334:HIS:HE2	1.64	0.63
1:A:939:ILE:O	1:A:1013:GLY:HA2	1.99	0.62
1:A:1176:SER:HA	1:S:964:LEU:HD13	1.80	0.62
2:B:664:SER:OG	2:B:667:TYR:HB2	1.99	0.62
1:S:855:THR:HG22	1:S:858:SER:OG	1.99	0.62
2:B:674:VAL:O	2:B:678:GLU:N	2.27	0.62
1:S:1033:ASP:CG	1:S:1093:SER:HB2	2.19	0.62
2:B:277:CYS:SG	2:B:278:GLN:N	2.71	0.62
8:P:196:VAL:N	8:P:244:GLY:O	2.28	0.62
1:S:835:LYS:HG2	1:S:903:TRP:CE3	2.33	0.62
11:U:909:LEU:HA	11:U:912:LEU:HD12	1.82	0.62
12:V:561:LYS:O	12:V:564:SER:OG	2.17	0.62
11:U:115:ALA:HB1	11:U:121:LEU:HD21	1.82	0.62
8:P:130:LEU:CA	8:P:144:VAL:HG23	2.29	0.62
8:P:253:VAL:HG23	8:P:272:VAL:HA	1.82	0.62
3:C:220:PHE:CD2	3:C:246:HIS:HB3	2.35	0.62
11:U:306:SER:N	11:U:309:SER:OG	2.33	0.62
8:P:156:GLU:O	8:P:166:PRO:O	2.16	0.62
8:P:203:SER:OG	8:P:222:ASP:OD1	2.17	0.61
6:H:388:PRO:HD2	6:H:389:PRO:CD	2.29	0.61
6:H:388:PRO:CD	6:H:389:PRO:HD3	2.30	0.61
1:A:1143:LEU:HD21	1:A:1185:TRP:CZ3	2.35	0.61
5:F:133:LEU:N	5:F:133:LEU:HD23	2.14	0.61
12:V:1128:PHE:CZ	12:V:1185:LEU:HD22	2.35	0.61
4:E:73:VAL:HB	4:E:75:GLN:HE21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:354:ILE:HG12	7:M:369:LYS:HG2	1.83	0.61
1:A:35:TYR:HE1	6:H:311:ASN:CG	2.02	0.61
6:H:564:ARG:O	6:H:568:THR:OG1	2.18	0.61
8:P:29:LEU:HB2	8:P:36:PHE:HB2	1.82	0.61
8:Q:30:CYS:SG	8:Q:404:VAL:HB	2.41	0.61
2:B:18:TYR:CE2	2:B:92:PRO:HD3	2.35	0.61
6:G:147:ALA:HB1	6:G:159:LEU:HD11	1.82	0.61
5:F:189:LEU:HA	5:F:192:LEU:HD12	1.83	0.61
1:A:770:ARG:NH1	1:A:820:SER:O	2.34	0.60
2:O:614:TYR:CG	8:Q:639:CYS:HB3	2.37	0.60
12:V:234:LEU:O	12:V:238:ASN:N	2.34	0.60
6:G:67:LEU:HD21	6:G:103:VAL:HG22	1.83	0.60
2:B:711:THR:O	2:B:713:PHE:N	2.34	0.60
4:E:500:TYR:HA	4:E:503:ASN:HD22	1.67	0.60
6:H:306:LEU:CD2	6:H:346:THR:HG21	2.32	0.60
11:U:134:LEU:HD11	11:U:160:LEU:HD23	1.83	0.60
2:B:393:PRO:HA	7:L:131:THR:O	2.01	0.60
2:O:401:CYS:SG	7:M:107:PRO:CG	2.88	0.60
1:S:830:LEU:HD23	1:S:871:LEU:CD2	2.31	0.60
7:M:354:ILE:HG13	7:M:369:LYS:HG2	1.82	0.60
1:A:32:ARG:CD	6:H:343:GLN:HE22	2.08	0.60
2:B:19:ASN:HA	8:P:428:ARG:NH1	2.16	0.60
3:C:196:VAL:C	3:C:198:PRO:HD2	2.22	0.60
3:C:240:VAL:CG2	3:C:284:ALA:HA	2.31	0.60
6:G:249:TYR:HA	6:G:252:LEU:HD12	1.83	0.60
6:G:252:LEU:HD13	6:G:268:TYR:CE1	2.37	0.60
8:P:51:GLY:O	8:P:53:LEU:N	2.34	0.60
2:B:487:LEU:O	2:B:581:VAL:HA	2.02	0.60
2:O:248:ILE:O	2:O:249:LYS:O	2.20	0.60
11:U:931:LEU:HD23	11:U:934:LEU:HD12	1.82	0.60
1:A:1174:TRP:HB3	1:A:1204:ARG:NH1	2.17	0.60
4:E:462:VAL:N	4:E:500:TYR:OH	2.34	0.60
11:U:487:TYR:O	11:U:491:LEU:HG	2.01	0.60
2:B:392:PRO:HB2	7:L:131:THR:HG22	1.82	0.60
1:A:185:LEU:HD12	1:A:191:VAL:HG22	1.82	0.60
3:C:269:LEU:HD21	3:C:313:ALA:HB1	1.83	0.60
4:E:487:MET:HG2	12:V:202:ILE:CG2	2.32	0.60
4:E:516:LEU:HD22	4:E:527:LEU:HD13	1.82	0.60
5:F:98:LEU:O	5:F:101:ARG:NH2	2.35	0.60
8:P:362:THR:HB	8:P:363:PRO:HD2	1.83	0.60
7:M:275:ASP:OD2	7:M:278:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:102:GLY:HA3	11:U:144:LEU:HD22	1.82	0.60
12:V:382:LEU:O	12:V:385:LEU:N	2.34	0.60
2:O:93:TYR:CE2	2:O:136:VAL:HG21	2.36	0.59
7:M:185:SER:O	7:M:188:SER:OG	2.15	0.59
10:X:36:ALA:HB3	10:X:53:LEU:HB2	1.82	0.59
1:A:818:PHE:CE1	1:A:864:LEU:HG	2.36	0.59
6:H:72:THR:O	6:H:76:ASN:ND2	2.35	0.59
8:Q:603:PHE:HA	8:Q:638:VAL:O	2.02	0.59
11:U:1060:ILE:HD11	11:U:1149:VAL:O	2.01	0.59
1:S:736:VAL:HG21	9:W:80:VAL:HG21	1.83	0.59
12:V:417:LEU:HD22	12:V:453:PHE:CE1	2.37	0.59
1:A:868:PHE:CZ	1:A:910:LEU:HD23	2.37	0.59
1:S:513:LEU:O	1:S:516:THR:OG1	2.18	0.59
12:V:820:VAL:HG21	12:V:964:GLU:HA	1.82	0.59
2:O:489:VAL:HG21	2:O:508:LEU:HD21	1.83	0.59
8:P:143:LEU:HD12	8:P:197:LEU:HD21	1.84	0.59
8:P:195:PRO:HB2	8:P:245:LEU:HD23	1.84	0.59
1:A:108:PRO:HG2	1:A:111:ILE:HD12	1.84	0.59
2:B:308:ALA:HB3	2:B:325:LEU:CD1	2.33	0.59
4:E:315:LEU:HA	4:E:318:GLU:HG2	1.85	0.59
5:F:196:LEU:HD21	5:F:201:PHE:CD1	2.38	0.59
6:H:244:VAL:O	6:H:248:VAL:HG23	2.02	0.59
11:U:450:THR:OG1	12:V:356:TYR:CG	2.55	0.59
1:A:474:PHE:CD2	1:A:510:TYR:CZ	2.90	0.59
2:B:259:LEU:HD11	2:B:284:PRO:HB2	1.84	0.59
2:B:521:LEU:O	8:P:565:TYR:HA	2.03	0.59
3:C:197:ASP:N	3:C:198:PRO:CD	2.66	0.59
8:Q:517:LEU:O	8:Q:519:THR:N	2.35	0.59
10:X:138:ALA:O	10:X:142:ASN:ND2	2.36	0.59
4:E:497:MET:O	4:E:501:GLN:HG2	2.02	0.59
6:G:266:LEU:O	6:G:270:VAL:HG23	2.03	0.59
1:S:1131:THR:HG22	1:S:1177:LEU:HD11	1.85	0.59
11:U:21:LEU:HD22	11:U:64:ARG:HG2	1.85	0.59
1:S:1020:ARG:O	1:S:1023:GLU:HB2	2.03	0.58
2:B:122:LEU:HD21	2:B:155:SER:HA	1.85	0.58
6:G:146:GLN:NE2	6:G:150:TRP:CE2	2.69	0.58
6:G:397:PHE:CE1	8:P:235:LEU:HD22	2.37	0.58
12:V:684:TYR:O	12:V:815:ARG:NH1	2.35	0.58
4:E:497:MET:O	4:E:501:GLN:HG3	2.02	0.58
11:U:982:ALA:O	11:U:986:VAL:HG23	2.02	0.58
1:A:1101:ILE:HG21	1:A:1154:PHE:CZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:306:LEU:HD21	6:G:346:THR:CG2	2.33	0.58
11:U:533:ARG:HD2	11:U:597:GLN:HE22	1.69	0.58
5:F:294:TRP:NE1	5:F:349:ASP:OD2	2.36	0.58
6:G:89:THR:OG1	6:G:90:GLU:N	2.36	0.58
1:S:795:ARG:HD2	1:S:815:PRO:HD3	1.84	0.58
1:S:1025:VAL:HG21	1:S:1085:LEU:HD13	1.86	0.58
3:C:188:VAL:HG22	3:C:219:PHE:HA	1.85	0.58
3:C:366:GLN:HE21	7:L:272:HIS:CE1	2.22	0.58
8:P:655:PHE:CE2	8:P:754:ILE:HD12	2.39	0.58
12:V:60:LYS:NZ	12:V:64:SER:OG	2.36	0.58
12:V:432:CYS:HA	12:V:465:PHE:CE2	2.38	0.58
12:V:1115:VAL:HG21	12:V:1142:LEU:HD21	1.85	0.58
2:B:426:LEU:O	2:B:429:LEU:HB3	2.04	0.58
4:E:497:MET:CG	4:E:512:LEU:HD13	2.34	0.58
7:M:349:ARG:HD3	11:U:273:LEU:CD2	2.34	0.58
11:U:317:THR:HA	11:U:323:GLN:HA	1.85	0.58
11:U:443:GLN:OE1	11:U:447:ARG:NH2	2.36	0.58
1:A:663:SER:HB3	1:A:676:GLN:HE22	1.68	0.58
3:C:134:PHE:HE2	5:F:166:GLN:HB3	1.67	0.58
2:O:669:LEU:O	2:O:709:GLN:NE2	2.36	0.58
8:P:20:GLY:HA3	8:P:425:ALA:O	2.03	0.58
1:S:664:MET:HG2	1:S:729:ASN:HD22	1.67	0.58
1:A:392:PHE:CE1	1:A:396:LEU:HD13	2.38	0.58
2:O:394:LEU:HD11	7:M:115:ILE:HD11	1.85	0.58
8:P:253:VAL:HG23	8:P:272:VAL:HG23	1.85	0.58
12:V:343:ILE:O	12:V:346:LEU:HB3	2.04	0.58
6:G:453:SER:HB2	6:G:483:LEU:CD2	2.34	0.57
11:U:928:GLN:OE1	11:U:954:ARG:NE	2.37	0.57
11:U:1075:VAL:HG13	11:U:1080:ALA:HB2	1.85	0.57
12:V:385:LEU:HD22	12:V:399:ILE:HG23	1.86	0.57
3:C:60:VAL:HG23	3:C:64:PHE:CZ	2.39	0.57
3:C:308:ALA:HB1	4:E:171:LEU:HD21	1.86	0.57
1:S:424:LEU:O	1:S:428:VAL:HG23	2.04	0.57
12:V:175:LEU:O	12:V:178:SER:OG	2.17	0.57
8:P:735:TRP:O	8:P:807:ARG:NH1	2.37	0.57
1:S:1139:LEU:CD2	1:S:1181:LEU:HD22	2.34	0.57
7:M:354:ILE:HA	7:M:368:LEU:O	2.05	0.57
12:V:64:SER:O	12:V:112:ASN:ND2	2.38	0.57
2:B:525:ASN:HD22	2:B:525:ASN:N	2.03	0.57
1:A:1118:ASN:HA	1:A:1324:PRO:HB3	1.87	0.57
5:F:345:SER:HB3	5:F:348:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:365:GLU:HG3	1:S:29:ARG:HH22	1.70	0.57
8:P:335:VAL:HG13	8:P:336:PRO:HD2	1.85	0.57
1:S:993:GLN:HG3	1:S:1073:ARG:HD3	1.85	0.57
1:A:300:GLY:O	1:A:303:SER:OG	2.18	0.57
1:A:1025:VAL:HG21	1:A:1085:LEU:HD13	1.86	0.57
7:M:303:PHE:CZ	7:M:305:MET:HB3	2.39	0.57
3:C:179:ARG:NH2	5:F:152:ARG:HG3	2.19	0.57
5:F:160:ASP:O	5:F:164:LYS:HB2	2.05	0.57
11:U:395:PRO:HD2	11:U:458:HIS:ND1	2.20	0.57
12:V:412:ILE:HG23	12:V:416:LEU:CD1	2.34	0.57
4:E:524:ARG:HA	4:E:527:LEU:HD12	1.87	0.57
11:U:503:VAL:HG13	11:U:506:LEU:HD12	1.87	0.57
1:A:944:ASP:OD2	1:A:951:ARG:NH1	2.37	0.57
1:A:1252:GLU:O	1:A:1298:ARG:NH1	2.38	0.57
2:B:360:THR:OG1	2:B:362:LEU:N	2.38	0.57
3:C:170:ASN:ND2	7:L:345:LEU:O	2.36	0.57
4:E:387:LEU:CD1	4:E:391:CYS:SG	2.89	0.57
7:L:110:PHE:O	7:L:114:LEU:HD23	2.03	0.57
8:P:390:LEU:N	8:P:390:LEU:HD23	2.20	0.57
1:S:988:LEU:HD21	1:S:1077:MET:HE3	1.85	0.57
1:A:474:PHE:CD2	1:A:510:TYR:CE2	2.93	0.57
1:A:1075:LEU:HD11	1:A:1115:GLU:HB3	1.86	0.57
2:B:146:HIS:O	2:B:148:LYS:N	2.38	0.57
5:F:317:ALA:HB1	5:F:318:PRO:HD2	1.87	0.57
6:G:450:LEU:HD13	6:G:512:LEU:HD22	1.87	0.57
8:P:471:PHE:CD1	8:P:471:PHE:C	2.78	0.57
7:M:25:TYR:HB2	7:M:40:ILE:HG23	1.85	0.57
11:U:1213:ILE:HD11	11:U:1253:LEU:CD2	2.32	0.57
4:E:510:LEU:O	4:E:513:ALA:HB3	2.05	0.56
5:F:201:PHE:O	5:F:204:VAL:HB	2.05	0.56
2:O:634:LEU:HD21	2:O:647:ASP:CG	2.25	0.56
8:P:361:SER:HB2	8:P:398:SER:O	2.02	0.56
1:S:1183:CYS:SG	1:S:1184:ARG:N	2.78	0.56
12:V:431:MET:N	12:V:431:MET:SD	2.78	0.56
12:V:524:ILE:CG2	12:V:528:GLN:HB2	2.35	0.56
1:A:494:LEU:HD11	1:A:518:LEU:HD13	1.87	0.56
2:B:534:PRO:HA	2:B:572:LYS:CE	2.35	0.56
11:U:1092:ALA:HB2	11:U:1144:PHE:CZ	2.40	0.56
12:V:1119:GLN:HE21	12:V:1158:LEU:HD13	1.68	0.56
1:A:835:LYS:HE2	1:A:903:TRP:CE2	2.40	0.56
2:B:298:PHE:CE1	2:B:312:TRP:CD1	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:651:LEU:HD22	2:B:655:PHE:CE2	2.41	0.56
4:E:364:THR:HG23	4:E:368:PHE:CD2	2.40	0.56
7:M:158:TYR:O	7:M:161:GLU:O	2.24	0.56
11:U:169:TRP:CE3	11:U:177:LEU:HD23	2.40	0.56
12:V:196:ILE:O	12:V:199:LEU:HB3	2.06	0.56
12:V:439:ALA:HB2	12:V:457:LEU:HD23	1.86	0.56
2:B:16:LEU:HD23	2:B:17:CYS:C	2.26	0.56
6:H:306:LEU:HD22	6:H:346:THR:HG21	1.87	0.56
8:P:352:CYS:O	8:P:403:SER:HB3	2.05	0.56
1:A:288:GLU:HA	1:A:292:HIS:CB	2.35	0.56
2:B:703:THR:HG22	2:B:705:PHE:CE1	2.37	0.56
2:O:590:PHE:O	2:O:592:LYS:N	2.39	0.56
12:V:431:MET:HB3	12:V:434:SER:OG	2.06	0.56
5:F:201:PHE:O	5:F:205:ILE:HD13	2.06	0.56
6:G:374:LEU:O	6:G:377:SER:OG	2.24	0.56
6:G:399:GLU:HG3	6:G:592:TYR:HB3	1.88	0.56
2:O:520:LEU:HD11	8:Q:565:TYR:HB3	1.88	0.56
2:O:711:THR:O	2:O:713:PHE:N	2.39	0.56
1:S:1343:HIS:HE2	1:S:1349:ARG:HG3	1.71	0.56
7:M:207:ILE:HG12	7:M:281:LEU:HD21	1.88	0.56
12:V:263:ARG:HD2	12:V:267:MET:CE	2.36	0.56
12:V:568:PHE:O	12:V:572:LEU:HB2	2.06	0.56
8:P:519:THR:OG1	8:P:520:GLN:OE1	2.14	0.56
7:M:168:ASP:HB2	7:M:221:ARG:HB2	1.87	0.56
12:V:443:LEU:HD22	12:V:451:ILE:HG23	1.88	0.56
2:O:514:HIS:ND1	2:O:593:PHE:HA	2.20	0.56
2:O:710:ARG:NH1	2:O:714:GLU:OE1	2.39	0.56
1:S:923:GLU:N	1:S:923:GLU:OE2	2.36	0.56
11:U:1267:LEU:HD23	11:U:1275:LEU:CD1	2.36	0.56
11:U:314:LEU:HD21	11:U:330:LEU:CD1	2.35	0.56
1:A:194:GLN:HG3	1:A:241:MET:SD	2.45	0.56
2:B:298:PHE:CE1	2:B:312:TRP:HD1	2.23	0.56
2:B:170:ILE:O	2:B:170:ILE:HG23	2.05	0.55
2:O:170:ILE:O	2:O:170:ILE:HG22	2.06	0.55
8:P:151:LYS:HE3	8:P:153:GLN:HE21	1.71	0.55
11:U:770:ASP:O	11:U:774:LEU:HG	2.06	0.55
1:A:474:PHE:CE2	1:A:510:TYR:CE2	2.94	0.55
1:A:1239:GLU:HG3	1:A:1283:LYS:HG2	1.88	0.55
3:C:244:LEU:HD21	3:C:287:HIS:HE2	1.72	0.55
4:E:38:GLU:OE1	4:E:38:GLU:N	2.38	0.55
6:H:128:ALA:HA	6:H:131:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:346:TRP:CE2	1:S:387:GLN:HG2	2.41	0.55
11:U:369:LYS:O	11:U:372:VAL:HG23	2.06	0.55
12:V:172:ILE:HB	12:V:173:PRO:HD3	1.88	0.55
12:V:425:TYR:O	12:V:429:LYS:N	2.39	0.55
1:A:824:CYS:O	1:A:939:ILE:HG22	2.06	0.55
2:B:19:ASN:HA	8:P:428:ARG:HH12	1.71	0.55
2:B:521:LEU:HD11	2:B:587:LEU:HD21	1.88	0.55
4:E:494:LEU:O	4:E:498:THR:HG23	2.06	0.55
6:H:193:ALA:HB1	6:H:194:PRO:HD2	1.88	0.55
2:O:533:ASN:O	2:O:572:LYS:NZ	2.33	0.55
8:P:243:CYS:SG	8:P:251:CYS:CB	2.87	0.55
1:S:964:LEU:N	1:S:964:LEU:HD23	2.21	0.55
11:U:1177:VAL:HG13	11:U:1267:LEU:HD22	1.88	0.55
2:B:642:ILE:HD11	2:B:693:PHE:CE2	2.41	0.55
3:C:224:ASN:HD22	3:C:249:SER:CB	2.20	0.55
4:E:41:ARG:O	4:E:44:LEU:N	2.39	0.55
2:O:18:TYR:OH	2:O:90:ASN:O	2.12	0.55
8:Q:505:PRO:HB3	8:Q:533:SER:HB3	1.87	0.55
1:S:163:ARG:NE	1:S:190:ILE:O	2.38	0.55
7:M:117:GLU:O	7:M:121:LEU:HG	2.06	0.55
11:U:379:THR:HA	11:U:382:LEU:HD12	1.89	0.55
11:U:494:GLN:H	11:U:494:GLN:CD	2.10	0.55
11:U:1099:VAL:HA	11:U:1102:LEU:HD12	1.88	0.55
12:V:676:PHE:CD2	12:V:680:VAL:HG21	2.42	0.55
6:G:497:PHE:CE2	8:P:254:ILE:HG13	2.42	0.55
6:H:69:LEU:O	6:H:73:VAL:HG23	2.06	0.55
1:S:430:ALA:O	1:S:434:VAL:HG23	2.05	0.55
4:E:446:TRP:CH2	4:E:454:LEU:CD2	2.89	0.55
2:O:768:VAL:HG22	8:Q:841:LEU:HD21	1.89	0.55
8:Q:487:ASN:ND2	7:M:13:PRO:O	2.37	0.55
11:U:885:TYR:CG	11:U:909:LEU:HD11	2.41	0.55
1:A:191:VAL:HG21	1:A:196:LEU:HD11	1.88	0.55
2:B:240:VAL:HG11	2:B:256:LEU:HD11	1.89	0.55
4:E:379:ALA:HB2	4:E:419:LEU:HD11	1.88	0.55
4:E:497:MET:HG2	4:E:512:LEU:HD13	1.89	0.55
2:O:590:PHE:C	2:O:592:LYS:N	2.60	0.55
8:Q:505:PRO:CB	8:Q:533:SER:HB3	2.36	0.55
11:U:272:ILE:CG2	11:U:312:LEU:HA	2.37	0.55
2:B:521:LEU:CD1	2:B:587:LEU:HD21	2.36	0.55
8:P:141:VAL:CG1	8:P:152:MET:SD	2.95	0.55
8:P:361:SER:OG	8:P:398:SER:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:450:THR:OG1	12:V:356:TYR:HB3	2.07	0.55
12:V:1313:LEU:HD22	12:V:1324:VAL:HG22	1.89	0.55
4:E:33:LEU:HB2	4:E:94:CYS:SG	2.47	0.55
6:G:450:LEU:HD21	6:G:509:LEU:HD13	1.89	0.55
8:P:43:LEU:HB3	8:P:45:TYR:CE1	2.42	0.55
7:M:8:LEU:HD21	7:M:25:TYR:CE2	2.42	0.55
12:V:1025:ASN:HD22	12:V:1097:ARG:HG2	1.71	0.55
1:A:286:GLN:C	1:A:288:GLU:N	2.61	0.54
3:C:81:LEU:HD21	3:C:121:ILE:HG23	1.89	0.54
3:C:149:LEU:HD12	5:F:165:THR:HG21	1.89	0.54
11:U:202:PHE:CZ	11:U:214:VAL:HG22	2.41	0.54
4:E:48:ARG:NH2	7:L:215:GLU:OE2	2.36	0.54
7:L:62:ILE:HG12	7:L:102:TYR:OH	2.07	0.54
1:S:1404:LEU:HD21	1:S:1432:VAL:HG22	1.89	0.54
2:B:79:CYS:HB3	2:B:94:ILE:CD1	2.38	0.54
8:Q:491:ASN:HB3	8:Q:535:PHE:CE1	2.42	0.54
11:U:718:LEU:HB3	11:U:723:LEU:HB2	1.89	0.54
12:V:1142:LEU:HD22	12:V:1151:ASN:CG	2.27	0.54
1:A:193:LEU:HD23	1:A:197:LEU:HD11	1.90	0.54
1:A:375:LEU:HD21	1:A:392:PHE:CE1	2.42	0.54
5:F:278:LEU:HD13	5:F:311:PHE:CE2	2.42	0.54
1:S:384:VAL:HG11	1:S:386:TRP:CE3	2.42	0.54
1:S:428:VAL:HG22	1:S:476:PHE:CZ	2.43	0.54
1:A:21:ALA:HA	6:H:415:THR:HG22	1.89	0.54
2:B:79:CYS:HB3	2:B:94:ILE:HD12	1.88	0.54
2:B:675:TRP:HA	2:B:679:HIS:CG	2.43	0.54
3:C:210:GLU:N	3:C:210:GLU:OE1	2.41	0.54
3:C:348:LEU:HD23	3:C:396:LEU:HD23	1.89	0.54
4:E:327:LEU:HD11	4:E:331:LEU:HD21	1.87	0.54
4:E:381:ARG:HB3	4:E:381:ARG:CZ	2.37	0.54
4:E:386:ALA:O	4:E:389:SER:OG	2.19	0.54
1:S:1063:TRP:CH2	1:S:1329:ARG:CZ	2.91	0.54
7:M:19:ASN:OD1	7:M:20:ARG:N	2.41	0.54
11:U:490:PHE:HD1	11:U:529:GLN:HE22	1.55	0.54
11:U:504:GLN:OE1	11:U:546:ASN:HB2	2.07	0.54
6:G:128:ALA:HA	6:G:131:LEU:HD12	1.88	0.54
2:O:840:LEU:HD21	8:Q:812:VAL:HG12	1.88	0.54
8:P:196:VAL:O	8:P:244:GLY:N	2.34	0.54
1:S:830:LEU:HD23	1:S:871:LEU:HD21	1.89	0.54
11:U:316:VAL:CG1	11:U:326:VAL:HG21	2.37	0.54
11:U:364:ILE:O	11:U:367:VAL:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:1089:LEU:HD21	11:U:1148:LEU:HD13	1.89	0.54
3:C:135:THR:HG22	5:F:169:LEU:CD1	2.38	0.54
4:E:505:THR:N	4:E:508:GLN:OE1	2.39	0.54
6:H:414:LEU:HD13	6:H:463:TRP:CZ2	2.42	0.54
8:Q:653:LEU:HD23	8:Q:758:ALA:HA	1.90	0.54
12:V:212:ILE:O	12:V:215:LEU:HG	2.07	0.54
2:B:700:PHE:O	2:B:703:THR:HB	2.08	0.54
2:B:711:THR:O	2:B:714:GLU:N	2.41	0.54
2:B:854:GLN:NE2	8:P:594:LEU:O	2.41	0.54
5:F:205:ILE:HG23	5:F:237:LEU:HD13	1.89	0.54
6:H:388:PRO:CD	6:H:389:PRO:CD	2.86	0.54
2:O:146:HIS:O	2:O:148:LYS:N	2.40	0.54
11:U:528:ASN:N	11:U:528:ASN:OD1	2.40	0.54
12:V:1351:THR:HA	12:V:1354:THR:HG22	1.90	0.54
6:H:177:LEU:HB2	6:H:211:PHE:CE2	2.42	0.54
1:S:1412:LYS:HG2	1:S:1443:ALA:HA	1.89	0.54
11:U:858:HIS:HB2	11:U:864:GLY:O	2.07	0.54
11:U:1081:ALA:HB3	11:U:1082:PRO:HD3	1.90	0.54
12:V:113:CYS:SG	12:V:136:ILE:HG13	2.47	0.54
2:B:700:PHE:O	2:B:703:THR:CB	2.56	0.53
4:E:321:PRO:O	4:E:325:ASP:N	2.35	0.53
4:E:364:THR:HG23	4:E:368:PHE:CE2	2.43	0.53
6:H:345:GLN:O	6:H:349:ILE:HG12	2.08	0.53
8:P:349:CYS:SG	8:P:399:LEU:HA	2.48	0.53
6:H:266:LEU:O	6:H:270:VAL:HG23	2.08	0.53
6:H:412:ASP:O	6:H:415:THR:OG1	2.24	0.53
8:P:346:PRO:HG2	8:P:363:PRO:HD3	1.89	0.53
11:U:1042:PRO:O	11:U:1046:LEU:HG	2.09	0.53
12:V:347:PHE:O	12:V:351:LYS:HG3	2.08	0.53
5:F:302:VAL:HG23	5:F:306:GLU:HB3	1.90	0.53
2:O:517:ARG:HB3	2:O:517:ARG:HH11	1.73	0.53
1:S:26:LEU:HA	1:S:29:ARG:CG	2.38	0.53
1:S:736:VAL:CG2	9:W:80:VAL:HG21	2.38	0.53
1:A:1266:MET:HE2	1:A:1266:MET:HA	1.91	0.53
7:L:295:ARG:HD2	7:L:298:LEU:HD13	1.91	0.53
11:U:314:LEU:HD21	11:U:330:LEU:HD13	1.90	0.53
11:U:1132:LYS:O	11:U:1136:MET:HG2	2.09	0.53
12:V:1186:LEU:HD11	12:V:1234:PHE:CD1	2.43	0.53
1:A:137:LEU:HD12	1:A:137:LEU:O	2.09	0.53
2:B:514:HIS:ND1	2:B:593:PHE:HA	2.24	0.53
4:E:63:LEU:O	4:E:67:LEU:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:840:LEU:HD22	8:Q:869:VAL:HG13	1.91	0.53
12:V:575:ILE:O	12:V:579:VAL:HG23	2.08	0.53
2:B:687:GLU:OE1	2:B:687:GLU:N	2.36	0.53
6:H:547:ASN:HD22	6:H:550:THR:HG22	1.73	0.53
8:Q:28:VAL:HG23	8:Q:400:ASN:HD21	1.74	0.53
1:S:1368:PHE:CZ	1:S:1392:PRO:HB2	2.44	0.53
11:U:1096:LEU:HD21	11:U:1141:LEU:HD11	1.90	0.53
12:V:439:ALA:CA	12:V:457:LEU:HD23	2.39	0.53
12:V:1299:ARG:HB3	12:V:1360:LEU:HA	1.91	0.53
1:A:1302:TRP:O	1:A:1305:LEU:HG	2.08	0.53
2:B:239:TYR:CE1	2:B:240:VAL:O	2.61	0.53
2:B:704:LEU:C	2:B:705:PHE:HD1	2.12	0.53
2:B:707:TRP:CH2	2:B:715:GLY:HA3	2.44	0.53
12:V:406:LYS:HG2	12:V:412:ILE:HD11	1.91	0.53
1:A:364:VAL:HG12	2:B:824:LEU:HD12	1.90	0.53
1:A:737:ALA:HB3	1:A:738:PRO:HD3	1.90	0.53
1:A:815:PRO:HA	1:A:818:PHE:CE2	2.43	0.53
1:A:1271:SER:OG	1:A:1280:ASP:OD1	2.27	0.53
4:E:382:LEU:HD11	12:V:309:HIS:ND1	2.23	0.53
2:O:488:VAL:HG11	2:O:650:ALA:HA	1.90	0.53
8:P:84:GLY:O	8:P:130:LEU:HD21	2.08	0.53
8:Q:529:LEU:HD21	8:Q:572:LEU:HD21	1.90	0.53
1:S:982:THR:HG23	1:S:1051:ILE:HD11	1.90	0.53
10:X:57:ILE:HG23	10:X:61:TYR:CG	2.43	0.53
12:V:267:MET:HA	12:V:270:LEU:HB2	1.91	0.53
12:V:1125:ILE:HD11	12:V:1134:LEU:HD13	1.90	0.53
1:A:746:ALA:O	1:A:750:VAL:HG23	2.07	0.53
2:B:89:ILE:HA	8:P:14:PHE:HA	1.91	0.53
2:B:749:SER:O	2:B:755:LEU:HD21	2.09	0.53
7:L:137:LYS:HA	7:L:150:ILE:O	2.09	0.53
8:P:27:ARG:C	8:P:400:ASN:HD21	2.13	0.53
12:V:98:SER:O	12:V:101:GLU:HG2	2.08	0.53
2:B:176:ILE:CG2	2:B:245:THR:HG21	2.38	0.53
2:B:602:MET:N	2:B:602:MET:SD	2.82	0.53
8:P:596:VAL:HG13	8:P:647:VAL:HB	1.91	0.53
7:M:270:ASN:ND2	7:M:287:VAL:O	2.42	0.53
11:U:428:GLU:O	11:U:432:ILE:HG12	2.09	0.53
12:V:1246:VAL:HG22	12:V:1268:TRP:CH2	2.44	0.53
4:E:492:LEU:O	4:E:496:VAL:HG23	2.09	0.52
6:G:21:ASP:OD1	6:G:25:ARG:NH1	2.42	0.52
2:O:229:ILE:HG23	2:O:256:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:130:LEU:HA	8:P:144:VAL:HG23	1.91	0.52
11:U:595:LEU:O	11:U:602:ARG:NE	2.41	0.52
12:V:277:ASP:O	12:V:280:VAL:HG22	2.08	0.52
12:V:820:VAL:HG11	12:V:964:GLU:HA	1.90	0.52
1:A:320:PHE:CD2	1:A:362:LEU:HD23	2.44	0.52
4:E:375:LEU:HD22	4:E:377:SER:O	2.09	0.52
6:H:345:GLN:HG2	6:H:386:PRO:CG	2.40	0.52
8:P:504:ARG:O	8:P:532:SER:OG	2.26	0.52
10:X:45:PRO:O	10:X:144:ARG:HA	2.08	0.52
11:U:386:GLY:HA3	11:U:426:LEU:HD11	1.92	0.52
2:B:176:ILE:HG23	2:B:245:THR:HG21	1.90	0.52
6:G:411:GLN:OE1	6:G:466:LEU:HD11	2.10	0.52
2:O:390:VAL:O	2:O:390:VAL:HG12	2.09	0.52
8:Q:478:GLN:HE21	8:Q:610:VAL:CG2	2.22	0.52
8:Q:492:VAL:HG22	8:Q:535:PHE:CG	2.45	0.52
1:S:868:PHE:CE2	1:S:910:LEU:HD22	2.44	0.52
1:A:264:GLN:O	1:A:268:ASP:HB2	2.09	0.52
2:B:315:SER:O	2:B:315:SER:OG	2.23	0.52
3:C:135:THR:HG22	5:F:169:LEU:HD12	1.92	0.52
3:C:169:PHE:HA	3:C:209:ARG:NH1	2.24	0.52
8:Q:572:LEU:HG	8:Q:572:LEU:O	2.09	0.52
1:S:665:THR:HA	9:W:80:VAL:HG22	1.91	0.52
7:M:311:TYR:HE1	7:M:361:TYR:OH	1.92	0.52
11:U:992:LEU:HD23	11:U:995:LEU:HD12	1.92	0.52
2:B:240:VAL:CG1	2:B:256:LEU:HD11	2.40	0.52
2:O:13:GLU:CD	2:O:353:CYS:SG	2.88	0.52
1:S:993:GLN:OE1	1:S:1074:GLU:HB2	2.10	0.52
7:M:300:LYS:HB2	7:M:303:PHE:HB3	1.92	0.52
10:X:70:PHE:HE2	10:X:79:ILE:HD13	1.73	0.52
10:X:78:ASN:ND2	10:X:119:ASN:O	2.43	0.52
11:U:86:VAL:HA	11:U:89:ILE:HG22	1.90	0.52
2:B:534:PRO:HA	2:B:572:LYS:HE2	1.92	0.52
8:P:134:THR:OG1	8:P:135:LEU:N	2.42	0.52
8:Q:531:ASN:O	8:Q:575:GLY:N	2.42	0.52
12:V:508:MET:O	12:V:508:MET:HE3	2.08	0.52
1:A:28:GLY:C	1:A:30:VAL:H	2.12	0.52
2:B:489:VAL:O	2:B:579:THR:HA	2.10	0.52
3:C:190:LEU:HD22	5:F:142:ALA:HB2	1.91	0.52
11:U:280:LYS:O	12:V:479:THR:HG23	2.09	0.52
11:U:447:ARG:HD3	11:U:459:PHE:CZ	2.45	0.52
2:B:846:GLN:OE1	8:P:874:ARG:NH2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:424:VAL:HA	4:E:429:LEU:CD2	2.40	0.52
2:O:145:ARG:HG3	2:O:150:PHE:CZ	2.45	0.52
8:P:150:TRP:HZ3	8:P:195:PRO:HG3	1.74	0.52
8:P:674:ASP:OD2	8:P:677:ALA:N	2.43	0.52
1:S:288:GLU:HB3	1:S:292:HIS:CB	2.37	0.52
11:U:885:TYR:CZ	11:U:909:LEU:HD21	2.44	0.52
2:B:710:ARG:O	2:B:711:THR:OG1	2.28	0.52
8:P:253:VAL:HG23	8:P:272:VAL:CB	2.40	0.52
7:M:164:ASP:HB3	7:M:166:PHE:CE1	2.45	0.52
11:U:202:PHE:HZ	11:U:214:VAL:HG22	1.75	0.52
12:V:1313:LEU:HD21	12:V:1327:LEU:HD23	1.90	0.52
4:E:391:CYS:SG	4:E:423:LEU:CD2	2.95	0.52
5:F:339:PHE:HD2	5:F:344:LEU:HB3	1.74	0.52
7:M:212:TRP:CD2	7:M:295:ARG:HA	2.45	0.52
10:X:40:GLY:N	10:X:49:GLY:O	2.43	0.52
11:U:630:GLN:HE21	11:U:662:GLU:HG2	1.75	0.52
11:U:1213:ILE:CD1	11:U:1253:LEU:HD23	2.39	0.52
12:V:284:PHE:O	12:V:288:SER:N	2.33	0.52
2:B:85:PHE:CZ	2:B:156:GLN:HG2	2.45	0.51
4:E:474:GLU:O	4:E:477:CYS:SG	2.60	0.51
2:O:829:LYS:N	8:Q:824:ASP:O	2.43	0.51
1:S:824:CYS:O	1:S:830:LEU:HD11	2.10	0.51
7:M:206:GLU:HG2	7:M:281:LEU:HD12	1.92	0.51
7:M:314:GLN:HE22	7:M:317:GLY:HA2	1.75	0.51
11:U:488:LEU:O	11:U:488:LEU:HD23	2.11	0.51
12:V:487:ALA:O	12:V:491:THR:OG1	2.27	0.51
3:C:138:LEU:O	5:F:173:ARG:NH2	2.43	0.51
3:C:199:LEU:O	3:C:202:ALA:HB3	2.11	0.51
2:O:252:LEU:CD1	2:O:254:ILE:HG23	2.41	0.51
8:P:134:THR:O	8:P:135:LEU:HG	2.11	0.51
8:Q:143:LEU:HB2	8:Q:197:LEU:HD11	1.92	0.51
8:Q:475:ALA:O	8:Q:479:ARG:HG2	2.10	0.51
7:M:157:LYS:HB3	7:M:160:ALA:HB3	1.92	0.51
7:M:311:TYR:CD2	10:X:6:ARG:HD2	2.45	0.51
7:M:342:LEU:HD22	7:M:357:GLY:HA3	1.91	0.51
1:A:288:GLU:HA	1:A:292:HIS:HB3	1.93	0.51
2:B:265:LEU:C	2:B:266:ILE:HG13	2.30	0.51
6:G:100:LEU:HD22	6:G:125:VAL:HG21	1.92	0.51
7:M:124:ASP:OD1	7:M:125:LYS:NZ	2.37	0.51
12:V:456:LEU:O	12:V:460:TYR:CD2	2.64	0.51
12:V:1186:LEU:HB3	12:V:1237:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:VAL:O	2:B:83:SER:OG	2.29	0.51
3:C:204:LEU:HD12	3:C:238:ALA:HB1	1.92	0.51
7:L:121:LEU:HD23	7:L:184:ILE:HD13	1.93	0.51
7:L:133:PHE:O	7:L:133:PHE:CD1	2.63	0.51
2:O:237:VAL:CG1	2:O:258:ALA:HB1	2.41	0.51
1:S:933:LEU:HD21	1:S:984:LEU:HD12	1.93	0.51
11:U:202:PHE:HA	11:U:205:MET:HE2	1.92	0.51
2:B:65:PHE:CE2	2:B:110:LEU:HD13	2.45	0.51
4:E:117:VAL:HA	4:E:120:ILE:HD12	1.93	0.51
6:G:552:PHE:CE2	6:G:602:PRO:HG3	2.45	0.51
1:S:739:PRO:HG2	1:S:846:CYS:HB3	1.92	0.51
1:S:1368:PHE:CZ	1:S:1392:PRO:CB	2.93	0.51
11:U:670:CYS:O	11:U:674:CYS:SG	2.66	0.51
12:V:146:GLN:NE2	12:V:186:VAL:HA	2.05	0.51
12:V:1242:LEU:HD22	12:V:1278:LEU:HD12	1.93	0.51
1:A:351:THR:HG21	1:A:391:SER:CB	2.41	0.51
1:A:818:PHE:CD1	1:A:864:LEU:HG	2.45	0.51
2:B:228:ILE:HG22	2:B:229:ILE:H	1.75	0.51
2:B:651:LEU:HD22	2:B:655:PHE:CZ	2.46	0.51
3:C:151:LYS:O	3:C:155:LEU:HD12	2.11	0.51
3:C:232:ILE:HG23	3:C:233:SER:N	2.26	0.51
8:P:328:TRP:HA	8:P:334:LEU:HA	1.93	0.51
1:S:719:VAL:HA	1:S:722:LEU:HD12	1.93	0.51
7:M:214:LEU:HB3	7:M:227:ARG:O	2.10	0.51
7:M:279:SER:O	7:M:283:ASN:ND2	2.42	0.51
2:B:17:CYS:SG	2:B:331:ASP:OD2	2.68	0.51
3:C:140:TYR:HE2	5:F:169:LEU:HB3	1.75	0.51
2:O:82:VAL:HG13	2:O:83:SER:H	1.75	0.51
8:P:344:PRO:HB2	8:P:362:THR:HG21	1.93	0.51
8:P:866:LEU:HA	8:P:869:VAL:HG23	1.92	0.51
8:Q:733:LEU:HD22	8:Q:746:VAL:HG11	1.92	0.51
11:U:50:ILE:O	11:U:54:SER:N	2.43	0.51
12:V:177:VAL:CG2	12:V:218:ILE:HD11	2.41	0.51
3:C:64:PHE:N	3:C:65:PRO:HD2	2.26	0.51
3:C:243:TRP:CB	3:C:290:ILE:HD11	2.41	0.51
5:F:95:LEU:O	5:F:99:GLU:HG2	2.11	0.51
6:G:147:ALA:CB	6:G:159:LEU:HD11	2.41	0.51
2:O:391:VAL:HB	2:O:392:PRO:HD3	1.93	0.51
11:U:590:SER:O	11:U:593:ARG:HB3	2.11	0.51
11:U:885:TYR:CD2	11:U:909:LEU:HD11	2.45	0.51
12:V:199:LEU:O	12:V:202:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:294:THR:O	12:V:297:VAL:HG12	2.11	0.51
12:V:412:ILE:HG23	12:V:416:LEU:HD12	1.93	0.51
3:C:224:ASN:C	3:C:224:ASN:OD1	2.49	0.51
4:E:284:ILE:O	4:E:288:LEU:N	2.44	0.51
6:H:99:SER:O	6:H:103:VAL:HG23	2.11	0.51
6:H:241:PRO:HD2	6:H:244:VAL:CG2	2.40	0.51
6:H:388:PRO:N	6:H:389:PRO:CD	2.74	0.51
11:U:533:ARG:CD	11:U:597:GLN:HE22	2.24	0.51
1:A:351:THR:HG21	1:A:391:SER:HB3	1.93	0.51
5:F:207:VAL:HG12	5:F:211:GLN:NE2	2.26	0.51
1:S:117:VAL:HG13	1:S:148:LEU:HD21	1.93	0.51
1:S:1349:ARG:HD3	1:S:1406:LEU:HD21	1.91	0.51
11:U:210:ILE:O	11:U:214:VAL:HG23	2.11	0.51
2:B:308:ALA:HB3	2:B:325:LEU:HD13	1.92	0.50
2:B:705:PHE:N	2:B:705:PHE:CD1	2.79	0.50
8:Q:249:GLN:HA	8:Q:277:HIS:HA	1.92	0.50
11:U:504:GLN:O	11:U:507:LEU:N	2.41	0.50
11:U:533:ARG:HD2	11:U:597:GLN:NE2	2.27	0.50
11:U:1031:LEU:HD12	11:U:1035:LEU:HD23	1.92	0.50
12:V:209:HIS:NE2	12:V:244:PRO:HG3	2.26	0.50
12:V:491:THR:O	12:V:495:VAL:HG23	2.11	0.50
12:V:820:VAL:HG12	12:V:967:PHE:HB3	1.94	0.50
1:A:1161:THR:O	1:A:1321:ARG:NH2	2.44	0.50
7:L:236:ILE:HD12	7:L:253:PHE:HE1	1.76	0.50
8:Q:339:ARG:NE	7:M:101:LEU:HD21	2.27	0.50
1:S:667:PRO:HB2	1:S:742:GLN:O	2.11	0.50
10:X:56:ILE:HB	10:X:67:GLN:HG2	1.92	0.50
11:U:306:SER:N	11:U:309:SER:HG	2.09	0.50
11:U:1092:ALA:O	11:U:1095:VAL:HB	2.11	0.50
12:V:417:LEU:HD13	12:V:453:PHE:CZ	2.46	0.50
1:A:428:VAL:HG22	1:A:476:PHE:CE1	2.46	0.50
1:A:818:PHE:O	1:A:821:LEU:HB3	2.11	0.50
6:H:411:GLN:O	6:H:415:THR:HG23	2.11	0.50
2:O:585:SER:N	2:O:586:PRO:HD3	2.25	0.50
8:P:717:ALA:HB3	8:P:815:GLN:HE22	1.75	0.50
11:U:723:LEU:HD23	11:U:739:ASN:HD22	1.76	0.50
11:U:1162:LEU:HD23	11:U:1212:PHE:CE2	2.46	0.50
3:C:243:TRP:HB2	3:C:290:ILE:HD11	1.92	0.50
4:E:130:ASP:OD2	4:E:133:LEU:HB2	2.11	0.50
1:S:959:ILE:HD12	1:S:1020:ARG:HD2	1.94	0.50
11:U:504:GLN:O	11:U:504:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:874:LEU:HD22	11:U:915:ILE:HG23	1.93	0.50
2:B:600:GLN:NE2	8:P:546:GLN:OE1	2.44	0.50
2:B:673:LYS:O	2:B:677:LEU:HD22	2.11	0.50
3:C:405:GLU:OE1	3:C:405:GLU:N	2.43	0.50
3:C:412:LEU:HD11	3:C:493:ASN:HB3	1.94	0.50
4:E:67:LEU:HD23	4:E:87:LEU:HD12	1.92	0.50
6:G:159:LEU:HD23	6:G:177:LEU:HD23	1.94	0.50
6:G:426:SER:HB2	8:P:223:ALA:HA	1.93	0.50
8:P:288:LEU:HG	8:P:311:CYS:SG	2.52	0.50
8:Q:596:VAL:HG13	8:Q:647:VAL:HB	1.94	0.50
1:S:1033:ASP:OD2	1:S:1093:SER:CB	2.58	0.50
12:V:1190:LEU:O	12:V:1196:ILE:HG12	2.12	0.50
2:B:362:LEU:O	8:P:468:ARG:NH1	2.41	0.50
6:G:417:CYS:HB3	6:G:459:GLN:HE21	1.75	0.50
2:O:277:CYS:HB2	2:O:316:PHE:HB3	1.94	0.50
8:P:517:LEU:O	8:P:519:THR:N	2.37	0.50
7:M:230:LEU:HD22	7:M:236:ILE:HG22	1.93	0.50
7:M:248:LEU:HB3	11:U:509:VAL:HG13	1.93	0.50
1:A:1020:ARG:O	1:A:1023:GLU:HB3	2.12	0.50
1:A:1305:LEU:HA	1:A:1308:LEU:HD21	1.93	0.50
3:C:60:VAL:O	3:C:64:PHE:CD2	2.64	0.50
2:O:480:TYR:CD2	2:O:620:VAL:HG12	2.47	0.50
8:P:384:GLU:O	8:P:385:GLU:HG3	2.12	0.50
8:Q:496:LEU:HD23	8:Q:505:PRO:HG2	1.93	0.50
8:Q:707:SER:HB3	8:Q:788:GLN:HG3	1.94	0.50
12:V:1246:VAL:CG2	12:V:1268:TRP:CZ3	2.95	0.50
1:A:30:VAL:HG21	6:H:372:ALA:CB	2.42	0.50
2:B:673:LYS:O	2:B:677:LEU:HB2	2.12	0.50
5:F:201:PHE:CZ	5:F:205:ILE:HD11	2.46	0.50
6:G:447:TYR:CD1	6:G:490:GLU:HB3	2.46	0.50
6:H:345:GLN:CD	6:H:386:PRO:HA	2.32	0.50
8:Q:541:TRP:CE2	8:Q:604:TYR:HD1	2.30	0.50
1:S:1261:PHE:CZ	1:S:1292:LEU:HD21	2.46	0.50
7:M:21:SER:O	7:M:23:THR:N	2.43	0.50
3:C:141:ALA:O	3:C:144:ASP:OD1	2.29	0.50
4:E:396:TYR:HB3	4:E:397:PRO:HD3	1.93	0.50
8:P:130:LEU:N	8:P:144:VAL:HG23	2.27	0.50
8:P:147:PRO:O	8:P:149:ARG:N	2.44	0.50
1:S:944:ASP:OD2	1:S:951:ARG:NH2	2.40	0.50
1:A:831:PHE:CE1	1:A:899:PRO:HD2	2.47	0.49
3:C:35:CYS:O	3:C:38:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:451:PHE:O	4:E:454:LEU:N	2.44	0.49
4:E:495:THR:HG22	12:V:162:PHE:CZ	2.46	0.49
6:G:469:GLN:HE22	6:G:526:ALA:HB1	1.77	0.49
6:H:62:ALA:HB1	6:H:106:THR:HG22	1.92	0.49
12:V:146:GLN:HE22	12:V:186:VAL:CA	2.08	0.49
2:B:297:LEU:O	2:B:313:LYS:HB3	2.12	0.49
4:E:382:LEU:HD11	12:V:309:HIS:CE1	2.47	0.49
5:F:274:TYR:CE2	5:F:314:LEU:HD21	2.46	0.49
2:O:312:TRP:CD1	2:O:319:ALA:HB2	2.48	0.49
11:U:210:ILE:N	11:U:211:PRO:HD2	2.27	0.49
11:U:443:GLN:O	11:U:447:ARG:NE	2.44	0.49
3:C:184:SER:OG	3:C:215:LEU:HD22	2.12	0.49
8:Q:491:ASN:HD22	7:M:9:LEU:HD11	1.76	0.49
11:U:900:LYS:HD3	11:U:903:SER:HB2	1.93	0.49
12:V:686:LEU:HD13	12:V:811:LYS:HG2	1.92	0.49
12:V:820:VAL:HG21	12:V:964:GLU:CA	2.43	0.49
1:A:481:VAL:O	1:A:485:SER:OG	2.27	0.49
1:A:1404:LEU:HD21	1:A:1432:VAL:HG22	1.93	0.49
3:C:162:ARG:NH1	3:C:166:LEU:HD11	2.27	0.49
6:H:406:GLN:HE22	6:H:599:TRP:HB2	1.78	0.49
7:L:105:PRO:O	7:L:107:PRO:HD3	2.12	0.49
7:L:357:GLY:O	7:L:366:ILE:HG22	2.12	0.49
8:P:346:PRO:HD2	8:P:363:PRO:HD2	1.94	0.49
8:Q:175:LEU:HD23	8:Q:272:VAL:HG21	1.93	0.49
1:S:1343:HIS:CE1	1:S:1348:ILE:HB	2.46	0.49
12:V:382:LEU:HD21	12:V:412:ILE:HG21	1.94	0.49
1:A:30:VAL:HG21	6:H:372:ALA:HB3	1.94	0.49
1:A:944:ASP:HB3	1:A:946:LEU:O	2.13	0.49
2:B:90:ASN:O	2:B:91:LEU:HD23	2.12	0.49
5:F:282:GLY:HA3	5:F:347:TRP:CH2	2.47	0.49
6:G:140:HIS:NE2	6:G:166:LEU:HD21	2.28	0.49
6:G:371:LEU:O	6:G:375:LEU:HD12	2.13	0.49
6:H:544:CYS:O	6:H:544:CYS:SG	2.70	0.49
2:O:265:LEU:CD2	2:O:311:VAL:HG21	2.43	0.49
8:P:679:PHE:CD2	8:P:679:PHE:C	2.82	0.49
1:S:139:VAL:HG12	1:S:140:GLU:H	1.77	0.49
1:S:815:PRO:HA	1:S:818:PHE:CE2	2.47	0.49
7:M:312:ALA:HB2	10:X:5:SER:HB2	1.94	0.49
12:V:614:LEU:HA	12:V:617:VAL:HG12	1.93	0.49
2:B:132:ASP:N	2:B:132:ASP:OD1	2.46	0.49
4:E:471:VAL:HA	4:E:474:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:500:TYR:HA	4:E:503:ASN:ND2	2.28	0.49
2:O:506:LEU:O	2:O:525:ASN:ND2	2.42	0.49
8:P:366:LEU:HD23	8:P:366:LEU:C	2.33	0.49
1:S:817:LEU:HD23	1:S:818:PHE:CE1	2.47	0.49
7:M:311:TYR:HB3	10:X:9:ARG:HD2	1.95	0.49
11:U:533:ARG:CZ	11:U:597:GLN:HE22	2.26	0.49
11:U:1068:LYS:HG2	11:U:1070:ASN:OD1	2.13	0.49
4:E:383:LEU:HA	4:E:386:ALA:CB	2.41	0.49
6:G:296:THR:O	6:G:299:GLU:HB3	2.12	0.49
2:O:79:CYS:O	2:O:79:CYS:SG	2.70	0.49
8:P:35:VAL:O	8:P:46:VAL:HA	2.13	0.49
8:P:451:ALA:O	8:P:454:LYS:HB3	2.13	0.49
8:P:599:SER:HB3	8:P:644:ARG:HG2	1.93	0.49
11:U:470:ALA:O	11:U:473:VAL:HG12	2.12	0.49
12:V:819:ILE:HG21	12:V:967:PHE:CZ	2.48	0.49
1:A:462:TYR:CG	1:A:462:TYR:O	2.65	0.49
2:B:18:TYR:O	2:B:21:GLU:HG2	2.13	0.49
2:B:700:PHE:CD1	2:B:700:PHE:N	2.81	0.49
6:G:306:LEU:CD2	6:G:346:THR:HG21	2.40	0.49
2:O:656:HIS:CE1	2:O:724:GLN:HG3	2.48	0.49
8:P:143:LEU:CD1	8:P:197:LEU:HD21	2.42	0.49
8:P:198:CYS:N	8:P:242:LEU:O	2.43	0.49
12:V:145:LEU:HB3	12:V:149:ILE:HD11	1.95	0.49
12:V:1142:LEU:HD13	12:V:1151:ASN:HB3	1.95	0.49
3:C:179:ARG:CZ	5:F:152:ARG:HG3	2.43	0.49
3:C:188:VAL:CG2	3:C:219:PHE:HA	2.43	0.49
4:E:358:SER:O	4:E:361:THR:HB	2.13	0.49
4:E:379:ALA:CB	4:E:419:LEU:HD11	2.43	0.49
5:F:290:GLN:O	6:G:485:ARG:NH2	2.45	0.49
8:Q:11:LEU:C	8:Q:11:LEU:HD12	2.32	0.49
8:Q:570:ASP:OD1	8:Q:578:ARG:NH1	2.46	0.49
1:S:940:GLN:NE2	1:S:1011:ARG:HD3	2.28	0.49
1:S:1143:LEU:HD21	1:S:1185:TRP:CZ3	2.47	0.49
1:S:1419:ALA:HB2	1:S:1440:GLN:HE22	1.77	0.49
12:V:246:LEU:HD22	12:V:284:PHE:CD2	2.48	0.49
8:P:260:THR:HG21	8:P:266:GLY:CA	2.43	0.49
2:B:315:SER:HB2	8:P:471:PHE:CE2	2.48	0.48
3:C:74:ALA:O	3:C:77:ASN:HB3	2.13	0.48
4:E:469:PHE:CE1	4:E:500:TYR:HB3	2.47	0.48
6:H:461:GLN:OE1	6:H:465:GLN:NE2	2.46	0.48
8:Q:149:ARG:HG2	8:Q:176:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:855:THR:CG2	1:S:858:SER:OG	2.62	0.48
7:M:234:VAL:HG11	7:M:259:VAL:CG1	2.39	0.48
12:V:301:LEU:HG	12:V:305:LEU:HD12	1.94	0.48
1:A:470:LEU:O	1:A:474:PHE:CD2	2.66	0.48
1:A:1139:LEU:HD23	1:A:1181:LEU:HD22	1.94	0.48
3:C:3:GLN:HB2	3:C:6:VAL:HG12	1.96	0.48
3:C:352:LEU:HB3	3:C:400:PHE:CG	2.48	0.48
6:G:81:ARG:NE	6:G:91:ASP:OD1	2.46	0.48
6:G:159:LEU:HD23	6:G:177:LEU:CD2	2.43	0.48
8:P:543:LEU:HB3	8:P:567:ILE:HG22	1.95	0.48
1:S:575:ARG:O	1:S:579:TYR:N	2.45	0.48
1:S:1045:GLU:OE2	1:S:1104:ARG:N	2.45	0.48
1:S:1143:LEU:HD11	1:S:1185:TRP:HA	1.95	0.48
11:U:874:LEU:HA	11:U:877:LEU:HD12	1.95	0.48
11:U:983:LEU:O	11:U:986:VAL:HB	2.12	0.48
12:V:436:LEU:HD11	12:V:461:ALA:HB1	1.94	0.48
4:E:363:LEU:O	4:E:367:LEU:N	2.34	0.48
8:P:25:LYS:O	8:P:27:ARG:NH1	2.45	0.48
8:P:645:HIS:CE1	8:P:651:GLN:HE22	2.30	0.48
11:U:610:TYR:CD1	11:U:610:TYR:C	2.86	0.48
11:U:1060:ILE:HG23	11:U:1215:TYR:CG	2.48	0.48
12:V:207:LEU:O	12:V:211:ILE:HG12	2.13	0.48
12:V:820:VAL:HG12	12:V:967:PHE:CD2	2.48	0.48
1:A:263:PRO:O	1:A:267:VAL:HG23	2.13	0.48
1:A:1322:VAL:HG12	1:A:1323:ALA:N	2.29	0.48
8:P:243:CYS:N	8:P:251:CYS:O	2.31	0.48
11:U:319:ILE:HG22	11:U:322:PHE:H	1.78	0.48
3:C:334:ARG:HD3	7:L:252:PHE:CE2	2.49	0.48
4:E:421:CYS:SG	4:E:422:CYS:N	2.86	0.48
5:F:339:PHE:CD2	5:F:344:LEU:HD13	2.48	0.48
6:G:248:VAL:O	6:G:251:ALA:HB3	2.13	0.48
2:O:208:TRP:HA	2:O:226:ILE:O	2.13	0.48
8:P:151:LYS:CE	8:P:153:GLN:HE21	2.27	0.48
12:V:466:ASP:OD1	12:V:469:CYS:N	2.36	0.48
1:A:1291:ILE:HG22	1:A:1295:LEU:HD12	1.95	0.48
3:C:87:GLN:O	3:C:91:ILE:HG12	2.13	0.48
3:C:348:LEU:HD23	3:C:396:LEU:HD21	1.94	0.48
6:G:62:ALA:CB	6:G:102:ARG:HD2	2.39	0.48
7:L:69:ILE:HG21	7:L:90:LEU:HD11	1.96	0.48
7:L:104:LEU:HD12	7:L:104:LEU:HA	1.70	0.48
8:P:594:LEU:HD22	8:P:596:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1167:LEU:O	1:S:1171:LEU:HG	2.14	0.48
11:U:306:SER:HG	11:U:309:SER:H	1.57	0.48
11:U:448:VAL:HA	11:U:456:ILE:HD12	1.95	0.48
11:U:1095:VAL:O	11:U:1099:VAL:HG23	2.13	0.48
12:V:235:LEU:HD23	12:V:262:VAL:CG2	2.43	0.48
12:V:439:ALA:CB	12:V:457:LEU:HD23	2.44	0.48
1:A:765:LEU:HD11	1:A:787:LEU:HD21	1.95	0.48
1:A:1272:HIS:ND1	1:A:1281:LEU:HD11	2.29	0.48
6:G:416:LEU:HD13	1:S:22:TRP:CZ3	2.49	0.48
6:H:193:ALA:HB1	6:H:194:PRO:CD	2.43	0.48
7:L:305:MET:O	7:L:320:PRO:HG2	2.14	0.48
8:P:594:LEU:CD2	8:P:596:VAL:HG12	2.44	0.48
8:P:778:PRO:HD3	8:P:824:ASP:O	2.14	0.48
7:M:168:ASP:O	7:M:222:SER:HB3	2.13	0.48
11:U:271:ILE:O	11:U:275:ILE:HG23	2.13	0.48
2:B:423:TYR:CZ	8:P:606:LEU:HB3	2.49	0.48
2:B:705:PHE:HD1	2:B:705:PHE:N	2.11	0.48
1:S:57:LEU:HD11	1:S:101:GLN:HB2	1.96	0.48
11:U:169:TRP:HB3	11:U:174:VAL:HG12	1.96	0.48
1:A:874:ARG:NH1	1:A:939:ILE:HD13	2.28	0.48
1:A:1075:LEU:CD1	1:A:1119:PHE:HD2	2.26	0.48
1:A:1326:GLN:OE1	1:A:1326:GLN:N	2.46	0.48
3:C:170:ASN:OD1	7:L:346:LEU:HA	2.13	0.48
3:C:330:SER:HB2	3:C:334:ARG:HB3	1.96	0.48
4:E:46:VAL:O	4:E:50:LEU:HG	2.13	0.48
4:E:391:CYS:SG	4:E:398:VAL:CG1	2.80	0.48
5:F:20:THR:O	5:F:100:ASN:ND2	2.47	0.48
5:F:346:ILE:O	5:F:349:ASP:HB2	2.14	0.48
6:G:414:LEU:HD21	6:G:462:ALA:CB	2.44	0.48
2:O:599:LEU:O	2:O:599:LEU:HD23	2.14	0.48
8:P:284:PHE:CD2	8:P:350:ALA:CB	2.96	0.48
8:P:368:VAL:O	8:P:390:LEU:CB	2.62	0.48
8:Q:492:VAL:HG22	8:Q:535:PHE:CB	2.43	0.48
1:S:973:CYS:SG	1:S:980:ALA:HA	2.53	0.48
7:M:55:CYS:SG	7:M:59:LEU:HD23	2.53	0.48
2:B:331:ASP:O	2:B:333:PHE:CE2	2.67	0.48
2:B:517:ARG:CZ	2:B:517:ARG:HB2	2.43	0.48
4:E:387:LEU:O	4:E:391:CYS:SG	2.71	0.48
4:E:518:PRO:O	4:E:521:THR:OG1	2.18	0.48
6:G:454:ALA:O	6:G:457:LEU:N	2.47	0.48
6:H:240:CYS:SG	6:H:245:LEU:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:274:TRP:CE3	7:L:283:ASN:HB3	2.48	0.48
8:Q:243:CYS:SG	8:Q:251:CYS:HB2	2.54	0.48
7:M:334:HIS:HB2	7:M:337:CYS:SG	2.54	0.48
12:V:375:SER:HA	12:V:411:CYS:SG	2.54	0.48
1:A:375:LEU:HD11	1:A:392:PHE:HE1	1.79	0.47
3:C:146:TYR:CB	3:C:147:PRO:HD3	2.44	0.47
6:H:239:LEU:HD11	6:H:241:PRO:HG3	1.96	0.47
7:L:105:PRO:HG2	7:L:111:TYR:HE1	1.79	0.47
8:Q:48:ASP:O	8:Q:51:GLY:O	2.32	0.47
12:V:1135:ILE:HG21	12:V:1188:ILE:HG21	1.95	0.47
1:A:348:PHE:CZ	1:A:356:THR:HG23	2.50	0.47
1:A:1060:THR:HG23	1:A:1067:ALA:HB1	1.96	0.47
1:A:1328:THR:O	1:A:1331:LEU:HB2	2.14	0.47
4:E:88:LEU:HD22	4:E:123:GLN:HE21	1.79	0.47
6:H:589:LEU:HB3	6:H:594:GLU:HG3	1.95	0.47
8:Q:143:LEU:HD12	8:Q:197:LEU:HD21	1.96	0.47
1:S:665:THR:HA	9:W:80:VAL:HA	1.96	0.47
11:U:990:THR:HA	11:U:1031:LEU:HD13	1.96	0.47
12:V:439:ALA:HA	12:V:457:LEU:HD23	1.95	0.47
4:E:91:PRO:O	4:E:93:ILE:N	2.47	0.47
4:E:156:LEU:HD13	4:E:160:CYS:SG	2.54	0.47
4:E:321:PRO:HB3	4:E:362:VAL:HG21	1.95	0.47
6:G:191:LEU:O	6:G:193:ALA:N	2.47	0.47
6:G:449:PRO:O	6:G:450:LEU:C	2.53	0.47
6:H:542:GLN:OE1	6:H:542:GLN:N	2.47	0.47
8:P:151:LYS:HA	8:P:174:GLU:HA	1.97	0.47
8:Q:569:VAL:HG12	8:Q:572:LEU:HD22	1.97	0.47
1:S:34:LYS:O	1:S:39:ARG:NH2	2.46	0.47
11:U:827:GLU:OE1	11:U:827:GLU:N	2.39	0.47
12:V:435:ILE:CD1	12:V:465:PHE:HZ	2.27	0.47
12:V:1240:ALA:HB2	12:V:1297:TYR:CZ	2.49	0.47
4:E:522:PHE:CB	4:E:523:LEU:HG	2.44	0.47
6:G:480:LEU:O	6:G:484:PHE:HD2	1.98	0.47
6:G:483:LEU:HD12	6:G:513:ARG:HG2	1.96	0.47
6:H:66:VAL:O	6:H:69:LEU:HB3	2.14	0.47
6:H:538:LEU:O	6:H:542:GLN:OE1	2.33	0.47
2:O:18:TYR:CE2	2:O:92:PRO:HD3	2.49	0.47
8:P:141:VAL:HG11	8:P:152:MET:SD	2.55	0.47
8:P:368:VAL:HG12	8:P:391:PRO:O	2.15	0.47
8:P:733:LEU:CD2	8:P:746:VAL:HG11	2.45	0.47
12:V:345:LEU:O	12:V:349:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:N	1:A:31:LYS:HD3	2.29	0.47
1:A:275:ILE:HG23	1:A:330:HIS:CE1	2.49	0.47
1:A:474:PHE:HD2	1:A:510:TYR:CZ	2.31	0.47
2:B:14:ARG:HD2	2:B:79:CYS:SG	2.54	0.47
2:B:90:ASN:OD1	8:P:14:PHE:O	2.32	0.47
3:C:342:PRO:HD2	3:C:343:TYR:CE2	2.49	0.47
6:G:267:LEU:HD21	1:S:60:LEU:HD11	1.95	0.47
2:O:176:ILE:HD12	2:O:182:VAL:HG21	1.95	0.47
2:O:475:VAL:HG21	2:O:615:VAL:HG11	1.96	0.47
8:P:70:LEU:HD11	8:P:135:LEU:HD22	1.96	0.47
8:P:268:PRO:O	8:P:269:ASN:C	2.52	0.47
8:P:341:TYR:N	8:P:341:TYR:CD1	2.80	0.47
8:P:366:LEU:N	8:P:395:CYS:O	2.38	0.47
1:S:491:VAL:HA	1:S:494:LEU:HD12	1.97	0.47
1:S:649:PRO:O	1:S:653:LEU:HD12	2.15	0.47
12:V:534:TYR:CD1	12:V:534:TYR:C	2.88	0.47
2:B:700:PHE:O	2:B:703:THR:OG1	2.29	0.47
4:E:327:LEU:O	4:E:331:LEU:N	2.45	0.47
6:H:100:LEU:HD21	6:H:122:TRP:CZ3	2.49	0.47
2:O:651:LEU:CD2	2:O:704:LEU:HD13	2.45	0.47
8:Q:510:THR:OG1	8:Q:645:HIS:CD2	2.67	0.47
1:S:1410:CYS:SG	1:S:1414:SER:OG	2.63	0.47
11:U:199:LEU:HD21	11:U:217:LEU:HD13	1.96	0.47
11:U:467:VAL:HG12	11:U:471:PRO:HB3	1.96	0.47
12:V:243:VAL:CG2	12:V:244:PRO:HD3	2.45	0.47
1:A:102:ALA:CB	1:A:109:VAL:HG23	2.44	0.47
1:A:276:PHE:CZ	1:A:291:THR:HG23	2.50	0.47
1:A:835:LYS:HE2	1:A:903:TRP:CZ2	2.50	0.47
1:A:1045:GLU:OE2	1:A:1104:ARG:N	2.48	0.47
2:B:81:CYS:CB	2:B:90:ASN:HD22	2.28	0.47
2:B:479:TRP:CH2	2:B:490:GLY:HA3	2.50	0.47
4:E:61:GLY:HA3	7:L:166:PHE:CE2	2.49	0.47
4:E:322:SER:HG	4:E:323:GLN:H	1.62	0.47
4:E:379:ALA:HB3	4:E:419:LEU:HD21	1.97	0.47
6:G:160:ALA:O	6:G:164:GLU:HB2	2.15	0.47
7:L:333:PHE:HE2	7:L:360:PRO:HG2	1.79	0.47
2:O:145:ARG:HG3	2:O:150:PHE:CE2	2.50	0.47
8:P:24:GLY:O	8:P:27:ARG:NH1	2.47	0.47
8:P:527:CYS:SG	8:P:580:VAL:HB	2.55	0.47
1:S:286:GLN:CA	1:S:288:GLU:HG2	2.44	0.47
1:S:392:PHE:CE2	1:S:396:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:456:PHE:HA	1:S:460:ARG:HB3	1.95	0.47
1:S:1063:TRP:CZ2	1:S:1329:ARG:HD3	2.50	0.47
7:M:244:HIS:O	7:M:247:MET:HB3	2.15	0.47
11:U:32:LEU:O	11:U:36:GLN:N	2.47	0.47
1:A:135:VAL:HG11	1:A:217:LEU:HG	1.97	0.47
2:B:103:ASN:O	2:B:127:GLY:O	2.33	0.47
2:B:633:LEU:O	2:B:634:LEU:HD23	2.15	0.47
3:C:115:GLN:HE22	5:F:98:LEU:HA	1.80	0.47
4:E:68:CYS:HA	4:E:85:PRO:HB2	1.96	0.47
6:H:191:LEU:HD12	6:H:192:ASP:N	2.30	0.47
6:H:206:VAL:HG13	6:H:325:VAL:HG22	1.97	0.47
1:S:927:LEU:CD2	1:S:932:TRP:HB2	2.44	0.47
1:S:998:TYR:HB3	1:S:1007:VAL:HG13	1.97	0.47
11:U:306:SER:OG	11:U:309:SER:N	2.35	0.47
11:U:448:VAL:O	11:U:456:ILE:HD13	2.15	0.47
12:V:278:LEU:N	12:V:279:PRO:CD	2.78	0.47
1:A:1330:LEU:O	1:A:1333:PHE:HB3	2.15	0.47
3:C:60:VAL:CG2	3:C:64:PHE:CZ	2.97	0.47
3:C:224:ASN:HD22	3:C:249:SER:CA	2.28	0.47
6:H:100:LEU:HD21	6:H:122:TRP:CH2	2.50	0.47
6:H:257:ARG:HG3	6:H:289:LEU:HD12	1.97	0.47
1:S:731:MET:CE	9:W:85:PHE:HB3	2.45	0.47
1:S:923:GLU:N	1:S:923:GLU:CD	2.67	0.47
7:M:127:VAL:HG21	7:M:149:LEU:HD22	1.97	0.47
11:U:100:PHE:CD2	11:U:104:LEU:HD11	2.50	0.47
12:V:639:ILE:HG23	12:V:649:LEU:HD21	1.97	0.47
1:A:324:LEU:HD11	1:A:392:PHE:CE2	2.50	0.47
1:A:486:PRO:CG	1:A:489:LEU:HD12	2.45	0.47
4:E:320:SER:HG	4:E:322:SER:HG	1.61	0.47
4:E:381:ARG:O	4:E:384:THR:HB	2.15	0.47
2:O:344:LEU:HD12	2:O:354:LEU:HA	1.96	0.47
2:O:585:SER:OG	2:O:586:PRO:HD3	2.15	0.47
12:V:278:LEU:HD22	12:V:282:ILE:HD11	1.96	0.47
3:C:188:VAL:N	3:C:189:PRO:HD2	2.29	0.46
3:C:300:CYS:SG	4:E:164:LEU:HD23	2.55	0.46
7:L:60:ARG:HD3	7:L:67:HIS:HE1	1.80	0.46
2:O:257:ILE:CD1	2:O:299:PHE:CE1	2.97	0.46
8:P:28:VAL:HG22	8:P:37:LEU:HA	1.95	0.46
8:P:359:TYR:CD2	8:P:420:LEU:HD23	2.50	0.46
8:Q:339:ARG:NE	8:Q:385:GLU:O	2.47	0.46
7:M:247:MET:HG3	11:U:509:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:214:VAL:HG13	11:U:233:ILE:HD11	1.98	0.46
11:U:533:ARG:NE	11:U:597:GLN:HE22	2.13	0.46
11:U:913:GLN:HA	11:U:988:VAL:HG22	1.97	0.46
12:V:347:PHE:O	12:V:351:LYS:N	2.41	0.46
12:V:820:VAL:HG21	12:V:964:GLU:CG	2.45	0.46
1:A:835:LYS:HG2	1:A:903:TRP:CZ3	2.50	0.46
1:A:1056:LEU:O	1:A:1071:ARG:NH2	2.48	0.46
2:B:38:THR:HG23	2:B:39:LYS:HG2	1.96	0.46
2:B:624:LEU:HD23	2:O:732:HIS:HB2	1.97	0.46
6:G:453:SER:CB	6:G:483:LEU:HD23	2.45	0.46
2:O:155:SER:O	2:O:156:GLN:CB	2.63	0.46
1:S:362:LEU:O	1:S:366:LEU:HD12	2.16	0.46
1:S:568:VAL:CG2	1:S:1069:LEU:HD11	2.45	0.46
11:U:130:LEU:N	11:U:131:PRO:CD	2.78	0.46
12:V:572:LEU:O	12:V:575:ILE:HB	2.16	0.46
12:V:613:LEU:O	12:V:616:LEU:HG	2.15	0.46
1:A:651:GLY:O	1:A:654:THR:OG1	2.31	0.46
1:A:835:LYS:HD3	1:A:903:TRP:CE3	2.51	0.46
2:B:81:CYS:HB3	2:B:90:ASN:HD22	1.79	0.46
6:H:224:ASN:C	6:H:226:ASP:H	2.19	0.46
8:P:474:LYS:O	8:P:477:ASP:HB2	2.16	0.46
8:Q:709:LYS:HB2	8:Q:879:ILE:HG22	1.96	0.46
1:S:584:LEU:HB2	1:S:585:PRO:CD	2.46	0.46
12:V:965:LEU:O	12:V:969:LEU:HG	2.16	0.46
1:A:1333:PHE:CD1	1:A:1333:PHE:C	2.89	0.46
3:C:489:HIS:CE1	3:C:525:PHE:HB2	2.50	0.46
4:E:486:SER:O	4:E:489:TYR:HB3	2.16	0.46
6:H:531:THR:OG1	6:H:532:LYS:N	2.49	0.46
7:L:167:VAL:HG21	7:L:190:PHE:CE1	2.50	0.46
2:O:774:SER:CB	8:Q:834:HIS:HB2	2.46	0.46
8:P:28:VAL:N	8:P:400:ASN:OD1	2.49	0.46
8:Q:130:LEU:CB	8:Q:144:VAL:HG22	2.46	0.46
8:Q:478:GLN:HE21	8:Q:610:VAL:HG21	1.79	0.46
1:S:1328:THR:O	1:S:1331:LEU:HD12	2.15	0.46
7:M:187:TYR:CE2	7:M:191:LEU:HD21	2.51	0.46
13:Y:11:DC:H2"	13:Y:12:DA:C8	2.50	0.46
1:A:486:PRO:HG2	1:A:489:LEU:HB2	1.96	0.46
1:A:822:LEU:HD23	1:A:822:LEU:C	2.36	0.46
2:B:585:SER:HB3	2:O:724:GLN:HB3	1.96	0.46
2:B:735:ILE:HD11	8:P:684:ARG:HG3	1.98	0.46
3:C:25:ALA:O	3:C:31:GLN:NE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:196:VAL:C	3:C:198:PRO:CD	2.84	0.46
5:F:196:LEU:HD11	5:F:201:PHE:HB2	1.96	0.46
2:O:588:LEU:O	2:O:590:PHE:N	2.49	0.46
1:S:1340:SER:HA	1:S:1402:PHE:CE2	2.51	0.46
11:U:503:VAL:O	11:U:506:LEU:CG	2.50	0.46
11:U:1025:CYS:SG	11:U:1074:ILE:HG22	2.56	0.46
12:V:1282:ILE:HG12	12:V:1294:CYS:SG	2.56	0.46
2:B:854:GLN:O	2:B:858:ASN:HB2	2.15	0.46
3:C:140:TYR:HD2	5:F:169:LEU:HD13	1.80	0.46
4:E:372:ILE:CD1	4:E:402:LEU:HD22	2.45	0.46
2:O:252:LEU:HD11	2:O:254:ILE:HG23	1.97	0.46
8:P:543:LEU:HD23	8:P:601:THR:O	2.15	0.46
1:S:1056:LEU:O	1:S:1071:ARG:NH2	2.48	0.46
1:S:1063:TRP:HA	1:S:1063:TRP:CE3	2.49	0.46
12:V:640:GLN:O	12:V:743:ARG:NH2	2.45	0.46
1:A:1330:LEU:C	1:A:1332:PRO:HD2	2.36	0.46
2:B:389:LEU:HD13	7:L:128:TYR:HA	1.98	0.46
2:B:828:LEU:HD22	8:P:826:ARG:HA	1.89	0.46
4:E:30:LEU:HD22	4:E:90:LEU:CD1	2.45	0.46
4:E:315:LEU:CA	4:E:318:GLU:HG2	2.45	0.46
6:G:249:TYR:O	6:G:252:LEU:HB2	2.16	0.46
6:H:537:PHE:O	6:H:540:SER:OG	2.27	0.46
2:O:229:ILE:CG2	2:O:256:LEU:HD21	2.46	0.46
8:P:139:VAL:CG1	8:P:154:LEU:HD11	2.45	0.46
8:P:280:GLU:OE2	8:P:318:HIS:N	2.47	0.46
8:P:470:SER:O	8:P:473:LYS:HB2	2.15	0.46
8:P:726:VAL:HB	8:P:727:PRO:HD3	1.97	0.46
11:U:418:ALA:O	11:U:421:LEU:HB3	2.15	0.46
1:A:242:PHE:O	1:A:266:THR:HG21	2.15	0.46
1:A:824:CYS:SG	1:A:825:ARG:N	2.89	0.46
1:A:992:HIS:O	1:A:1073:ARG:NH2	2.49	0.46
1:A:1397:THR:O	1:A:1401:LEU:HG	2.16	0.46
2:B:231:PRO:O	2:B:234:SER:OG	2.24	0.46
3:C:224:ASN:ND2	3:C:249:SER:HA	2.30	0.46
6:G:346:THR:HA	6:G:349:ILE:HG12	1.98	0.46
6:H:402:VAL:O	6:H:406:GLN:HG2	2.15	0.46
2:O:651:LEU:HD22	2:O:704:LEU:HD13	1.98	0.46
8:P:288:LEU:HB2	8:P:311:CYS:SG	2.56	0.46
8:Q:531:ASN:ND2	8:Q:573:GLY:O	2.49	0.46
1:A:78:ILE:HG23	1:A:123:GLN:HE22	1.81	0.46
3:C:41:PHE:CE2	3:C:45:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:242:ARG:O	6:H:246:VAL:HG23	2.16	0.46
8:P:74:ARG:HD2	8:P:90:LEU:HD12	1.97	0.46
8:P:274:ILE:O	8:P:274:ILE:HG23	2.16	0.46
8:Q:252:CYS:SG	8:Q:275:LEU:HD11	2.55	0.46
10:X:34:LEU:HB2	10:X:55:VAL:HB	1.98	0.46
11:U:742:SER:HA	11:U:745:LEU:HD12	1.97	0.46
1:A:320:PHE:CG	1:A:366:LEU:HD11	2.51	0.46
2:B:472:GLU:OE2	2:B:474:LEU:HD13	2.16	0.46
3:C:188:VAL:HB	3:C:189:PRO:CD	2.45	0.46
4:E:516:LEU:HD11	4:E:527:LEU:HD22	1.97	0.46
6:G:267:LEU:CD2	1:S:60:LEU:HD11	2.46	0.46
6:H:100:LEU:HD22	6:H:125:VAL:HG21	1.98	0.46
2:O:83:SER:HA	2:O:90:ASN:HA	1.98	0.46
2:O:242:ILE:HG21	8:Q:18:LEU:HD13	1.98	0.46
8:Q:311:CYS:SG	8:Q:312:LEU:N	2.89	0.46
8:Q:565:TYR:N	8:Q:565:TYR:CD1	2.84	0.46
1:S:665:THR:CA	9:W:80:VAL:HG22	2.46	0.46
1:S:728:GLN:NE2	9:W:87:TRP:CE2	2.84	0.46
1:S:935:LEU:O	1:S:939:ILE:HD12	2.16	0.46
11:U:322:PHE:O	11:U:323:GLN:C	2.52	0.46
1:A:320:PHE:CB	1:A:366:LEU:HD11	2.46	0.45
1:A:1261:PHE:HB2	1:A:1291:ILE:HG21	1.98	0.45
1:A:1376:VAL:HG11	1:A:1392:PRO:HG3	1.98	0.45
2:B:828:LEU:HD23	8:P:826:ARG:C	2.37	0.45
3:C:394:TRP:CH2	3:C:398:ILE:HD11	2.51	0.45
4:E:357:LEU:HD13	4:E:397:PRO:HG3	1.98	0.45
1:S:568:VAL:HG23	1:S:1069:LEU:HD11	1.97	0.45
1:S:731:MET:SD	9:W:87:TRP:HD1	2.39	0.45
11:U:4:LYS:O	11:U:8:LEU:HD13	2.15	0.45
12:V:813:LEU:HD22	12:V:935:ILE:HG23	1.98	0.45
1:A:818:PHE:CD1	1:A:819:ASP:N	2.84	0.45
1:A:1329:ARG:O	1:A:1332:PRO:HD2	2.16	0.45
2:B:280:PRO:HB2	2:B:281:PHE:CD1	2.51	0.45
3:C:209:ARG:HA	4:E:91:PRO:HB3	1.98	0.45
7:L:127:VAL:HG22	7:L:137:LYS:O	2.15	0.45
2:O:65:PHE:HB2	2:O:118:PHE:CD1	2.51	0.45
2:O:409:ARG:O	2:O:413:LEU:HG	2.16	0.45
8:P:71:ALA:N	8:P:72:PRO:CD	2.79	0.45
1:S:737:ALA:HB1	1:S:738:PRO:CD	2.44	0.45
7:M:62:ILE:HG21	7:M:95:LEU:HD21	1.99	0.45
7:M:80:LEU:O	7:M:83:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:672:GLN:HE21	11:U:756:TYR:HA	1.82	0.45
12:V:412:ILE:HG23	12:V:416:LEU:HD13	1.97	0.45
12:V:1024:CYS:HA	12:V:1027:LEU:HD12	1.99	0.45
1:A:414:LEU:HG	1:A:426:SER:HB2	1.98	0.45
1:A:1075:LEU:CD1	1:A:1119:PHE:CD2	2.95	0.45
6:H:387:SER:HB2	6:H:388:PRO:CD	2.47	0.45
7:L:185:SER:O	7:L:188:SER:OG	2.24	0.45
7:L:333:PHE:CZ	7:L:360:PRO:HD2	2.51	0.45
8:P:520:GLN:OE1	8:P:520:GLN:N	2.49	0.45
8:P:649:MET:HE2	8:P:799:ARG:HB2	1.99	0.45
1:S:550:ASP:OD2	1:S:578:TYR:OH	2.35	0.45
7:M:266:LYS:HG2	7:M:270:ASN:ND2	2.32	0.45
7:M:326:ASN:HD22	7:M:364:LYS:HG3	1.80	0.45
11:U:364:ILE:O	11:U:368:VAL:HG23	2.16	0.45
11:U:471:PRO:O	11:U:472:LEU:C	2.51	0.45
12:V:205:GLU:CA	12:V:208:GLN:HG2	2.42	0.45
2:B:759:MET:O	2:B:762:THR:OG1	2.34	0.45
6:G:458:LEU:HD22	6:G:596:TYR:CD2	2.52	0.45
8:P:11:LEU:HD13	8:P:431:THR:HG23	1.97	0.45
8:P:339:ARG:HB3	8:P:341:TYR:CE1	2.52	0.45
8:P:658:LEU:HD21	8:P:745:VAL:HG12	1.97	0.45
8:Q:130:LEU:HA	8:Q:144:VAL:HA	1.98	0.45
1:S:184:HIS:HA	1:S:187:VAL:HG12	1.98	0.45
1:S:1076:LEU:HD23	1:S:1120:CYS:SG	2.56	0.45
7:M:146:ARG:HD3	7:M:205:ASP:OD2	2.17	0.45
7:M:158:TYR:OH	7:M:182:SER:HA	2.16	0.45
7:M:256:ALA:HA	7:M:323:VAL:CG2	2.47	0.45
10:X:61:TYR:CD1	10:X:62:PRO:HA	2.51	0.45
12:V:193:THR:O	12:V:196:ILE:HG22	2.17	0.45
12:V:765:LEU:HD21	12:V:785:LEU:HD23	1.99	0.45
1:A:818:PHE:HZ	1:A:861:SER:HB2	1.81	0.45
2:B:479:TRP:CZ2	2:B:490:GLY:HA3	2.51	0.45
6:G:227:LYS:O	6:G:230:SER:OG	2.33	0.45
7:L:326:ASN:HD22	7:L:364:LYS:HG3	1.80	0.45
1:S:822:LEU:HD23	1:S:822:LEU:HA	1.82	0.45
1:S:1186:ARG:HB3	1:S:1190:GLN:HE22	1.82	0.45
11:U:502:ALA:O	11:U:505:PRO:HD2	2.17	0.45
1:A:1176:SER:HA	1:S:964:LEU:CD1	2.46	0.45
2:B:31:ASN:O	2:B:38:THR:N	2.49	0.45
2:B:682:CYS:HB3	2:B:692:TYR:HB3	1.99	0.45
5:F:285:LEU:HB3	5:F:294:TRP:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:186:PRO:HG2	6:H:201:GLN:HG2	1.98	0.45
6:H:240:CYS:O	6:H:242:ARG:N	2.50	0.45
2:O:419:ILE:CG1	8:Q:483:LEU:HD12	2.47	0.45
8:P:23:ALA:HB2	8:P:399:LEU:HD12	1.99	0.45
11:U:195:VAL:HG11	11:U:220:LEU:HD22	1.99	0.45
11:U:548:LYS:HZ3	11:U:550:LEU:HA	1.82	0.45
3:C:312:ILE:O	3:C:316:GLN:HG3	2.17	0.45
4:E:427:GLU:N	4:E:427:GLU:CD	2.70	0.45
6:G:461:GLN:NE2	6:G:596:TYR:OH	2.41	0.45
6:G:487:THR:HA	6:G:488:PRO:HD2	1.90	0.45
6:H:360:ALA:HB1	6:H:406:GLN:HB2	1.97	0.45
2:O:429:LEU:HD11	8:Q:490:MET:CE	2.46	0.45
2:O:501:LEU:O	2:O:604:ARG:HG3	2.16	0.45
8:P:86:TYR:N	8:P:86:TYR:CD1	2.84	0.45
1:A:1224:TRP:CZ3	1:A:1225:LEU:HD13	2.51	0.45
3:C:366:GLN:NE2	7:L:272:HIS:CE1	2.85	0.45
4:E:87:LEU:HD22	4:E:117:VAL:HG13	1.99	0.45
5:F:143:VAL:HG12	5:F:144:HIS:N	2.32	0.45
6:G:280:GLY:N	6:G:281:PRO:CD	2.79	0.45
6:G:457:LEU:HD13	6:G:479:CYS:SG	2.56	0.45
6:H:264:ARG:O	6:H:267:LEU:HB2	2.16	0.45
6:H:544:CYS:HG	6:H:550:THR:HG21	1.82	0.45
7:L:320:PRO:HA	7:L:333:PHE:O	2.17	0.45
2:O:830:VAL:HG22	8:Q:826:ARG:HG3	1.99	0.45
8:P:253:VAL:HG23	8:P:272:VAL:CG2	2.47	0.45
8:P:510:THR:OG1	8:P:645:HIS:CD2	2.70	0.45
8:Q:175:LEU:CD2	8:Q:272:VAL:HG21	2.47	0.45
1:S:291:THR:HA	1:S:294:ILE:HD12	1.98	0.45
1:S:563:ASN:HA	1:S:564:ILE:HD12	1.99	0.45
10:X:2:GLN:OE1	10:X:2:GLN:N	2.45	0.45
11:U:382:LEU:O	11:U:385:LEU:HB3	2.17	0.45
11:U:448:VAL:HA	11:U:456:ILE:CD1	2.46	0.45
11:U:636:GLU:O	11:U:712:ARG:NH2	2.50	0.45
11:U:707:GLU:O	11:U:711:ASN:ND2	2.50	0.45
11:U:1021:ASP:OD1	11:U:1078:ARG:NH2	2.45	0.45
12:V:1095:SER:HA	12:V:1113:GLN:HG3	1.98	0.45
1:A:1280:ASP:OD1	1:A:1280:ASP:N	2.49	0.45
2:B:487:LEU:HB2	2:B:584:LEU:CD2	2.46	0.45
8:P:154:LEU:CD2	8:P:258:LEU:HD23	2.43	0.45
8:P:423:LEU:HA	8:P:428:ARG:O	2.16	0.45
11:U:56:CYS:SG	11:U:65:ARG:NE	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:450:THR:OG1	12:V:356:TYR:CB	2.65	0.45
12:V:149:ILE:O	12:V:153:LEU:HB2	2.17	0.45
12:V:178:SER:HA	12:V:181:LYS:HG3	1.99	0.45
1:A:384:VAL:HG13	1:A:389:VAL:HG21	1.98	0.45
1:A:815:PRO:HA	1:A:818:PHE:CZ	2.51	0.45
1:A:823:THR:HG21	1:A:829:SER:HB2	1.98	0.45
1:A:1097:ALA:HB3	1:A:1100:PRO:HD2	1.99	0.45
2:B:346:LYS:O	2:B:349:LEU:HD12	2.16	0.45
2:B:526:ARG:HH21	2:B:653:ALA:C	2.20	0.45
2:B:739:PRO:HD2	2:B:742:CYS:SG	2.57	0.45
4:E:389:SER:HG	4:E:390:PHE:H	1.64	0.45
6:H:345:GLN:NE2	6:H:386:PRO:HA	2.32	0.45
2:O:254:ILE:HD12	2:O:256:LEU:HD13	1.98	0.45
2:O:750:GLY:HA2	8:Q:556:LEU:HD12	1.99	0.45
8:P:12:ALA:O	8:P:429:LEU:N	2.35	0.45
1:S:583:PHE:HZ	1:S:613:ILE:HG23	1.82	0.45
7:M:125:LYS:O	7:M:139:LYS:HB3	2.17	0.45
12:V:149:ILE:O	12:V:152:THR:HG22	2.16	0.45
12:V:489:VAL:O	12:V:493:LEU:HD23	2.17	0.45
12:V:1135:ILE:CD1	12:V:1185:LEU:HD11	2.47	0.45
2:B:752:GLU:CD	8:P:859:SER:O	2.55	0.44
3:C:150:LEU:CD2	5:F:139:ARG:HG2	2.47	0.44
5:F:147:ARG:HG3	5:F:148:PHE:CE1	2.52	0.44
6:H:257:ARG:HD2	6:H:289:LEU:HA	1.98	0.44
2:O:602:MET:HG2	8:Q:644:ARG:NH1	2.32	0.44
7:M:365:PRO:CB	11:U:266:HIS:NE2	2.76	0.44
10:X:56:ILE:HB	10:X:67:GLN:CG	2.47	0.44
11:U:3:GLN:HA	11:U:6:LEU:HG	1.99	0.44
11:U:474:LEU:CD2	11:U:506:LEU:HD11	2.43	0.44
11:U:494:GLN:CD	11:U:494:GLN:N	2.70	0.44
11:U:990:THR:O	11:U:993:SER:OG	2.33	0.44
12:V:51:LEU:HD21	12:V:83:LEU:HG	1.99	0.44
12:V:446:LEU:HG	12:V:447:ASP:N	2.32	0.44
1:A:1034:LEU:HD22	1:S:1188:HIS:CG	2.53	0.44
2:B:259:LEU:CD1	2:B:284:PRO:HB2	2.47	0.44
2:B:326:SER:OG	2:B:346:LYS:HA	2.17	0.44
4:E:359:ASN:C	4:E:363:LEU:HD23	2.37	0.44
6:G:370:LEU:O	6:G:373:LEU:HB2	2.17	0.44
6:G:480:LEU:O	6:G:484:PHE:CD2	2.70	0.44
8:P:60:PHE:CD1	8:P:60:PHE:N	2.84	0.44
8:P:224:LEU:O	8:P:227:LEU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:730:CYS:O	8:Q:734:GLN:HG2	2.17	0.44
1:S:139:VAL:HG12	1:S:140:GLU:N	2.32	0.44
1:S:855:THR:O	1:S:858:SER:N	2.46	0.44
1:S:1008:PHE:CG	1:S:1008:PHE:O	2.70	0.44
1:S:1258:VAL:HG13	1:S:1305:LEU:HD21	1.99	0.44
7:M:125:LYS:O	7:M:139:LYS:N	2.43	0.44
12:V:246:LEU:CD2	12:V:284:PHE:CD2	3.00	0.44
12:V:752:ILE:O	12:V:755:LEU:N	2.49	0.44
1:A:21:ALA:HA	6:H:415:THR:CG2	2.46	0.44
1:A:1305:LEU:C	1:A:1308:LEU:HD21	2.37	0.44
3:C:184:SER:OG	3:C:215:LEU:CD2	2.65	0.44
3:C:337:LEU:HD12	3:C:341:PHE:CD2	2.52	0.44
4:E:29:LEU:O	4:E:32:ALA:HB3	2.17	0.44
5:F:275:LEU:HD22	5:F:325:VAL:HG23	2.00	0.44
8:P:137:ASP:N	8:P:137:ASP:OD1	2.50	0.44
8:P:278:LEU:HD12	8:P:282:VAL:HG22	1.99	0.44
8:Q:776:LEU:HD13	8:Q:879:ILE:HD12	1.98	0.44
1:S:289:SER:HA	1:S:293:LYS:HE3	1.98	0.44
1:S:798:LEU:HB3	1:S:799:PRO:HD2	1.99	0.44
1:S:1304:ALA:O	1:S:1308:LEU:HD23	2.18	0.44
11:U:459:PHE:O	11:U:463:LEU:HB2	2.16	0.44
12:V:348:ASP:HA	12:V:351:LYS:HB2	1.99	0.44
12:V:435:ILE:HG22	12:V:436:LEU:HD12	1.99	0.44
1:A:1167:LEU:HB3	1:A:1225:LEU:HD11	2.00	0.44
2:B:534:PRO:HD2	2:B:689:PRO:HG2	1.99	0.44
2:B:667:TYR:CE2	6:H:239:LEU:CD1	2.92	0.44
3:C:248:PRO:O	3:C:252:LYS:HB2	2.17	0.44
4:E:341:LEU:HD22	4:E:371:ARG:NE	2.32	0.44
4:E:407:LEU:HD21	4:E:420:LEU:HD13	1.99	0.44
6:H:541:VAL:HG21	6:H:554:LEU:HD22	1.99	0.44
1:S:26:LEU:HA	1:S:29:ARG:HG2	1.99	0.44
7:M:361:TYR:CD1	10:X:101:SER:HB3	2.53	0.44
11:U:322:PHE:O	11:U:326:VAL:HG23	2.16	0.44
12:V:346:LEU:HD11	12:V:350:ILE:HD11	2.00	0.44
12:V:554:ASP:O	12:V:557:LEU:HB3	2.16	0.44
1:A:1103:ALA:O	1:A:1104:ARG:HB2	2.18	0.44
3:C:188:VAL:HB	3:C:189:PRO:HD2	1.99	0.44
3:C:241:CYS:SG	4:E:37:PRO:HG3	2.57	0.44
3:C:315:ILE:HG21	3:C:399:HIS:HA	2.00	0.44
4:E:68:CYS:SG	4:E:120:ILE:HD11	2.58	0.44
4:E:397:PRO:O	4:E:400:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:346:ILE:HG23	5:F:347:TRP:CD2	2.53	0.44
6:G:453:SER:CB	6:G:483:LEU:CD2	2.96	0.44
2:O:585:SER:N	2:O:586:PRO:CD	2.80	0.44
8:P:284:PHE:HZ	8:P:352:CYS:HG	1.64	0.44
8:Q:726:VAL:HA	8:Q:727:PRO:HD2	1.65	0.44
1:S:222:GLU:N	1:S:222:GLU:OE1	2.51	0.44
1:S:453:LYS:CE	1:S:496:PRO:HG3	2.47	0.44
11:U:214:VAL:HA	11:U:217:LEU:HD12	1.99	0.44
11:U:331:LYS:O	11:U:334:VAL:HB	2.18	0.44
11:U:450:THR:O	11:U:450:THR:HG22	2.17	0.44
11:U:1138:LEU:HA	11:U:1141:LEU:HD23	1.98	0.44
12:V:555:MET:HA	12:V:558:VAL:HG12	1.98	0.44
1:A:88:ASN:HD22	1:A:93:PHE:HE2	1.64	0.44
1:A:481:VAL:O	1:A:521:LEU:HD11	2.18	0.44
1:A:504:ARG:HE	1:A:504:ARG:N	2.16	0.44
3:C:367:THR:HG21	3:C:403:TRP:CH2	2.53	0.44
6:G:147:ALA:HA	6:G:159:LEU:CD1	2.48	0.44
6:G:416:LEU:HD13	1:S:22:TRP:CH2	2.51	0.44
6:G:524:TRP:CD1	6:G:532:LYS:HB3	2.53	0.44
7:L:234:VAL:HG11	7:L:259:VAL:HG11	1.98	0.44
8:P:366:LEU:C	8:P:366:LEU:CD2	2.86	0.44
11:U:240:LEU:HD13	11:U:264:LEU:CD1	2.47	0.44
11:U:1141:LEU:HA	11:U:1144:PHE:HB3	1.99	0.44
12:V:1332:GLN:HA	12:V:1335:THR:HB	2.00	0.44
2:B:139:GLY:O	2:B:141:LEU:HB2	2.17	0.44
2:B:828:LEU:N	2:B:828:LEU:HD12	2.33	0.44
4:E:68:CYS:SG	4:E:120:ILE:CD1	3.06	0.44
4:E:465:THR:OG1	4:E:467:GLU:HB3	2.17	0.44
5:F:147:ARG:O	5:F:151:TYR:HB3	2.17	0.44
7:L:228:ILE:HD12	7:L:238:ILE:HD12	2.00	0.44
8:Q:14:PHE:N	8:Q:427:GLY:O	2.49	0.44
8:Q:49:GLN:O	8:Q:50:GLU:HB2	2.18	0.44
8:Q:538:ASP:O	8:Q:570:ASP:O	2.35	0.44
1:S:242:PHE:HB3	1:S:266:THR:HG23	2.00	0.44
1:S:817:LEU:HD23	1:S:818:PHE:CD1	2.53	0.44
7:M:201:TRP:CZ3	7:M:221:ARG:HD2	2.53	0.44
11:U:1092:ALA:O	11:U:1096:LEU:HG	2.17	0.44
11:U:1181:LEU:CD2	11:U:1270:LYS:HB2	2.47	0.44
12:V:1204:ALA:HB2	12:V:1238:MET:HE3	1.99	0.44
1:A:923:GLU:OE1	1:A:923:GLU:HA	2.18	0.44
1:A:973:CYS:SG	1:A:980:ALA:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:TYR:O	3:C:148:GLY:N	2.51	0.44
4:E:333:LEU:N	4:E:334:PRO:CD	2.81	0.44
6:G:424:THR:O	6:G:428:LEU:HG	2.17	0.44
8:P:129:ALA:O	8:P:145:GLN:CB	2.66	0.44
8:Q:39:THR:OG1	8:Q:41:SER:HB3	2.18	0.44
1:S:116:MET:HE3	1:S:116:MET:HB3	1.86	0.44
11:U:272:ILE:HG23	11:U:312:LEU:HA	1.99	0.44
12:V:149:ILE:HA	12:V:152:THR:HG22	1.98	0.44
12:V:232:SER:HG	12:V:258:PHE:HE1	1.63	0.44
12:V:281:ILE:O	12:V:284:PHE:HB3	2.18	0.44
14:Z:53:DT:H2"	14:Z:54:DG:C8	2.53	0.44
1:A:279:ASP:O	1:A:283:ALA:HB3	2.17	0.44
8:P:253:VAL:HG23	8:P:272:VAL:CA	2.47	0.44
8:Q:153:GLN:HB3	8:Q:172:GLU:HG3	2.00	0.44
8:Q:450:SER:O	8:Q:453:GLN:NE2	2.51	0.44
8:Q:548:LEU:HB2	8:Q:597:THR:HG22	2.00	0.44
7:M:244:HIS:HB3	7:M:247:MET:HB2	2.00	0.44
7:M:320:PRO:HA	7:M:333:PHE:O	2.17	0.44
11:U:964:ARG:HA	11:U:967:LEU:HD12	2.00	0.44
11:U:1095:VAL:HG13	11:U:1137:GLN:HE21	1.80	0.44
12:V:629:ALA:N	12:V:729:CYS:SG	2.91	0.44
3:C:140:TYR:CE2	5:F:169:LEU:HD22	2.53	0.43
6:H:53:LEU:O	6:H:57:LEU:HG	2.18	0.43
2:O:237:VAL:HG11	2:O:258:ALA:HB1	2.00	0.43
8:P:173:VAL:HG12	8:P:268:PRO:HB3	2.00	0.43
8:Q:514:TRP:CZ2	8:Q:523:LEU:HD21	2.53	0.43
1:S:759:PRO:O	1:S:763:THR:HG23	2.17	0.43
11:U:817:LEU:HD22	11:U:839:MET:HE1	1.99	0.43
12:V:1246:VAL:HG22	12:V:1268:TRP:CZ3	2.52	0.43
1:A:818:PHE:HA	1:A:821:LEU:HB3	1.99	0.43
1:A:835:LYS:HB2	1:A:903:TRP:CZ3	2.52	0.43
1:A:1153:ASP:HA	1:A:1196:GLU:HG3	2.00	0.43
2:B:422:SER:HB3	7:L:18:GLN:OE1	2.18	0.43
2:B:584:LEU:HB2	2:O:725:THR:CG2	2.47	0.43
5:F:248:PHE:CE1	5:F:270:LEU:CD1	3.00	0.43
6:H:597:LEU:O	6:H:601:ARG:HG3	2.18	0.43
2:O:139:GLY:O	2:O:141:LEU:N	2.51	0.43
2:O:706:THR:OG1	2:O:718:ILE:HB	2.18	0.43
8:P:135:LEU:HD21	8:P:140:LEU:HD12	1.99	0.43
8:P:343:LEU:HD13	8:P:360:HIS:CE1	2.54	0.43
1:S:599:SER:OG	1:S:600:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:651:GLY:O	1:S:654:THR:OG1	2.31	0.43
1:S:948:ASP:OD1	1:S:952:GLN:NE2	2.51	0.43
12:V:1142:LEU:HD22	12:V:1151:ASN:ND2	2.32	0.43
1:A:1249:LEU:HD12	1:A:1252:GLU:HB2	2.01	0.43
2:B:41:PRO:HB2	2:B:74:LEU:HD12	1.99	0.43
2:B:481:ARG:O	2:B:488:VAL:HG23	2.18	0.43
2:B:828:LEU:CD2	8:P:826:ARG:CA	2.77	0.43
4:E:487:MET:HG2	12:V:202:ILE:HG22	1.99	0.43
5:F:290:GLN:C	6:G:485:ARG:HH22	2.22	0.43
6:G:473:ILE:HD11	6:G:523:GLU:HB3	2.01	0.43
6:H:209:THR:HG21	6:H:325:VAL:HG21	1.99	0.43
7:L:19:ASN:OD1	7:L:20:ARG:N	2.51	0.43
2:O:660:PHE:HE1	8:Q:676:VAL:HG11	1.83	0.43
1:S:485:SER:OG	1:S:521:LEU:HD22	2.18	0.43
1:S:1324:PRO:O	1:S:1328:THR:OG1	2.36	0.43
11:U:32:LEU:HD11	11:U:68:ILE:CD1	2.48	0.43
11:U:767:ARG:HA	11:U:770:ASP:OD2	2.18	0.43
11:U:856:THR:OG1	11:U:858:HIS:O	2.36	0.43
1:A:428:VAL:HG22	1:A:476:PHE:CZ	2.54	0.43
1:A:713:PRO:O	1:A:717:MET:HG2	2.19	0.43
6:H:239:LEU:HD12	6:H:239:LEU:C	2.38	0.43
7:L:107:PRO:N	7:L:108:PRO:CD	2.81	0.43
2:O:594:CYS:HA	2:O:620:VAL:O	2.17	0.43
2:O:771:SER:HB2	8:Q:834:HIS:CE1	2.52	0.43
8:P:51:GLY:C	8:P:53:LEU:H	2.21	0.43
8:P:60:PHE:N	8:P:60:PHE:HD1	2.16	0.43
11:U:507:LEU:HA	11:U:510:SER:OG	2.17	0.43
12:V:1014:HIS:ND1	12:V:1086:LEU:HD21	2.33	0.43
1:A:424:LEU:O	1:A:428:VAL:HG23	2.18	0.43
1:A:868:PHE:CE1	1:A:872:MET:HG2	2.53	0.43
1:A:928:THR:HG23	1:A:971:GLY:HA3	2.01	0.43
1:A:1084:ARG:NH2	1:S:952:GLN:OE1	2.52	0.43
2:B:16:LEU:HD11	2:B:80:ASN:CA	2.48	0.43
3:C:280:SER:HB3	3:C:283:GLN:HB2	2.01	0.43
6:H:69:LEU:O	6:H:72:THR:HB	2.19	0.43
8:P:346:PRO:O	8:P:362:THR:HA	2.18	0.43
1:S:458:SER:OG	1:S:462:TYR:OH	2.35	0.43
11:U:924:GLN:HA	11:U:927:ILE:HD11	1.99	0.43
3:C:146:TYR:CE2	5:F:143:VAL:HG11	2.54	0.43
4:E:67:LEU:HB3	4:E:87:LEU:HD13	2.00	0.43
6:H:241:PRO:HD2	6:H:244:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:248:ILE:HD12	2:O:253:ARG:HD2	2.01	0.43
8:P:10:TYR:CE1	8:P:430:MET:HB3	2.53	0.43
8:P:527:CYS:SG	8:P:527:CYS:O	2.76	0.43
1:S:1139:LEU:HD12	1:S:1139:LEU:HA	1.96	0.43
7:M:215:GLU:CB	7:M:227:ARG:HB3	2.47	0.43
11:U:134:LEU:HD12	11:U:157:LYS:CG	2.48	0.43
11:U:430:PHE:CZ	11:U:466:ILE:HG23	2.54	0.43
11:U:460:LEU:HA	11:U:463:LEU:HB3	2.01	0.43
1:A:1241:ASN:OD1	1:A:1241:ASN:N	2.50	0.43
1:S:57:LEU:HD12	1:S:101:GLN:HE21	1.84	0.43
1:S:547:ALA:HB1	1:S:582:HIS:HA	2.00	0.43
1:S:736:VAL:HG12	1:S:737:ALA:HB2	1.99	0.43
7:M:248:LEU:HD13	7:M:271:ILE:HD11	2.00	0.43
11:U:347:SER:O	11:U:351:GLN:NE2	2.52	0.43
11:U:602:ARG:O	11:U:605:LEU:N	2.44	0.43
2:B:163:VAL:HG11	2:B:191:LEU:HD11	2.00	0.43
4:E:429:LEU:HG	4:E:434:GLN:HG3	2.00	0.43
6:G:404:LEU:HD23	6:G:404:LEU:HA	1.91	0.43
8:P:866:LEU:O	8:P:869:VAL:HG23	2.18	0.43
1:S:1112:VAL:HG11	1:S:1163:CYS:SG	2.59	0.43
7:M:191:LEU:O	7:M:195:GLU:HG3	2.19	0.43
11:U:548:LYS:NZ	11:U:577:SER:OG	2.46	0.43
12:V:157:LEU:N	12:V:158:PRO:CD	2.81	0.43
12:V:406:LYS:HG2	12:V:412:ILE:CD1	2.49	0.43
12:V:1279:ILE:HG22	12:V:1337:LEU:HD23	2.00	0.43
1:A:371:LEU:HD23	1:A:396:LEU:HD11	2.00	0.43
1:A:1060:THR:HG23	1:A:1067:ALA:CB	2.49	0.43
2:B:40:THR:HG23	2:B:70:GLU:HA	2.01	0.43
2:B:130:MET:HG3	2:B:144:TRP:CD1	2.54	0.43
2:B:277:CYS:SG	2:B:279:LEU:HD12	2.59	0.43
2:B:364:LYS:HB2	2:B:365:ILE:HD12	2.01	0.43
6:G:273:LEU:HD23	6:G:279:TRP:HB2	2.00	0.43
8:P:33:ALA:O	8:P:49:GLN:HB2	2.19	0.43
8:Q:11:LEU:HD23	8:Q:431:THR:HG21	2.01	0.43
8:Q:529:LEU:O	8:Q:577:ARG:HA	2.19	0.43
1:S:299:PHE:CE2	1:S:358:LEU:HB2	2.54	0.43
1:S:463:HIS:CD2	1:S:473:LEU:HD21	2.53	0.43
1:S:1220:PRO:O	1:S:1253:ARG:NH2	2.51	0.43
1:S:1295:LEU:HD23	1:S:1300:ILE:HD12	2.01	0.43
7:M:128:TYR:HB3	7:M:137:LYS:HB2	2.00	0.43
10:X:14:LEU:HD13	10:X:24:CYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:646:LYS:HG3	11:U:649:ALA:HB3	2.00	0.43
11:U:1037:VAL:HA	11:U:1040:LYS:O	2.18	0.43
1:A:1213:PRO:O	1:A:1215:ALA:N	2.52	0.43
2:B:682:CYS:HA	2:B:693:PHE:O	2.19	0.43
3:C:95:CYS:O	3:C:98:ILE:HG22	2.19	0.43
2:O:588:LEU:HD13	2:O:624:LEU:HD11	2.00	0.43
8:Q:542:THR:HG23	8:Q:603:PHE:HB3	2.00	0.43
1:S:911:TRP:CE3	1:S:917:ARG:NH1	2.87	0.43
11:U:170:ASP:O	11:U:174:VAL:HG13	2.18	0.43
12:V:111:ARG:HG2	12:V:115:LEU:HD12	2.00	0.43
12:V:403:LEU:O	12:V:407:ILE:HG22	2.19	0.43
1:A:659:GLU:HG2	1:A:676:GLN:HE21	1.83	0.42
4:E:391:CYS:O	4:E:395:THR:CA	2.67	0.42
8:P:243:CYS:SG	8:P:251:CYS:O	2.75	0.42
1:S:342:MET:HB3	1:S:346:TRP:CZ2	2.54	0.42
1:S:1186:ARG:O	1:S:1190:GLN:NE2	2.52	0.42
11:U:582:THR:HG23	11:U:583:PHE:CD1	2.54	0.42
11:U:1210:TYR:CE1	11:U:1254:ILE:HD12	2.54	0.42
12:V:110:PHE:CE2	12:V:114:LEU:HD11	2.54	0.42
1:A:167:CYS:SG	1:A:196:LEU:HD23	2.59	0.42
2:B:738:LEU:HD23	2:B:738:LEU:HA	1.83	0.42
3:C:20:SER:HA	3:C:73:LYS:HD2	2.01	0.42
4:E:67:LEU:CD2	4:E:87:LEU:CD1	2.96	0.42
4:E:360:ALA:O	4:E:364:THR:OG1	2.29	0.42
4:E:476:LEU:HD13	4:E:492:LEU:CD2	2.48	0.42
6:H:499:CYS:SG	6:H:500:GLU:N	2.92	0.42
8:P:17:PRO:HD2	8:P:21:LEU:HD23	2.01	0.42
8:Q:484:THR:OG1	8:Q:485:SER:N	2.52	0.42
1:S:598:ASP:HB2	1:S:1008:PHE:HE1	1.83	0.42
1:S:788:ALA:HB1	1:S:818:PHE:CE1	2.54	0.42
11:U:1193:ASN:O	11:U:1196:LYS:HB3	2.18	0.42
12:V:198:GLN:O	12:V:202:ILE:HG23	2.19	0.42
12:V:307:LEU:N	12:V:307:LEU:HD23	2.33	0.42
12:V:435:ILE:CD1	12:V:465:PHE:CZ	3.02	0.42
12:V:809:LYS:O	12:V:813:LEU:HG	2.19	0.42
12:V:813:LEU:CD2	12:V:935:ILE:HG12	2.49	0.42
1:A:348:PHE:CE1	1:A:356:THR:HG23	2.53	0.42
1:A:1168:THR:HG23	1:A:1228:ALA:HB1	2.01	0.42
1:A:1231:HIS:CD2	1:A:1232:PHE:CE1	3.07	0.42
4:E:394:TYR:HB3	4:E:397:PRO:HG2	2.00	0.42
4:E:402:LEU:O	4:E:406:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:255:LEU:HB3	5:F:256:PRO:HD2	2.01	0.42
6:G:374:LEU:HD12	6:G:393:MET:HE1	2.01	0.42
8:P:11:LEU:HD23	8:P:429:LEU:HD23	2.00	0.42
8:P:28:VAL:HA	8:P:36:PHE:O	2.19	0.42
8:P:284:PHE:HD2	8:P:350:ALA:HB3	1.82	0.42
8:P:866:LEU:HA	8:P:869:VAL:CG2	2.48	0.42
8:Q:517:LEU:O	8:Q:518:GLN:C	2.58	0.42
1:S:330:HIS:O	1:S:388:ARG:NH1	2.48	0.42
7:M:361:TYR:HA	10:X:101:SER:CB	2.49	0.42
12:V:820:VAL:CB	12:V:964:GLU:HA	2.50	0.42
1:A:922:GLU:N	1:A:923:GLU:HG2	2.34	0.42
1:A:1262:PHE:CD1	1:A:1319:LEU:HD23	2.55	0.42
2:B:754:PHE:CG	8:P:555:ASP:HB2	2.55	0.42
6:H:598:SER:HA	6:H:601:ARG:HD2	2.01	0.42
8:P:14:PHE:HZ	8:P:37:LEU:HD11	1.85	0.42
8:P:228:LEU:HD11	8:P:312:LEU:HD22	2.02	0.42
8:P:361:SER:OG	8:P:397:ALA:HA	2.19	0.42
8:P:800:ALA:O	8:P:803:ALA:HB3	2.19	0.42
1:S:346:TRP:NE1	1:S:387:GLN:HG2	2.34	0.42
7:M:254:LEU:HD12	7:M:254:LEU:N	2.34	0.42
11:U:395:PRO:CD	11:U:458:HIS:ND1	2.82	0.42
12:V:628:SER:O	12:V:632:TYR:CD2	2.72	0.42
12:V:820:VAL:HG21	12:V:964:GLU:HG3	2.00	0.42
1:A:1127:THR:HG22	1:A:1129:ASP:H	1.85	0.42
5:F:339:PHE:CD2	5:F:344:LEU:HB3	2.54	0.42
6:G:419:GLU:HG2	1:S:22:TRP:CE2	2.54	0.42
6:H:67:LEU:N	6:H:68:PRO:HD2	2.35	0.42
7:L:307:CYS:O	7:L:333:PHE:HA	2.20	0.42
2:O:724:GLN:O	2:O:727:MET:HB3	2.18	0.42
8:Q:492:VAL:HG22	8:Q:535:PHE:CD2	2.54	0.42
7:M:144:SER:OG	7:M:198:LYS:NZ	2.31	0.42
7:M:182:SER:OG	7:M:184:ILE:HG22	2.20	0.42
7:M:282:GLN:O	7:M:282:GLN:NE2	2.53	0.42
7:M:354:ILE:HD11	11:U:435:MET:HG3	2.01	0.42
11:U:272:ILE:HG21	11:U:312:LEU:HA	2.01	0.42
11:U:628:LEU:O	11:U:631:LEU:HB3	2.19	0.42
11:U:919:VAL:HG13	11:U:923:TYR:HB2	2.01	0.42
12:V:699:LEU:HD21	12:V:788:LEU:HD23	2.02	0.42
1:A:54:HIS:CE1	6:H:298:ALA:HB2	2.54	0.42
2:B:728:PHE:CZ	8:P:676:VAL:HG22	2.55	0.42
6:H:67:LEU:O	6:H:71:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:89:THR:N	6:H:92:GLN:OE1	2.48	0.42
7:L:259:VAL:O	7:L:263:LEU:HD12	2.19	0.42
2:O:141:LEU:HD11	2:O:152:PHE:HB2	2.01	0.42
8:P:523:LEU:HD21	8:P:652:CYS:SG	2.59	0.42
8:P:860:CYS:SG	8:P:861:ALA:N	2.91	0.42
8:Q:239:PRO:HG2	8:Q:255:LEU:HD12	2.02	0.42
8:Q:710:VAL:HG23	8:Q:880:LEU:HB2	2.01	0.42
1:S:239:VAL:HG11	1:S:301:VAL:HG22	2.01	0.42
1:S:963:PHE:HD1	1:S:963:PHE:HA	1.66	0.42
11:U:113:ILE:HD11	11:U:160:LEU:HD12	2.01	0.42
11:U:275:ILE:HD11	11:U:312:LEU:HD21	2.01	0.42
11:U:524:ALA:HB3	11:U:536:ALA:HB2	2.01	0.42
11:U:593:ARG:O	11:U:596:SER:OG	2.28	0.42
11:U:746:VAL:HA	11:U:749:VAL:HB	2.01	0.42
1:A:247:PHE:CE2	1:A:319:PHE:HB2	2.55	0.42
1:A:286:GLN:HB2	1:A:288:GLU:OE1	2.20	0.42
1:A:1334:ALA:HA	1:A:1337:SER:OG	2.19	0.42
4:E:67:LEU:HA	4:E:86:LEU:CB	2.49	0.42
2:O:582:THR:HG22	2:O:583:SER:O	2.19	0.42
1:S:305:HIS:ND1	1:S:306:THR:HG23	2.34	0.42
11:U:280:LYS:HG2	12:V:479:THR:OG1	2.20	0.42
12:V:61:THR:OG1	12:V:62:GLY:N	2.52	0.42
12:V:139:LEU:HB3	12:V:149:ILE:HD13	2.01	0.42
1:A:291:THR:HA	1:A:294:ILE:HD12	2.02	0.42
3:C:79:PHE:HA	5:F:145:MET:HE3	2.01	0.42
3:C:140:TYR:CD2	5:F:169:LEU:HD13	2.55	0.42
4:E:486:SER:O	4:E:489:TYR:CB	2.68	0.42
5:F:158:GLN:HA	5:F:207:VAL:HG13	2.01	0.42
6:G:305:LEU:O	1:S:43:LEU:HD21	2.20	0.42
6:G:458:LEU:HD22	6:G:596:TYR:CE2	2.55	0.42
2:O:154:SER:OG	2:O:155:SER:O	2.30	0.42
1:S:795:ARG:HD2	1:S:815:PRO:CD	2.49	0.42
7:M:338:LEU:HD23	7:M:368:LEU:HD13	2.02	0.42
11:U:506:LEU:O	11:U:509:VAL:HB	2.19	0.42
11:U:900:LYS:HE2	11:U:900:LYS:HA	2.02	0.42
11:U:1132:LYS:HE2	11:U:1193:ASN:HD21	1.85	0.42
12:V:96:PHE:CD1	12:V:145:LEU:HD21	2.54	0.42
12:V:241:LEU:HG	12:V:241:LEU:O	2.20	0.42
12:V:465:PHE:N	12:V:465:PHE:HD1	2.18	0.42
1:A:395:ALA:O	1:A:399:CYS:HB2	2.20	0.42
1:A:742:GLN:HB3	1:A:745:TRP:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:ARG:HG2	2:B:711:THR:HG23	2.01	0.42
3:C:140:TYR:CE1	5:F:173:ARG:NH2	2.88	0.42
5:F:275:LEU:CD2	5:F:325:VAL:HG23	2.50	0.42
8:P:170:ILE:CG2	8:P:259:VAL:HA	2.50	0.42
8:P:175:LEU:HD23	8:P:272:VAL:HG21	2.00	0.42
8:P:193:PHE:CE2	8:P:281:PRO:HG2	2.55	0.42
8:P:861:ALA:O	8:P:865:ARG:HB2	2.20	0.42
1:S:495:HIS:HB3	1:S:496:PRO:HD3	2.02	0.42
1:S:936:GLU:HA	1:S:939:ILE:HD13	2.02	0.42
11:U:221:SER:HB2	11:U:229:VAL:HG21	2.02	0.42
11:U:240:LEU:HD13	11:U:264:LEU:HD11	2.02	0.42
1:A:1255:GLU:O	1:A:1259:PHE:HD2	2.03	0.42
2:B:276:VAL:HG12	2:B:277:CYS:O	2.20	0.42
3:C:55:MET:SD	3:C:60:VAL:HG21	2.59	0.42
3:C:224:ASN:HD22	3:C:249:SER:HB3	1.85	0.42
4:E:67:LEU:HD23	4:E:87:LEU:CD1	2.49	0.42
4:E:434:GLN:O	4:E:437:MET:HB2	2.20	0.42
4:E:519:ASN:HD22	4:E:519:ASN:N	2.17	0.42
6:H:563:ARG:HD3	6:H:567:ALA:HB3	2.01	0.42
8:P:129:ALA:O	8:P:145:GLN:HB3	2.20	0.42
1:S:384:VAL:HG13	1:S:389:VAL:HG21	2.00	0.42
7:M:55:CYS:HB3	7:M:59:LEU:HB3	2.02	0.42
11:U:1028:LEU:CD1	11:U:1074:ILE:HD13	2.50	0.42
12:V:300:GLU:O	12:V:304:LYS:HG2	2.20	0.42
1:A:43:LEU:HD23	6:H:309:ALA:HB2	2.02	0.41
2:B:750:GLY:HA2	8:P:556:LEU:HD12	2.02	0.41
4:E:396:TYR:HB3	4:E:397:PRO:CD	2.50	0.41
4:E:500:TYR:CA	4:E:503:ASN:HD22	2.32	0.41
4:E:525:LYS:HB2	12:V:155:GLU:CG	2.50	0.41
5:F:69:GLU:HB2	5:F:74:ARG:NH2	2.34	0.41
6:G:420:LEU:CD2	6:G:455:THR:OG1	2.68	0.41
6:G:448:CYS:HB2	6:G:486:ALA:CB	2.50	0.41
6:H:355:LEU:HD11	6:H:406:GLN:HG3	2.02	0.41
8:P:288:LEU:CG	8:P:311:CYS:SG	3.08	0.41
8:P:367:CYS:HA	8:P:392:PRO:HA	2.02	0.41
8:P:516:ARG:HG2	8:Q:581:THR:HG23	2.02	0.41
8:P:733:LEU:HD22	8:P:746:VAL:HG11	2.02	0.41
8:Q:707:SER:CB	8:Q:788:GLN:HG3	2.50	0.41
8:Q:707:SER:OG	8:Q:875:HIS:O	2.30	0.41
11:U:342:GLN:HE22	11:U:414:PRO:HD3	1.85	0.41
1:A:1343:HIS:HE2	1:A:1349:ARG:HG3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:GLU:OE1	2:B:71:ASN:ND2	2.53	0.41
3:C:134:PHE:CD2	5:F:166:GLN:HB3	2.54	0.41
6:G:89:THR:N	6:G:92:GLN:OE1	2.48	0.41
6:G:559:LYS:HD2	6:G:608:PHE:CE1	2.55	0.41
8:P:86:TYR:N	8:P:86:TYR:HD1	2.18	0.41
8:P:339:ARG:NH1	8:P:385:GLU:O	2.53	0.41
1:S:914:ARG:O	1:S:918:GLU:OE1	2.39	0.41
11:U:422:GLY:HA2	11:U:425:ILE:HD12	2.02	0.41
12:V:348:ASP:O	12:V:351:LYS:HB2	2.20	0.41
12:V:456:LEU:HB3	12:V:460:TYR:CE2	2.55	0.41
12:V:1328:LEU:HD13	12:V:1371:VAL:HG22	2.02	0.41
1:A:768:LEU:O	1:A:772:GLN:C	2.58	0.41
2:B:674:VAL:O	2:B:678:GLU:HB3	2.20	0.41
3:C:89:ILE:O	3:C:93:CYS:SG	2.70	0.41
3:C:407:VAL:HG13	3:C:422:LEU:HD22	2.01	0.41
6:G:99:SER:O	6:G:103:VAL:HG23	2.20	0.41
6:G:458:LEU:N	6:G:458:LEU:HD23	2.35	0.41
2:O:768:VAL:CG2	8:Q:841:LEU:HD21	2.51	0.41
8:P:77:TYR:N	8:P:77:TYR:CD1	2.88	0.41
8:P:390:LEU:HD23	8:P:390:LEU:H	1.83	0.41
1:S:218:CYS:HB3	1:S:294:ILE:HA	2.02	0.41
1:S:556:MET:SD	1:S:1010:GLY:HA3	2.61	0.41
1:S:880:ARG:HB2	1:S:881:GLN:OE1	2.20	0.41
1:S:974:ASP:O	1:S:975:GLY:C	2.58	0.41
1:S:1022:GLN:HA	1:S:1085:LEU:HD22	2.02	0.41
10:X:51:PHE:CD2	10:X:72:THR:HG21	2.55	0.41
10:X:52:LYS:HB3	10:X:71:LEU:HD12	2.02	0.41
11:U:267:VAL:HG22	11:U:271:ILE:HD12	2.01	0.41
11:U:966:LEU:O	11:U:970:LEU:HG	2.19	0.41
11:U:1076:ASN:HB3	11:U:1077:LEU:HD23	2.02	0.41
12:V:67:GLN:HA	12:V:118:GLU:HB3	2.03	0.41
2:B:331:ASP:O	2:B:333:PHE:CD2	2.72	0.41
6:G:450:LEU:HD22	6:G:450:LEU:HA	1.88	0.41
6:H:164:GLU:HG2	6:H:171:SER:O	2.20	0.41
6:H:218:GLN:O	6:H:222:THR:OG1	2.15	0.41
2:O:344:LEU:CD1	2:O:354:LEU:HA	2.51	0.41
2:O:486:SER:HA	2:O:582:THR:O	2.20	0.41
8:P:481:LYS:O	8:P:484:THR:OG1	2.34	0.41
8:P:577:ARG:O	8:Q:664:ARG:NH2	2.54	0.41
1:S:328:LEU:HD22	1:S:389:VAL:CG2	2.50	0.41
1:S:731:MET:HE2	9:W:85:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1261:PHE:HB2	1:S:1291:ILE:HG21	2.02	0.41
1:S:1276:ASN:O	1:S:1279:THR:OG1	2.22	0.41
1:S:1418:VAL:O	1:S:1421:LEU:HB3	2.20	0.41
7:M:146:ARG:NH2	7:M:202:ASP:OD1	2.44	0.41
11:U:127:LEU:O	11:U:131:PRO:HD3	2.21	0.41
11:U:319:ILE:HG22	11:U:322:PHE:HB2	2.01	0.41
11:U:488:LEU:HD21	11:U:496:VAL:CG1	2.51	0.41
11:U:504:GLN:O	11:U:504:GLN:CG	2.67	0.41
11:U:623:VAL:O	11:U:627:LEU:HG	2.20	0.41
12:V:65:GLN:HG3	12:V:118:GLU:HB2	2.01	0.41
12:V:436:LEU:HD11	12:V:461:ALA:CB	2.51	0.41
12:V:969:LEU:HD13	12:V:1065:LEU:HG	2.01	0.41
1:A:486:PRO:HG2	1:A:489:LEU:HD12	2.01	0.41
1:A:1118:ASN:HA	1:A:1324:PRO:CB	2.49	0.41
1:A:1185:TRP:CZ2	1:A:1194:PRO:HD3	2.56	0.41
3:C:56:ASP:O	3:C:60:VAL:HG22	2.21	0.41
4:E:493:MET:HE1	4:E:512:LEU:HA	2.02	0.41
7:L:164:ASP:HB3	7:L:166:PHE:HE1	1.86	0.41
8:P:366:LEU:HD22	8:P:393:MET:CE	2.50	0.41
8:P:658:LEU:HD21	8:P:745:VAL:CG1	2.50	0.41
8:Q:276:HIS:NE2	7:M:61:THR:CG2	2.83	0.41
7:M:187:TYR:O	7:M:191:LEU:HD23	2.21	0.41
7:M:309:ILE:HD11	7:M:360:PRO:HG2	2.03	0.41
7:M:335:GLN:NE2	7:M:370:MET:HA	2.35	0.41
11:U:924:GLN:N	11:U:925:PRO:CD	2.84	0.41
12:V:556:HIS:O	12:V:559:ILE:HB	2.21	0.41
1:A:1281:LEU:HB3	1:A:1282:PRO:HD3	2.03	0.41
3:C:337:LEU:HD12	3:C:341:PHE:HD2	1.83	0.41
4:E:424:VAL:HG12	4:E:437:MET:SD	2.60	0.41
6:G:75:CYS:SG	6:G:142:LEU:HD12	2.61	0.41
7:L:29:ILE:HD12	7:L:84:MET:CE	2.50	0.41
2:O:257:ILE:HD11	2:O:299:PHE:CE1	2.56	0.41
2:O:521:LEU:HD23	2:O:523:CYS:SG	2.59	0.41
8:P:200:VAL:HA	8:P:218:PHE:O	2.20	0.41
1:S:108:PRO:HG2	1:S:111:ILE:HD12	2.03	0.41
1:S:992:HIS:CD2	1:S:1073:ARG:NH2	2.88	0.41
1:S:1263:PHE:CE1	1:S:1322:VAL:HG11	2.55	0.41
7:M:361:TYR:CD1	10:X:101:SER:CB	3.04	0.41
11:U:237:PHE:CE2	11:U:271:ILE:HD13	2.56	0.41
11:U:456:ILE:O	11:U:457:SER:C	2.58	0.41
11:U:517:LEU:HG	11:U:521:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:1180:TYR:O	11:U:1184:CYS:SG	2.79	0.41
12:V:161:PHE:CD1	12:V:207:LEU:HD13	2.55	0.41
12:V:525:SER:O	12:V:529:ILE:HG12	2.21	0.41
12:V:695:ILE:HG22	12:V:758:CYS:SG	2.61	0.41
2:B:86:ARG:CZ	2:B:121:ARG:NH2	2.84	0.41
2:B:526:ARG:NH2	2:B:653:ALA:C	2.72	0.41
3:C:191:ILE:HD12	3:C:200:VAL:HG21	2.02	0.41
5:F:171:LEU:N	5:F:171:LEU:HD23	2.36	0.41
6:H:60:LEU:O	6:H:102:ARG:NH2	2.53	0.41
1:S:818:PHE:HA	1:S:821:LEU:HD12	2.03	0.41
11:U:606:TYR:CE1	11:U:667:LEU:HD13	2.55	0.41
11:U:665:ASP:N	11:U:665:ASP:OD1	2.53	0.41
12:V:816:LEU:HD12	12:V:935:ILE:HG21	2.03	0.41
1:A:659:GLU:CG	1:A:676:GLN:HE21	2.33	0.41
1:A:898:LEU:HB3	1:A:899:PRO:CD	2.50	0.41
1:A:1075:LEU:HD12	1:A:1119:PHE:HD2	1.80	0.41
1:A:1367:LEU:HD22	1:A:1372:ASP:HB3	2.03	0.41
1:A:1403:LEU:HD23	1:A:1432:VAL:HG11	2.03	0.41
2:B:170:ILE:HD12	2:B:170:ILE:HA	1.97	0.41
2:B:277:CYS:SG	2:B:279:LEU:CD1	3.09	0.41
2:B:294:GLY:O	2:B:296:ASN:OD1	2.38	0.41
2:B:324:LYS:O	2:B:325:LEU:C	2.59	0.41
2:B:728:PHE:CE1	8:P:676:VAL:HG22	2.55	0.41
2:B:840:LEU:HD21	8:P:812:VAL:CG1	2.51	0.41
3:C:232:ILE:CG2	3:C:233:SER:N	2.84	0.41
5:F:18:SER:O	5:F:100:ASN:ND2	2.53	0.41
5:F:302:VAL:HG22	5:F:303:PRO:O	2.20	0.41
6:G:147:ALA:CA	6:G:159:LEU:HD11	2.51	0.41
8:Q:478:GLN:HB3	8:Q:610:VAL:HG21	2.01	0.41
1:S:37:PRO:O	1:S:40:ALA:HB3	2.21	0.41
1:S:711:LEU:HD11	9:W:94:LEU:HD12	2.02	0.41
1:S:982:THR:HG23	1:S:1051:ILE:CD1	2.50	0.41
1:S:1063:TRP:CZ3	1:S:1329:ARG:NH2	2.89	0.41
1:S:1333:PHE:CD1	1:S:1333:PHE:C	2.92	0.41
11:U:113:ILE:O	11:U:116:VAL:HG12	2.21	0.41
1:A:320:PHE:CD2	1:A:366:LEU:CD1	3.04	0.41
2:B:25:PHE:CD1	2:B:45:VAL:HG22	2.55	0.41
2:B:50:PHE:HB3	2:B:333:PHE:O	2.21	0.41
2:B:505:THR:HG22	8:P:548:LEU:HD21	2.03	0.41
2:B:577:ILE:HD13	2:B:649:PHE:CD1	2.55	0.41
3:C:131:VAL:HG21	5:F:162:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:LEU:N	3:C:282:PRO:CD	2.84	0.41
3:C:291:PHE:CE2	3:C:340:TYR:HB3	2.56	0.41
6:G:254:SER:O	6:G:258:LYS:HG2	2.21	0.41
6:G:303:LEU:O	6:G:306:LEU:HB3	2.20	0.41
6:H:179:LEU:O	6:H:183:THR:OG1	2.38	0.41
6:H:406:GLN:OE1	6:H:599:TRP:CG	2.73	0.41
6:H:538:LEU:HG	6:H:542:GLN:HE22	1.86	0.41
2:O:257:ILE:HD11	2:O:299:PHE:CZ	2.56	0.41
2:O:525:ASN:N	2:O:525:ASN:OD1	2.54	0.41
8:P:7:ARG:HG3	8:P:8:VAL:HG23	2.03	0.41
8:P:390:LEU:HG	8:P:390:LEU:O	2.21	0.41
1:S:145:LEU:HG	1:S:149:LEU:HD11	2.03	0.41
1:S:274:LEU:HD21	1:S:323:THR:HG23	2.02	0.41
1:S:739:PRO:HA	1:S:742:GLN:HB2	2.01	0.41
7:M:105:PRO:O	7:M:107:PRO:HD3	2.21	0.41
11:U:19:GLU:OE1	11:U:19:GLU:N	2.54	0.41
11:U:237:PHE:CZ	11:U:271:ILE:CD1	3.04	0.41
11:U:817:LEU:HD22	11:U:839:MET:CE	2.51	0.41
11:U:869:LYS:O	11:U:872:GLN:HB2	2.21	0.41
12:V:58:ILE:HD13	12:V:67:GLN:HB2	2.03	0.41
12:V:1016:VAL:O	12:V:1020:LEU:N	2.53	0.41
1:A:348:PHE:CZ	1:A:356:THR:CG2	3.04	0.41
1:A:385:HIS:CE1	1:A:387:GLN:HB2	2.55	0.41
1:A:422:CYS:HB3	1:A:472:PHE:CE2	2.56	0.41
2:B:658:SER:CB	2:B:727:MET:SD	3.09	0.41
3:C:188:VAL:CB	3:C:189:PRO:CD	2.99	0.41
4:E:327:LEU:O	4:E:330:GLN:N	2.54	0.41
6:G:309:ALA:O	6:G:312:VAL:HG12	2.20	0.41
6:H:139:LEU:O	6:H:142:LEU:HB2	2.21	0.41
6:H:181:LEU:HD22	6:H:207:LEU:HB3	2.03	0.41
6:H:480:LEU:O	6:H:483:LEU:HB3	2.21	0.41
7:L:41:VAL:HB	7:L:52:ARG:HB2	2.03	0.41
2:O:272:THR:O	2:O:274:LYS:HG3	2.21	0.41
8:P:28:VAL:O	8:P:29:LEU:HD23	2.21	0.41
8:P:346:PRO:HD2	8:P:363:PRO:CD	2.51	0.41
8:P:472:LEU:O	8:P:476:VAL:HG23	2.20	0.41
8:Q:733:LEU:CD2	8:Q:746:VAL:HG11	2.51	0.41
1:S:290:SER:OG	1:S:291:THR:N	2.54	0.41
11:U:809:PHE:CZ	11:U:813:LEU:HD13	2.56	0.41
11:U:953:GLN:HA	11:U:1002:GLN:HE21	1.86	0.41
12:V:1313:LEU:HB3	12:V:1324:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:PRO:HG2	1:A:1226:SER:CB	2.51	0.40
3:C:61:ILE:HA	3:C:64:PHE:HB2	2.02	0.40
3:C:224:ASN:HD22	3:C:249:SER:HA	1.86	0.40
4:E:514:MET:SD	4:E:514:MET:N	2.93	0.40
6:G:332:PRO:O	8:P:265:PRO:HG3	2.21	0.40
6:H:136:LEU:HA	6:H:139:LEU:HD12	2.02	0.40
6:H:213:TYR:CD1	6:H:329:LEU:HD22	2.56	0.40
2:O:322:TRP:HB2	2:O:325:LEU:HD11	2.03	0.40
2:O:394:LEU:CD1	7:M:115:ILE:HD11	2.48	0.40
2:O:522:LYS:C	2:O:523:CYS:SG	3.00	0.40
2:O:673:LYS:O	2:O:677:LEU:HD22	2.21	0.40
8:P:726:VAL:HB	8:P:727:PRO:CD	2.51	0.40
1:S:1199:LYS:HA	1:S:1202:GLU:HB2	2.03	0.40
1:S:1358:VAL:O	1:S:1362:LEU:HG	2.22	0.40
10:X:22:ILE:HD11	10:X:112:GLN:HE21	1.86	0.40
12:V:631:TYR:HD2	12:V:632:TYR:CD1	2.40	0.40
1:A:135:VAL:O	1:A:178:LEU:HD12	2.21	0.40
1:A:827:ARG:HA	1:A:830:LEU:HD12	2.03	0.40
2:B:74:LEU:HD22	2:B:98:LYS:HD3	2.04	0.40
2:B:660:PHE:CZ	2:B:731:LEU:HD11	2.56	0.40
3:C:364:TRP:CE3	3:C:406:MET:SD	3.14	0.40
4:E:63:LEU:HG	4:E:67:LEU:HD11	2.03	0.40
6:G:89:THR:O	6:G:149:LEU:HD21	2.20	0.40
6:G:346:THR:HA	6:G:349:ILE:CG1	2.51	0.40
8:P:679:PHE:O	8:P:679:PHE:CD1	2.74	0.40
8:Q:526:THR:HG22	8:Q:581:THR:HG22	2.02	0.40
8:Q:556:LEU:O	8:Q:557:ASP:HB2	2.21	0.40
8:Q:768:VAL:HG12	8:Q:787:ILE:CG1	2.51	0.40
1:S:552:GLU:HG2	1:S:1007:VAL:HG11	2.03	0.40
1:S:866:LYS:HE3	1:S:924:ASP:O	2.22	0.40
10:X:61:TYR:CG	10:X:62:PRO:HA	2.56	0.40
11:U:14:ALA:HB2	11:U:55:PRO:HG3	2.03	0.40
11:U:605:LEU:HB3	11:U:609:PHE:CE2	2.56	0.40
11:U:1014:CYS:HA	11:U:1074:ILE:HD12	2.02	0.40
12:V:224:HIS:O	12:V:227:VAL:HB	2.21	0.40
1:A:818:PHE:HA	1:A:821:LEU:CB	2.51	0.40
2:B:239:TYR:HB3	2:B:259:LEU:CD2	2.52	0.40
2:B:407:GLU:O	2:B:410:GLN:HB3	2.22	0.40
3:C:312:ILE:HG12	3:C:398:ILE:HD12	2.02	0.40
4:E:19:TRP:HD1	4:E:27:ARG:HG3	1.86	0.40
4:E:391:CYS:O	4:E:392:ALA:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:340:CYS:O	8:P:263:SER:OG	2.37	0.40
8:P:289:LYS:HB2	8:P:307:VAL:HG11	2.04	0.40
8:P:335:VAL:CG1	8:P:336:PRO:HD2	2.51	0.40
8:P:717:ALA:HB3	8:P:815:GLN:NE2	2.36	0.40
8:Q:529:LEU:HD13	8:Q:543:LEU:HD22	2.03	0.40
1:S:585:PRO:HA	1:S:588:LEU:HB2	2.03	0.40
1:S:1028:LEU:HD23	1:S:1028:LEU:HA	1.92	0.40
11:U:353:LEU:HD13	11:U:1102:LEU:HD21	2.03	0.40
11:U:474:LEU:HD23	11:U:481:VAL:HG11	2.04	0.40
11:U:500:LEU:HD22	11:U:517:LEU:HD21	2.03	0.40
11:U:844:ASN:HA	11:U:847:LEU:HD22	2.02	0.40
12:V:226:ASP:O	12:V:229:LYS:N	2.54	0.40
12:V:243:VAL:O	12:V:246:LEU:HB2	2.22	0.40
12:V:465:PHE:N	12:V:465:PHE:CD1	2.89	0.40
1:A:982:THR:OG1	1:A:1051:ILE:HD11	2.21	0.40
4:E:315:LEU:HA	4:E:318:GLU:CG	2.52	0.40
6:G:37:LEU:N	6:G:37:LEU:HD23	2.36	0.40
6:G:280:GLY:N	6:G:281:PRO:HD2	2.35	0.40
6:H:544:CYS:SG	6:H:550:THR:HG21	2.61	0.40
7:L:6:ALA:O	7:L:10:ARG:HG2	2.21	0.40
2:O:481:ARG:NE	2:O:647:ASP:OD1	2.55	0.40
8:P:42:GLU:C	8:P:43:LEU:HD22	2.42	0.40
8:P:143:LEU:C	8:P:143:LEU:HD23	2.41	0.40
8:P:238:SER:HB2	8:P:256:LYS:HG3	2.04	0.40
8:P:359:TYR:CD2	8:P:420:LEU:CD2	3.04	0.40
8:Q:279:GLU:N	8:Q:279:GLU:OE2	2.54	0.40
1:S:815:PRO:HB3	1:S:861:SER:HB3	2.03	0.40
11:U:642:LEU:O	11:U:716:SER:OG	2.27	0.40
11:U:1019:ARG:HB3	11:U:1024:PHE:CE2	2.57	0.40
1:A:730:LEU:HD22	1:A:783:GLY:HA2	2.03	0.40
2:B:408:LEU:O	2:B:411:HIS:HB3	2.22	0.40
2:B:656:HIS:CD2	2:B:656:HIS:C	2.94	0.40
2:B:773:LEU:HB2	2:B:838:ILE:HG21	2.03	0.40
4:E:418:GLU:OE2	12:V:237:GLU:O	2.40	0.40
6:G:547:ASN:HD22	6:G:550:THR:HG23	1.86	0.40
6:H:178:LEU:HD12	6:H:211:PHE:HD2	1.87	0.40
2:O:98:LYS:HB3	2:O:106:GLU:HG3	2.04	0.40
8:P:11:LEU:CD2	8:P:429:LEU:HD23	2.52	0.40
8:P:510:THR:OG1	8:P:645:HIS:HD2	2.04	0.40
8:P:546:GLN:HG3	8:P:599:SER:OG	2.22	0.40
8:P:795:ALA:O	8:P:798:CYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:676:GLN:O	1:S:679:VAL:HB	2.22	0.40
1:S:994:SER:OG	1:S:995:SER:N	2.54	0.40
7:M:309:ILE:HD11	7:M:333:PHE:CE1	2.56	0.40
11:U:915:ILE:O	11:U:919:VAL:HG23	2.22	0.40
12:V:173:PRO:HA	12:V:176:ILE:HG22	2.04	0.40
12:V:275:LEU:HD12	12:V:278:LEU:HD12	2.04	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%)	1041 (90%)	109 (9%)	10 (1%)	17 56
1	S	1224/1477 (83%)	1088 (89%)	125 (10%)	11 (1%)	17 56
2	B	685/884 (78%)	586 (86%)	82 (12%)	17 (2%)	5 35
2	O	685/884 (78%)	598 (87%)	72 (10%)	15 (2%)	6 38
3	C	546/583 (94%)	483 (88%)	61 (11%)	2 (0%)	34 72
4	E	411/555 (74%)	364 (89%)	45 (11%)	2 (0%)	29 68
5	F	336/399 (84%)	302 (90%)	32 (10%)	2 (1%)	25 64
6	G	567/641 (88%)	507 (89%)	58 (10%)	2 (0%)	34 72
6	H	532/641 (83%)	483 (91%)	44 (8%)	5 (1%)	17 56
7	L	368/394 (93%)	331 (90%)	35 (10%)	2 (0%)	29 68
7	M	368/394 (93%)	333 (90%)	29 (8%)	6 (2%)	9 45
8	P	726/906 (80%)	613 (84%)	95 (13%)	18 (2%)	5 35
8	Q	732/906 (81%)	629 (86%)	89 (12%)	14 (2%)	8 41
9	W	21/39 (54%)	13 (62%)	5 (24%)	3 (14%)	0 4
10	X	151/197 (77%)	146 (97%)	3 (2%)	2 (1%)	12 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	U	1163/1328 (88%)	1029 (88%)	128 (11%)	6 (0%)	29 68
12	V	1096/1451 (76%)	1011 (92%)	79 (7%)	6 (0%)	29 68
All	All	10771/13156 (82%)	9557 (89%)	1091 (10%)	123 (1%)	18 52

All (123) 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
6	G	192	ASP
6	H	192	ASP
6	H	242	ARG
2	O	83	SER
2	O	132	ASP
2	O	147	VAL
2	O	249	LYS
2	O	354	LEU
8	P	63	GLN
8	P	781	PRO
8	Q	50	GLU
8	Q	518	GLN
8	Q	557	ASP
8	Q	643	SER
1	S	288	GLU
1	S	947	SER
9	W	80	VAL
7	M	103	ALA
11	U	451	ARG
1	A	900	SER
1	A	972	GLY
2	B	826	THR
4	E	353	PRO
5	F	127	GLU
2	O	251	GLN
2	O	637	PRO
8	P	148	ALA
8	P	557	ASP

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Mol	Chain	Res	Type
8	P	782	ILE
8	Q	649	MET
1	S	975	GLY
7	M	22	LYS
7	M	296	ALA
11	U	449	VAL
11	U	548	LYS
11	U	808	LYS
12	V	411	CYS
1	A	26	LEU
1	A	29	ARG
1	A	1214	GLU
2	B	273	PRO
2	B	325	LEU
2	B	637	PRO
3	C	23	ASP
6	H	61	PRO
6	H	241	PRO
7	L	307	CYS
2	O	250	ASN
2	O	324	LYS
2	O	325	LEU
8	P	137	ASP
8	P	387	PRO
8	P	550	SER
8	P	857	ALA
8	P	860	CYS
8	Q	148	ALA
8	Q	397	ALA
8	Q	500	GLY
1	S	599	SER
1	S	1104	ARG
1	S	1214	GLU
9	W	86	SER
7	M	110	PHE
12	V	753	ASP
1	A	1104	ARG
2	B	140	PRO
2	B	314	GLU
2	B	316	PHE
8	P	52	GLY
1	S	564	ILE

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Mol	Chain	Res	Type
1	S	670	ARG
1	S	976	ASP
1	S	1023	GLU
11	U	170	ASP
1	A	220	GLN
2	B	631	LYS
2	B	734	LEU
4	E	23	GLU
6	H	63	ALA
2	O	70	GLU
2	O	636	PHE
8	P	383	PRO
8	Q	63	GLN
8	Q	550	SER
8	Q	608	GLU
8	Q	727	PRO
7	M	78	PRO
7	M	176	SER
11	U	77	GLU
12	V	206	ASN
2	B	83	SER
2	B	324	LYS
5	F	337	GLY
6	G	425	SER
2	O	138	ASN
2	O	631	LYS
8	Q	757	VAL
10	X	62	PRO
8	P	166	PRO
8	P	354	GLY
8	P	876	PRO
8	P	822	ALA
8	Q	19	GLY
9	W	74	PRO
10	X	94	PRO
12	V	559	ILE
12	V	645	ASP
1	A	1322	VAL
2	B	82	VAL
2	B	711	THR
3	C	232	ILE
2	O	140	PRO

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Mol	Chain	Res	Type
8	P	396	PRO
1	S	201	PRO
12	V	834	PRO
7	L	320	PRO
8	P	586	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%)	938 (91%)	96 (9%)	9 31
1	S	1092/1282 (85%)	986 (90%)	106 (10%)	8 29
2	B	644/810 (80%)	556 (86%)	88 (14%)	3 20
2	O	641/810 (79%)	569 (89%)	72 (11%)	6 25
3	C	480/507 (95%)	446 (93%)	34 (7%)	14 42
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%)	423 (88%)	60 (12%)	4 22
6	H	454/538 (84%)	400 (88%)	54 (12%)	5 23
7	L	334/354 (94%)	308 (92%)	26 (8%)	12 39
7	M	334/354 (94%)	319 (96%)	15 (4%)	27 54
8	P	627/749 (84%)	535 (85%)	92 (15%)	3 17
8	Q	630/749 (84%)	554 (88%)	76 (12%)	5 23
9	W	22/22 (100%)	20 (91%)	2 (9%)	9 32
10	X	136/175 (78%)	130 (96%)	6 (4%)	28 54
11	U	1076/1204 (89%)	1014 (94%)	62 (6%)	20 47
12	V	1036/1324 (78%)	992 (96%)	44 (4%)	30 55
All	All	9669/11501 (84%)	8772 (91%)	897 (9%)	12 31

All (897) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	50	LEU
1	A	60	LEU
1	A	93	PHE
1	A	100	ASP
1	A	109	VAL
1	A	139	VAL
1	A	145	LEU
1	A	148	LEU
1	A	153	GLN
1	A	163	ARG
1	A	169	GLU
1	A	179	LEU
1	A	182	VAL
1	A	185	LEU
1	A	192	SER
1	A	193	LEU
1	A	217	LEU
1	A	219	GLU
1	A	226	GLN
1	A	244	LEU
1	A	274	LEU
1	A	279	ASP
1	A	285	VAL
1	A	321	SER
1	A	333	VAL
1	A	342	MET
1	A	380	GLU
1	A	390	LEU
1	A	407	LEU
1	A	424	LEU
1	A	425	ASP
1	A	426	SER
1	A	434	VAL
1	A	447	SER
1	A	452	PHE
1	A	453	LYS
1	A	456	PHE
1	A	465	CYS
1	A	468	LYS
1	A	491	VAL
1	A	507	LEU
1	A	517	ARG

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Mol	Chain	Res	Type
1	A	653	LEU
1	A	660	LEU
1	A	666	ASP
1	A	668	SER
1	A	731	MET
1	A	758	LEU
1	A	782	LEU
1	A	793	GLU
1	A	817	LEU
1	A	826	THR
1	A	827	ARG
1	A	834	LEU
1	A	860	LEU
1	A	861	SER
1	A	877	SER
1	A	928	THR
1	A	944	ASP
1	A	949	THR
1	A	953	ASP
1	A	964	LEU
1	A	984	LEU
1	A	988	LEU
1	A	993	GLN
1	A	1014	ASN
1	A	1030	LEU
1	A	1053	ARG
1	A	1060	THR
1	A	1061	SER
1	A	1063	TRP
1	A	1073	ARG
1	A	1077	MET
1	A	1098	GLU
1	A	1105	CYS
1	A	1126	LEU
1	A	1130	ILE
1	A	1184	ARG
1	A	1188	HIS
1	A	1190	GLN
1	A	1231	HIS
1	A	1241	ASN
1	A	1258	VAL
1	A	1269	LEU

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Mol	Chain	Res	Type
1	A	1271	SER
1	A	1280	ASP
1	A	1331	LEU
1	A	1345	ASP
1	A	1360	MET
1	A	1367	LEU
1	A	1372	ASP
1	A	1391	ASN
1	A	1413	LYS
1	A	1421	LEU
1	A	1425	ARG
2	B	9	SER
2	B	11	GLU
2	B	13	GLU
2	B	17	CYS
2	B	29	LYS
2	B	40	THR
2	B	46	ARG
2	B	47	ARG
2	B	55	LYS
2	B	65	PHE
2	B	66	THR
2	B	70	GLU
2	B	90	ASN
2	B	102	ASN
2	B	112	LEU
2	B	155	SER
2	B	177	GLU
2	B	181	MET
2	B	187	LYS
2	B	245	THR
2	B	259	LEU
2	B	261	ARG
2	B	265	LEU
2	B	277	CYS
2	B	285	CYS
2	B	291	ASP
2	B	302	SER
2	B	307	ASN
2	B	309	CYS
2	B	311	VAL
2	B	331	ASP

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Mol	Chain	Res	Type
2	B	354	LEU
2	B	360	THR
2	B	390	VAL
2	B	403	SER
2	B	405	PHE
2	B	412	LEU
2	B	422	SER
2	B	483	ILE
2	B	484	ASP
2	B	486	SER
2	B	488	VAL
2	B	491	VAL
2	B	496	SER
2	B	503	ASP
2	B	507	SER
2	B	510	MET
2	B	518	PHE
2	B	519	ARG
2	B	525	ASN
2	B	526	ARG
2	B	531	SER
2	B	572	LYS
2	B	573	GLU
2	B	574	CYS
2	B	582	THR
2	B	585	SER
2	B	592	LYS
2	B	602	MET
2	B	606	SER
2	B	617	CYS
2	B	624	LEU
2	B	628	SER
2	B	635	THR
2	B	638	LYS
2	B	640	LYS
2	B	643	GLU
2	B	658	SER
2	B	659	CYS
2	B	670	ASN
2	B	673	LYS
2	B	677	LEU
2	B	690	GLU

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Mol	Chain	Res	Type
2	B	693	PHE
2	B	696	ARG
2	B	705	PHE
2	B	716	ILE
2	B	722	ARG
2	B	727	MET
2	B	748	LYS
2	B	751	SER
2	B	780	HIS
2	B	813	ARG
2	B	836	ARG
2	B	844	GLU
2	B	854	GLN
2	B	857	SER
2	B	858	ASN
3	C	10	CYS
3	C	19	LEU
3	C	42	GLN
3	C	63	ARG
3	C	65	PRO
3	C	86	SER
3	C	96	CYS
3	C	125	LEU
3	C	126	ARG
3	C	142	PRO
3	C	144	ASP
3	C	146	TYR
3	C	149	LEU
3	C	156	SER
3	C	162	ARG
3	C	172	GLN
3	C	173	ARG
3	C	205	ILE
3	C	213	GLU
3	C	218	GLU
3	C	224	ASN
3	C	260	LYS
3	C	283	GLN
3	C	294	VAL
3	C	302	LEU
3	C	304	GLU
3	C	327	GLU

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Mol	Chain	Res	Type
3	C	343	TYR
3	C	344	THR
3	C	345	SER
3	C	347	SER
3	C	493	ASN
3	C	509	ILE
3	C	528	GLN
4	E	28	LEU
4	E	78	ASP
4	E	86	LEU
4	E	87	LEU
4	E	98	LEU
4	E	101	LEU
4	E	114	LEU
4	E	116	SER
4	E	119	GLN
4	E	123	GLN
4	E	128	ASP
4	E	130	ASP
4	E	141	ARG
4	E	149	SER
4	E	150	MET
4	E	154	SER
4	E	155	PRO
4	E	276	GLU
4	E	293	GLN
4	E	300	GLU
4	E	318	GLU
4	E	347	TRP
4	E	352	SER
4	E	361	THR
4	E	387	LEU
4	E	390	PHE
4	E	395	THR
4	E	404	ASP
4	E	412	THR
4	E	419	LEU
4	E	428	SER
4	E	432	ASP
4	E	443	GLU
4	E	450	THR
4	E	459	GLU

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Mol	Chain	Res	Type
4	E	464	MET
4	E	474	GLU
4	E	484	THR
4	E	486	SER
4	E	494	LEU
4	E	496	VAL
4	E	507	THR
4	E	519	ASN
4	E	523	LEU
4	E	524	ARG
4	E	525	LYS
4	E	526	SER
5	F	10	ARG
5	F	90	ASP
5	F	136	LEU
5	F	138	ARG
5	F	143	VAL
5	F	164	LYS
5	F	196	LEU
5	F	210	LEU
5	F	215	SER
5	F	264	THR
5	F	270	LEU
5	F	288	ASP
5	F	300	GLN
5	F	302	VAL
5	F	315	CYS
5	F	336	ASP
5	F	355	ARG
6	G	12	CYS
6	G	13	LEU
6	G	14	ASP
6	G	35	LEU
6	G	37	LEU
6	G	57	LEU
6	G	67	LEU
6	G	71	LEU
6	G	89	THR
6	G	101	GLU
6	G	104	LEU
6	G	115	GLU
6	G	118	LEU

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Mol	Chain	Res	Type
6	G	124	SER
6	G	132	LEU
6	G	136	LEU
6	G	142	LEU
6	G	145	LEU
6	G	149	LEU
6	G	154	ASP
6	G	155	ARG
6	G	166	LEU
6	G	170	GLN
6	G	174	SER
6	G	176	ASP
6	G	179	LEU
6	G	180	LEU
6	G	189	GLU
6	G	207	LEU
6	G	226	ASP
6	G	234	GLU
6	G	240	CYS
6	G	250	THR
6	G	258	LYS
6	G	267	LEU
6	G	284	LEU
6	G	300	LEU
6	G	327	LEU
6	G	333	ASP
6	G	334	LEU
6	G	340	CYS
6	G	346	THR
6	G	352	SER
6	G	357	THR
6	G	405	ILE
6	G	437	ASP
6	G	448	CYS
6	G	450	LEU
6	G	459	GLN
6	G	474	SER
6	G	485	ARG
6	G	489	GLU
6	G	497	PHE
6	G	498	ASN
6	G	544	CYS

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Mol	Chain	Res	Type
6	G	566	GLU
6	G	578	THR
6	G	594	GLU
6	G	604	ASP
6	G	608	PHE
6	H	18	GLU
6	H	35	LEU
6	H	37	LEU
6	H	42	LEU
6	H	54	LEU
6	H	67	LEU
6	H	80	LEU
6	H	91	ASP
6	H	98	ARG
6	H	104	LEU
6	H	124	SER
6	H	130	CYS
6	H	136	LEU
6	H	145	LEU
6	H	158	ASP
6	H	159	LEU
6	H	174	SER
6	H	183	THR
6	H	191	LEU
6	H	192	ASP
6	H	226	ASP
6	H	250	THR
6	H	267	LEU
6	H	292	GLN
6	H	295	ASP
6	H	296	THR
6	H	297	THR
6	H	300	LEU
6	H	311	ASN
6	H	327	LEU
6	H	334	LEU
6	H	350	LEU
6	H	359	ARG
6	H	365	GLU
6	H	371	LEU
6	H	373	LEU
6	H	393	MET

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Mol	Chain	Res	Type
6	H	404	LEU
6	H	412	ASP
6	H	416	LEU
6	H	466	LEU
6	H	470	LYS
6	H	479	CYS
6	H	483	LEU
6	H	506	ASP
6	H	519	SER
6	H	523	GLU
6	H	530	ASP
6	H	559	LYS
6	H	568	THR
6	H	573	ARG
6	H	586	LEU
6	H	604	ASP
6	H	605	ARG
7	L	7	SER
7	L	39	ARG
7	L	44	GLU
7	L	46	LEU
7	L	56	SER
7	L	60	ARG
7	L	68	ARG
7	L	88	LYS
7	L	90	LEU
7	L	91	LEU
7	L	110	PHE
7	L	116	GLU
7	L	139	LYS
7	L	164	ASP
7	L	169	PHE
7	L	185	SER
7	L	227	ARG
7	L	243	ARG
7	L	251	CYS
7	L	268	SER
7	L	271	ILE
7	L	286	ASP
7	L	292	PHE
7	L	348	SER
7	L	349	ARG

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Mol	Chain	Res	Type
7	L	350	GLN
2	O	39	LYS
2	O	47	ARG
2	O	61	SER
2	O	72	SER
2	O	78	CYS
2	O	94	ILE
2	O	104	VAL
2	O	132	ASP
2	O	145	ARG
2	O	166	ASN
2	O	167	PHE
2	O	171	GLN
2	O	175	GLU
2	O	223	LEU
2	O	226	ILE
2	O	237	VAL
2	O	242	ILE
2	O	252	LEU
2	O	253	ARG
2	O	256	LEU
2	O	261	ARG
2	O	267	SER
2	O	279	LEU
2	O	283	ASP
2	O	287	VAL
2	O	300	VAL
2	O	315	SER
2	O	328	VAL
2	O	346	LYS
2	O	347	ASP
2	O	354	LEU
2	O	401	CYS
2	O	412	LEU
2	O	426	LEU
2	O	472	GLU
2	O	475	VAL
2	O	484	ASP
2	O	491	VAL
2	O	496	SER
2	O	503	ASP
2	O	506	LEU

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Mol	Chain	Res	Type
2	O	507	SER
2	O	509	LEU
2	O	510	MET
2	O	512	GLN
2	O	517	ARG
2	O	519	ARG
2	O	523	CYS
2	O	526	ARG
2	O	573	GLU
2	O	579	THR
2	O	583	SER
2	O	585	SER
2	O	587	LEU
2	O	591	SER
2	O	592	LYS
2	O	604	ARG
2	O	622	LEU
2	O	624	LEU
2	O	628	SER
2	O	631	LYS
2	O	635	THR
2	O	640	LYS
2	O	661	GLN
2	O	677	LEU
2	O	687	GLU
2	O	724	GLN
2	O	735	ILE
2	O	742	CYS
2	O	748	LYS
2	O	779	LYS
2	O	854	GLN
8	P	29	LEU
8	P	30	CYS
8	P	35	VAL
8	P	41	SER
8	P	69	LEU
8	P	74	ARG
8	P	76	LEU
8	P	82	ARG
8	P	91	ASP
8	P	118	VAL
8	P	119	ASP

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Mol	Chain	Res	Type
8	P	125	LEU
8	P	130	LEU
8	P	131	CYS
8	P	138	SER
8	P	145	GLN
8	P	155	PHE
8	P	159	CYS
8	P	162	GLU
8	P	165	ARG
8	P	169	GLN
8	P	170	ILE
8	P	173	VAL
8	P	195	PRO
8	P	196	VAL
8	P	198	CYS
8	P	201	SER
8	P	219	THR
8	P	224	LEU
8	P	232	ASP
8	P	234	THR
8	P	235	LEU
8	P	237	GLN
8	P	238	SER
8	P	246	PRO
8	P	253	VAL
8	P	269	ASN
8	P	274	ILE
8	P	285	ILE
8	P	305	GLU
8	P	310	ASP
8	P	311	CYS
8	P	321	MET
8	P	330	GLU
8	P	365	ASP
8	P	373	ARG
8	P	387	PRO
8	P	390	LEU
8	P	402	CYS
8	P	424	SER
8	P	450	SER
8	P	465	ILE
8	P	470	SER

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Mol	Chain	Res	Type
8	P	485	SER
8	P	515	SER
8	P	517	LEU
8	P	527	CYS
8	P	543	LEU
8	P	545	ILE
8	P	560	CYS
8	P	569	VAL
8	P	571	GLN
8	P	599	SER
8	P	600	CYS
8	P	638	VAL
8	P	639	CYS
8	P	642	LEU
8	P	646	THR
8	P	648	ASP
8	P	683	CYS
8	P	701	LEU
8	P	707	SER
8	P	732	THR
8	P	747	ARG
8	P	749	ARG
8	P	752	SER
8	P	768	VAL
8	P	782	ILE
8	P	789	VAL
8	P	793	SER
8	P	797	ILE
8	P	810	THR
8	P	811	MET
8	P	828	GLN
8	P	829	TYR
8	P	836	ASN
8	P	842	ARG
8	P	855	ASP
8	P	864	GLN
8	P	868	GLN
8	P	869	VAL
8	P	876	PRO
8	Q	16	CYS
8	Q	35	VAL
8	Q	69	LEU

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Mol	Chain	Res	Type
8	Q	89	SER
8	Q	91	ASP
8	Q	125	LEU
8	Q	130	LEU
8	Q	153	GLN
8	Q	159	CYS
8	Q	219	THR
8	Q	235	LEU
8	Q	242	LEU
8	Q	250	LEU
8	Q	253	VAL
8	Q	278	LEU
8	Q	307	VAL
8	Q	334	LEU
8	Q	337	GLU
8	Q	352	CYS
8	Q	362	THR
8	Q	365	ASP
8	Q	369	VAL
8	Q	373	ARG
8	Q	395	CYS
8	Q	402	CYS
8	Q	449	GLU
8	Q	450	SER
8	Q	465	ILE
8	Q	473	LYS
8	Q	481	LYS
8	Q	483	LEU
8	Q	490	MET
8	Q	498	SER
8	Q	507	SER
8	Q	508	CYS
8	Q	510	THR
8	Q	517	LEU
8	Q	521	ASP
8	Q	522	VAL
8	Q	542	THR
8	Q	546	GLN
8	Q	560	CYS
8	Q	566	THR
8	Q	569	VAL
8	Q	570	ASP

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Mol	Chain	Res	Type
8	Q	578	ARG
8	Q	582	LEU
8	Q	593	ASP
8	Q	598	VAL
8	Q	603	PHE
8	Q	607	ARG
8	Q	608	GLU
8	Q	638	VAL
8	Q	642	LEU
8	Q	645	HIS
8	Q	652	CYS
8	Q	683	CYS
8	Q	701	LEU
8	Q	732	THR
8	Q	739	GLU
8	Q	744	ASP
8	Q	745	VAL
8	Q	768	VAL
8	Q	782	ILE
8	Q	788	GLN
8	Q	789	VAL
8	Q	794	LEU
8	Q	807	ARG
8	Q	808	MET
8	Q	810	THR
8	Q	812	VAL
8	Q	838	GLU
8	Q	842	ARG
8	Q	855	ASP
8	Q	859	SER
8	Q	874	ARG
1	S	60	LEU
1	S	98	LEU
1	S	116	MET
1	S	142	ARG
1	S	148	LEU
1	S	169	GLU
1	S	174	GLN
1	S	175	SER
1	S	182	VAL
1	S	185	LEU
1	S	191	VAL

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Mol	Chain	Res	Type
1	S	194	GLN
1	S	222	GLU
1	S	239	VAL
1	S	245	ARG
1	S	267	VAL
1	S	274	LEU
1	S	287	GLU
1	S	290	SER
1	S	321	SER
1	S	333	VAL
1	S	334	LEU
1	S	337	SER
1	S	367	SER
1	S	370	GLU
1	S	376	GLN
1	S	383	GLU
1	S	396	LEU
1	S	407	LEU
1	S	423	GLN
1	S	424	LEU
1	S	425	ASP
1	S	427	MET
1	S	450	ASP
1	S	456	PHE
1	S	459	THR
1	S	460	ARG
1	S	466	SER
1	S	491	VAL
1	S	492	HIS
1	S	507	LEU
1	S	518	LEU
1	S	546	GLN
1	S	611	ASP
1	S	653	LEU
1	S	664	MET
1	S	666	ASP
1	S	668	SER
1	S	670	ARG
1	S	683	ARG
1	S	684	LEU
1	S	685	ARG
1	S	688	LEU

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Mol	Chain	Res	Type
1	S	714	ARG
1	S	723	LEU
1	S	735	SER
1	S	741	ARG
1	S	766	CYS
1	S	795	ARG
1	S	800	GLU
1	S	818	PHE
1	S	828	ASP
1	S	849	SER
1	S	856	LEU
1	S	859	CYS
1	S	911	TRP
1	S	912	THR
1	S	922	GLU
1	S	923	GLU
1	S	924	ASP
1	S	948	ASP
1	S	949	THR
1	S	973	CYS
1	S	984	LEU
1	S	992	HIS
1	S	993	GLN
1	S	1012	THR
1	S	1020	ARG
1	S	1027	ASP
1	S	1030	LEU
1	S	1045	GLU
1	S	1050	GLU
1	S	1053	ARG
1	S	1060	THR
1	S	1098	GLU
1	S	1105	CYS
1	S	1139	LEU
1	S	1142	CYS
1	S	1183	CYS
1	S	1202	GLU
1	S	1241	ASN
1	S	1251	CYS
1	S	1265	LEU
1	S	1274	THR
1	S	1282	PRO

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Mol	Chain	Res	Type
1	S	1301	SER
1	S	1320	LEU
1	S	1339	LEU
1	S	1345	ASP
1	S	1351	GLU
1	S	1369	VAL
1	S	1395	LEU
1	S	1403	LEU
1	S	1421	LEU
1	S	1425	ARG
1	S	1428	CYS
9	W	90	PHE
9	W	94	LEU
7	M	12	CYS
7	M	39	ARG
7	M	50	ASN
7	M	88	LYS
7	M	104	LEU
7	M	126	LEU
7	M	133	PHE
7	M	226	ARG
7	M	243	ARG
7	M	303	PHE
7	M	314	GLN
7	M	318	THR
7	M	343	ARG
7	M	347	THR
7	M	349	ARG
10	X	8	LYS
10	X	9	ARG
10	X	24	CYS
10	X	29	ASP
10	X	32	ASP
10	X	99	ARG
11	U	59	GLU
11	U	80	ASP
11	U	99	HIS
11	U	110	ASN
11	U	123	ASN
11	U	135	THR
11	U	165	CYS
11	U	231	GLU

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Mol	Chain	Res	Type
11	U	248	GLN
11	U	270	THR
11	U	275	ILE
11	U	276	VAL
11	U	281	LEU
11	U	284	GLU
11	U	285	LEU
11	U	316	VAL
11	U	323	GLN
11	U	398	VAL
11	U	424	ASN
11	U	442	GLU
11	U	451	ARG
11	U	454	SER
11	U	468	MET
11	U	476	SER
11	U	477	CYS
11	U	480	LYS
11	U	481	VAL
11	U	497	GLN
11	U	512	SER
11	U	514	ARG
11	U	515	ASP
11	U	528	ASN
11	U	546	ASN
11	U	547	PHE
11	U	576	ASN
11	U	590	SER
11	U	600	ASP
11	U	617	SER
11	U	640	ASP
11	U	652	LEU
11	U	659	SER
11	U	742	SER
11	U	760	ILE
11	U	762	SER
11	U	788	LYS
11	U	847	LEU
11	U	856	THR
11	U	870	ILE
11	U	890	THR
11	U	965	SER

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Mol	Chain	Res	Type
11	U	1006	MET
11	U	1020	GLU
11	U	1042	PRO
11	U	1043	VAL
11	U	1044	ILE
11	U	1100	ASP
11	U	1141	LEU
11	U	1143	THR
11	U	1144	PHE
11	U	1167	CYS
11	U	1199	LYS
11	U	1279	MET
12	V	45	ASP
12	V	89	TYR
12	V	104	ILE
12	V	175	LEU
12	V	198	GLN
12	V	201	SER
12	V	205	GLU
12	V	206	ASN
12	V	212	ILE
12	V	235	LEU
12	V	260	LEU
12	V	338	SER
12	V	348	ASP
12	V	355	ARG
12	V	359	THR
12	V	369	GLU
12	V	384	MET
12	V	406	LYS
12	V	412	ILE
12	V	421	PHE
12	V	424	HIS
12	V	430	ASP
12	V	431	MET
12	V	438	LEU
12	V	491	THR
12	V	513	PHE
12	V	525	SER
12	V	552	GLN
12	V	572	LEU
12	V	607	CYS

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Mol	Chain	Res	Type
12	V	662	ASP
12	V	770	LYS
12	V	771	LEU
12	V	803	GLU
12	V	929	ASP
12	V	931	GLU
12	V	1006	GLN
12	V	1036	CYS
12	V	1180	ASP
12	V	1227	THR
12	V	1257	SER
12	V	1294	CYS
12	V	1299	ARG
12	V	1320	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	123	GLN
1	A	153	GLN
1	A	168	GLN
1	A	188	GLN
1	A	248	GLN
1	A	676	GLN
1	A	978	GLN
1	A	1355	HIS
2	B	90	ASN
2	B	116	ASN
2	B	241	HIS
2	B	576	GLN
2	B	600	GLN
2	B	656	HIS
2	B	753	ASN
2	B	825	GLN
2	B	827	ASN
2	B	854	GLN
3	C	320	GLN
3	C	366	GLN
3	C	399	HIS
3	C	489	HIS
3	C	493	ASN

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Mol	Chain	Res	Type
3	C	520	HIS
3	C	557	GLN
4	E	75	GLN
4	E	95	GLN
4	E	97	ASN
4	E	287	GLN
4	E	434	GLN
4	E	503	ASN
4	E	519	ASN
4	E	533	HIS
5	F	63	HIS
5	F	130	GLN
5	F	283	GLN
5	F	300	GLN
5	F	308	HIS
6	G	31	GLN
6	G	94	GLN
6	G	97	GLN
6	G	167	ASN
6	G	320	GLN
6	G	406	GLN
6	G	459	GLN
6	G	461	GLN
6	G	465	GLN
6	G	498	ASN
6	G	510	GLN
6	G	547	ASN
6	H	31	GLN
6	H	58	GLN
6	H	107	GLN
6	H	343	GLN
6	H	406	GLN
6	H	411	GLN
6	H	465	GLN
6	H	547	ASN
7	L	67	HIS
7	L	272	HIS
2	O	26	GLN
2	O	178	ASN
2	O	386	ASN
2	O	524	GLN
2	O	600	GLN

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Mol	Chain	Res	Type
2	O	656	HIS
2	O	729	GLN
2	O	753	ASN
8	P	153	GLN
8	P	589	ASN
8	P	645	HIS
8	P	815	GLN
8	Q	277	HIS
8	Q	478	GLN
8	Q	491	ASN
8	Q	546	GLN
8	Q	589	ASN
8	Q	645	HIS
8	Q	788	GLN
8	Q	832	GLN
1	S	101	GLN
1	S	286	GLN
1	S	343	GLN
1	S	352	HIS
1	S	490	GLN
1	S	546	GLN
1	S	729	ASN
1	S	771	HIS
1	S	869	GLN
1	S	940	GLN
1	S	992	HIS
1	S	1190	GLN
1	S	1231	HIS
1	S	1326	GLN
1	S	1417	HIS
1	S	1440	GLN
7	M	18	GLN
7	M	148	HIS
7	M	180	GLN
7	M	270	ASN
7	M	272	HIS
7	M	278	ASN
7	M	282	GLN
7	M	331	GLN
7	M	335	GLN
10	X	26	GLN
10	X	37	GLN

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Mol	Chain	Res	Type
10	X	112	GLN
10	X	142	ASN
10	X	150	HIS
11	U	31	ASN
11	U	35	ASN
11	U	99	HIS
11	U	323	GLN
11	U	345	GLN
11	U	416	GLN
11	U	529	GLN
11	U	597	GLN
11	U	625	GLN
11	U	630	GLN
11	U	711	ASN
11	U	924	GLN
11	U	1017	ASN
11	U	1030	ASN
11	U	1137	GLN
11	U	1193	ASN
12	V	86	HIS
12	V	112	ASN
12	V	146	GLN
12	V	164	ASN
12	V	392	ASN
12	V	394	GLN
12	V	480	HIS
12	V	552	GLN
12	V	798	ASN
12	V	802	GLN
12	V	1025	ASN
12	V	1105	GLN
12	V	1113	GLN
12	V	1119	GLN
12	V	1181	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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

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	1

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	37.25
1	W	95:TRP	C	101:UNK	N	6.01
1	L	330:GLY	C	331:GLN	N	1.08

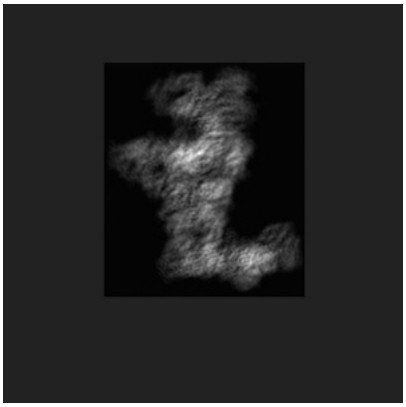
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23089. These allow visual inspection of the internal detail of the map and identification of artifacts.

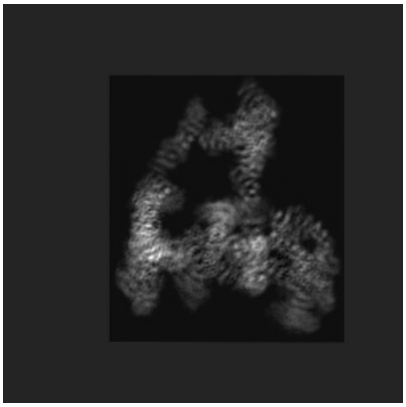
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

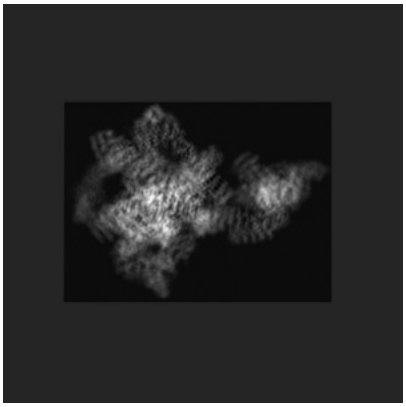
6.1.1 Primary map



X



Y

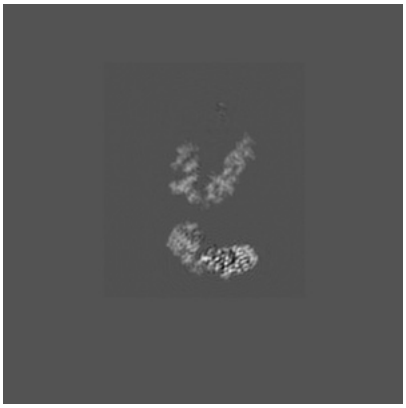


Z

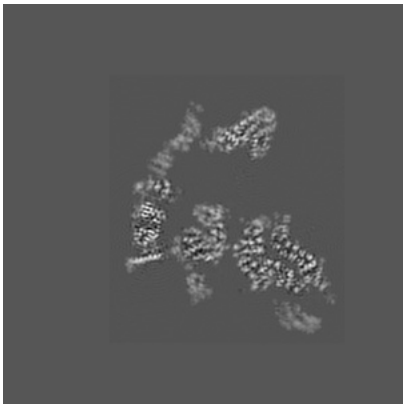
The images above show the map projected in three orthogonal directions.

6.2 Central slices

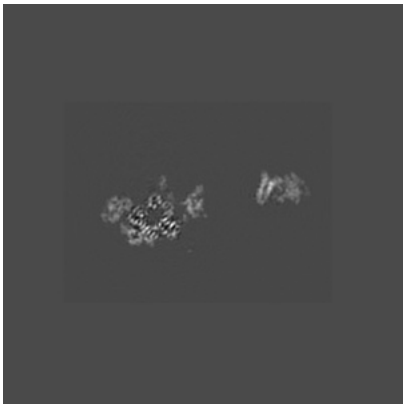
6.2.1 Primary map



X Index: 224



Y Index: 224



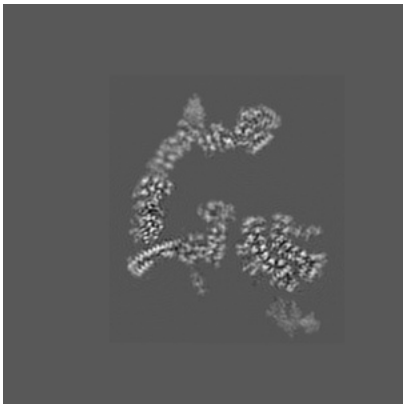
Z Index: 224

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

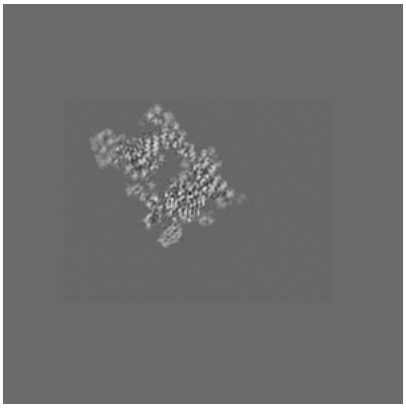
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 163



Y Index: 231



Z Index: 163

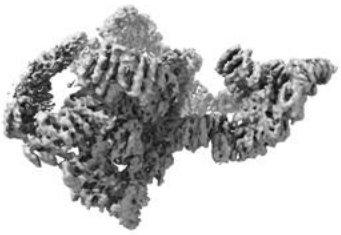
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

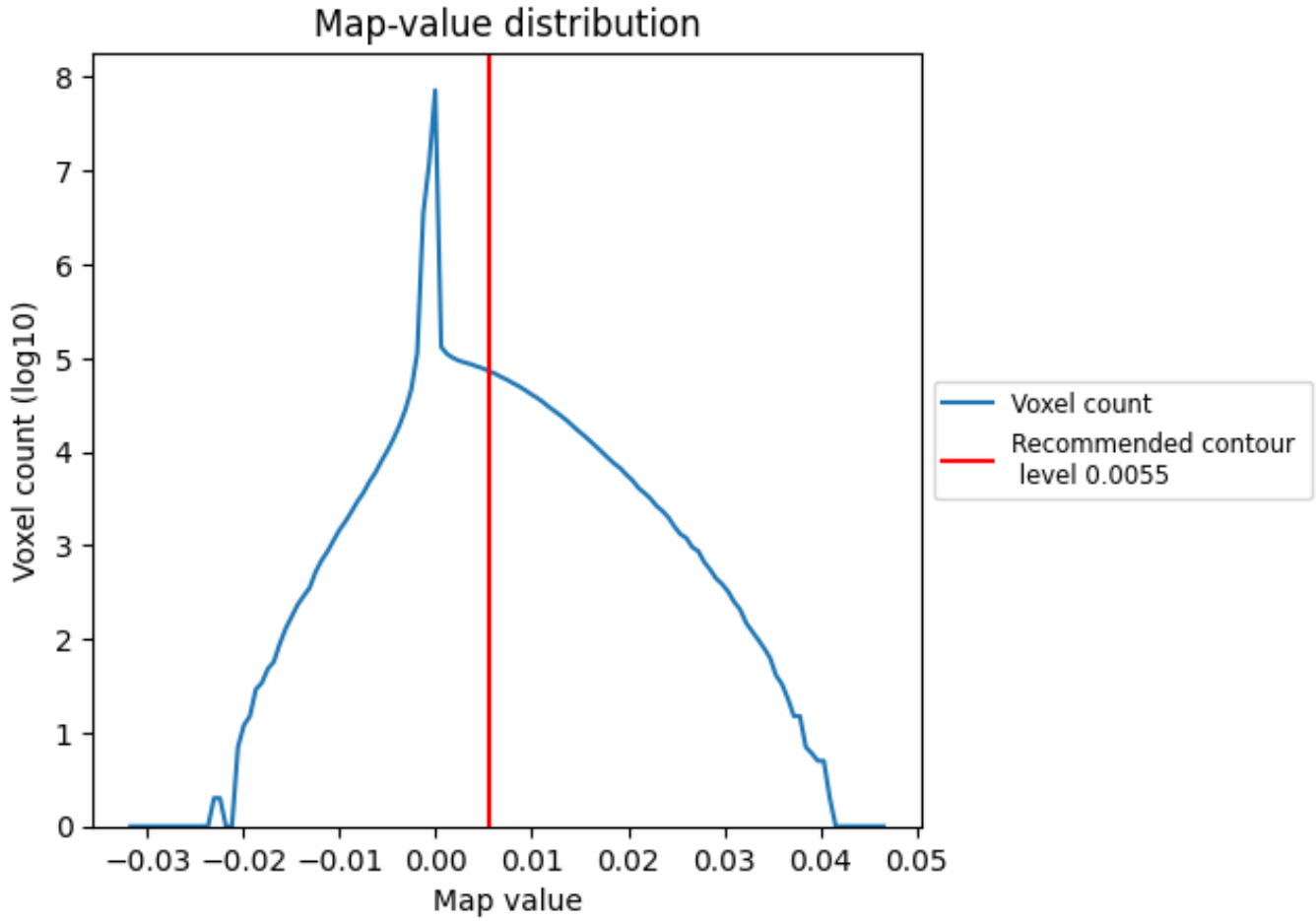
6.5 Mask visualisation (i)

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

7 Map analysis

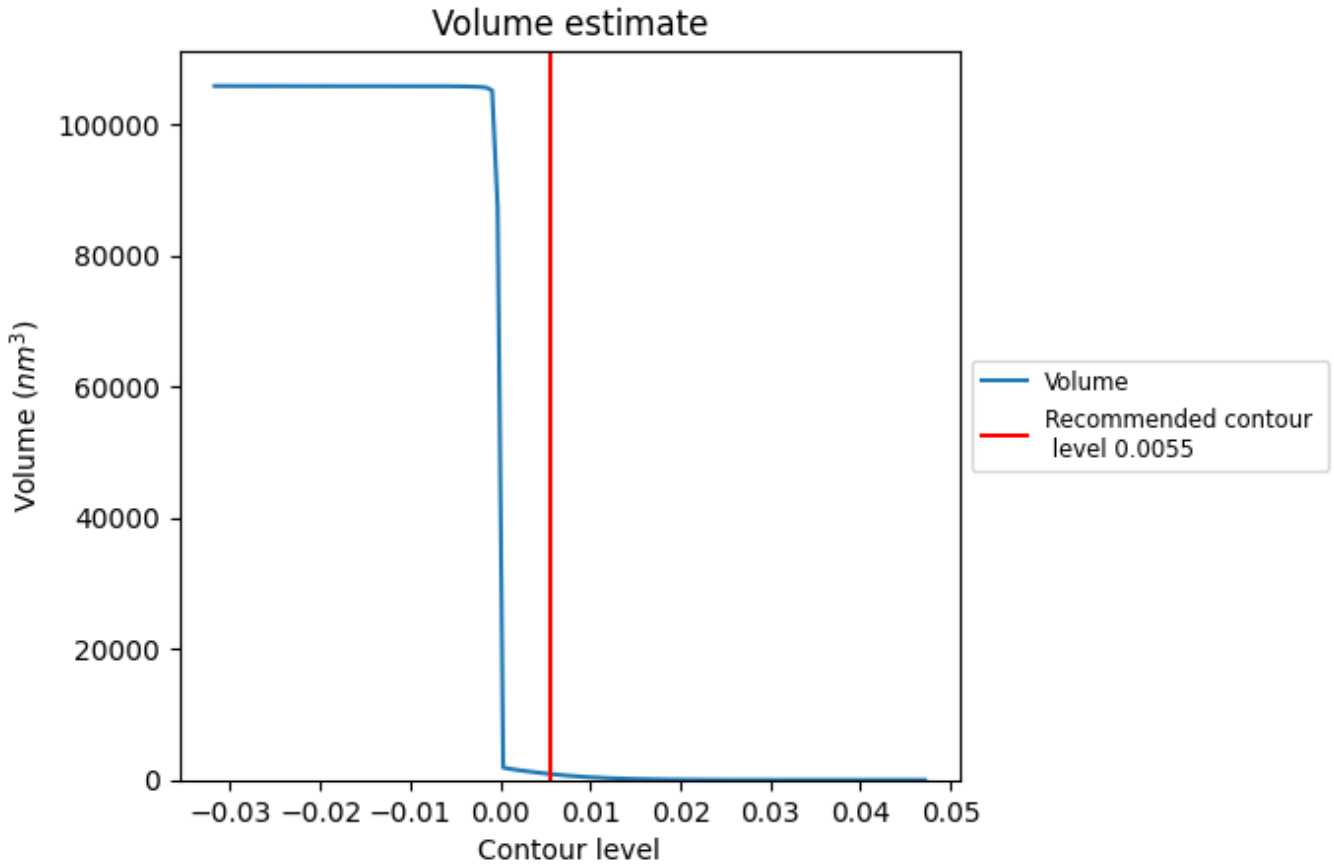
This section contains the results of statistical analysis of the map.

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.

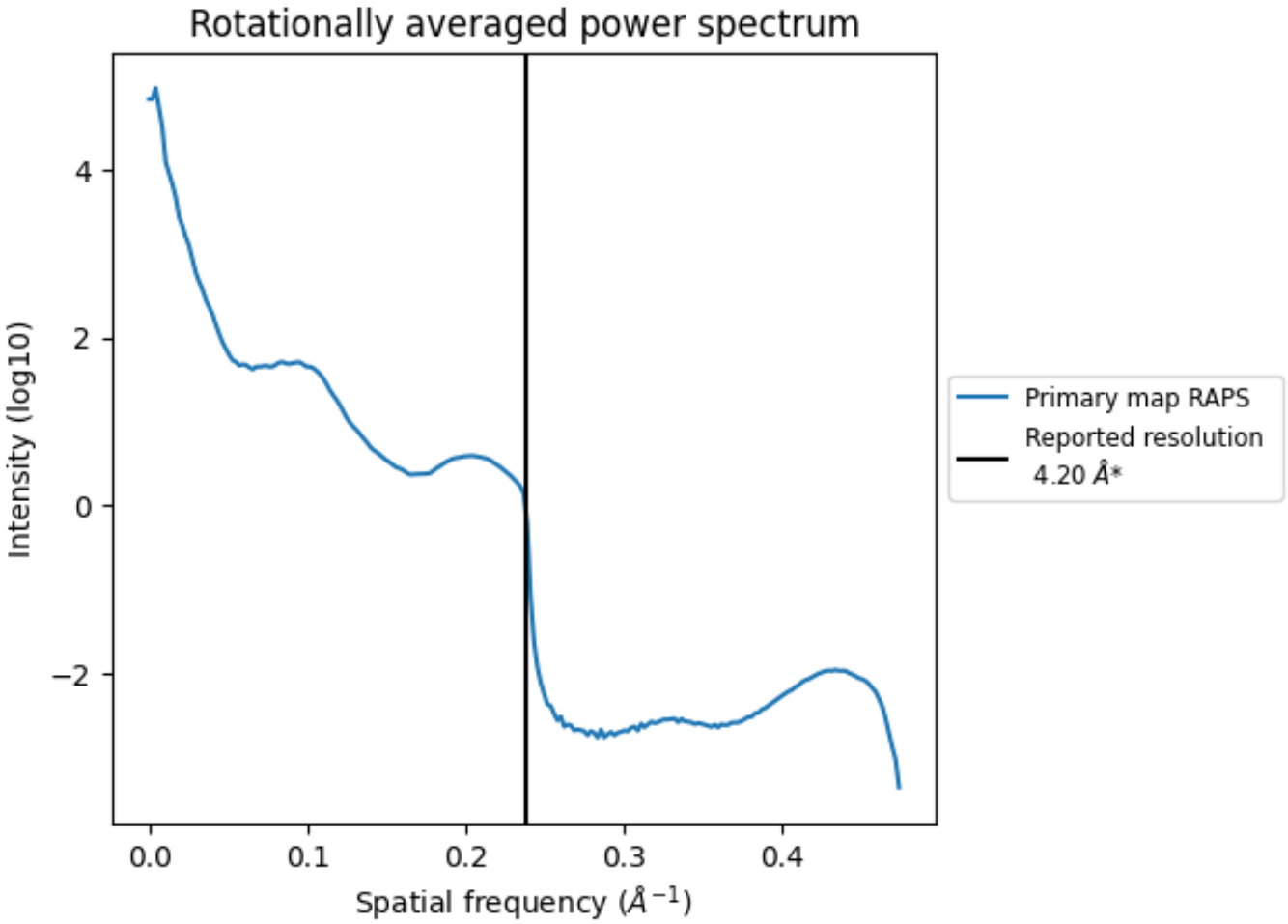
7.2 Volume estimate



The volume at the recommended contour level is 916 nm^3; this corresponds to an approximate mass of 827 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 $Å^{-1}$

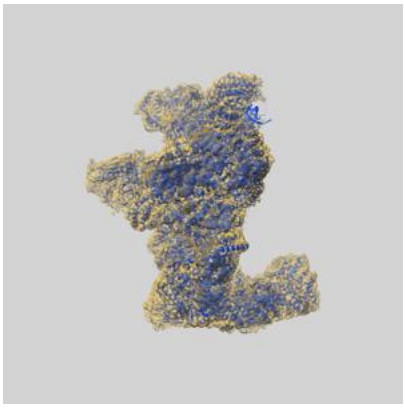
8 Fourier-Shell correlation

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

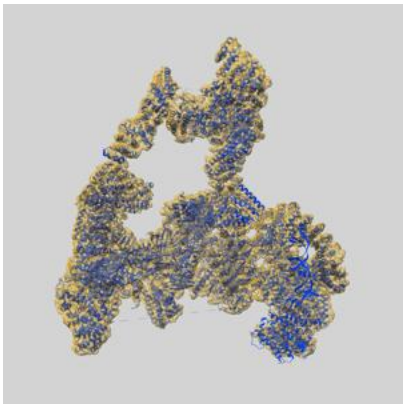
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23089 and PDB model 7KZT. Per-residue inclusion information can be found in section 3 on page 15.

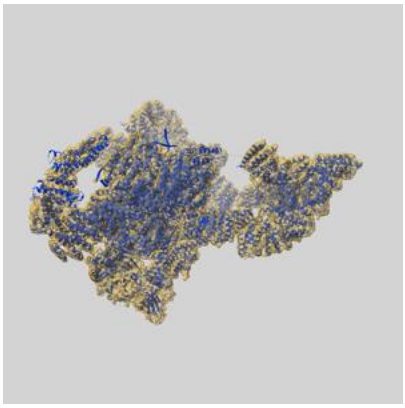
9.1 Map-model overlay



X



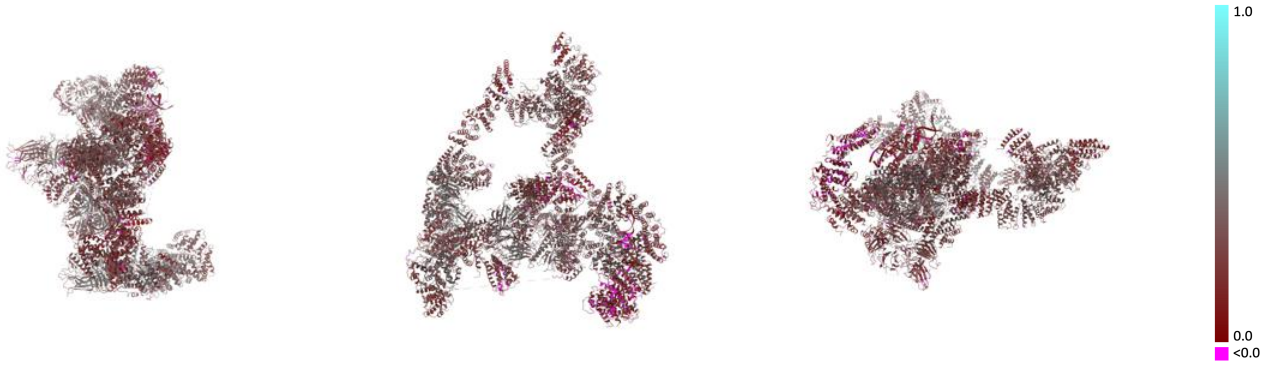
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0055 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.

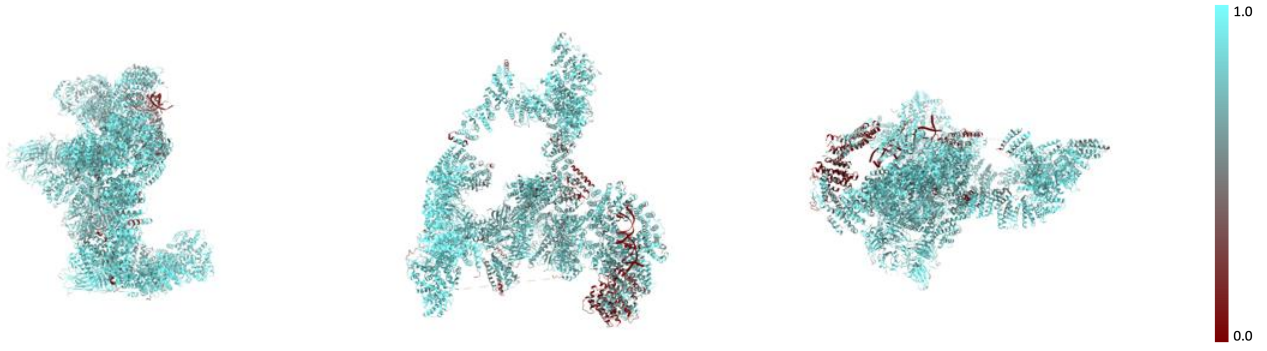
9.2 Q-score mapped to coordinate model (i)



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.

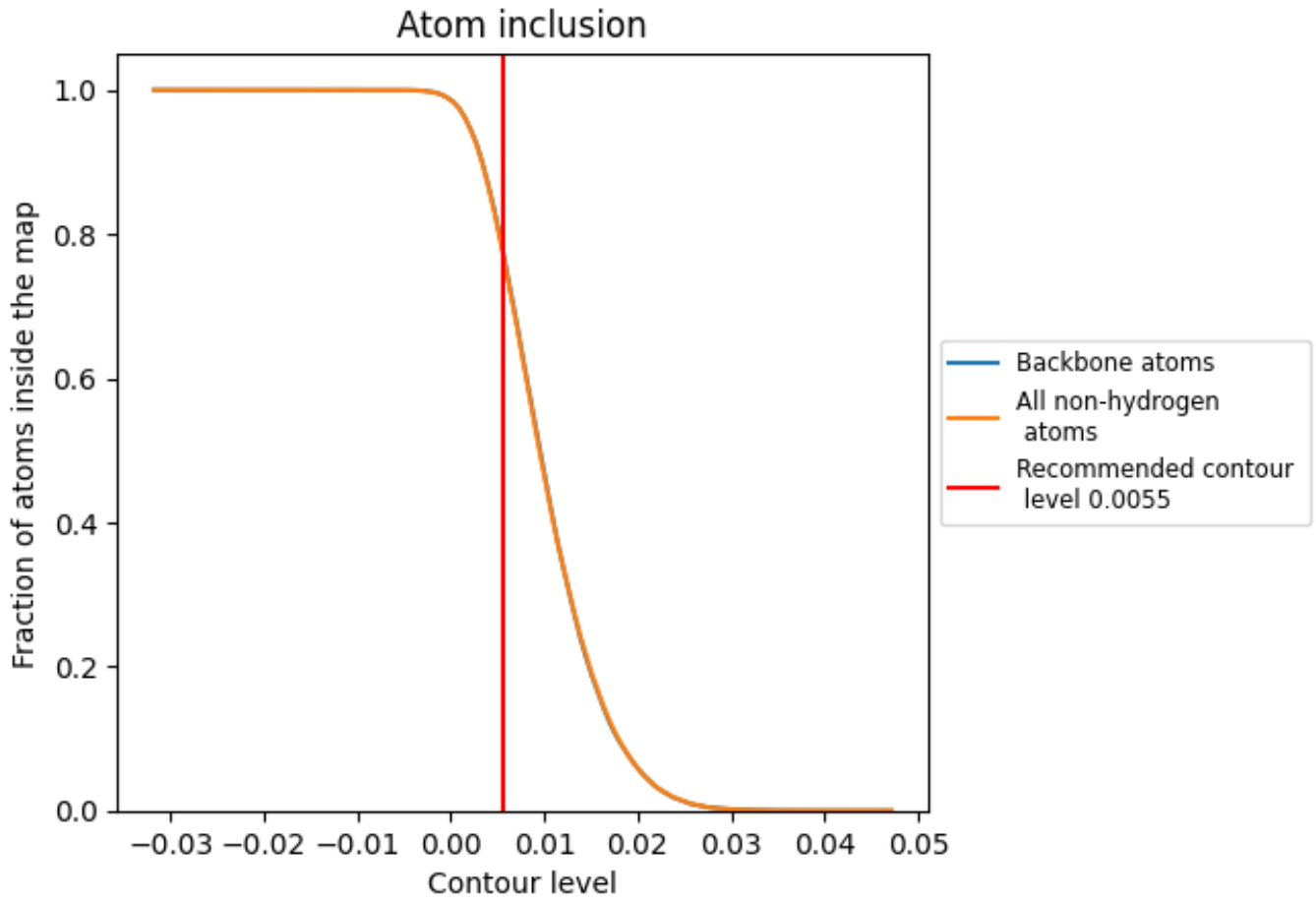
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0055).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.0055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7793	0.2970
A	0.7667	0.2690
B	0.8545	0.3580
C	0.8918	0.3400
E	0.8167	0.3290
F	0.9116	0.3520
G	0.8477	0.3220
H	0.7915	0.2560
L	0.8281	0.3290
M	0.7942	0.3110
O	0.8073	0.2790
P	0.8729	0.3790
Q	0.7619	0.2880
S	0.8312	0.2840
U	0.7700	0.2940
V	0.5894	0.2340
W	0.8178	0.3330
X	0.8151	0.2820
Y	0.0721	0.1240
Z	0.1149	0.1350