



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:31 AM UTC

PDB ID : 7KZT / pdb_00007kzt
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:

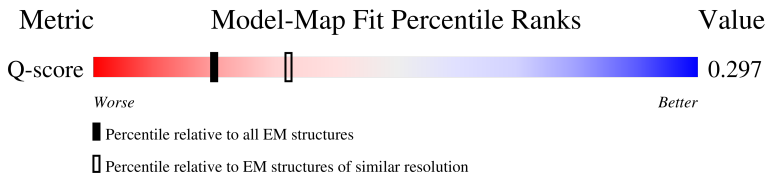
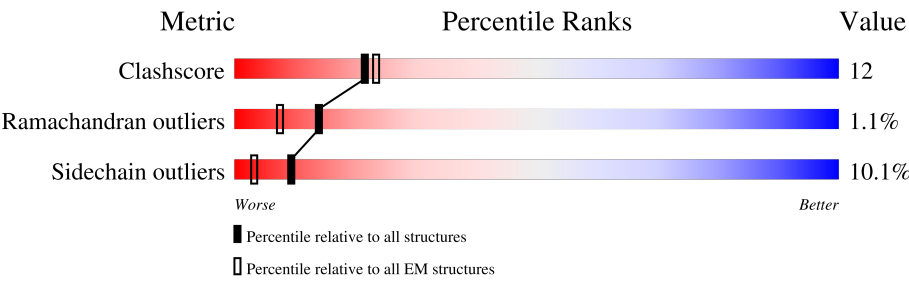
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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 $\leq 5\%$. 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% 55% 21% • 20%
1	S	1477	• 57% 23% • 15%
2	B	884	• 45% 27% 7% • 21%
2	O	884	• 56% 18% • 21%

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Mol	Chain	Length	Quality of chain
3	C	583	
4	E	555	
5	F	399	
6	G	641	
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

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
5	F	340	Total	C	H	N	O	S	0	0
			5466	1730	2740	506	483	7		

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		

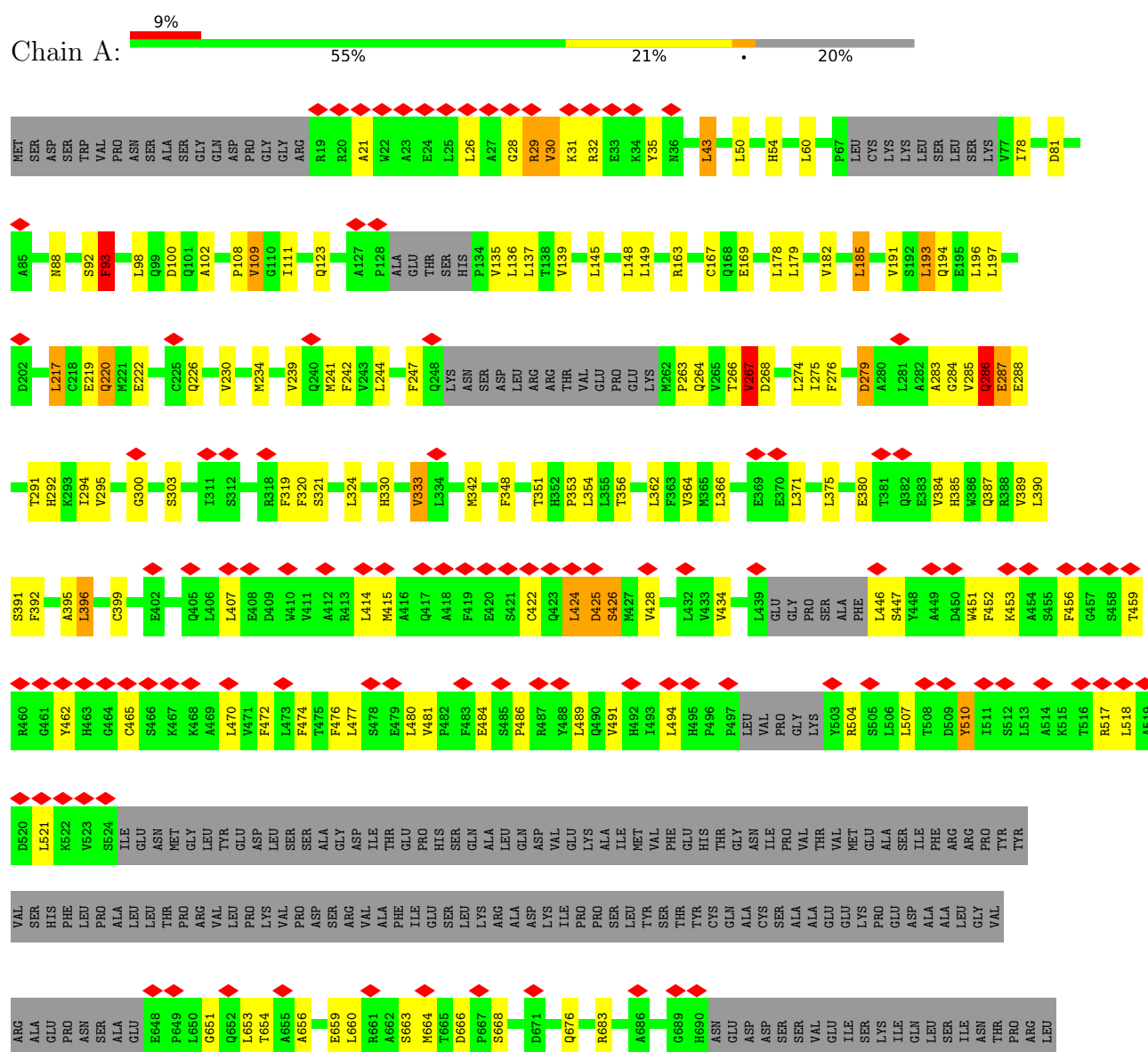
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

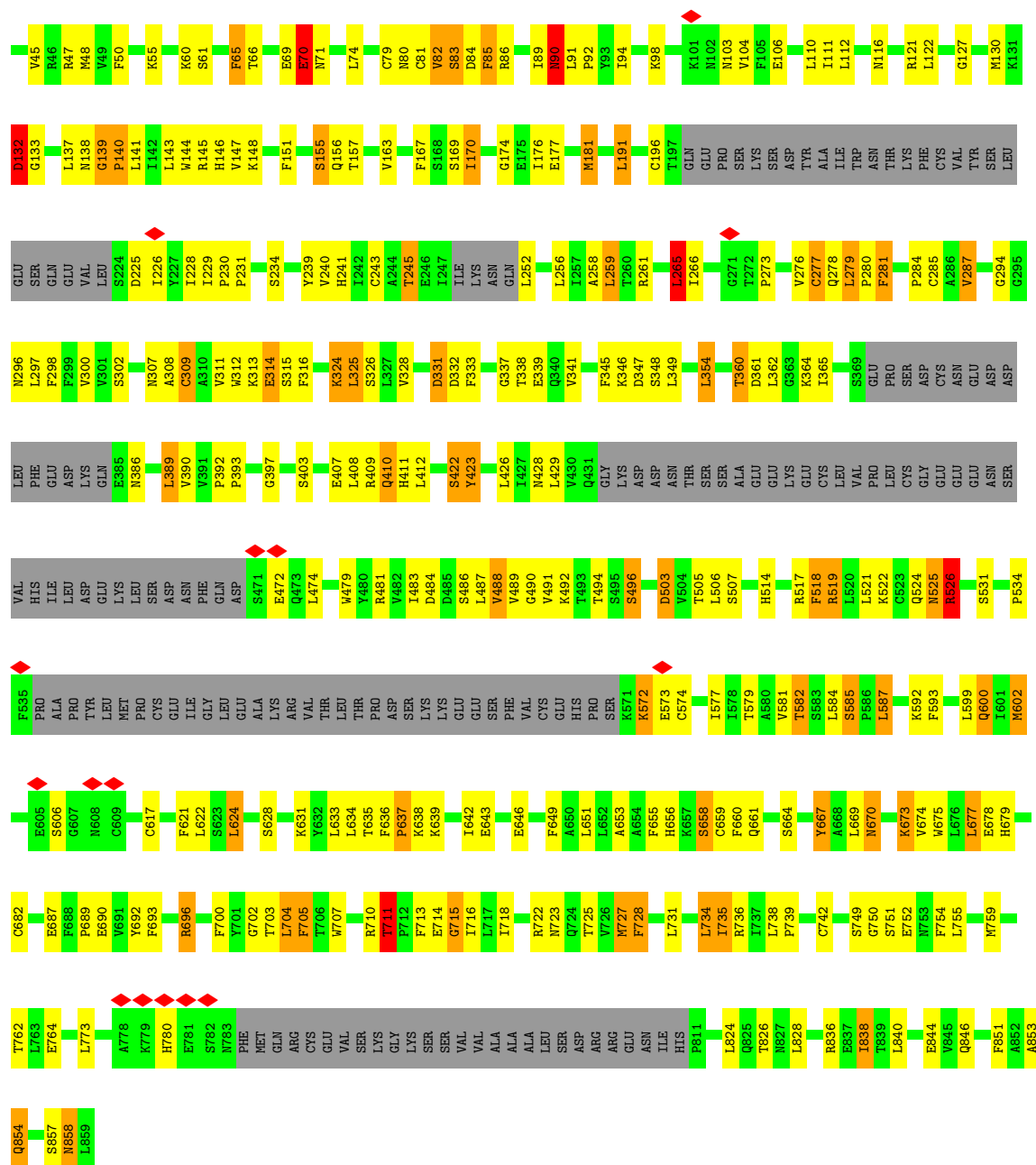
Mol	Chain	Residues	Atoms		AltConf
15	G	1	Total	Zn	0
			1	1	
15	L	2	Total	Zn	0
			2	2	
15	M	2	Total	Zn	0
			2	2	

3 Residue-property plots

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.

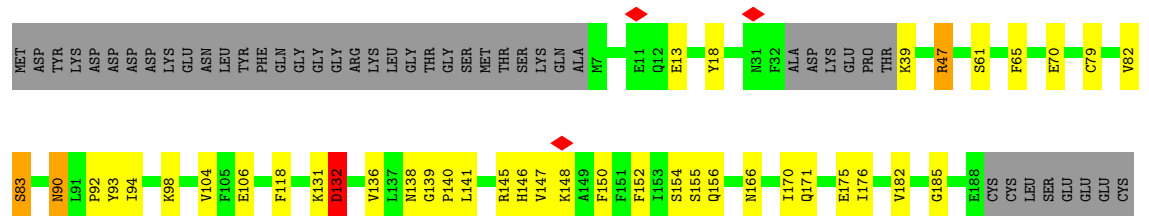
- Molecule 1: Fanconi anemia group A protein

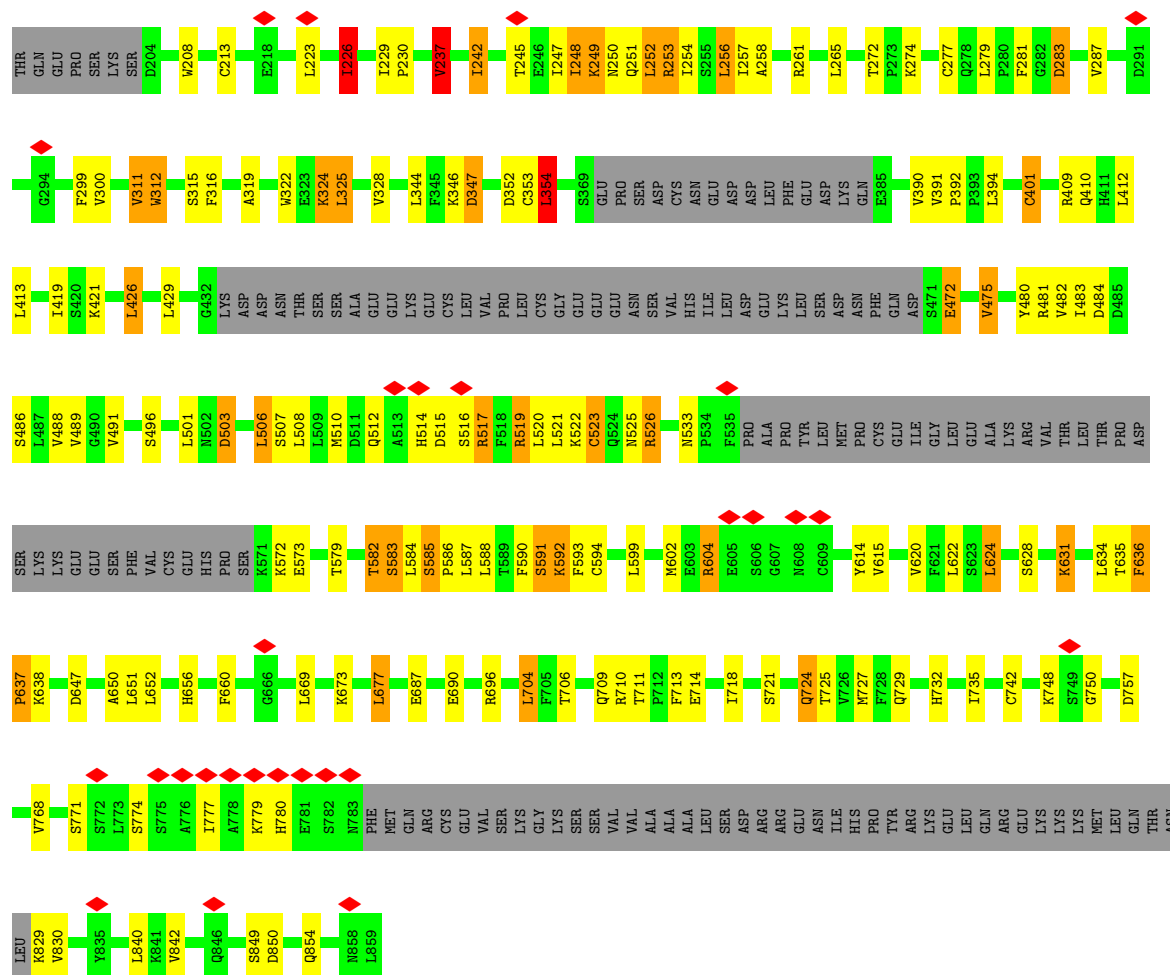




• Molecule 2: Fanconi anemia group B protein

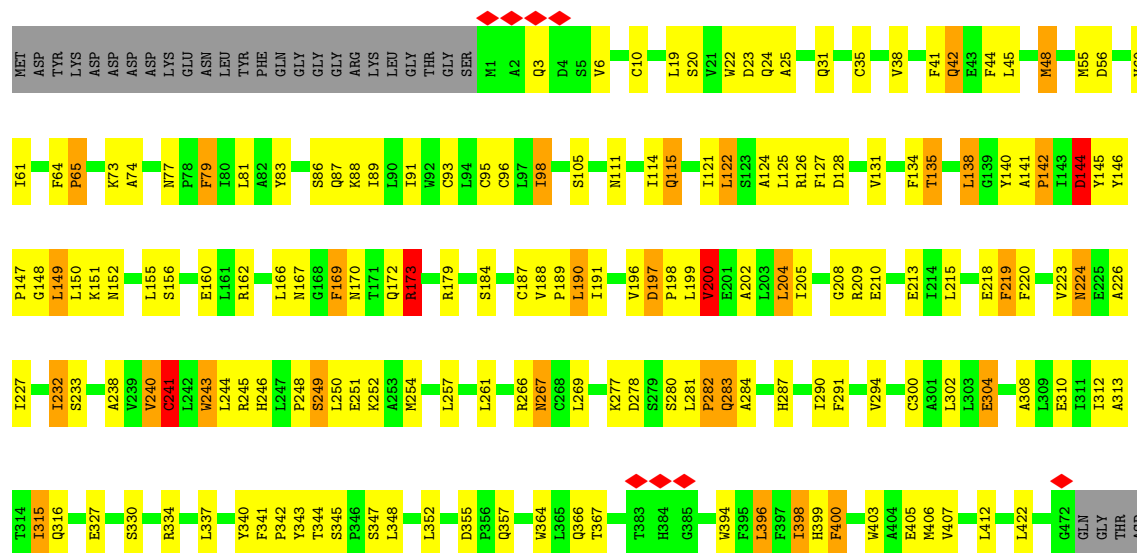
Chain O: 56% 18% 21%





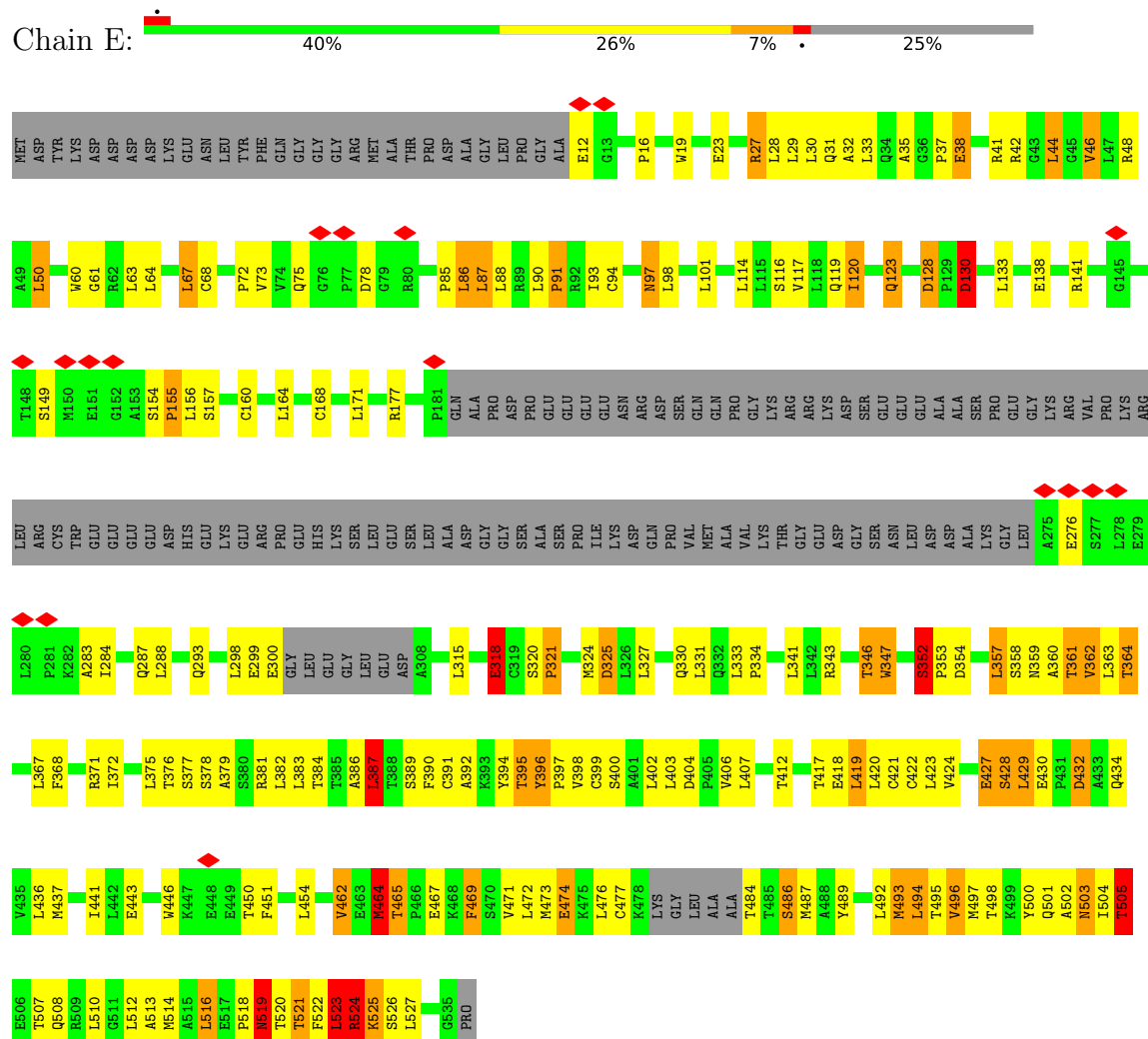
• Molecule 3: Fanconi anemia group C protein

Chain C: 63% 25% 5% • 6%

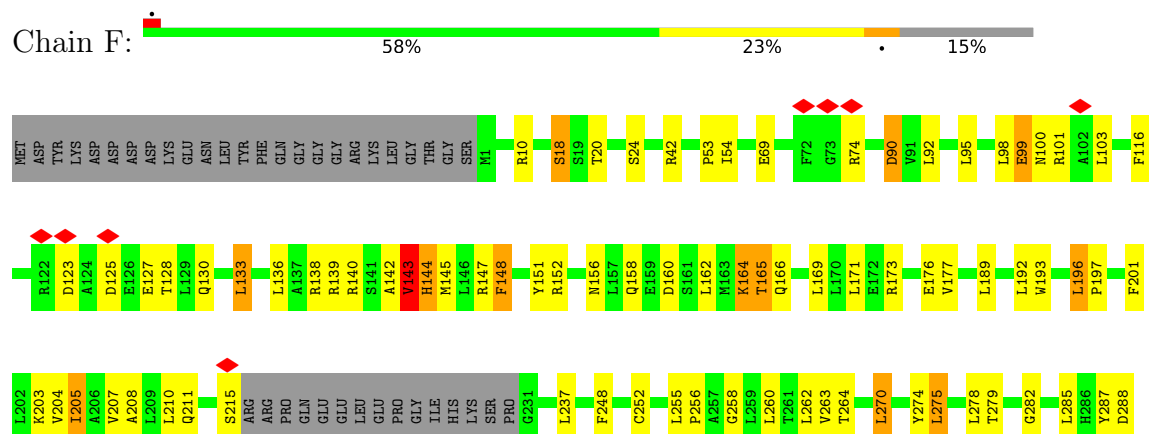


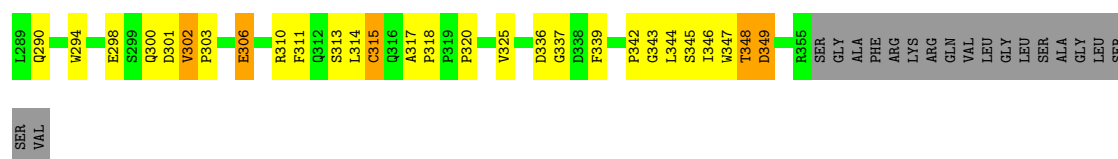


• Molecule 4: Fanconi anemia group E protein

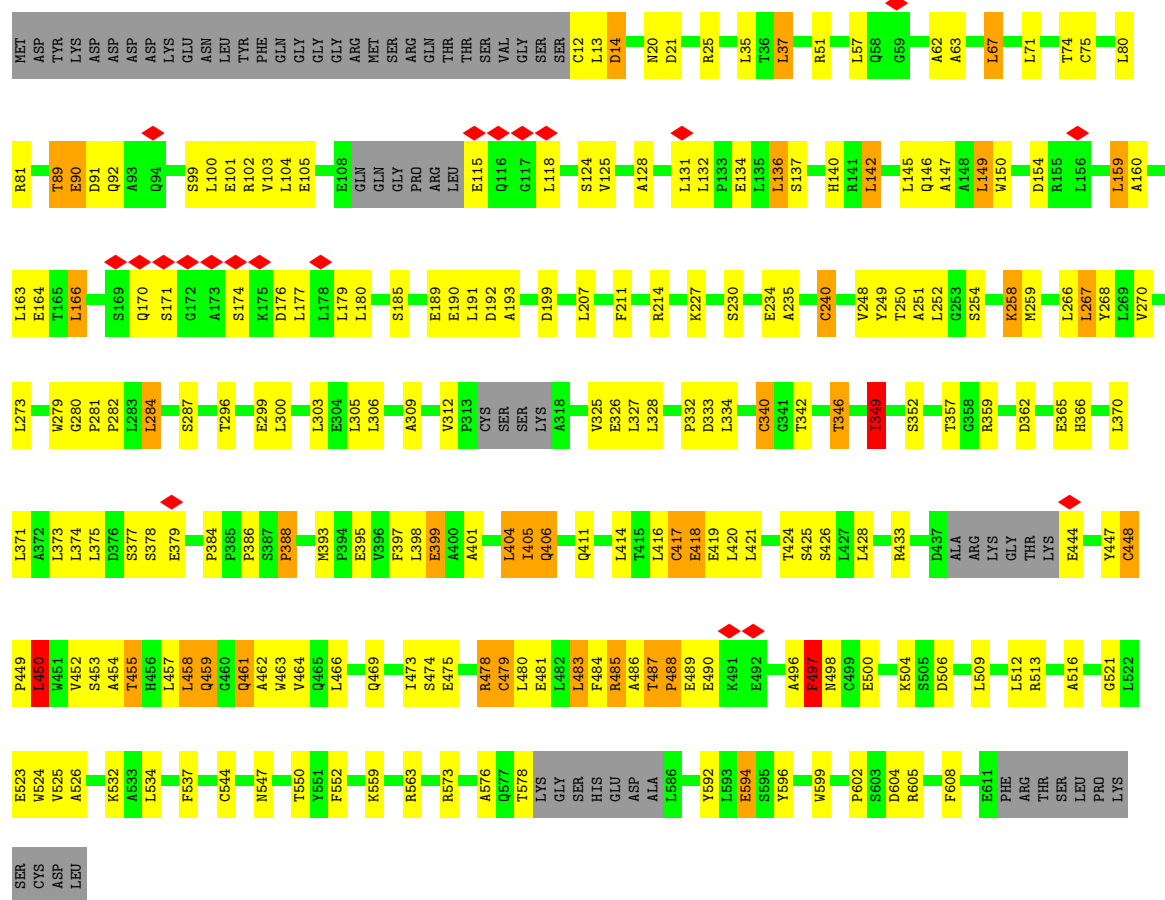


• Molecule 5: Fanconi anemia group F protein

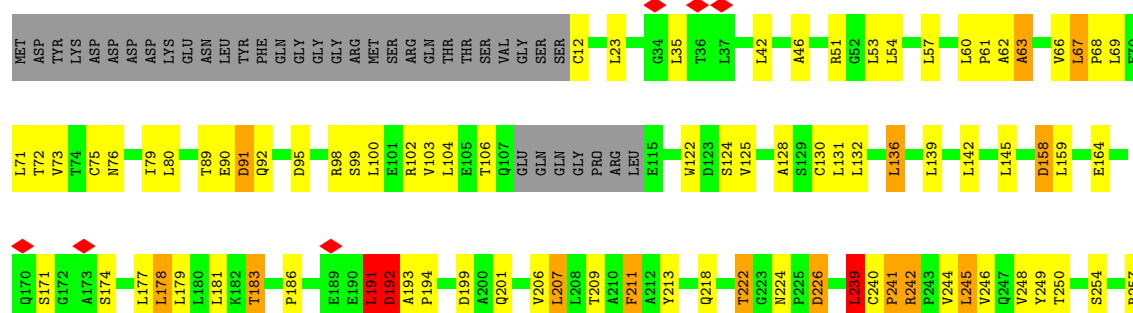




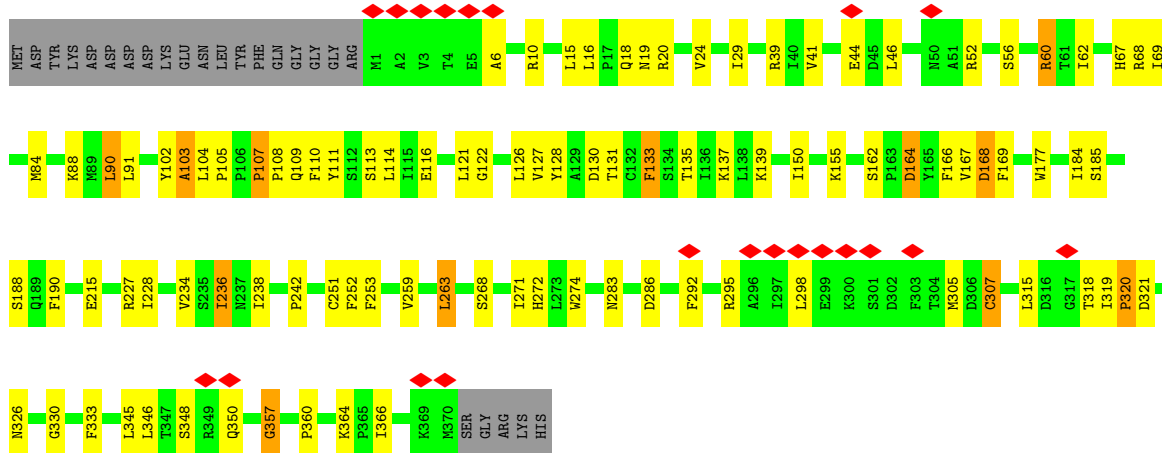
• Molecule 6: Fanconi anemia group G protein



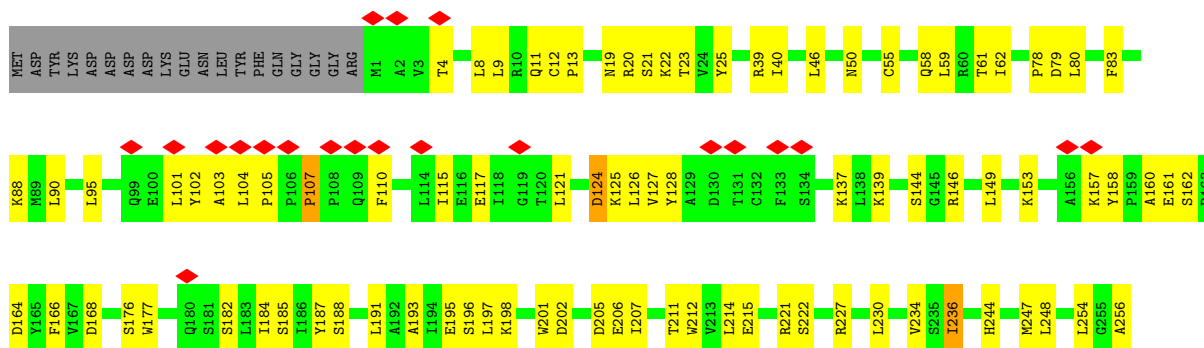
• Molecule 6: Fanconi anemia group G protein

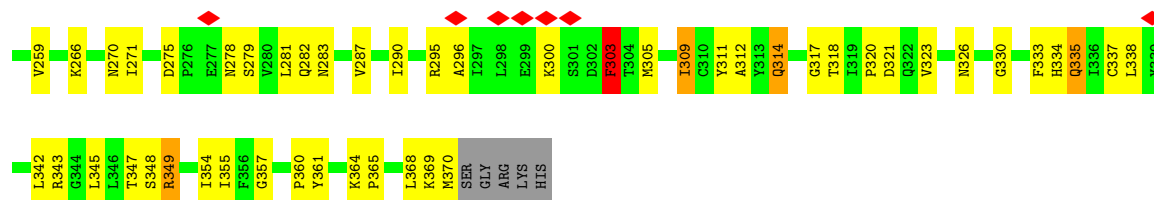


- Molecule 7: E3 ubiquitin-protein ligase FANCL

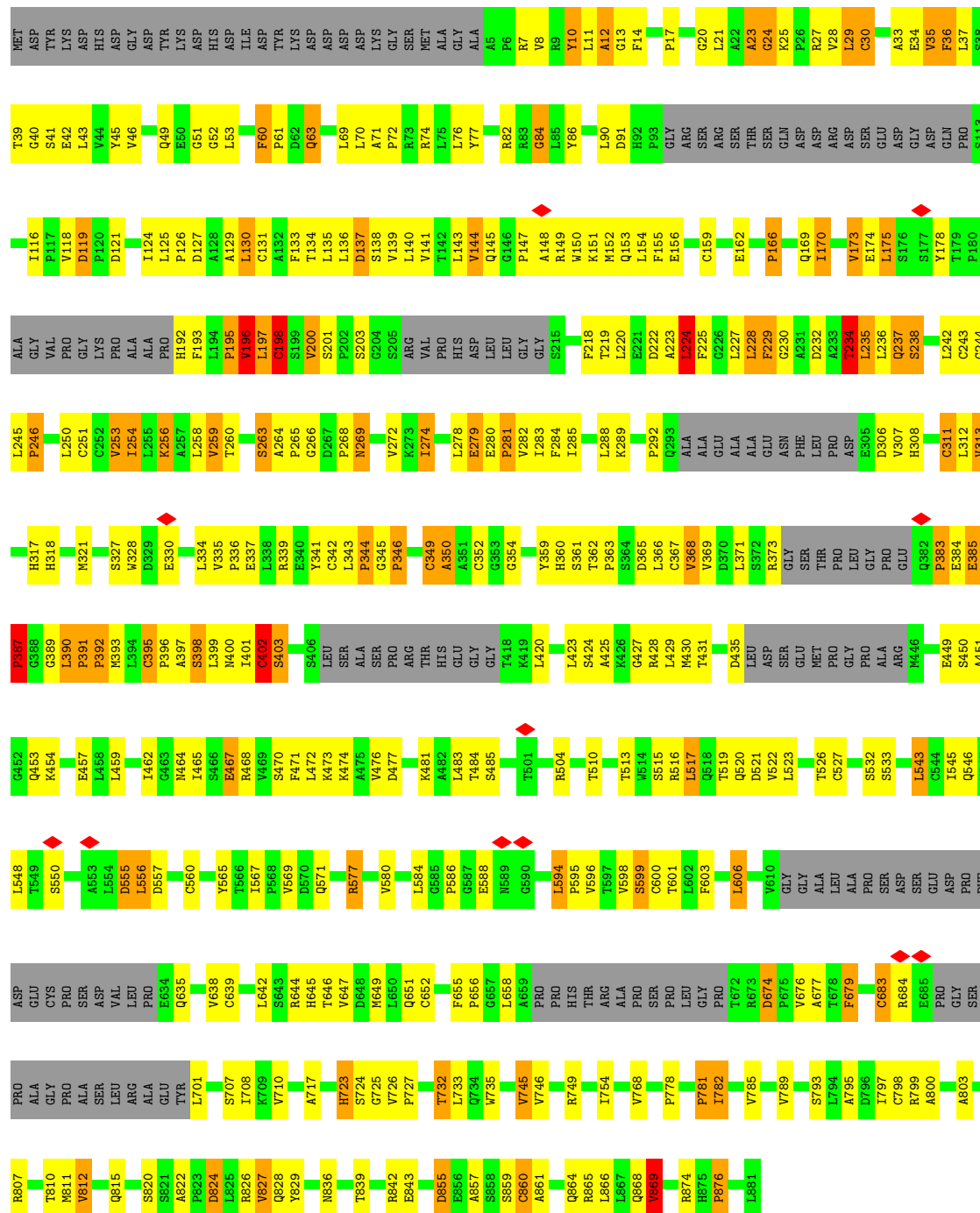


- Molecule 7: E3 ubiquitin-protein ligase FANCL

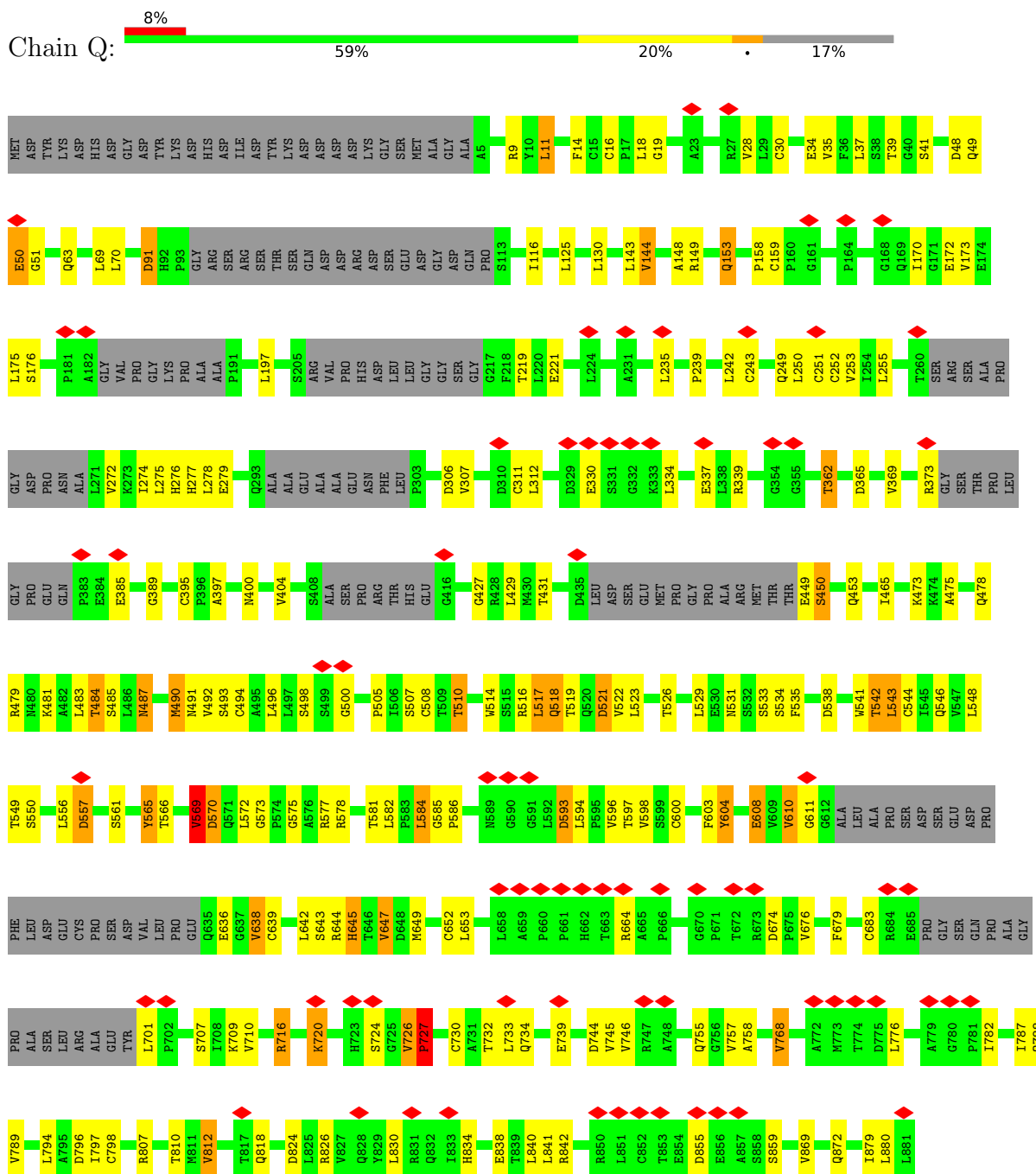




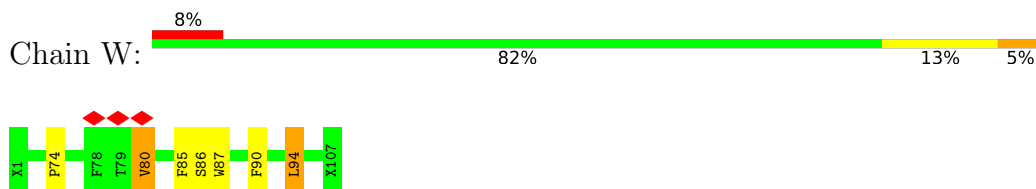
• Molecule 8: Fanconi anemia core complex-associated protein 100



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

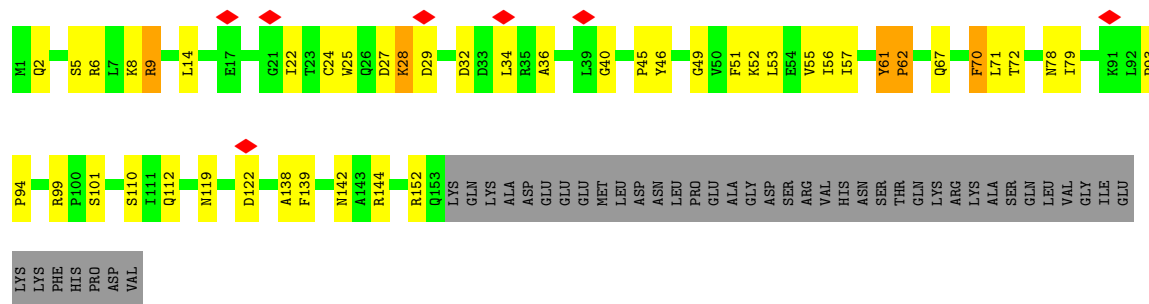


- Molecule 9: Fanconi anemia core complex-associated protein 20



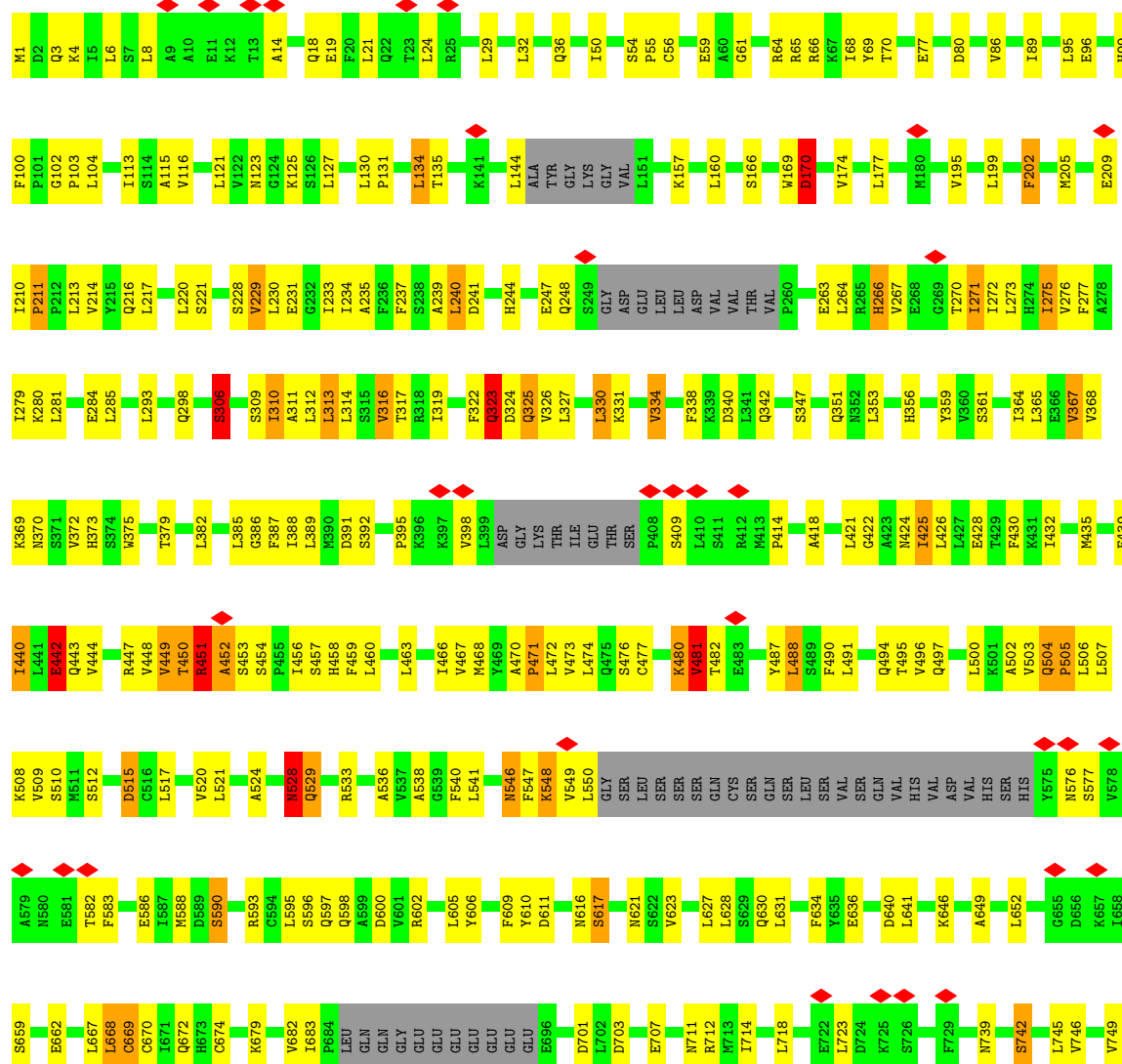
- Molecule 10: Ubiquitin-conjugating enzyme E2 T

Chain X: 



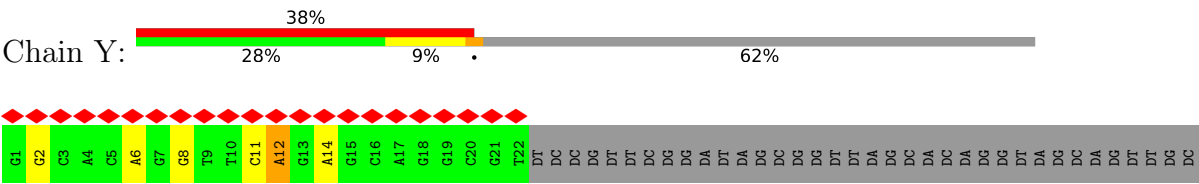
• Molecule 11: Fanconi anemia, complementation group I

Chain U: 

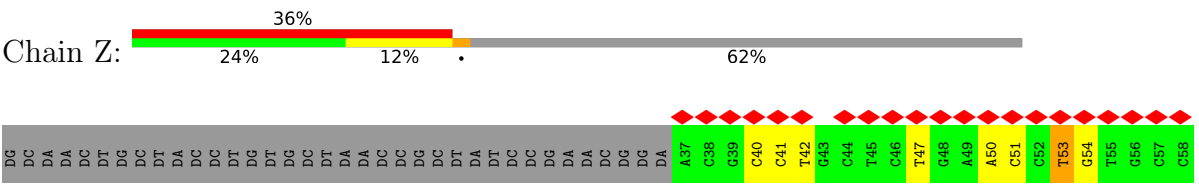




● Molecule 13: DNA (22-MER)



● Molecule 14: DNA (22-MER)



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	473.088, 473.088, 473.088	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	1.14	0/9605	1.74	50/13008 (0.4%)
1	S	1.12	1/10153 (0.0%)	1.76	74/13749 (0.5%)
2	B	1.15	0/5707	1.72	68/7686 (0.9%)
2	O	1.11	0/5701	1.58	32/7686 (0.4%)
3	C	1.16	3/4497 (0.1%)	1.83	44/6103 (0.7%)
4	E	1.17	4/3274 (0.1%)	1.93	60/4438 (1.4%)
5	F	1.17	0/2791	1.82	48/3790 (1.3%)
6	G	1.18	5/4568 (0.1%)	1.84	65/6215 (1.0%)
6	H	1.08	1/4293 (0.0%)	1.76	26/5840 (0.4%)
7	L	1.12	1/3050 (0.0%)	1.66	23/4143 (0.6%)
7	M	1.03	2/3050 (0.1%)	1.55	19/4143 (0.5%)
8	P	1.22	11/5697 (0.2%)	1.80	91/7752 (1.2%)
8	Q	1.13	2/5737 (0.0%)	1.61	34/7810 (0.4%)
9	W	0.99	0/202	1.44	1/281 (0.4%)
10	X	1.07	0/1267	1.56	9/1722 (0.5%)
11	U	1.18	2/9494 (0.0%)	1.93	139/12802 (1.1%)
12	V	1.20	2/9163 (0.0%)	1.87	102/12390 (0.8%)
13	Y	0.37	0/515	1.06	5/794 (0.6%)
14	Z	0.37	0/495	1.11	7/760 (0.9%)
All	All	1.14	34/89259 (0.0%)	1.76	897/121112 (0.7%)

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

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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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	330	GLY	C-N	-15.15	1.08	1.33
7	M	355	ILE	C-N	7.03	1.43	1.33
1	S	961	GLU	N-CA	6.35	1.54	1.46
12	V	671	VAL	N-CA	6.04	1.50	1.46
8	P	63	GLN	C-O	5.91	1.31	1.24
8	P	350	ALA	C-O	-5.88	1.16	1.23
8	P	259	VAL	C-O	5.85	1.30	1.24
3	C	250	LEU	N-CA	5.84	1.53	1.46
3	C	227	ILE	N-CA	5.67	1.53	1.46
8	P	283	ILE	C-O	5.57	1.30	1.24
8	P	387	PRO	C-O	-5.54	1.16	1.24
6	G	398	LEU	N-CA	5.53	1.52	1.46
8	Q	611	GLY	N-CA	5.53	1.49	1.45
8	Q	116	ILE	N-CA	5.38	1.50	1.45
6	G	418	GLU	N-CA	5.37	1.52	1.46
4	E	441	ILE	N-CA	5.32	1.53	1.46
6	G	405	ILE	N-CA	5.25	1.52	1.46
8	P	144	VAL	C-O	5.15	1.29	1.24
8	P	116	ILE	N-CA	5.14	1.49	1.45
11	U	471	PRO	C-O	-5.11	1.18	1.23
4	E	155	PRO	C-O	-5.11	1.17	1.24
6	G	379	GLU	N-CA	5.10	1.50	1.46
4	E	396	TYR	N-CA	5.09	1.50	1.46
8	P	196	VAL	N-CA	5.09	1.51	1.46
8	P	369	VAL	N-CA	5.05	1.51	1.46
8	P	126	PRO	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	321	PRO	C-O	-5.04	1.17	1.24
6	H	63	ALA	C-O	5.04	1.30	1.24
12	V	422	SER	N-CA	5.03	1.52	1.46
6	G	464	VAL	N-CA	5.02	1.52	1.46
8	P	827	VAL	N-CA	5.02	1.50	1.46
7	M	124	ASP	N-CA	5.01	1.52	1.46
3	C	128	ASP	N-CA	5.00	1.52	1.46
11	U	240	LEU	N-CA	5.00	1.52	1.46

All (897) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	321	ASP	CA-C-N	13.89	140.92	121.05
7	M	321	ASP	C-N-CA	13.89	140.92	121.05
7	L	357	GLY	O-C-N	-12.67	108.97	123.67
7	M	321	ASP	O-C-N	-11.96	107.95	121.95
7	L	168	ASP	CA-CB-CG	11.66	124.26	112.60
8	P	391	PRO	N-CA-C	11.15	124.30	110.70
6	G	481	GLU	CB-CG-CD	10.96	131.22	112.60
7	L	357	GLY	CA-C-N	10.92	138.25	122.09
7	L	357	GLY	C-N-CA	10.92	138.25	122.09
2	O	503	ASP	CA-CB-CG	10.44	123.04	112.60
11	U	450	THR	CA-CB-OG1	-10.40	94.00	109.60
3	C	128	ASP	CA-CB-CG	10.10	122.70	112.60
6	G	384	PRO	CB-CA-C	-10.03	98.68	110.92
6	G	384	PRO	N-CA-C	9.74	122.58	110.70
1	S	992	HIS	CA-CB-CG	-9.50	104.30	113.80
8	P	679	PHE	CA-CB-CG	-9.49	104.31	113.80
7	M	330	GLY	O-C-N	9.46	135.00	122.70
2	B	621	PHE	CA-CB-CG	9.46	123.26	113.80
10	X	122	ASP	CA-CB-CG	9.33	121.93	112.60
8	P	10	TYR	CA-C-N	9.00	133.15	122.44
8	P	10	TYR	C-N-CA	9.00	133.15	122.44
6	G	211	PHE	CA-CB-CG	-8.93	104.87	113.80
11	U	770	ASP	CA-CB-CG	8.91	121.52	112.60
1	S	960	HIS	CB-CA-C	8.89	123.50	111.14
4	E	325	ASP	CA-CB-CG	8.86	121.46	112.60
12	V	308	GLN	CA-C-N	8.84	132.13	120.28
12	V	308	GLN	C-N-CA	8.84	132.13	120.28
7	L	130	ASP	CA-CB-CG	8.74	121.34	112.60
4	E	354	ASP	CA-CB-CG	8.52	121.12	112.60
6	G	487	THR	CB-CA-C	8.40	120.76	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	277	PHE	CA-CB-CG	-8.37	105.43	113.80
8	Q	727	PRO	N-CD-CG	-8.33	90.71	103.20
6	G	388	PRO	N-CA-C	8.27	120.79	110.70
8	Q	362	THR	CB-CA-C	8.26	121.34	108.63
3	C	160	GLU	CB-CA-C	8.13	124.24	110.74
2	B	230	PRO	N-CA-C	8.12	118.26	110.47
1	S	948	ASP	CA-CB-CG	8.10	120.70	112.60
1	S	338	ASP	CA-CB-CG	8.09	120.69	112.60
11	U	783	ASP	CA-CB-CG	8.08	120.68	112.60
2	B	347	ASP	CA-CB-CG	8.07	120.67	112.60
1	S	1022	GLN	CB-CG-CD	-7.99	99.03	112.60
12	V	212	ILE	N-CA-C	-7.97	101.94	110.23
8	P	119	ASP	CA-CB-CG	7.96	120.56	112.60
5	F	279	THR	CB-CA-C	7.88	124.08	110.68
7	L	321	ASP	CA-C-N	7.88	132.77	121.50
7	L	321	ASP	C-N-CA	7.88	132.77	121.50
1	S	854	ASP	CA-CB-CG	7.87	120.47	112.60
6	H	158	ASP	CA-CB-CG	7.87	120.47	112.60
4	E	91	PRO	CB-CA-C	-7.86	101.74	111.64
12	V	293	ASP	CA-CB-CG	7.81	120.41	112.60
8	Q	674	ASP	CA-CB-CG	7.79	120.39	112.60
8	P	237	GLN	CB-CG-CD	7.75	125.78	112.60
12	V	513	PHE	CA-CB-CG	7.75	121.55	113.80
8	P	127	ASP	CA-CB-CG	7.73	120.33	112.60
11	U	266	HIS	CA-CB-CG	-7.72	106.08	113.80
8	P	464	ASN	CA-CB-CG	7.71	120.31	112.60
14	Z	50	DA	C2'-C3'-O3'	7.69	123.03	111.50
12	V	212	ILE	N-CA-CB	7.67	118.67	110.62
8	P	555	ASP	CA-CB-CG	7.66	120.26	112.60
8	P	839	THR	CB-CA-C	7.62	122.84	110.88
1	S	960	HIS	CA-C-N	7.62	135.90	122.42
1	S	960	HIS	C-N-CA	7.62	135.90	122.42
4	E	318	GLU	CB-CG-CD	7.58	125.48	112.60
4	E	523	LEU	CA-C-N	7.57	130.28	120.44
4	E	523	LEU	C-N-CA	7.57	130.28	120.44
2	O	515	ASP	CA-CB-CG	7.53	120.13	112.60
3	C	226	ALA	CA-C-O	-7.52	111.32	119.97
2	B	281	PHE	CA-C-N	7.49	127.80	122.33
2	B	281	PHE	C-N-CA	7.49	127.80	122.33
5	F	349	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	1372	ASP	CA-CB-CG	7.45	120.05	112.60
6	G	171	SER	CA-C-N	7.37	128.10	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	171	SER	C-N-CA	7.37	128.10	120.00
8	P	824	ASP	CA-CB-CG	7.35	119.95	112.60
3	C	144	ASP	CA-CB-CG	7.33	119.93	112.60
1	S	1021	LEU	CA-C-N	7.33	130.42	120.38
1	S	1021	LEU	C-N-CA	7.33	130.42	120.38
2	B	332	ASP	CA-CB-CG	7.31	119.91	112.60
8	P	121	ASP	CA-CB-CG	7.31	119.91	112.60
6	G	421	LEU	CA-C-N	7.31	129.94	120.44
6	G	421	LEU	C-N-CA	7.31	129.94	120.44
6	G	497	PHE	CA-CB-CG	7.31	121.11	113.80
3	C	127	PHE	CA-C-O	-7.29	113.48	121.28
6	G	506	ASP	CA-CB-CG	7.22	119.82	112.60
12	V	238	ASN	CA-C-N	7.19	130.22	120.44
12	V	238	ASN	C-N-CA	7.19	130.22	120.44
2	B	196	CYS	CA-C-N	7.16	134.59	121.70
2	B	196	CYS	C-N-CA	7.16	134.59	121.70
11	U	876	ASP	CB-CA-C	7.15	123.01	110.85
7	L	321	ASP	CA-CB-CG	7.14	119.74	112.60
8	P	178	TYR	CA-C-N	7.13	131.19	122.42
8	P	178	TYR	C-N-CA	7.13	131.19	122.42
11	U	529	GLN	CA-C-N	7.12	129.82	120.28
11	U	529	GLN	C-N-CA	7.12	129.82	120.28
12	V	359	THR	CB-CA-C	7.12	122.56	110.74
3	C	278	ASP	CA-CB-CG	7.12	119.72	112.60
8	P	30	CYS	CB-CA-C	7.08	122.68	109.71
8	P	869	VAL	N-CA-CB	7.08	120.16	110.54
8	Q	484	THR	CB-CA-C	-7.08	98.65	110.68
6	G	450	LEU	CA-C-O	-7.07	113.00	120.92
11	U	1144	PHE	CA-CB-CG	7.05	120.85	113.80
11	U	682	VAL	CA-C-N	7.03	125.95	120.33
11	U	682	VAL	C-N-CA	7.03	125.95	120.33
4	E	417	THR	CB-CA-C	7.02	122.45	110.79
3	C	204	LEU	CA-C-O	-7.02	111.90	119.97
2	B	503	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	93	PHE	CA-CB-CG	6.99	120.79	113.80
1	A	425	ASP	CA-CB-CG	6.95	119.55	112.60
12	V	216	PRO	N-CA-C	6.91	122.50	113.86
7	M	309	ILE	N-CA-C	-6.89	105.00	111.48
11	U	910	GLU	CA-C-N	6.87	127.43	119.94
11	U	910	GLU	C-N-CA	6.87	127.43	119.94
8	P	467	GLU	CB-CG-CD	6.87	124.27	112.60
3	C	304	GLU	CB-CG-CD	6.85	124.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	375	TRP	CA-CB-CG	6.84	126.60	113.60
11	U	515	ASP	CA-CB-CG	6.84	119.44	112.60
11	U	442	GLU	CB-CG-CD	6.83	124.21	112.60
3	C	357	GLN	CB-CA-C	-6.83	99.41	110.74
6	G	386	PRO	CA-C-N	6.81	131.02	120.60
6	G	386	PRO	C-N-CA	6.81	131.02	120.60
1	S	1133	HIS	CA-CB-CG	-6.81	106.99	113.80
5	F	165	THR	CA-CB-OG1	-6.81	99.39	109.60
3	C	398	ILE	N-CA-CB	6.79	118.02	110.62
13	Y	6	DA	C2'-C3'-O3'	6.79	121.68	111.50
2	O	347	ASP	CA-CB-CG	6.78	119.38	112.60
2	B	65	PHE	CA-CB-CG	6.78	120.58	113.80
2	O	283	ASP	CA-CB-CG	6.78	119.38	112.60
2	B	261	ARG	CG-CD-NE	6.78	126.91	112.00
7	M	303	PHE	CA-CB-CG	6.75	120.56	113.80
11	U	1100	ASP	CA-CB-CG	6.75	119.35	112.60
4	E	31	GLN	N-CA-C	-6.75	103.92	111.28
2	B	423	TYR	CB-CA-C	-6.74	100.31	110.88
4	E	432	ASP	CA-CB-CG	6.74	119.33	112.60
14	Z	53	DT	N1-C1'-C2'	6.73	123.60	113.50
1	A	286	GLN	CB-CA-C	6.72	121.39	110.37
4	E	357	LEU	CA-C-N	6.71	129.51	120.65
4	E	357	LEU	C-N-CA	6.71	129.51	120.65
8	P	350	ALA	CA-C-O	-6.71	111.96	120.14
12	V	150	ILE	N-CA-C	-6.70	103.99	110.42
5	F	287	TYR	CA-C-O	-6.70	113.42	121.05
11	U	452	ALA	CA-C-N	6.68	129.12	120.44
11	U	452	ALA	C-N-CA	6.68	129.12	120.44
11	U	391	ASP	CA-CB-CG	6.67	119.27	112.60
3	C	241	CYS	CA-C-O	-6.67	113.82	120.82
8	Q	796	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	923	GLU	N-CA-C	6.66	120.47	108.69
4	E	31	GLN	CA-C-N	6.65	129.08	120.44
4	E	31	GLN	C-N-CA	6.65	129.08	120.44
3	C	227	ILE	N-CA-CB	6.64	119.57	110.54
2	B	725	THR	N-CA-CB	6.61	119.83	110.12
11	U	310	ILE	CB-CA-C	6.60	120.25	111.94
3	C	135	THR	CB-CA-C	6.59	121.23	110.88
12	V	423	VAL	CA-C-O	-6.58	113.78	120.69
11	U	701	ASP	CA-CB-CG	6.58	119.18	112.60
5	F	298	GLU	CA-C-N	6.58	129.09	120.28
5	F	298	GLU	C-N-CA	6.58	129.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	728	PHE	CB-CA-C	6.56	121.19	110.88
4	E	503	ASN	CB-CA-C	6.55	120.71	109.24
3	C	251	GLU	CB-CG-CD	6.55	123.73	112.60
1	S	1095	PHE	CA-CB-CG	6.55	120.35	113.80
4	E	465	THR	N-CA-CB	6.54	120.25	109.98
6	G	399	GLU	CB-CG-CD	6.52	123.68	112.60
11	U	867	PRO	CA-C-N	6.52	129.85	120.79
11	U	867	PRO	C-N-CA	6.52	129.85	120.79
3	C	249	SER	CA-C-O	-6.50	112.11	119.79
11	U	598	GLN	CA-C-N	6.50	128.88	120.44
11	U	598	GLN	C-N-CA	6.50	128.88	120.44
4	E	72	PRO	N-CD-CG	-6.49	93.46	103.20
4	E	128	ASP	CA-CB-CG	6.49	119.09	112.60
4	E	502	ALA	N-CA-C	-6.47	104.65	112.54
12	V	466	ASP	CA-C-N	6.45	128.92	120.28
12	V	466	ASP	C-N-CA	6.45	128.92	120.28
8	P	175	LEU	CA-C-N	6.45	128.92	120.28
8	P	175	LEU	C-N-CA	6.45	128.92	120.28
6	G	488	PRO	N-CA-C	6.44	121.95	114.03
2	B	157	THR	CB-CA-C	6.44	120.93	110.95
8	P	346	PRO	CB-CA-C	6.43	122.18	111.56
3	C	169	PHE	CA-CB-CG	6.42	120.22	113.80
1	S	1024	MET	N-CA-C	-6.42	104.37	111.82
4	E	299	GLU	CB-CG-CD	6.42	123.51	112.60
11	U	621	ASN	CA-CB-CG	6.41	119.01	112.60
8	P	387	PRO	CB-CA-C	-6.39	101.02	111.56
6	G	378	SER	CA-C-N	6.38	126.92	119.83
6	G	378	SER	C-N-CA	6.38	126.92	119.83
2	B	386	ASN	CB-CA-C	6.38	120.89	110.24
8	P	281	PRO	CB-CA-C	-6.37	102.60	110.95
12	V	437	SER	CA-C-N	6.37	129.64	120.79
12	V	437	SER	C-N-CA	6.37	129.64	120.79
8	P	12	ALA	CA-C-N	6.36	127.83	122.17
8	P	12	ALA	C-N-CA	6.36	127.83	122.17
12	V	633	ASP	CA-CB-CG	6.35	118.95	112.60
8	Q	679	PHE	CA-CB-CG	-6.35	107.45	113.80
8	P	144	VAL	CA-C-N	6.35	129.88	120.87
8	P	144	VAL	C-N-CA	6.35	129.88	120.87
2	B	735	ILE	CA-C-N	6.34	128.78	120.28
2	B	735	ILE	C-N-CA	6.34	128.78	120.28
6	H	326	GLU	CA-C-N	6.33	128.67	120.44
6	H	326	GLU	C-N-CA	6.33	128.67	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	45	GLU	CB-CA-C	-6.32	100.70	110.81
5	F	306	GLU	CB-CA-C	6.32	120.92	110.81
12	V	1193	THR	CA-C-N	6.32	128.65	120.44
12	V	1193	THR	C-N-CA	6.32	128.65	120.44
1	S	480	LEU	CA-C-N	6.31	124.21	120.24
1	S	480	LEU	C-N-CA	6.31	124.21	120.24
4	E	97	ASN	CB-CA-C	6.30	122.34	109.55
8	P	603	PHE	CA-CB-CG	6.30	120.10	113.80
6	H	95	ASP	CA-CB-CG	6.29	118.89	112.60
6	G	14	ASP	CA-CB-CG	6.29	118.89	112.60
8	P	365	ASP	CA-CB-CG	6.29	118.89	112.60
4	E	493	MET	CA-C-N	6.29	129.53	120.79
4	E	493	MET	C-N-CA	6.29	129.53	120.79
8	P	398	SER	CB-CA-C	6.28	120.71	110.22
1	A	30	VAL	N-CA-C	-6.28	105.03	110.74
11	U	311	ALA	CA-C-N	6.28	128.60	120.44
11	U	311	ALA	C-N-CA	6.28	128.60	120.44
4	E	505	THR	N-CA-CB	6.27	118.97	110.38
1	A	480	LEU	CA-C-N	6.27	124.19	120.24
1	A	480	LEU	C-N-CA	6.27	124.19	120.24
11	U	634	PHE	CA-CB-CG	-6.27	107.53	113.80
1	A	1126	LEU	CA-C-N	6.26	131.35	122.09
1	A	1126	LEU	C-N-CA	6.26	131.35	122.09
2	B	526	ARG	CB-CG-CD	6.24	125.65	111.30
8	P	327	SER	CA-C-N	6.24	130.98	122.19
8	P	327	SER	C-N-CA	6.24	130.98	122.19
1	S	1184	ARG	CG-CD-NE	-6.23	98.30	112.00
8	Q	600	CYS	CB-CA-C	6.23	119.80	109.53
6	G	594	GLU	CB-CG-CD	6.22	123.17	112.60
8	P	435	ASP	CA-CB-CG	6.22	118.82	112.60
12	V	194	THR	CB-CA-C	6.21	121.42	110.85
4	E	523	LEU	N-CA-CB	-6.20	102.77	112.13
11	U	324	ASP	CB-CA-C	6.20	121.08	110.86
4	E	364	THR	N-CA-C	-6.19	104.44	111.07
6	G	452	VAL	CA-C-N	6.19	129.08	120.29
6	G	452	VAL	C-N-CA	6.19	129.08	120.29
12	V	421	PHE	CA-C-O	-6.19	111.79	119.28
1	S	1250	ASP	CA-CB-CG	6.18	118.78	112.60
8	P	225	PHE	O-C-N	6.18	128.44	122.07
1	S	425	ASP	CA-CB-CG	6.18	118.78	112.60
6	G	349	ILE	N-CA-CB	6.17	117.77	110.55
13	Y	8	DG	C2'-C3'-O3'	6.16	120.74	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	391	PRO	CB-CA-C	-6.14	103.42	110.92
8	Q	565	TYR	CA-C-O	-6.14	113.92	121.78
11	U	310	ILE	CA-C-O	-6.14	113.64	120.46
11	U	611	ASP	CA-CB-CG	6.14	118.74	112.60
8	P	606	LEU	CA-C-N	6.13	128.50	120.28
8	P	606	LEU	C-N-CA	6.13	128.50	120.28
6	G	417	CYS	CA-C-N	6.13	128.78	120.44
6	G	417	CYS	C-N-CA	6.13	128.78	120.44
1	S	940	GLN	CB-CA-C	6.13	118.29	108.91
7	M	343	ARG	CA-C-N	6.10	126.75	119.98
7	M	343	ARG	C-N-CA	6.10	126.75	119.98
14	Z	40	DC	C2'-C3'-O3'	6.09	120.64	111.50
2	B	314	GLU	CB-CG-CD	6.07	122.93	112.60
12	V	303	GLU	CB-CG-CD	6.07	122.92	112.60
10	X	110	SER	CA-C-N	6.07	128.12	120.72
10	X	110	SER	C-N-CA	6.07	128.12	120.72
11	U	340	ASP	CA-C-N	6.06	128.40	120.28
11	U	340	ASP	C-N-CA	6.06	128.40	120.28
12	V	217	GLU	CA-C-N	6.05	128.69	120.77
12	V	217	GLU	C-N-CA	6.05	128.69	120.77
2	O	483	ILE	N-CA-CB	-6.05	105.45	112.34
1	S	1394	GLU	CB-CA-C	-6.05	101.39	110.88
12	V	1342	CYS	CA-C-N	6.05	126.82	119.99
12	V	1342	CYS	C-N-CA	6.05	126.82	119.99
2	B	106	GLU	CB-CG-CD	6.04	122.86	112.60
2	O	226	ILE	CA-C-O	-6.04	115.43	120.80
7	L	319	ILE	N-CA-CB	-6.04	107.67	111.83
2	B	243	CYS	CB-CA-C	6.02	117.29	109.28
8	Q	727	PRO	N-CA-CB	-6.01	96.94	103.25
11	U	830	SER	CA-C-N	6.01	128.13	120.56
11	U	830	SER	C-N-CA	6.01	128.13	120.56
5	F	342	PRO	CB-CA-C	-6.00	102.16	111.22
5	F	205	ILE	N-CA-C	-6.00	104.66	110.42
8	P	595	PRO	N-CA-C	6.00	124.82	112.47
8	P	237	GLN	N-CA-C	-5.99	103.40	111.54
1	S	862	PRO	CA-C-N	5.99	126.73	120.03
1	S	862	PRO	C-N-CA	5.99	126.73	120.03
3	C	152	ASN	CB-CA-C	-5.99	100.85	110.79
8	P	254	ILE	CA-C-O	-5.99	114.03	120.85
12	V	287	HIS	CB-CA-C	5.98	119.71	109.24
13	Y	12	DA	C2'-C3'-O3'	5.98	120.47	111.50
8	P	674	ASP	CA-CB-CG	5.98	118.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	279	GLU	N-CA-C	-5.98	105.82	113.23
1	S	1420	GLU	CA-C-N	5.97	129.09	120.79
1	S	1420	GLU	C-N-CA	5.97	129.09	120.79
4	E	427	GLU	CB-CA-C	5.97	120.82	110.79
2	O	248	ILE	CA-C-O	-5.97	115.50	122.13
12	V	198	GLN	N-CA-C	-5.97	104.77	111.28
6	H	321	PHE	CB-CA-C	5.97	121.07	112.12
11	U	481	VAL	CA-C-O	-5.96	114.53	120.85
4	E	64	LEU	CA-C-N	5.95	128.18	120.44
4	E	64	LEU	C-N-CA	5.95	128.18	120.44
3	C	245	ARG	CB-CG-CD	5.95	124.97	111.30
5	F	279	THR	N-CA-C	-5.95	104.14	111.33
4	E	38	GLU	N-CA-C	-5.94	106.01	113.20
4	E	364	THR	CB-CA-C	5.94	120.21	110.88
12	V	765	LEU	CA-C-N	5.94	129.76	120.97
12	V	765	LEU	C-N-CA	5.94	129.76	120.97
8	P	313	VAL	CA-C-O	-5.94	114.16	120.39
1	S	598	ASP	CA-CB-CG	5.93	118.53	112.60
6	G	463	TRP	CA-C-O	-5.93	113.40	120.10
1	S	984	LEU	CA-C-O	-5.91	114.61	120.70
2	O	230	PRO	N-CA-C	5.91	117.91	110.70
8	Q	493	SER	CA-C-N	5.91	128.52	120.54
8	Q	493	SER	C-N-CA	5.91	128.52	120.54
3	C	197	ASP	CB-CA-C	5.91	121.81	110.17
12	V	386	PHE	CA-CB-CG	5.90	119.70	113.80
2	B	84	ASP	CA-CB-CG	5.90	118.50	112.60
2	B	151	PHE	CA-CB-CG	5.90	119.70	113.80
2	O	421	LYS	CB-CA-C	5.90	120.89	110.85
1	A	862	PRO	CA-C-N	5.90	126.66	119.99
1	A	862	PRO	C-N-CA	5.90	126.66	119.99
7	L	107	PRO	CB-CA-C	-5.90	103.72	110.92
8	P	308	HIS	CB-CA-C	5.90	121.59	111.68
8	P	402	CYS	CA-C-O	-5.90	114.21	121.11
1	A	510	TYR	CB-CA-C	-5.89	100.83	110.85
10	X	70	PHE	CA-CB-CG	5.89	119.69	113.80
3	C	105	SER	CA-C-N	5.87	126.61	120.03
3	C	105	SER	C-N-CA	5.87	126.61	120.03
8	P	843	GLU	CB-CA-C	5.87	120.10	110.88
12	V	213	THR	N-CA-C	-5.87	104.06	111.11
2	O	132	ASP	CA-CB-CG	5.87	118.47	112.60
14	Z	47	DT	C2'-C3'-O3'	5.87	120.31	111.50
4	E	42	ARG	N-CA-C	-5.87	104.23	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	91	ASP	CA-CB-CG	5.86	118.46	112.60
8	Q	726	VAL	CA-C-N	5.86	127.16	119.84
8	Q	726	VAL	C-N-CA	5.86	127.16	119.84
1	S	1402	PHE	CB-CA-C	-5.86	101.94	110.96
10	X	29	ASP	CA-CB-CG	5.85	118.45	112.60
3	C	42	GLN	CB-CA-C	5.85	120.06	110.88
7	L	242	PRO	N-CA-C	5.84	121.23	113.40
8	P	234	THR	CA-C-N	5.84	128.39	120.44
8	P	234	THR	C-N-CA	5.84	128.39	120.44
8	Q	565	TYR	N-CA-C	-5.84	101.55	110.14
8	P	279	GLU	CB-CG-CD	5.84	122.53	112.60
11	U	263	GLU	CB-CG-CD	5.83	122.52	112.60
6	G	479	CYS	CA-C-O	-5.83	114.66	120.90
1	S	928	THR	CB-CA-C	-5.83	99.33	109.64
3	C	160	GLU	CB-CG-CD	5.82	122.49	112.60
4	E	60	TRP	CA-C-N	5.82	126.55	120.03
4	E	60	TRP	C-N-CA	5.82	126.55	120.03
2	B	111	ILE	CB-CA-C	5.82	119.29	110.62
6	G	63	ALA	CA-C-N	5.81	124.98	120.33
6	G	63	ALA	C-N-CA	5.81	124.98	120.33
12	V	522	ASP	CA-CB-CG	5.81	118.41	112.60
8	P	198	CYS	CA-C-N	5.81	130.14	121.72
8	P	198	CYS	C-N-CA	5.81	130.14	121.72
7	L	103	ALA	CA-C-N	-5.80	114.37	122.66
7	L	103	ALA	C-N-CA	-5.80	114.37	122.66
2	B	764	GLU	CB-CG-CD	5.80	122.45	112.60
1	S	292	HIS	CB-CA-C	-5.80	101.53	110.81
2	B	90	ASN	CA-CB-CG	5.79	118.39	112.60
1	S	561	THR	CA-CB-OG1	-5.79	100.91	109.60
1	S	320	PHE	CA-CB-CG	5.79	119.59	113.80
12	V	707	ASP	CA-CB-CG	5.79	118.39	112.60
11	U	481	VAL	CA-C-N	5.79	128.31	120.38
11	U	481	VAL	C-N-CA	5.79	128.31	120.38
6	G	20	ASN	CA-C-N	5.78	127.95	120.44
6	G	20	ASN	C-N-CA	5.78	127.95	120.44
8	Q	818	GLN	CA-C-N	5.78	125.83	120.34
8	Q	818	GLN	C-N-CA	5.78	125.83	120.34
11	U	367	VAL	CB-CA-C	-5.77	104.49	111.88
6	G	573	ARG	CB-CA-C	-5.77	101.22	110.79
5	F	90	ASP	CA-CB-CG	5.76	118.36	112.60
2	B	851	PHE	CA-CB-CG	-5.75	108.05	113.80
8	P	306	ASP	CA-CB-CG	5.75	118.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1250	ASP	CA-CB-CG	5.75	118.35	112.60
8	P	34	GLU	CB-CG-CD	5.75	122.37	112.60
11	U	235	ALA	CA-C-N	5.74	128.23	120.65
11	U	235	ALA	C-N-CA	5.74	128.23	120.65
11	U	244	HIS	CA-C-N	5.74	127.90	120.44
11	U	244	HIS	C-N-CA	5.74	127.90	120.44
12	V	1079	SER	CA-C-N	5.74	129.04	120.83
12	V	1079	SER	C-N-CA	5.74	129.04	120.83
3	C	127	PHE	CA-C-N	5.74	130.51	121.56
3	C	127	PHE	C-N-CA	5.74	130.51	121.56
11	U	230	LEU	CA-C-O	-5.74	114.34	120.42
4	E	130	ASP	CA-CB-CG	5.74	118.33	112.60
4	E	521	THR	CB-CA-C	5.73	118.44	109.84
2	O	757	ASP	CA-C-N	5.73	128.28	120.54
2	O	757	ASP	C-N-CA	5.73	128.28	120.54
12	V	424	HIS	CB-CA-C	-5.73	104.17	111.22
8	Q	487	ASN	CA-CB-CG	5.72	118.32	112.60
4	E	352	SER	CB-CA-C	5.71	116.59	108.76
2	B	70	GLU	CB-CG-CD	5.71	122.31	112.60
1	A	452	PHE	CA-CB-CG	5.71	119.51	113.80
3	C	88	LYS	CB-CA-C	5.70	120.25	110.79
8	P	337	GLU	CB-CG-CD	5.70	122.28	112.60
8	P	200	VAL	CA-C-O	-5.69	113.67	120.78
1	S	287	GLU	CA-C-N	5.68	132.40	121.54
1	S	287	GLU	C-N-CA	5.68	132.40	121.54
6	H	565	ASP	CA-CB-CG	5.68	118.28	112.60
2	B	167	PHE	CA-CB-CG	5.68	119.48	113.80
11	U	170	ASP	CA-CB-CG	5.68	118.28	112.60
12	V	504	PRO	CA-C-N	5.68	128.16	120.38
12	V	504	PRO	C-N-CA	5.68	128.16	120.38
8	P	39	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	81	ASP	CA-CB-CG	5.67	118.27	112.60
11	U	1108	GLY	CA-C-N	5.67	128.20	120.54
11	U	1108	GLY	C-N-CA	5.67	128.20	120.54
5	F	125	ASP	CA-CB-CG	5.67	118.27	112.60
7	L	133	PHE	CA-C-N	5.67	128.13	120.65
7	L	133	PHE	C-N-CA	5.67	128.13	120.65
11	U	703	ASP	CA-CB-CG	5.67	118.27	112.60
8	P	453	GLN	N-CA-C	-5.66	105.11	111.28
11	U	549	VAL	CA-C-N	5.65	131.88	121.70
11	U	549	VAL	C-N-CA	5.65	131.88	121.70
6	H	359	ARG	CA-C-N	5.65	128.12	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	359	ARG	C-N-CA	5.65	128.12	120.38
2	B	90	ASN	N-CA-C	-5.65	101.48	109.96
1	S	1266	MET	CA-C-N	5.65	126.10	119.94
1	S	1266	MET	C-N-CA	5.65	126.10	119.94
12	V	350	ILE	N-CA-C	-5.64	105.00	110.42
5	F	177	VAL	CA-C-N	5.64	126.36	119.99
5	F	177	VAL	C-N-CA	5.64	126.36	119.99
12	V	662	ASP	CA-CB-CG	5.64	118.24	112.60
6	H	605	ARG	CB-CA-C	5.63	120.16	110.86
12	V	268	ASP	CA-CB-CG	5.63	118.23	112.60
11	U	1054	HIS	CA-C-N	5.63	126.35	119.99
11	U	1054	HIS	C-N-CA	5.63	126.35	119.99
2	B	661	GLN	CB-CG-CD	-5.62	103.04	112.60
11	U	103	PRO	N-CA-C	5.62	121.23	113.98
3	C	187	CYS	CB-CA-C	-5.62	99.24	110.42
4	E	436	LEU	CA-C-N	5.62	128.60	120.79
4	E	436	LEU	C-N-CA	5.62	128.60	120.79
8	P	533	SER	CA-C-N	5.61	127.80	120.28
8	P	533	SER	C-N-CA	5.61	127.80	120.28
8	P	462	ILE	CA-C-N	5.61	126.33	119.99
8	P	462	ILE	C-N-CA	5.61	126.33	119.99
7	L	130	ASP	CA-C-N	5.60	127.79	120.28
7	L	130	ASP	C-N-CA	5.60	127.79	120.28
12	V	243	VAL	CA-CB-CG2	5.60	119.92	110.40
5	F	348	THR	O-C-N	5.60	128.07	122.08
12	V	150	ILE	O-C-N	5.60	127.39	121.91
12	V	378	LYS	CA-C-N	5.59	128.41	120.53
12	V	378	LYS	C-N-CA	5.59	128.41	120.53
11	U	1044	ILE	CA-C-N	5.59	127.70	120.44
11	U	1044	ILE	C-N-CA	5.59	127.70	120.44
14	Z	51	DC	C2'-C3'-O3'	5.58	119.88	111.50
7	L	263	LEU	CA-C-N	5.58	126.18	119.98
7	L	263	LEU	C-N-CA	5.58	126.18	119.98
11	U	616	ASN	CA-C-N	5.58	127.69	120.44
11	U	616	ASN	C-N-CA	5.58	127.69	120.44
2	O	410	GLN	CA-C-N	5.58	128.07	120.54
2	O	410	GLN	C-N-CA	5.58	128.07	120.54
6	H	239	LEU	CA-C-O	-5.58	115.37	120.95
8	P	229	PHE	CA-C-O	-5.58	113.11	119.41
7	M	335	GLN	CA-C-N	5.58	127.67	120.70
7	M	335	GLN	C-N-CA	5.58	127.67	120.70
3	C	398	ILE	O-C-N	5.56	127.67	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	974	GLU	CA-C-N	5.56	128.51	120.79
11	U	974	GLU	C-N-CA	5.56	128.51	120.79
11	U	858	HIS	CA-CB-CG	5.55	119.35	113.80
12	V	60	LYS	CA-C-N	5.55	127.99	120.44
12	V	60	LYS	C-N-CA	5.55	127.99	120.44
12	V	211	ILE	N-CA-C	-5.55	104.92	110.30
12	V	344	ILE	N-CA-C	-5.55	105.09	110.42
2	B	397	GLY	CA-C-N	5.54	128.03	120.54
2	B	397	GLY	C-N-CA	5.54	128.03	120.54
5	F	279	THR	CA-C-O	-5.54	114.64	120.63
12	V	1334	ASP	CA-CB-CG	5.54	118.14	112.60
11	U	325	GLN	CA-C-N	5.54	127.54	120.56
11	U	325	GLN	C-N-CA	5.54	127.54	120.56
4	E	16	PRO	N-CA-C	-5.54	102.44	111.68
2	B	492	LYS	CB-CA-C	5.53	118.77	109.48
1	S	963	PHE	CA-CB-CG	-5.53	108.27	113.80
3	C	219	PHE	CA-C-O	-5.53	115.02	120.82
11	U	1170	TYR	CA-C-N	5.53	127.69	120.28
11	U	1170	TYR	C-N-CA	5.53	127.69	120.28
1	S	960	HIS	CA-CB-CG	5.52	119.32	113.80
2	O	582	THR	CA-C-N	5.52	128.68	120.95
2	O	582	THR	C-N-CA	5.52	128.68	120.95
6	H	483	LEU	N-CA-CB	-5.52	101.80	110.30
11	U	440	ILE	CA-C-N	5.52	127.95	120.44
11	U	440	ILE	C-N-CA	5.52	127.95	120.44
12	V	781	PHE	CA-CB-CG	5.52	119.32	113.80
11	U	409	SER	CA-C-N	5.52	127.93	120.65
11	U	409	SER	C-N-CA	5.52	127.93	120.65
6	H	79	ILE	N-CA-C	-5.51	104.95	110.30
1	S	673	ILE	N-CA-C	-5.51	105.72	110.74
10	X	27	ASP	CA-CB-CG	5.51	118.11	112.60
12	V	105	GLU	CB-CG-CD	5.51	121.96	112.60
2	B	338	THR	CB-CA-C	-5.51	100.08	110.16
8	P	246	PRO	N-CA-C	5.50	121.79	113.81
11	U	306	SER	N-CA-C	5.50	113.17	108.22
2	B	428	ASN	CA-C-N	5.50	127.59	120.44
2	B	428	ASN	C-N-CA	5.50	127.59	120.44
1	A	800	GLU	CB-CG-CD	5.50	121.95	112.60
11	U	387	PHE	CA-C-O	-5.49	112.62	119.38
1	A	820	SER	CA-C-N	5.49	127.90	120.38
1	A	820	SER	C-N-CA	5.49	127.90	120.38
11	U	1212	PHE	CA-C-O	-5.49	115.04	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	99	GLU	CB-CG-CD	5.49	121.93	112.60
5	F	258	GLY	CA-C-N	5.49	127.57	120.44
5	F	258	GLY	C-N-CA	5.49	127.57	120.44
6	G	105	GLU	CB-CG-CD	5.48	121.92	112.60
4	E	376	THR	N-CA-C	-5.48	105.64	112.93
6	G	401	ALA	CA-C-O	-5.48	114.62	120.42
8	P	61	PRO	CB-CA-C	5.47	118.11	110.17
11	U	216	GLN	CB-CG-CD	5.47	121.91	112.60
3	C	167	ASN	CB-CA-C	-5.47	104.43	111.22
4	E	138	GLU	CB-CG-CD	5.47	121.90	112.60
8	Q	726	VAL	N-CA-CB	5.47	115.17	110.08
12	V	458	TYR	CA-C-O	-5.47	114.76	120.55
1	S	22	TRP	CA-C-O	-5.46	115.27	120.90
12	V	106	ASP	CA-C-N	5.46	128.05	120.29
12	V	106	ASP	C-N-CA	5.46	128.05	120.29
12	V	308	GLN	N-CA-C	-5.46	106.55	113.43
4	E	346	THR	CA-C-N	5.46	128.04	120.29
4	E	346	THR	C-N-CA	5.46	128.04	120.29
12	V	273	ILE	CA-C-O	-5.46	113.92	121.51
11	U	370	ASN	CA-CB-CG	5.46	118.06	112.60
6	G	185	SER	N-CA-C	-5.46	103.30	110.39
6	H	51	ARG	CB-CA-C	-5.45	102.25	110.92
8	P	40	GLY	CA-C-N	5.45	129.35	122.16
8	P	40	GLY	C-N-CA	5.45	129.35	122.16
4	E	399	CYS	N-CA-C	-5.45	106.14	112.89
4	E	429	LEU	CB-CA-C	5.44	117.62	110.06
5	F	156	ASN	CA-C-O	-5.43	115.99	122.13
5	F	42	ARG	CA-C-N	5.43	127.50	120.44
5	F	42	ARG	C-N-CA	5.43	127.50	120.44
10	X	28	LYS	CA-C-N	5.43	128.10	120.28
10	X	28	LYS	C-N-CA	5.43	128.10	120.28
11	U	234	ILE	CA-C-O	-5.43	115.48	121.29
5	F	143	VAL	O-C-N	5.43	127.53	121.94
8	P	855	ASP	CA-CB-CG	5.43	118.03	112.60
6	G	576	ALA	CA-C-N	5.42	127.81	120.65
6	G	576	ALA	C-N-CA	5.42	127.81	120.65
1	S	190	ILE	N-CA-C	-5.42	105.81	110.74
11	U	757	ASN	CB-CA-C	-5.42	101.84	110.84
2	B	410	GLN	CB-CA-C	5.42	119.38	110.88
5	F	336	ASP	CA-CB-CG	5.42	118.02	112.60
2	O	131	LYS	CA-C-N	5.41	131.88	121.54
2	O	131	LYS	C-N-CA	5.41	131.88	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	1213	ILE	N-CA-CB	5.41	117.89	110.54
3	C	22	TRP	CA-C-O	-5.40	115.33	120.90
11	U	298	GLN	CA-C-N	5.40	127.08	120.22
11	U	298	GLN	C-N-CA	5.40	127.08	120.22
10	X	122	ASP	CB-CA-C	5.40	119.40	110.87
1	A	396	LEU	CA-C-N	5.40	127.56	120.60
1	A	396	LEU	C-N-CA	5.40	127.56	120.60
5	F	262	LEU	CA-C-O	-5.39	114.70	120.42
12	V	283	LYS	CA-C-N	5.39	127.82	120.54
12	V	283	LYS	C-N-CA	5.39	127.82	120.54
6	G	461	GLN	N-CA-C	-5.39	105.51	111.71
1	S	486	PRO	CA-C-O	-5.39	115.46	121.23
11	U	330	LEU	O-C-N	5.39	127.62	122.07
3	C	282	PRO	CA-C-N	5.39	127.81	120.54
3	C	282	PRO	C-N-CA	5.39	127.81	120.54
8	P	224	LEU	CA-C-N	5.39	127.44	120.44
8	P	224	LEU	C-N-CA	5.39	127.44	120.44
5	F	320	PRO	CB-CA-C	-5.38	103.27	112.26
11	U	239	ALA	CA-C-O	-5.38	115.14	120.90
2	O	47	ARG	CB-CA-C	5.38	118.91	110.19
8	Q	389	GLY	CA-C-O	-5.38	116.23	120.91
1	A	1401	LEU	CA-C-N	5.38	127.43	120.44
1	A	1401	LEU	C-N-CA	5.38	127.43	120.44
4	E	399	CYS	CB-CA-C	5.38	121.22	109.99
3	C	514	HIS	CA-CB-CG	5.37	119.17	113.80
12	V	387	ILE	N-CA-C	-5.37	105.27	110.42
2	B	241	HIS	CB-CA-C	5.37	118.45	110.62
13	Y	2	DG	C4'-C3'-O3'	-5.37	101.95	110.00
1	S	961	GLU	CB-CA-C	-5.36	99.60	109.15
12	V	1286	ASP	CA-CB-CG	5.36	117.96	112.60
1	S	1306	PHE	CB-CA-C	5.36	118.41	109.56
11	U	528	ASN	CB-CA-C	5.35	120.35	110.88
11	U	1213	ILE	CA-CB-CG1	5.35	119.50	110.40
1	A	923	GLU	CA-C-N	5.35	127.98	120.28
1	A	923	GLU	C-N-CA	5.35	127.98	120.28
1	A	899	PRO	CB-CA-C	-5.35	104.22	111.12
6	H	353	ARG	CA-C-N	5.35	127.89	120.29
6	H	353	ARG	C-N-CA	5.35	127.89	120.29
8	Q	565	TYR	CB-CA-C	5.35	119.88	110.36
11	U	228	SER	CA-C-O	-5.34	115.21	120.82
12	V	287	HIS	N-CA-C	-5.34	106.89	113.41
11	U	1042	PRO	N-CA-CB	-5.34	97.64	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	V	466	ASP	CA-CB-CG	5.34	117.94	112.60
6	G	455	THR	CA-CB-OG1	-5.34	101.59	109.60
13	Y	14	DA	C2'-C3'-O3'	5.34	119.50	111.50
2	O	842	VAL	CA-C-O	-5.33	115.41	120.95
5	F	275	LEU	CA-C-N	5.33	126.01	119.99
5	F	275	LEU	C-N-CA	5.33	126.01	119.99
6	G	404	LEU	CA-C-N	5.33	127.38	120.56
6	G	404	LEU	C-N-CA	5.33	127.38	120.56
2	B	348	SER	CA-C-N	5.33	127.68	120.65
2	B	348	SER	C-N-CA	5.33	127.68	120.65
12	V	391	THR	CB-CA-C	5.33	121.02	110.42
12	V	565	SER	CA-C-N	5.32	127.41	120.28
12	V	565	SER	C-N-CA	5.32	127.41	120.28
8	P	453	GLN	CB-CG-CD	5.32	121.65	112.60
8	P	403	SER	CA-C-N	5.32	128.52	120.75
8	P	403	SER	C-N-CA	5.32	128.52	120.75
11	U	202	PHE	CA-CB-CG	5.32	119.12	113.80
6	G	605	ARG	CB-CA-C	5.32	120.29	110.88
11	U	504	GLN	CB-CA-C	-5.32	100.74	111.80
8	P	723	HIS	CA-CB-CG	5.31	119.11	113.80
11	U	1161	THR	CB-CA-C	5.31	120.86	110.67
2	B	90	ASN	N-CA-CB	5.30	117.75	109.85
11	U	505	PRO	CA-C-N	5.30	127.70	120.54
11	U	505	PRO	C-N-CA	5.30	127.70	120.54
1	S	1084	ARG	CB-CG-CD	5.30	123.50	111.30
2	B	409	ARG	N-CA-C	-5.30	105.50	111.28
8	P	526	THR	CB-CA-C	5.30	118.98	110.29
1	S	543	PRO	CA-C-N	5.30	128.37	120.31
1	S	543	PRO	C-N-CA	5.30	128.37	120.31
12	V	363	ALA	CA-C-O	-5.30	114.93	120.55
4	E	157	SER	CA-C-N	5.30	127.33	120.44
4	E	157	SER	C-N-CA	5.30	127.33	120.44
8	P	256	LYS	CA-C-O	-5.30	115.23	120.90
12	V	224	HIS	CA-C-N	5.30	127.38	120.28
12	V	224	HIS	C-N-CA	5.30	127.38	120.28
2	B	715	GLY	CA-C-O	-5.29	116.47	121.60
7	L	292	PHE	CA-CB-CG	5.29	119.09	113.80
7	M	153	LYS	CB-CA-C	5.29	118.95	110.16
8	Q	158	PRO	CA-C-N	5.29	126.70	120.09
8	Q	158	PRO	C-N-CA	5.29	126.70	120.09
6	G	163	LEU	CA-C-N	5.29	127.37	120.28
6	G	163	LEU	C-N-CA	5.29	127.37	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	656	PRO	CA-C-N	5.29	126.94	120.22
8	P	656	PRO	C-N-CA	5.29	126.94	120.22
8	Q	611	GLY	N-CA-C	5.29	115.02	110.21
11	U	669	CYS	CA-C-N	5.29	127.63	120.65
11	U	669	CYS	C-N-CA	5.29	127.63	120.65
2	B	169	SER	CA-C-O	-5.29	115.28	121.46
1	S	1023	GLU	CA-CB-CG	5.29	124.67	114.10
11	U	271	ILE	CA-C-O	-5.29	115.57	121.17
11	U	338	PHE	N-CA-C	-5.29	105.19	111.69
12	V	1180	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	339	GLU	CA-C-N	5.28	132.41	123.01
2	B	339	GLU	C-N-CA	5.28	132.41	123.01
6	H	199	ASP	CA-C-N	5.28	127.67	120.54
6	H	199	ASP	C-N-CA	5.28	127.67	120.54
2	O	849	SER	CA-C-N	5.28	127.31	120.44
2	O	849	SER	C-N-CA	5.28	127.31	120.44
5	F	342	PRO	N-CA-C	5.28	118.61	111.22
4	E	387	LEU	N-CA-C	-5.28	105.44	111.14
11	U	1161	THR	CA-C-O	-5.28	113.90	119.97
1	A	287	GLU	CA-C-N	5.27	129.85	122.36
1	A	287	GLU	C-N-CA	5.27	129.85	122.36
1	A	757	VAL	N-CA-C	-5.27	107.02	111.56
12	V	153	LEU	CA-C-N	5.27	127.35	120.28
12	V	153	LEU	C-N-CA	5.27	127.35	120.28
5	F	148	PHE	CB-CA-C	5.27	119.50	110.01
8	P	238	SER	CA-C-O	-5.27	115.07	119.76
12	V	392	ASN	CB-CA-C	5.27	118.44	109.80
5	F	205	ILE	O-C-N	5.27	127.07	121.91
6	G	459	GLN	CA-C-N	5.27	125.68	119.94
6	G	459	GLN	C-N-CA	5.27	125.68	119.94
6	G	342	THR	CB-CA-C	5.26	119.04	109.83
1	S	29	ARG	CA-C-N	5.26	127.55	120.50
1	S	29	ARG	C-N-CA	5.26	127.55	120.50
11	U	439	GLU	CB-CG-CD	5.26	121.55	112.60
1	A	1314	ARG	CA-C-O	-5.26	115.48	120.90
1	S	575	ARG	CA-C-N	5.26	126.30	119.78
1	S	575	ARG	C-N-CA	5.26	126.30	119.78
6	H	191	LEU	CA-C-O	-5.25	115.78	121.87
8	P	136	LEU	N-CA-C	-5.25	102.39	109.95
1	A	1345	ASP	CA-CB-CG	5.25	117.85	112.60
5	F	263	VAL	CA-C-N	5.25	127.58	120.44
5	F	263	VAL	C-N-CA	5.25	127.58	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	726	VAL	CB-CA-C	5.24	116.55	110.89
1	S	1126	LEU	CA-C-N	5.24	128.92	121.42
1	S	1126	LEU	C-N-CA	5.24	128.92	121.42
3	C	200	VAL	N-CA-C	-5.24	104.78	110.23
5	F	103	LEU	CA-C-N	5.23	125.31	120.34
5	F	103	LEU	C-N-CA	5.23	125.31	120.34
6	H	91	ASP	N-CA-CB	5.23	117.81	110.12
2	B	639	LYS	CA-C-N	5.23	125.63	119.83
2	B	639	LYS	C-N-CA	5.23	125.63	119.83
6	G	362	ASP	CA-CB-CG	5.23	117.83	112.60
12	V	1231	PHE	CA-C-O	-5.22	115.01	120.55
4	E	27	ARG	CB-CG-CD	5.22	123.31	111.30
1	A	1276	ASN	CA-CB-CG	5.22	117.82	112.60
7	M	11	GLN	CB-CA-C	5.22	117.84	109.07
11	U	450	THR	CB-CA-C	-5.22	100.65	110.67
12	V	212	ILE	CA-CB-CG1	5.22	119.27	110.40
1	A	1263	PHE	CA-CB-CG	5.22	119.02	113.80
6	G	452	VAL	CA-C-O	-5.22	115.53	120.95
11	U	209	GLU	CA-C-N	5.22	124.50	120.33
11	U	209	GLU	C-N-CA	5.22	124.50	120.33
11	U	820	ASP	CA-CB-CG	5.22	117.82	112.60
12	V	562	GLN	CA-C-N	5.22	127.53	120.38
12	V	562	GLN	C-N-CA	5.22	127.53	120.38
2	B	85	PHE	CA-C-N	5.21	127.72	120.63
2	B	85	PHE	C-N-CA	5.21	127.72	120.63
11	U	356	HIS	CB-CA-C	5.21	118.60	110.67
12	V	396	LYS	N-CA-C	-5.21	105.24	111.03
5	F	193	TRP	CA-C-N	5.21	127.22	120.44
5	F	193	TRP	C-N-CA	5.21	127.22	120.44
1	A	136	LEU	CA-C-N	5.21	129.74	121.72
1	A	136	LEU	C-N-CA	5.21	129.74	121.72
5	F	123	ASP	CA-CB-CG	5.21	117.81	112.60
6	G	325	VAL	CA-C-N	5.21	128.63	120.82
6	G	325	VAL	C-N-CA	5.21	128.63	120.82
3	C	267	ASN	CB-CA-C	5.21	118.48	111.82
8	P	349	CYS	CA-C-O	-5.21	115.71	121.28
12	V	263	ARG	CG-CD-NE	5.21	123.45	112.00
8	Q	593	ASP	CA-C-O	-5.20	114.76	120.69
4	E	469	PHE	CA-CB-CG	-5.20	108.60	113.80
12	V	396	LYS	CB-CA-C	5.20	119.01	110.95
12	V	963	PRO	CA-C-N	5.20	127.56	120.54
12	V	963	PRO	C-N-CA	5.20	127.56	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	CA-C-N	5.20	127.22	120.88
1	A	29	ARG	C-N-CA	5.20	127.22	120.88
1	A	353	PRO	CA-C-N	5.20	127.20	120.44
1	A	353	PRO	C-N-CA	5.20	127.20	120.44
1	A	1012	THR	CB-CA-C	5.20	120.54	109.10
6	H	254	SER	CA-C-O	-5.20	115.36	120.82
4	E	31	GLN	O-C-N	5.20	127.63	122.12
6	H	124	SER	CA-C-N	5.20	127.11	120.56
6	H	124	SER	C-N-CA	5.20	127.11	120.56
2	O	237	VAL	N-CA-CB	5.20	117.09	110.13
6	G	366	HIS	CB-CA-C	5.19	119.03	110.88
2	B	174	GLY	CA-C-N	5.19	128.25	120.87
2	B	174	GLY	C-N-CA	5.19	128.25	120.87
1	S	406	LEU	CA-C-N	5.19	127.69	120.63
1	S	406	LEU	C-N-CA	5.19	127.69	120.63
14	Z	41	DC	C2'-C3'-O3'	5.19	119.29	111.50
2	B	519	ARG	CB-CA-C	5.19	118.29	109.84
4	E	403	LEU	CA-C-N	5.18	127.18	120.44
4	E	403	LEU	C-N-CA	5.18	127.18	120.44
1	A	149	LEU	CA-C-N	5.18	127.48	120.38
1	A	149	LEU	C-N-CA	5.18	127.48	120.38
6	G	51	ARG	CA-C-N	5.18	125.73	119.98
6	G	51	ARG	C-N-CA	5.18	125.73	119.98
8	P	577	ARG	CB-CA-C	5.18	118.65	109.89
1	S	561	THR	CA-CB-CG2	5.18	119.31	110.50
1	S	1089	VAL	CA-C-N	5.18	127.68	120.63
1	S	1089	VAL	C-N-CA	5.18	127.68	120.63
2	O	472	GLU	CB-CA-C	5.18	118.79	110.29
12	V	300	GLU	N-CA-C	-5.18	105.53	111.07
4	E	177	ARG	CB-CA-C	5.17	119.06	110.74
7	L	286	ASP	CA-CB-CG	5.17	117.77	112.60
8	P	317	HIS	CA-CB-CG	-5.17	108.63	113.80
11	U	852	GLN	CB-CA-C	-5.17	102.21	110.79
12	V	281	ILE	O-C-N	5.16	126.97	121.91
1	S	671	ASP	CA-CB-CG	5.16	117.76	112.60
1	S	1073	ARG	CB-CA-C	-5.16	102.78	110.88
11	U	495	THR	CA-C-N	5.16	127.26	120.60
11	U	495	THR	C-N-CA	5.16	127.26	120.60
12	V	216	PRO	CB-CA-C	-5.16	104.15	111.68
1	S	1012	THR	CB-CA-C	5.16	120.67	111.03
11	U	998	PRO	N-CA-C	5.15	120.54	113.84
1	S	1406	LEU	CA-C-N	5.15	125.38	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	1406	LEU	C-N-CA	5.15	125.38	120.43
11	U	340	ASP	CA-CB-CG	5.15	117.75	112.60
12	V	177	VAL	N-CA-CB	5.15	117.55	110.54
12	V	359	THR	CA-C-O	-5.15	115.15	120.92
8	P	84	GLY	N-CA-C	5.15	114.89	110.21
11	U	1103	ILE	CA-C-O	-5.15	115.39	120.85
7	M	107	PRO	N-CA-C	5.14	116.97	110.70
11	U	241	ASP	CA-CB-CG	5.14	117.74	112.60
12	V	478	VAL	O-C-N	5.14	126.95	121.91
4	E	168	CYS	CA-C-N	5.14	128.53	120.82
4	E	168	CYS	C-N-CA	5.14	128.53	120.82
6	G	406	GLN	CA-C-N	5.14	127.17	120.28
6	G	406	GLN	C-N-CA	5.14	127.17	120.28
8	P	12	ALA	O-C-N	5.14	128.66	123.26
7	L	107	PRO	N-CA-C	5.14	116.97	110.70
11	U	1009	TRP	CA-C-N	5.14	127.93	120.79
11	U	1009	TRP	C-N-CA	5.14	127.93	120.79
1	A	333	VAL	CA-C-O	-5.13	117.62	121.68
2	B	60	LYS	CB-CA-C	5.13	119.81	110.11
12	V	200	ILE	O-C-N	5.13	127.08	121.94
6	G	444	GLU	CB-CG-CD	5.13	121.33	112.60
1	A	267	VAL	CA-C-N	5.13	127.92	120.79
1	A	267	VAL	C-N-CA	5.13	127.92	120.79
7	M	4	THR	CA-C-N	5.13	127.41	120.44
7	M	4	THR	C-N-CA	5.13	127.41	120.44
11	U	770	ASP	N-CA-CB	5.13	117.58	109.94
11	U	361	SER	O-C-N	5.13	127.35	122.07
12	V	237	GLU	CA-C-O	-5.13	115.44	120.82
2	B	702	GLY	CA-C-N	5.12	128.95	121.31
2	B	702	GLY	C-N-CA	5.12	128.95	121.31
14	Z	42	DT	C2'-C3'-O3'	5.12	119.19	111.50
2	B	736	ARG	CA-C-N	5.12	128.76	121.02
2	B	736	ARG	C-N-CA	5.12	128.76	121.02
12	V	300	GLU	CB-CG-CD	5.12	121.31	112.60
8	P	457	GLU	CB-CG-CD	5.12	121.31	112.60
12	V	241	LEU	N-CA-CB	-5.12	103.41	111.39
3	C	79	PHE	CA-C-N	5.12	127.09	120.70
3	C	79	PHE	C-N-CA	5.12	127.09	120.70
8	Q	306	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	899	PRO	N-CA-C	5.11	119.27	111.34
4	E	120	ILE	O-C-N	5.11	127.22	121.90
5	F	24	SER	CA-C-N	5.11	127.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	24	SER	C-N-CA	5.11	127.64	120.28
8	Q	487	ASN	N-CA-CB	5.11	117.59	109.82
11	U	327	LEU	O-C-N	5.11	127.54	122.12
2	B	600	GLN	CB-CA-C	5.11	118.06	109.48
5	F	53	PRO	CA-C-N	5.11	126.99	120.56
5	F	53	PRO	C-N-CA	5.11	126.99	120.56
12	V	1206	VAL	CA-C-N	5.11	126.56	120.13
12	V	1206	VAL	C-N-CA	5.11	126.56	120.13
8	Q	716	ARG	CA-C-O	-5.10	115.64	121.00
11	U	61	GLY	CA-C-N	5.10	127.54	120.29
11	U	61	GLY	C-N-CA	5.10	127.54	120.29
2	B	38	THR	CB-CA-C	5.10	120.33	109.10
2	B	646	GLU	CB-CG-CD	5.10	121.27	112.60
6	H	211	PHE	N-CA-CB	5.10	117.62	110.12
6	H	249	TYR	CA-C-O	-5.10	115.45	120.70
11	U	311	ALA	O-C-N	5.10	127.53	122.12
2	B	225	ASP	CA-CB-CG	5.10	117.70	112.60
5	F	348	THR	CA-CB-OG1	5.10	117.25	109.60
6	G	326	GLU	CA-C-N	5.10	128.47	120.82
6	G	326	GLU	C-N-CA	5.10	128.47	120.82
2	O	516	SER	CA-C-N	5.10	129.38	122.19
2	O	516	SER	C-N-CA	5.10	129.38	122.19
7	M	330	GLY	CA-C-N	-5.09	114.07	121.20
7	M	330	GLY	C-N-CA	-5.09	114.07	121.20
2	B	332	ASP	CB-CA-C	5.09	119.66	111.05
2	B	667	TYR	CA-C-O	-5.09	115.98	121.38
11	U	870	ILE	N-CA-CB	5.09	118.22	110.58
5	F	18	SER	CA-C-N	5.09	128.74	120.60
5	F	18	SER	C-N-CA	5.09	128.74	120.60
9	W	90	PHE	CA-CB-CG	5.09	118.89	113.80
5	F	128	THR	CA-C-N	5.09	127.05	120.44
5	F	128	THR	C-N-CA	5.09	127.05	120.44
1	S	29	ARG	CB-CG-CD	5.09	123.00	111.30
6	G	525	VAL	CA-C-O	-5.08	115.66	120.95
6	H	245	LEU	CA-C-N	5.08	127.16	120.60
6	H	245	LEU	C-N-CA	5.08	127.16	120.60
8	P	521	ASP	CB-CA-C	5.08	118.13	109.84
1	S	140	GLU	N-CA-C	-5.08	106.59	112.89
1	A	1127	THR	CB-CA-C	-5.08	101.15	109.53
1	S	367	SER	CA-C-N	5.08	127.04	120.44
1	S	367	SER	C-N-CA	5.08	127.04	120.44
6	G	433	ARG	CA-C-N	5.07	128.43	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	433	ARG	C-N-CA	5.07	128.43	120.82
11	U	211	PRO	N-CA-C	5.07	116.88	110.70
11	U	538	ALA	CA-C-N	5.07	125.60	119.98
11	U	538	ALA	C-N-CA	5.07	125.60	119.98
7	L	60	ARG	CA-C-O	-5.07	115.18	120.55
2	O	185	GLY	CA-C-O	-5.07	117.35	121.76
12	V	87	PRO	CB-CA-C	-5.07	104.58	111.12
2	O	352	ASP	CA-CB-CG	5.06	117.66	112.60
1	S	791	LEU	CA-C-N	5.06	126.47	120.14
1	S	791	LEU	C-N-CA	5.06	126.47	120.14
2	B	704	LEU	N-CA-C	5.06	117.65	108.69
4	E	524	ARG	O-C-N	5.06	127.28	122.07
2	O	281	PHE	CA-C-N	5.06	127.62	122.66
2	O	281	PHE	C-N-CA	5.06	127.62	122.66
1	S	826	THR	CB-CA-C	-5.05	99.34	109.35
7	M	345	LEU	CA-C-N	5.05	127.01	120.44
7	M	345	LEU	C-N-CA	5.05	127.01	120.44
3	C	243	TRP	CA-CB-CG	5.05	123.20	113.60
6	G	199	ASP	CA-C-N	5.05	127.05	120.28
6	G	199	ASP	C-N-CA	5.05	127.05	120.28
11	U	1202	GLY	CA-C-N	5.05	127.32	120.65
11	U	1202	GLY	C-N-CA	5.05	127.32	120.65
12	V	400	ASP	CB-CA-C	5.05	118.88	110.90
3	C	173	ARG	CB-CG-CD	5.05	122.92	111.30
12	V	364	TRP	N-CA-CB	5.05	117.46	109.94
8	Q	636	GLU	CB-CG-CD	5.04	121.18	112.60
5	F	144	HIS	CA-CB-CG	-5.04	108.76	113.80
3	C	277	LYS	CA-C-N	5.04	127.30	120.65
3	C	277	LYS	C-N-CA	5.04	127.30	120.65
1	S	558	PHE	CA-CB-CG	-5.04	108.76	113.80
11	U	1183	VAL	CA-C-O	-5.04	114.87	120.46
8	Q	70	LEU	CA-C-N	5.04	126.02	119.78
8	Q	70	LEU	C-N-CA	5.04	126.02	119.78
11	U	166	SER	CA-C-N	5.04	126.22	120.53
11	U	166	SER	C-N-CA	5.04	126.22	120.53
2	O	248	ILE	N-CA-C	-5.03	104.52	110.21
11	U	125	LYS	CA-C-N	5.03	127.02	120.28
11	U	125	LYS	C-N-CA	5.03	127.02	120.28
12	V	1223	PHE	CA-CB-CG	5.03	118.83	113.80
8	P	785	VAL	CA-C-O	-5.03	116.30	121.93
11	U	29	LEU	CA-C-N	5.03	127.02	120.28
11	U	29	LEU	C-N-CA	5.03	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	732	THR	CB-CA-C	-5.03	102.98	110.88
11	U	279	ILE	CA-C-N	5.03	127.27	120.38
11	U	279	ILE	C-N-CA	5.03	127.27	120.38
12	V	414	GLU	CB-CG-CD	5.03	121.15	112.60
11	U	851	GLN	CB-CA-C	5.02	118.77	110.88
2	O	721	SER	CA-C-O	-5.02	115.72	121.40
1	S	169	GLU	CB-CG-CD	5.02	121.14	112.60
4	E	352	SER	N-CA-C	-5.02	102.74	110.32
2	B	723	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	1132	ALA	CA-C-O	-5.02	115.23	120.55
8	P	197	LEU	CA-C-O	-5.02	114.94	120.36
11	U	617	SER	CA-C-N	5.01	127.50	120.28
11	U	617	SER	C-N-CA	5.01	127.50	120.28
11	U	1261	GLU	CA-C-O	-5.01	115.21	120.63
8	Q	221	GLU	CA-C-N	5.01	127.00	120.28
8	Q	221	GLU	C-N-CA	5.01	127.00	120.28
1	S	980	ALA	CA-C-O	-5.01	115.74	121.00
1	A	92	SER	CA-C-N	5.01	127.75	120.79
1	A	92	SER	C-N-CA	5.01	127.75	120.79
11	U	425	ILE	N-CA-CB	5.01	115.88	110.62
3	C	138	LEU	CA-C-N	5.00	128.36	121.26
3	C	138	LEU	C-N-CA	5.00	128.36	121.26
8	P	386	GLY	CA-C-N	5.00	126.09	119.84
8	P	386	GLY	C-N-CA	5.00	126.09	119.84
11	U	1108	GLY	O-C-N	5.00	126.98	122.18
12	V	171	ASN	CA-C-N	5.00	124.33	120.33
12	V	171	ASN	C-N-CA	5.00	124.33	120.33

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	GLY	Peptide
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	Mainchain,Peptide
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
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

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Mol	Chain	Res	Type	Group
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 ⓘ

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	212	0
1	S	9933	10028	9969	223	0
2	B	5605	5790	5768	175	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	5594	5759	5740	109	0
3	C	4396	4442	4427	118	0
4	E	3224	3390	3384	141	0
5	F	2726	2740	2729	73	0
6	G	4483	4537	4523	111	0
6	H	4216	4288	4273	112	0
7	L	2974	2977	2971	50	0
7	M	2974	2977	2972	102	0
8	P	5598	5681	5652	220	0
8	Q	5631	5724	5694	102	0
9	W	271	242	196	11	0
10	X	1233	1251	1248	26	0
11	U	9350	9739	9708	243	0
12	V	8997	9224	9173	206	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	88352	2058	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 12.

All (2058) 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
1:A:900:SER:HG	1:A:903:TRP:CD1	1.71	1.08
12:V:146:GLN:HE22	12:V:186:VAL:HA	1.20	1.05
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
1:S:988:LEU:HD21	1:S:1077:MET:HE2	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:286:GLN:C	1:A:288:GLU:H	1.88	0.81
6:G:306:LEU:HD21	6:G:346:THR:HG21	1.63	0.81
8:P:402:CYS:O	8:P:402:CYS:SG	2.36	0.80
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:S:988:LEU:HD21	1:S:1077:MET:CE	2.13	0.77
5:F:255:LEU:HD12	5:F:260:LEU:HD21	1.67	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
1:S:731:MET:HE2	9:W:85:PHE:HB3	1.70	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: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
11:U:668:LEU:C	11:U:752:VAL:HG11	2.14	0.72
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:M:162:SER:HG	7:M:177:TRP:CD1	2.07	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:989:MET:HE1	1:S:1077:MET:HB3	1.73	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
4:E:522:PHE:C	4:E:523:LEU:HG	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1033:ASP:CG	1:S:1093:SER:HB2	2.19	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
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
2:O:155:SER:O	2:O:156:GLN:HB3	1.92	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
1:A:35:TYR:HE1	6:H:311:ASN:CG	2.02	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
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
1:A:286:GLN:HB3	1:A:288:GLU:HG3	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:196:VAL:C	3:C:198:PRO:HD2	2.22	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:988:LEU:CD2	1:S:1077:MET:HE2	2.23	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
5:F:116:PHE:HA	5:F:130:GLN:HE21	1.62	0.64
2:O:18:TYR:OH	2:O:90:ASN:O	2.12	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
11:U:817:LEU:HD22	11:U:839:MET:HE1	1.80	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
6:G:457:LEU:HD11	6:G:516:ALA:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:V:938:CYS:HG	12:V:960:LEU:N	1.96	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
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
12:V:175:LEU:O	12:V:178:SER:OG	2.17	0.61
4:E:464:MET:HE3	4:E:469:PHE:CD1	2.36	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
8:P:471:PHE:CD1	8:P:471:PHE:C	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:O:634:LEU:HD21	2:O:647:ASP:CG	2.25	0.61
7:M:354:ILE:HG12	7:M:369:LYS:HG2	1.83	0.61
2:B:16:LEU:HD23	2:B:17:CYS:C	2.26	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: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
11:U:494:GLN:H	11:U:494:GLN:CD	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:V:1142:LEU:HD22	12:V:1151:ASN:CG	2.27	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
12:V:427:VAL:HG12	12:V:431:MET:HE1	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
10:X:25:TRP:CD1	10:X:28:LYS:HZ3	2.22	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
2:O:590:PHE:C	2:O:592:LYS:N	2.60	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:B:704:LEU:C	2:B:705:PHE:HD1	2.12	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
1:A:1266:MET:HE2	1:A:1266:MET:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:LYS:HZ3	1:A:903:TRP:CD1	2.21	0.57
6:G:89:THR:OG1	6:G:90:GLU:N	2.36	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
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:835:LYS:HZ3	1:A:903:TRP:CG	2.22	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
2:O:13:GLU:CD	2:O:353:CYS:SG	2.88	0.57
8:P:390:LEU:N	8:P:390:LEU:HD23	2.20	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:137:LEU:HB3	2:B:181:MET:HE2	1.87	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:27:ARG:C	8:P:400:ASN:HD21	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:GLY:C	1:A:30:VAL:H	2.12	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
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
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:B:265:LEU:C	2:B:266:ILE:HG13	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:P:649:MET:HE2	8:P:799:ARG:HB2	1.87	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:224:ASN:C	3:C:224:ASN:OD1	2.49	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
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
12:V:428:LEU:HD23	12:V:431:MET:HE2	1.87	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
8:Q:11:LEU:C	8:Q:11:LEU:HD12	2.32	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
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
1:A:230:VAL:HG12	1:A:234:MET:HE3	1.89	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
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
6:H:345:GLN:CD	6:H:386:PRO:HA	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:381:ARG:HB3	4:E:381:ARG:CZ	2.37	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
4:E:518:PRO:O	4:E:521:THR:OG1	2.18	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
8:P:366:LEU:HD23	8:P:366:LEU:C	2.33	0.54
8:P:679:PHE:CD2	8:P:679:PHE:C	2.82	0.54
1:S:361:ARG:C	1:S:365:MET:HE2	2.33	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
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
1:S:57:LEU:HB2	1:S:116:MET:HE1	1.89	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:OD1	11:U:528:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:U:1:MET:HE1	11:U:24:LEU:HD11	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:610:TYR:CD1	11:U:610:TYR:C	2.86	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
6:H:537:PHE:O	6:H:540:SER:OG	2.27	0.53
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:315:SER:O	2:B:315:SER:OG	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:988:LEU:HD22	1:A:1077:MET:HE3	1.91	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
1:A:286:GLN:C	1:A:288:GLU:N	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:G:449:PRO:O	6:G:450:LEU:C	2.53	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
11:U:205:MET:HE1	11:U:213:LEU:HD23	1.92	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
8:P:268:PRO:O	8:P:269:ASN:C	2.52	0.52
1:S:923:GLU:N	1:S:923:GLU:CD	2.67	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
12:V:534:TYR:CD1	12:V:534:TYR:C	2.88	0.52
2:B:846:GLN:OE1	8:P:874:ARG:NH2	2.38	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
1:A:1333:PHE:CD1	1:A:1333:PHE:C	2.89	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
6:H:224:ASN:C	6:H:226:ASP:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:E:464:MET:HE3	4:E:469:PHE:HD1	1.74	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
1:A:822:LEU:HD23	1:A:822:LEU:C	2.36	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
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:196:VAL:C	3:C:198:PRO:CD	2.84	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
1:A:1330:LEU:C	1:A:1332:PRO:HD2	2.36	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
11:U:817:LEU:HB3	11:U:839:MET:HE1	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:828:LEU:HD23	8:P:826:ARG:C	2.37	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:322:PHE:O	11:U:323:GLN:C	2.52	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
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
3:C:232:ILE:HG23	3:C:233:SER:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:471:PRO:O	11:U:472:LEU:C	2.51	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
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
4:E:427:GLU:N	4:E:427:GLU:CD	2.70	0.49
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:1404:LEU:HD21	1:A:1432:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:ARG:HH21	2:B:653:ALA:C	2.20	0.49
2:B:752:GLU:CD	8:P:859:SER:O	2.55	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
1:A:1305:LEU:C	1:A:1308:LEU:HD21	2.37	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:SG	6:H:544:CYS:O	2.70	0.49
2:O:265:LEU:CD2	2:O:311:VAL:HG21	2.43	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
11:U:494:GLN:CD	11:U:494:GLN:N	2.70	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
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
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:359:ASN:C	4:E:363:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:669:LEU:C	2:B:670:ASN:CG	2.81	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: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
12:V:263:ARG:HD2	12:V:267:MET:HE2	1.95	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:P:366:LEU:C	8:P:366:LEU:CD2	2.86	0.48
8:Q:149:ARG:HG2	8:Q:176:SER:HA	1.96	0.48
1:S:855:THR:CG2	1:S:858:SER:OG	2.62	0.48
1:S:989:MET:HE1	1:S:1077:MET:CB	2.40	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:320:PHE:CZ	1:S:365:MET:HE3	2.48	0.48
1:S:575:ARG:O	1:S:579:TYR:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
5:F:290:GLN:C	6:G:485:ARG:HH22	2.22	0.48
5:F:310:ARG:O	5:F:313:SER:OG	2.28	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
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
6:H:239:LEU:HD12	6:H:239:LEU:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:305:MET:O	7:L:320:PRO:HG2	2.14	0.48
8:P:51:GLY:C	8:P:53:LEU:H	2.21	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
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
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
1:S:361:ARG:O	1:S:365:MET:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:992:HIS:CB	1:A:1077:MET:HE1	2.43	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
4:E:421:CYS:SG	4:E:422:CYS:N	2.86	0.47
6:G:191:LEU:O	6:G:193:ALA:N	2.47	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
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
1:A:768:LEU:O	1:A:772:GLN:C	2.58	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
4:E:386:ALA:O	4:E:389:SER:OG	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
8:Q:517:LEU:O	8:Q:518:GLN:C	2.58	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:U:670:CYS:O	11:U:674:CYS:SG	2.66	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
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
2:B:82:VAL:O	2:B:83:SER:OG	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:M:207:ILE:O	7:M:211:THR:OG1	2.32	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
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
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
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
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:974:ASP:O	1:S:975:GLY:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1063:TRP:HA	1:S:1063:TRP:CE3	2.49	0.46
12:V:247:ASP:O	12:V:250:SER:OG	2.28	0.46
12:V:640:GLN:O	12:V:743:ARG:NH2	2.45	0.46
2:B:389:LEU:HD13	7:L:128:TYR:HA	1.98	0.46
2:B:759:MET:HE1	2:B:853:ALA:HB2	1.97	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
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:143:LEU:C	8:P:143:LEU:HD23	2.41	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
2:B:727:MET:HE2	2:B:727:MET:HB2	1.82	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:S:57:LEU:CB	1:S:116:MET:HE1	2.46	0.46
1:S:1410:CYS:SG	1:S:1414:SER:OG	2.63	0.46
11:U:456:ILE:O	11:U:457:SER:C	2.58	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
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:324:LYS:O	2:B:325:LEU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:S:1333:PHE:C	1:S:1333:PHE:CD1	2.92	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:526:ARG:NH2	2:B:653:ALA:C	2.72	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
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
2:B:700:PHE:O	2:B:703:THR:OG1	2.29	0.45
6:H:387:SER:HB2	6:H:388:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:C:79:PHE:CD1	5:F:145:MET:HE2	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
4:E:391:CYS:O	4:E:392:ALA:C	2.58	0.45
5:F:285:LEU:HB3	5:F:294:TRP:HE3	1.81	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:312:ILE:O	3:C:316:GLN:HG3	2.17	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
2:B:656:HIS:CD2	2:B:656:HIS:C	2.94	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
4:E:430:GLU:C	4:E:434:GLN:HE21	2.25	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
7:L:320:PRO:HA	7:L:333:PHE:O	2.17	0.45
2:O:522:LYS:C	2:O:523:CYS:SG	3.00	0.45
2:O:830:VAL:HG22	8:Q:826:ARG:HG3	1.99	0.45
8:P:42:GLU:C	8:P:43:LEU:HD22	2.42	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
1:S:975:GLY:O	1:S:976:ASP:C	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:1204:ALA:HB2	12:V:1238:MET:HE3	1.98	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:739:PRO:HD2	2:B:742:CYS:SG	2.57	0.45
6:G:279:TRP:C	6:G:282:PRO:HD2	2.42	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:415:MET:HE2	1:S:419:PHE:CE2	2.52	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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:295:LEU:O	12:V:296:GLU:C	2.60	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:342:LEU:O	7:M:348:SER:OG	2.33	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:205:GLU:C	12:V:205:GLU:CD	2.85	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
11:U:240:LEU:HD13	11:U:264:LEU:CD1	2.47	0.44
11:U:442:GLU:O	11:U:442:GLU:CD	2.61	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
1:A:664:MET:HE2	1:A:733:ALA:HB2	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:807:MET:HE3	11:U:859:VAL:HG21	1.98	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
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
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
2:O:590:PHE:C	2:O:592:LYS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:728:GLN:HE21	9:W:87:TRP:CG	2.36	0.44
1:S:989:MET:HE2	1:S:1074:GLU:HG3	2.00	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: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
2:B:524:GLN:C	2:B:525:ASN:HD22	2.25	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
4:E:38:GLU:H	4:E:38:GLU:CD	2.26	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
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
7:L:162:SER:HG	7:L:177:TRP:CD1	2.36	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
1:S:651:GLY:O	1:S:654:THR:OG1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:992:HIS:HB2	1:A:1077:MET:HE1	2.00	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
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
7:L:315:LEU:O	7:L:318:THR:OG1	2.33	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
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
2:B:494:THR:OG1	2:B:496:SER:OG	2.36	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:60:PHE:N	8:P:60:PHE:HD1	2.16	0.43
7:M:157:LYS:O	7:M:161:GLU:CD	2.62	0.43
11:U:507:LEU:HA	11:U:510:SER:OG	2.17	0.43
12:V:446:LEU:HG	12:V:447:ASP:N	2.32	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:220:LEU:C	11:U:220:LEU:HD23	2.43	0.43
11:U:388:ILE:O	11:U:392:SER:OG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:O:248:ILE:HD12	2:O:253:ARG:HD2	2.01	0.43
2:O:426:LEU:HG	8:Q:490:MET:HE3	1.99	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:733:ALA:HB1	1:S:742:GLN:CD	2.44	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
1:A:1372:ASP:CG	1:A:1372:ASP:O	2.62	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
6:H:192:ASP:CG	6:H:192:ASP:O	2.62	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
6:G:496:ALA:HB1	8:P:229:PHE:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:529:LEU:O	8:Q:577:ARG:HA	2.19	0.43
1:S:203:MET:HE3	1:S:265:VAL:CG2	2.48	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
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:415:MET:HE2	1:A:451:TRP:CH2	2.54	0.42
1:A:659:GLU:HG2	1:A:676:GLN:HE21	1.83	0.42
2:B:599:LEU:HD23	2:B:599:LEU:C	2.43	0.42
4:E:389:SER:HG	4:E:390:PHE:H	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:197:LEU:O	7:M:198:LYS:C	2.62	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
5:F:255:LEU:HB3	5:F:256:PRO:HD2	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
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
4:E:464:MET:HE1	4:E:472:LEU:CD2	2.49	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:508:MET:O	12:V:508:MET:HE3	2.19	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
4:E:428:SER:O	4:E:429:LEU:C	2.62	0.42
4:E:493:MET:HE1	4:E:512:LEU:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:H:89:THR:N	6:H:92:GLN:OE1	2.48	0.42
6:H:450:LEU:O	6:H:453:SER:OG	2.36	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
8:Q:585:GLY:O	8:Q:586:PRO:C	2.63	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:140:TYR:CD2	5:F:169:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:G:596:TYR:CD1	6:G:596:TYR:C	2.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:69:GLU:OE1	2:B:71:ASN:ND2	2.53	0.41
3:C:44:PHE:CZ	3:C:48:MET:HE3	2.55	0.41
3:C:134:PHE:CD2	5:F:166:GLN:HB3	2.54	0.41
3:C:254:MET:HE1	3:C:257:LEU:HD23	2.01	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
11:U:451:ARG:C	11:U:453:SER:H	2.28	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:220:GLN:C	1:A:222:GLU:H	2.28	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:731:MET:CE	9:W:85:PHE:HB3	2.45	0.41
1:S:880:ARG:HB2	1:S:881:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1022:GLN:HA	1:S:1085:LEU:HD22	2.02	0.41
10:X:46:TYR:HH	10:X:139:PHE:HZ	1.68	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:324:LYS:O	2:O:325:LEU:C	2.63	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:1261:PHE:HB2	1:S:1291:ILE:HG21	2.02	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
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:442:GLU:CD	11:U:442:GLU:C	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:924:GLN:N	11:U:925:PRO:CD	2.84	0.41
12:V:211:ILE:O	12:V:212:ILE:C	2.64	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
2:B:846:GLN:CD	8:P:874:ARG:HH22	2.27	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:517:LEU:HG	11:U:521:LEU:HD11	2.02	0.41
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
3:C:191:ILE:HD12	3:C:200:VAL:HG21	2.02	0.41
4:E:473:MET:HE3	4:E:496:VAL:HG11	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
12:V:816:LEU:HD12	12:V:935:ILE:HG21	2.03	0.41
12:V:1189:TYR:O	12:V:1193:THR:OG1	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:U:113:ILE:O	11:U:116:VAL:HG12	2.21	0.41
11:U:540:PHE:O	11:U:541:LEU:C	2.63	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
3:C:232:ILE:CG2	3:C:233:SER:N	2.84	0.41
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:284:LEU:O	6:G:287:SER:OG	2.32	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:OD1	2:O:525:ASN:N	2.54	0.41
8:P:7:ARG:HG3	8:P:8:VAL:HG23	2.03	0.41
8:P:243:CYS:HG	8:P:251:CYS:C	2.28	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
1:S:855:THR:O	1:S:858:SER:OG	2.26	0.41
1:S:910:LEU:HD23	1:S:910:LEU:C	2.46	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: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:344:ILE:O	12:V:345:LEU:C	2.64	0.41
12:V:1016:VAL:O	12:V:1020:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:SER:HA	12:V:101:GLU:CD	2.45	0.41
12:V:1313:LEU:HB3	12:V:1324:VAL:HG13	2.03	0.41
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
6:H:345:GLN:CD	6:H:386:PRO:HB3	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:H:226:ASP:OD1	6:H:259:MET:HE3	2.21	0.40
2:O:725:THR:C	2:O:729:GLN:HE21	2.29	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
1:A:1351:GLU:CD	1:A:1352:ALA:N	2.79	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
6:G:340:CYS:O	8:P:263:SER:OG	2.37	0.40
6:G:592:TYR:CD2	6:G:592:TYR:C	2.99	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:664:MET:HE2	1:S:733:ALA:HB2	2.01	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
1:A:1305:LEU:C	1:A:1308:LEU:CD2	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:TYR:O	3:C:146:TYR:C	2.64	0.40
4:E:33:LEU:C	4:E:35:ALA:N	2.78	0.40
4:E:315:LEU:HA	4:E:318:GLU:CG	2.52	0.40
4:E:427:GLU:CD	4:E:427:GLU:H	2.29	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
6:H:571:TRP:HH2	6:H:610:GLU:C	2.30	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: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:P:390:LEU:O	8:P:390:LEU:HG	2.21	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: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:83:SER:OG	2:B:83:SER:O	2.39	0.40
2:B:408:LEU:O	2:B:411:HIS:HB3	2.22	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
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:212:ILE:O	12:V:213:THR:C	2.63	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	14	49
1	S	1224/1477 (83%)	1088 (89%)	125 (10%)	11 (1%)	14	49
2	B	685/884 (78%)	586 (86%)	82 (12%)	17 (2%)	4	27
2	O	685/884 (78%)	598 (87%)	72 (10%)	15 (2%)	5	29
3	C	546/583 (94%)	483 (88%)	61 (11%)	2 (0%)	30	66
4	E	411/555 (74%)	364 (89%)	45 (11%)	2 (0%)	24	62
5	F	336/399 (84%)	302 (90%)	32 (10%)	2 (1%)	21	58
6	G	567/641 (88%)	507 (89%)	58 (10%)	2 (0%)	30	66
6	H	532/641 (83%)	483 (91%)	44 (8%)	5 (1%)	14	49
7	L	368/394 (93%)	331 (90%)	35 (10%)	2 (0%)	24	62
7	M	368/394 (93%)	333 (90%)	29 (8%)	6 (2%)	7	37
8	P	726/906 (80%)	613 (84%)	95 (13%)	18 (2%)	4	27
8	Q	732/906 (81%)	629 (86%)	89 (12%)	14 (2%)	6	32
9	W	21/39 (54%)	13 (62%)	5 (24%)	3 (14%)	0	3
10	X	151/197 (77%)	146 (97%)	3 (2%)	2 (1%)	9	41
11	U	1163/1328 (88%)	1029 (88%)	128 (11%)	6 (0%)	24	62
12	V	1096/1451 (76%)	1011 (92%)	79 (7%)	6 (0%)	24	62
All	All	10771/13156 (82%)	9557 (89%)	1091 (10%)	123 (1%)	14	45

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	926 (90%)	108 (10%)	7	23
1	S	1092/1282 (85%)	974 (89%)	118 (11%)	6	22
2	B	644/810 (80%)	553 (86%)	91 (14%)	3	16
2	O	641/810 (79%)	572 (89%)	69 (11%)	6	22
3	C	480/507 (95%)	438 (91%)	42 (9%)	9	30
4	E	358/467 (77%)	304 (85%)	54 (15%)	3	14
5	F	288/336 (86%)	267 (93%)	21 (7%)	13	35
6	G	483/538 (90%)	414 (86%)	69 (14%)	3	16
6	H	454/538 (84%)	393 (87%)	61 (13%)	4	17
7	L	334/354 (94%)	314 (94%)	20 (6%)	17	40
7	M	334/354 (94%)	319 (96%)	15 (4%)	24	47
8	P	627/749 (84%)	526 (84%)	101 (16%)	2	13
8	Q	630/749 (84%)	550 (87%)	80 (13%)	4	18
9	W	22/22 (100%)	21 (96%)	1 (4%)	24	47
10	X	136/175 (78%)	132 (97%)	4 (3%)	37	58
11	U	1076/1204 (89%)	1001 (93%)	75 (7%)	14	37
12	V	1036/1324 (78%)	987 (95%)	49 (5%)	23	46
All	All	9669/11501 (84%)	8691 (90%)	978 (10%)	9	24

All (978) 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	98	LEU
1	A	100	ASP
1	A	109	VAL
1	A	139	VAL
1	A	145	LEU
1	A	148	LEU
1	A	163	ARG
1	A	169	GLU
1	A	179	LEU
1	A	182	VAL
1	A	185	LEU

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	217	LEU
1	A	219	GLU
1	A	226	GLN
1	A	239	VAL
1	A	244	LEU
1	A	267	VAL
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	446	LEU
1	A	447	SER
1	A	453	LYS
1	A	456	PHE
1	A	459	THR
1	A	465	CYS
1	A	491	VAL
1	A	507	LEU
1	A	517	ARG
1	A	653	LEU
1	A	660	LEU
1	A	666	ASP
1	A	668	SER
1	A	719	VAL
1	A	731	MET
1	A	750	VAL
1	A	782	LEU
1	A	793	GLU
1	A	817	LEU
1	A	826	THR
1	A	827	ARG
1	A	834	LEU

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Mol	Chain	Res	Type
1	A	860	LEU
1	A	861	SER
1	A	877	SER
1	A	878	GLU
1	A	881	GLN
1	A	928	THR
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	1031	GLN
1	A	1053	ARG
1	A	1060	THR
1	A	1061	SER
1	A	1063	TRP
1	A	1069	LEU
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	1139	LEU
1	A	1155	ILE
1	A	1184	ARG
1	A	1188	HIS
1	A	1190	GLN
1	A	1231	HIS
1	A	1241	ASN
1	A	1250	ASP
1	A	1258	VAL
1	A	1265	LEU
1	A	1269	LEU
1	A	1271	SER
1	A	1280	ASP
1	A	1309	THR
1	A	1330	LEU
1	A	1331	LEU

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Mol	Chain	Res	Type
1	A	1345	ASP
1	A	1360	MET
1	A	1367	LEU
1	A	1369	VAL
1	A	1391	ASN
1	A	1403	LEU
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	40	THR
2	B	47	ARG
2	B	55	LYS
2	B	66	THR
2	B	70	GLU
2	B	90	ASN
2	B	104	VAL
2	B	112	LEU
2	B	143	LEU
2	B	155	SER
2	B	170	ILE
2	B	177	GLU
2	B	181	MET
2	B	226	ILE
2	B	245	THR
2	B	252	LEU
2	B	259	LEU
2	B	265	LEU
2	B	277	CYS
2	B	279	LEU
2	B	285	CYS
2	B	287	VAL
2	B	300	VAL
2	B	302	SER
2	B	307	ASN
2	B	309	CYS
2	B	311	VAL
2	B	328	VAL
2	B	331	ASP

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Mol	Chain	Res	Type
2	B	341	VAL
2	B	354	LEU
2	B	360	THR
2	B	389	LEU
2	B	390	VAL
2	B	403	SER
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	506	LEU
2	B	507	SER
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	587	LEU
2	B	592	LYS
2	B	602	MET
2	B	606	SER
2	B	617	CYS
2	B	622	LEU
2	B	624	LEU
2	B	628	SER
2	B	635	THR
2	B	638	LYS
2	B	643	GLU
2	B	658	SER
2	B	659	CYS
2	B	670	ASN
2	B	673	LYS

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Mol	Chain	Res	Type
2	B	677	LEU
2	B	690	GLU
2	B	696	ARG
2	B	705	PHE
2	B	716	ILE
2	B	718	ILE
2	B	722	ARG
2	B	727	MET
2	B	751	SER
2	B	780	HIS
2	B	836	ARG
2	B	838	ILE
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	48	MET
3	C	65	PRO
3	C	86	SER
3	C	96	CYS
3	C	98	ILE
3	C	115	GLN
3	C	122	LEU
3	C	125	LEU
3	C	126	ARG
3	C	142	PRO
3	C	144	ASP
3	C	149	LEU
3	C	156	SER
3	C	172	GLN
3	C	173	ARG
3	C	190	LEU
3	C	200	VAL
3	C	205	ILE
3	C	213	GLU
3	C	218	GLU
3	C	223	VAL
3	C	224	ASN
3	C	240	VAL

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Mol	Chain	Res	Type
3	C	241	CYS
3	C	261	LEU
3	C	283	GLN
3	C	294	VAL
3	C	302	LEU
3	C	304	GLU
3	C	315	ILE
3	C	327	GLU
3	C	344	THR
3	C	345	SER
3	C	347	SER
3	C	396	LEU
3	C	493	ASN
3	C	509	ILE
3	C	528	GLN
3	C	552	LYS
4	E	12	GLU
4	E	28	LEU
4	E	44	LEU
4	E	46	VAL
4	E	67	LEU
4	E	78	ASP
4	E	86	LEU
4	E	87	LEU
4	E	97	ASN
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	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

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Mol	Chain	Res	Type
4	E	352	SER
4	E	361	THR
4	E	362	VAL
4	E	378	SER
4	E	387	LEU
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	462	VAL
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	504	ILE
4	E	505	THR
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	54	ILE
5	F	90	ASP
5	F	92	LEU
5	F	133	LEU
5	F	136	LEU
5	F	138	ARG
5	F	143	VAL
5	F	164	LYS
5	F	176	GLU
5	F	196	LEU
5	F	197	PRO
5	F	210	LEU
5	F	215	SER

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Mol	Chain	Res	Type
5	F	264	THR
5	F	270	LEU
5	F	288	ASP
5	F	300	GLN
5	F	301	ASP
5	F	302	VAL
5	F	315	CYS
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	74	THR
6	G	80	LEU
6	G	89	THR
6	G	90	GLU
6	G	101	GLU
6	G	104	LEU
6	G	115	GLU
6	G	118	LEU
6	G	124	SER
6	G	132	LEU
6	G	134	GLU
6	G	136	LEU
6	G	142	LEU
6	G	145	LEU
6	G	149	LEU
6	G	154	ASP
6	G	159	LEU
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	234	GLU
6	G	240	CYS

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Mol	Chain	Res	Type
6	G	250	THR
6	G	258	LYS
6	G	259	MET
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	349	ILE
6	G	352	SER
6	G	357	THR
6	G	359	ARG
6	G	395	GLU
6	G	405	ILE
6	G	418	GLU
6	G	448	CYS
6	G	450	LEU
6	G	458	LEU
6	G	474	SER
6	G	478	ARG
6	G	483	LEU
6	G	485	ARG
6	G	489	GLU
6	G	497	PHE
6	G	498	ASN
6	G	504	LYS
6	G	534	LEU
6	G	544	CYS
6	G	578	THR
6	G	594	GLU
6	G	604	ASP
6	H	12	CYS
6	H	35	LEU
6	H	42	LEU
6	H	54	LEU
6	H	67	LEU
6	H	80	LEU
6	H	90	GLU
6	H	91	ASP

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Mol	Chain	Res	Type
6	H	98	ARG
6	H	104	LEU
6	H	130	CYS
6	H	132	LEU
6	H	136	LEU
6	H	145	LEU
6	H	158	ASP
6	H	159	LEU
6	H	174	SER
6	H	178	LEU
6	H	183	THR
6	H	191	LEU
6	H	192	ASP
6	H	207	LEU
6	H	222	THR
6	H	226	ASP
6	H	239	LEU
6	H	250	THR
6	H	267	LEU
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	333	ASP
6	H	334	LEU
6	H	359	ARG
6	H	365	GLU
6	H	370	LEU
6	H	371	LEU
6	H	373	LEU
6	H	393	MET
6	H	395	GLU
6	H	404	LEU
6	H	405	ILE
6	H	412	ASP
6	H	416	LEU
6	H	466	LEU
6	H	470	LYS
6	H	479	CYS
6	H	483	LEU

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Mol	Chain	Res	Type
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	578	THR
6	H	586	LEU
6	H	604	ASP
6	H	605	ARG
7	L	15	LEU
7	L	24	VAL
7	L	39	ARG
7	L	44	GLU
7	L	46	LEU
7	L	56	SER
7	L	68	ARG
7	L	88	LYS
7	L	90	LEU
7	L	91	LEU
7	L	116	GLU
7	L	139	LYS
7	L	164	ASP
7	L	227	ARG
7	L	236	ILE
7	L	251	CYS
7	L	268	SER
7	L	271	ILE
7	L	348	SER
7	L	350	GLN
2	O	39	LYS
2	O	47	ARG
2	O	61	SER
2	O	90	ASN
2	O	94	ILE
2	O	104	VAL
2	O	132	ASP
2	O	166	ASN
2	O	171	GLN
2	O	175	GLU
2	O	223	LEU

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Mol	Chain	Res	Type
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	279	LEU
2	O	283	ASP
2	O	287	VAL
2	O	300	VAL
2	O	311	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
2	O	507	SER
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

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Mol	Chain	Res	Type
2	O	622	LEU
2	O	624	LEU
2	O	628	SER
2	O	631	LYS
2	O	635	THR
2	O	638	LYS
2	O	677	LEU
2	O	687	GLU
2	O	690	GLU
2	O	704	LEU
2	O	724	GLN
2	O	735	ILE
2	O	742	CYS
2	O	779	LYS
2	O	780	HIS
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	76	LEU
8	P	82	ARG
8	P	91	ASP
8	P	118	VAL
8	P	119	ASP
8	P	124	ILE
8	P	125	LEU
8	P	130	LEU
8	P	131	CYS
8	P	138	SER
8	P	155	PHE
8	P	159	CYS
8	P	162	GLU
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

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Mol	Chain	Res	Type
8	P	224	LEU
8	P	228	LEU
8	P	232	ASP
8	P	234	THR
8	P	235	LEU
8	P	237	GLN
8	P	246	PRO
8	P	250	LEU
8	P	253	VAL
8	P	269	ASN
8	P	274	ILE
8	P	279	GLU
8	P	285	ILE
8	P	311	CYS
8	P	313	VAL
8	P	321	MET
8	P	330	GLU
8	P	342	CYS
8	P	368	VAL
8	P	373	ARG
8	P	385	GLU
8	P	387	PRO
8	P	390	LEU
8	P	395	CYS
8	P	402	CYS
8	P	424	SER
8	P	450	SER
8	P	459	LEU
8	P	465	ILE
8	P	467	GLU
8	P	485	SER
8	P	515	SER
8	P	517	LEU
8	P	522	VAL
8	P	543	LEU
8	P	545	ILE
8	P	560	CYS
8	P	569	VAL
8	P	571	GLN
8	P	584	LEU
8	P	588	GLU
8	P	598	VAL

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Mol	Chain	Res	Type
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	683	CYS
8	P	701	LEU
8	P	707	SER
8	P	708	ILE
8	P	710	VAL
8	P	723	HIS
8	P	732	THR
8	P	745	VAL
8	P	749	ARG
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	812	VAL
8	P	827	VAL
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	9	ARG
8	Q	11	LEU
8	Q	16	CYS
8	Q	34	GLU
8	Q	35	VAL
8	Q	69	LEU
8	Q	91	ASP
8	Q	125	LEU
8	Q	144	VAL

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Mol	Chain	Res	Type
8	Q	153	GLN
8	Q	159	CYS
8	Q	170	ILE
8	Q	173	VAL
8	Q	219	THR
8	Q	235	LEU
8	Q	242	LEU
8	Q	250	LEU
8	Q	253	VAL
8	Q	274	ILE
8	Q	278	LEU
8	Q	307	VAL
8	Q	330	GLU
8	Q	334	LEU
8	Q	337	GLU
8	Q	362	THR
8	Q	365	ASP
8	Q	369	VAL
8	Q	373	ARG
8	Q	395	CYS
8	Q	449	GLU
8	Q	450	SER
8	Q	465	ILE
8	Q	473	LYS
8	Q	481	LYS
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	543	LEU
8	Q	544	CYS
8	Q	546	GLN
8	Q	561	SER
8	Q	566	THR
8	Q	569	VAL
8	Q	570	ASP
8	Q	582	LEU

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Mol	Chain	Res	Type
8	Q	584	LEU
8	Q	593	ASP
8	Q	598	VAL
8	Q	608	GLU
8	Q	610	VAL
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	755	GLN
8	Q	768	VAL
8	Q	782	ILE
8	Q	789	VAL
8	Q	794	LEU
8	Q	797	ILE
8	Q	807	ARG
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	872	GLN
1	S	60	LEU
1	S	61	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	179	LEU
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	244	LEU
1	S	267	VAL
1	S	271	GLN
1	S	274	LEU
1	S	285	VAL
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	371	LEU
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	459	THR
1	S	466	SER
1	S	491	VAL
1	S	507	LEU
1	S	518	LEU
1	S	546	GLN
1	S	566	VAL
1	S	573	ILE
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

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Mol	Chain	Res	Type
1	S	685	ARG
1	S	688	LEU
1	S	714	ARG
1	S	723	LEU
1	S	735	SER
1	S	753	MET
1	S	758	LEU
1	S	766	CYS
1	S	782	LEU
1	S	795	ARG
1	S	800	GLU
1	S	814	VAL
1	S	818	PHE
1	S	828	ASP
1	S	834	LEU
1	S	849	SER
1	S	856	LEU
1	S	859	CYS
1	S	878	GLU
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	964	LEU
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	1053	ARG
1	S	1060	THR
1	S	1098	GLU
1	S	1105	CYS
1	S	1126	LEU
1	S	1129	ASP

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Mol	Chain	Res	Type
1	S	1139	LEU
1	S	1142	CYS
1	S	1183	CYS
1	S	1190	GLN
1	S	1202	GLU
1	S	1241	ASN
1	S	1251	CYS
1	S	1258	VAL
1	S	1274	THR
1	S	1301	SER
1	S	1320	LEU
1	S	1330	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	94	LEU
7	M	12	CYS
7	M	39	ARG
7	M	46	LEU
7	M	50	ASN
7	M	88	LYS
7	M	90	LEU
7	M	104	LEU
7	M	126	LEU
7	M	236	ILE
7	M	290	ILE
7	M	303	PHE
7	M	314	GLN
7	M	318	THR
7	M	347	THR
7	M	349	ARG
10	X	8	LYS
10	X	9	ARG
10	X	32	ASP
10	X	99	ARG
11	U	18	GLN

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Mol	Chain	Res	Type
11	U	59	GLU
11	U	80	ASP
11	U	95	LEU
11	U	99	HIS
11	U	123	ASN
11	U	134	LEU
11	U	135	THR
11	U	229	VAL
11	U	231	GLU
11	U	247	GLU
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	310	ILE
11	U	313	LEU
11	U	316	VAL
11	U	323	GLN
11	U	325	GLN
11	U	334	VAL
11	U	365	LEU
11	U	389	LEU
11	U	398	VAL
11	U	442	GLU
11	U	449	VAL
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	482	THR
11	U	497	GLN
11	U	512	SER
11	U	515	ASP
11	U	520	VAL
11	U	528	ASN
11	U	546	ASN
11	U	576	ASN

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Mol	Chain	Res	Type
11	U	586	GLU
11	U	588	MET
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	668	LEU
11	U	742	SER
11	U	760	ILE
11	U	769	GLU
11	U	847	LEU
11	U	856	THR
11	U	870	ILE
11	U	880	VAL
11	U	890	THR
11	U	965	SER
11	U	1006	MET
11	U	1020	GLU
11	U	1042	PRO
11	U	1043	VAL
11	U	1044	ILE
11	U	1053	ILE
11	U	1100	ASP
11	U	1141	LEU
11	U	1143	THR
11	U	1158	CYS
11	U	1167	CYS
11	U	1199	LYS
11	U	1254	ILE
11	U	1279	MET
12	V	45	ASP
12	V	104	ILE
12	V	105	GLU
12	V	150	ILE
12	V	175	LEU
12	V	190	LYS
12	V	198	GLN
12	V	201	SER
12	V	202	ILE
12	V	205	GLU

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Mol	Chain	Res	Type
12	V	206	ASN
12	V	212	ILE
12	V	234	LEU
12	V	235	LEU
12	V	239	THR
12	V	260	LEU
12	V	292	MET
12	V	307	LEU
12	V	338	SER
12	V	359	THR
12	V	369	GLU
12	V	384	MET
12	V	387	ILE
12	V	402	VAL
12	V	403	LEU
12	V	412	ILE
12	V	421	PHE
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	551	ILE
12	V	572	LEU
12	V	607	CYS
12	V	644	LEU
12	V	662	ASP
12	V	688	GLU
12	V	756	LEU
12	V	803	GLU
12	V	929	ASP
12	V	931	GLU
12	V	960	LEU
12	V	1006	GLN
12	V	1227	THR
12	V	1257	SER
12	V	1294	CYS
12	V	1368	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (228) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	58	ASN
1	A	88	ASN
1	A	101	GLN
1	A	123	GLN
1	A	153	GLN
1	A	188	GLN
1	A	248	GLN
1	A	322	HIS
1	A	330	HIS
1	A	376	GLN
1	A	423	GLN
1	A	676	GLN
1	A	771	HIS
1	A	962	HIS
1	A	1014	ASN
1	A	1160	GLN
1	A	1190	GLN
1	A	1201	GLN
1	A	1235	GLN
1	A	1355	HIS
2	B	44	HIS
2	B	90	ASN
2	B	102	ASN
2	B	116	ASN
2	B	241	HIS
2	B	366	ASN
2	B	473	GLN
2	B	576	GLN
2	B	600	GLN
2	B	644	HIS
2	B	656	HIS
2	B	753	ASN
2	B	825	GLN
2	B	827	ASN
2	B	854	GLN
3	C	13	GLN
3	C	69	GLN
3	C	320	GLN
3	C	366	GLN
3	C	399	HIS
3	C	465	GLN
3	C	520	HIS

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Mol	Chain	Res	Type
3	C	557	GLN
4	E	75	GLN
4	E	95	GLN
4	E	97	ASN
4	E	287	GLN
4	E	314	GLN
4	E	332	GLN
4	E	335	GLN
4	E	434	GLN
4	E	461	GLN
4	E	503	ASN
4	E	519	ASN
4	E	533	HIS
5	F	36	GLN
5	F	43	HIS
5	F	63	HIS
5	F	114	GLN
5	F	130	GLN
5	F	283	GLN
5	F	300	GLN
5	F	308	HIS
5	F	312	GLN
5	F	316	GLN
6	G	31	GLN
6	G	58	GLN
6	G	94	GLN
6	G	97	GLN
6	G	167	ASN
6	G	256	HIS
6	G	311	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	547	ASN
6	H	58	GLN
6	H	201	GLN
6	H	233	HIS
6	H	291	GLN
6	H	343	GLN

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Mol	Chain	Res	Type
6	H	461	GLN
6	H	465	GLN
6	H	511	GLN
6	H	547	ASN
7	L	75	GLN
7	L	99	GLN
7	L	272	HIS
7	L	328	GLN
2	O	12	GLN
2	O	26	GLN
2	O	59	GLN
2	O	71	ASN
2	O	178	ASN
2	O	264	GLN
2	O	278	GLN
2	O	317	GLN
2	O	350	ASN
2	O	386	ASN
2	O	428	ASN
2	O	524	GLN
2	O	600	GLN
2	O	656	HIS
2	O	729	GLN
2	O	732	HIS
2	O	733	ASN
2	O	746	ASN
2	O	753	ASN
2	O	780	HIS
8	P	92	HIS
8	P	153	GLN
8	P	169	GLN
8	P	464	ASN
8	P	571	GLN
8	P	645	HIS
8	P	723	HIS
8	P	763	ASN
8	P	788	GLN
8	P	815	GLN
8	Q	63	GLN
8	Q	478	GLN
8	Q	491	ASN
8	Q	571	GLN

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Mol	Chain	Res	Type
8	Q	788	GLN
8	Q	868	GLN
1	S	101	GLN
1	S	153	GLN
1	S	240	GLN
1	S	271	GLN
1	S	322	HIS
1	S	330	HIS
1	S	341	GLN
1	S	343	GLN
1	S	387	GLN
1	S	405	GLN
1	S	490	GLN
1	S	546	GLN
1	S	729	ASN
1	S	869	GLN
1	S	940	GLN
1	S	992	HIS
1	S	1107	GLN
1	S	1118	ASN
1	S	1190	GLN
1	S	1231	HIS
1	S	1417	HIS
1	S	1440	GLN
7	M	11	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	283	ASN
7	M	328	GLN
7	M	331	GLN
7	M	335	GLN
10	X	26	GLN
10	X	112	GLN
10	X	150	HIS
11	U	31	ASN
11	U	35	ASN
11	U	99	HIS

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Mol	Chain	Res	Type
11	U	143	ASN
11	U	159	GLN
11	U	162	ASN
11	U	298	GLN
11	U	323	GLN
11	U	342	GLN
11	U	345	GLN
11	U	416	GLN
11	U	465	ASN
11	U	475	GLN
11	U	497	GLN
11	U	529	GLN
11	U	597	GLN
11	U	598	GLN
11	U	630	GLN
11	U	711	ASN
11	U	739	ASN
11	U	865	GLN
11	U	872	GLN
11	U	924	GLN
11	U	958	GLN
11	U	961	GLN
11	U	963	GLN
11	U	1017	ASN
11	U	1030	ASN
11	U	1127	ASN
11	U	1137	GLN
11	U	1185	GLN
11	U	1193	ASN
12	V	86	HIS
12	V	112	ASN
12	V	146	GLN
12	V	208	GLN
12	V	308	GLN
12	V	370	ASN
12	V	394	GLN
12	V	480	HIS
12	V	550	HIS
12	V	552	GLN
12	V	637	ASN
12	V	641	HIS
12	V	658	ASN

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Mol	Chain	Res	Type
12	V	706	GLN
12	V	802	GLN
12	V	1025	ASN
12	V	1056	HIS
12	V	1105	GLN
12	V	1113	GLN
12	V	1119	GLN
12	V	1120	ASN
12	V	1129	GLN
12	V	1150	GLN
12	V	1176	ASN
12	V	1179	ASN
12	V	1181	GLN
12	V	1192	HIS
12	V	1213	ASN
12	V	1332	GLN
12	V	1379	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 [i](#)

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.

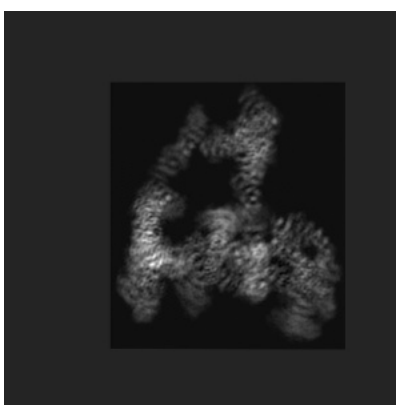
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

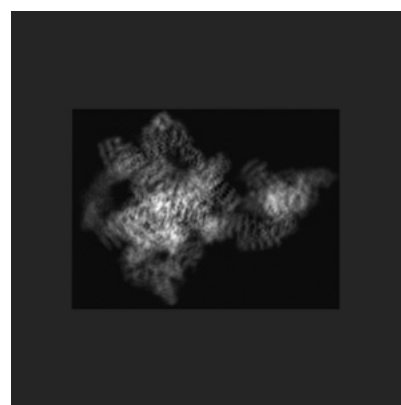
6.1.1 Primary map



X



Y

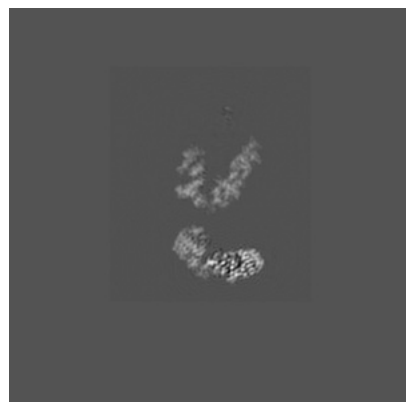


Z

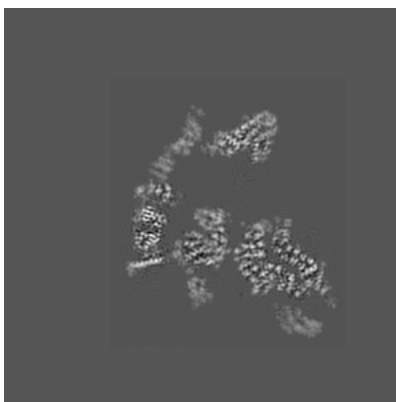
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

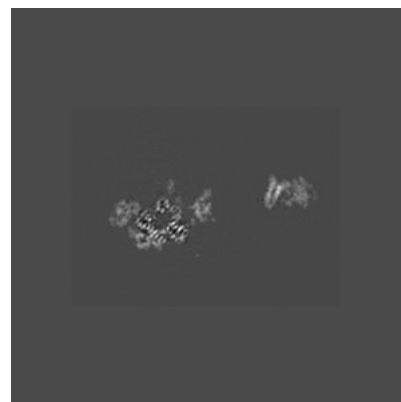
6.2.1 Primary map



X Index: 224



Y Index: 224

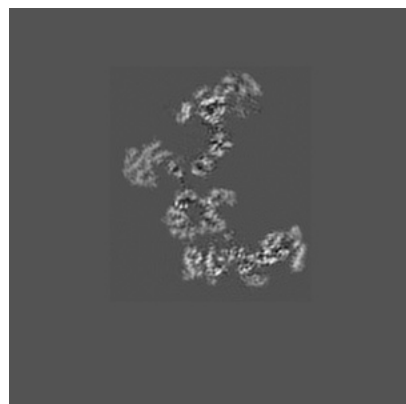


Z Index: 224

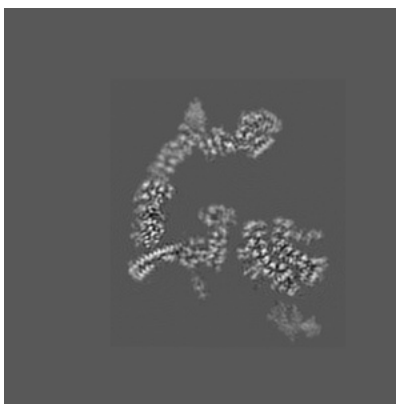
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 163



Y Index: 231



Z Index: 163

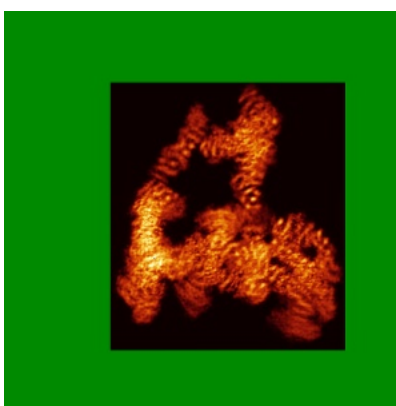
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

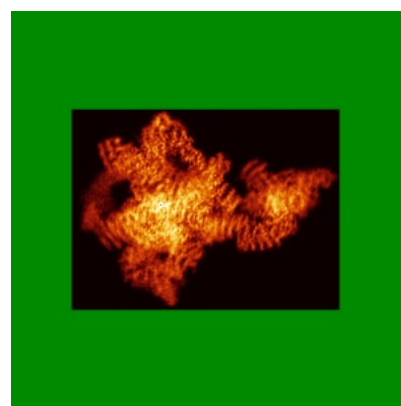
6.4.1 Primary map



X



Y

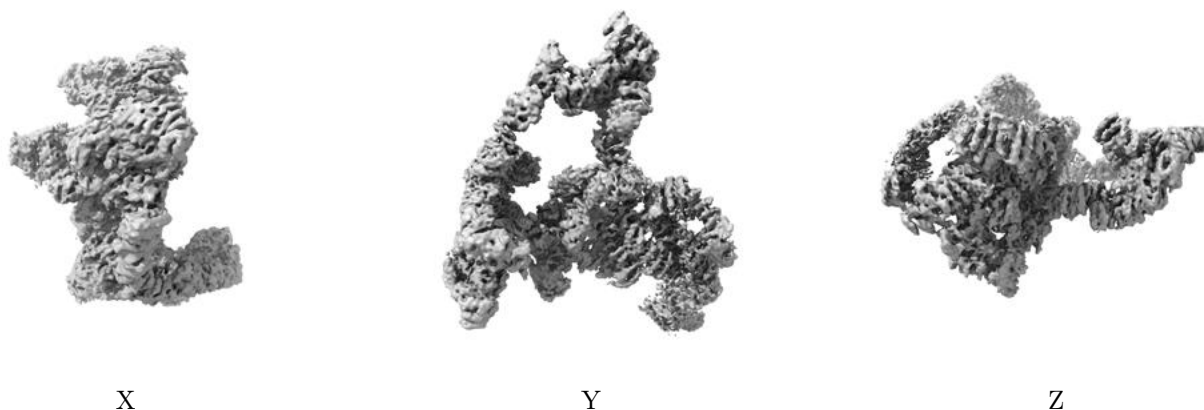


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

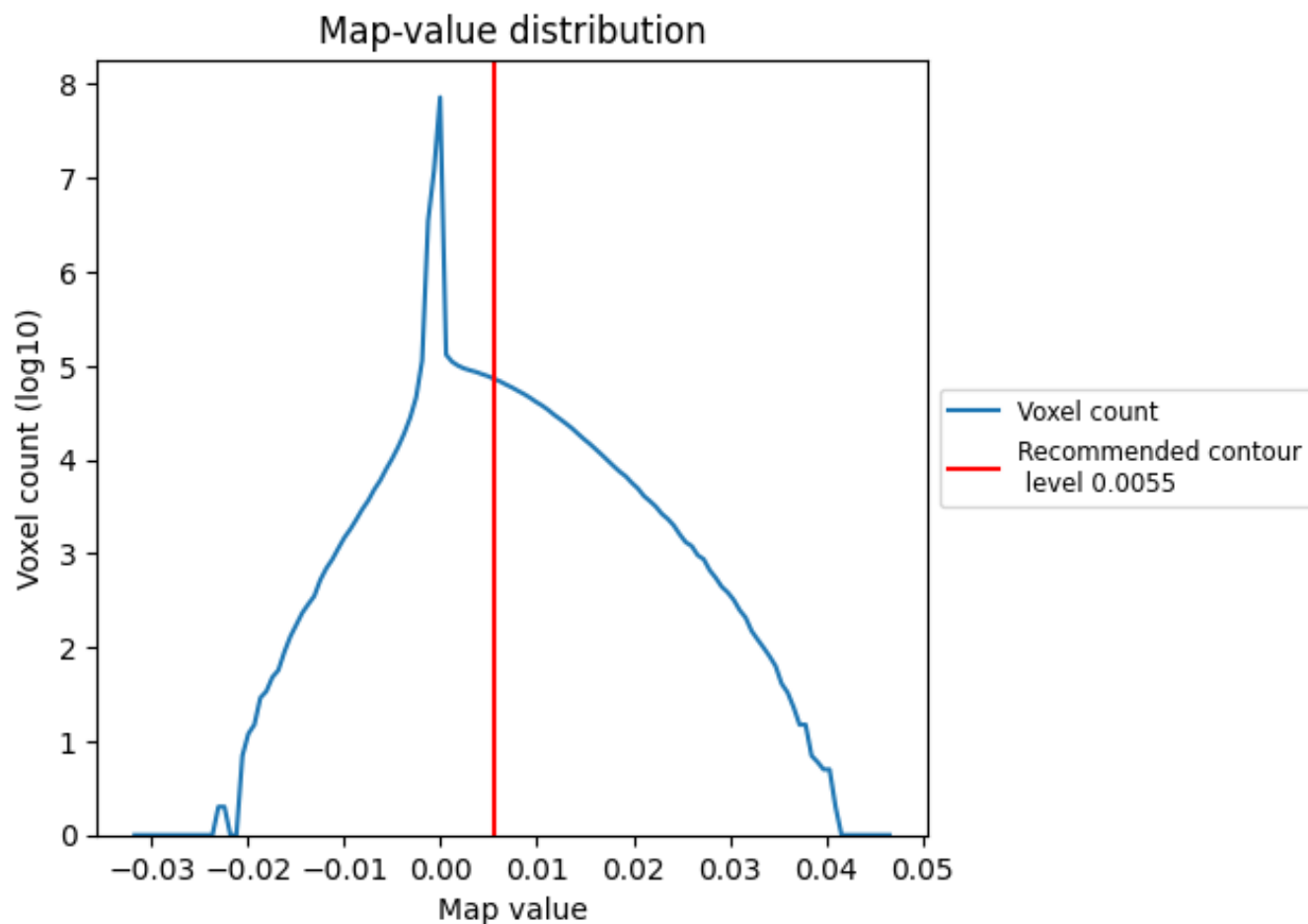
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

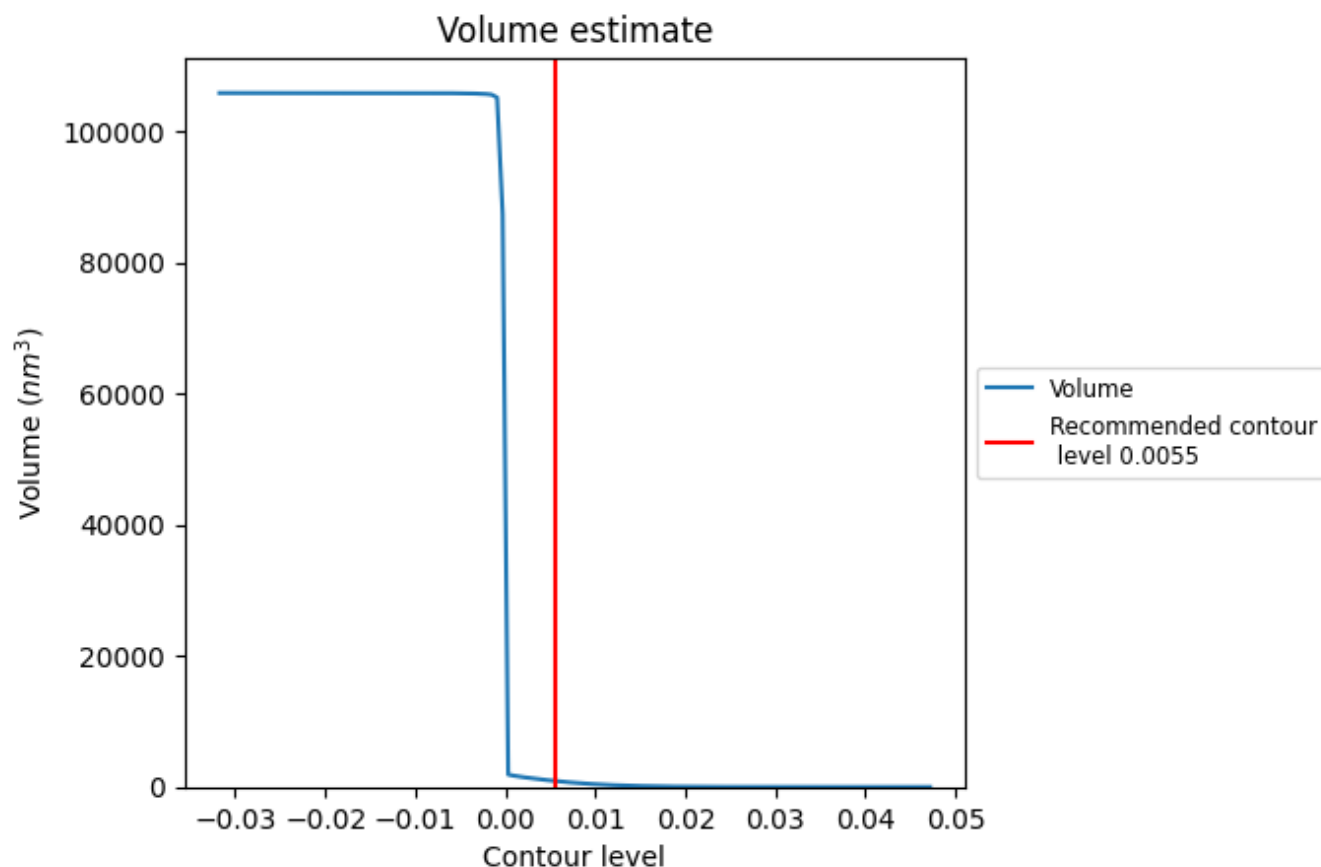
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

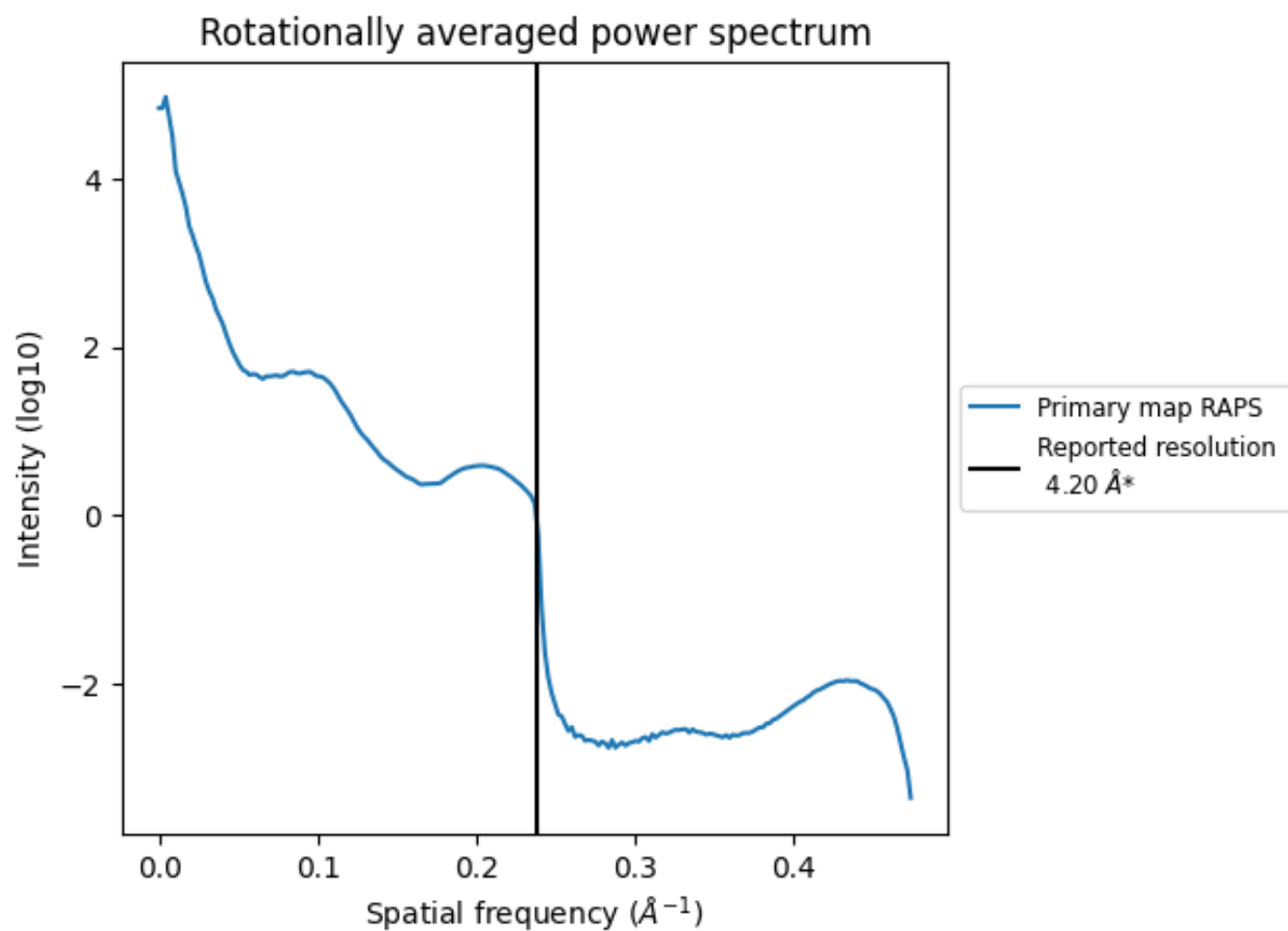
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 916 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

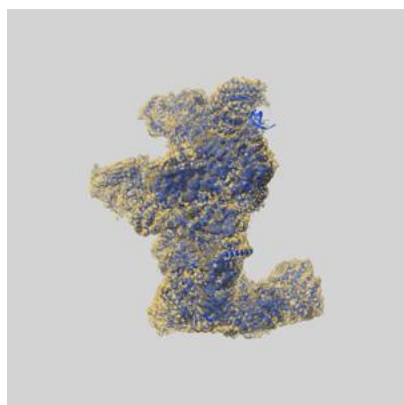
8 Fourier-Shell correlation

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

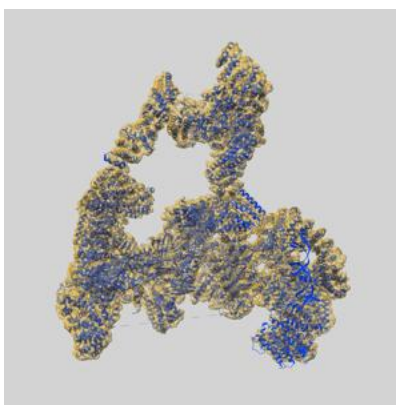
9 Map-model fit [i](#)

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.

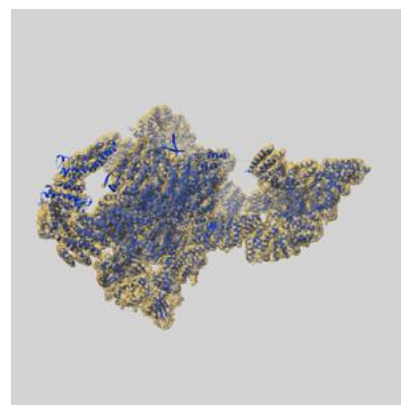
9.1 Map-model overlay [i](#)



X



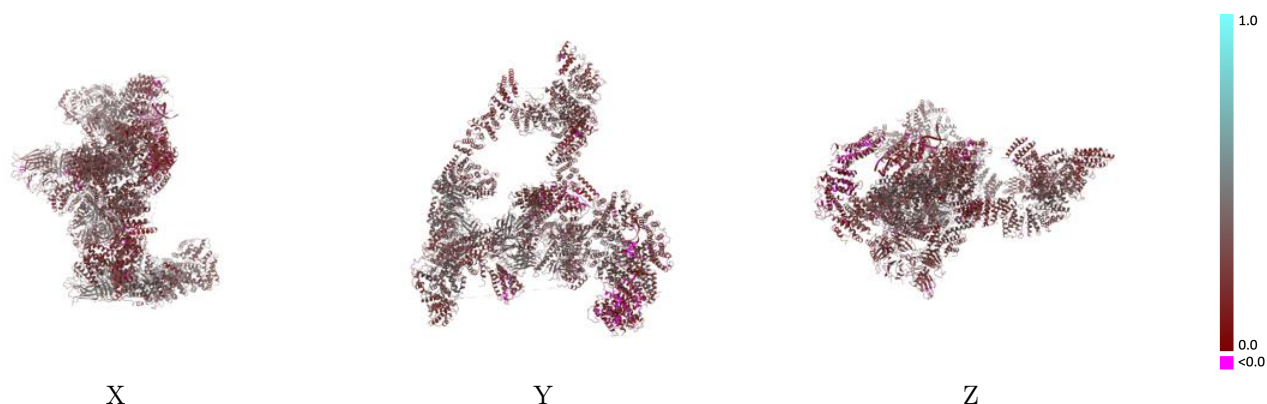
Y



Z

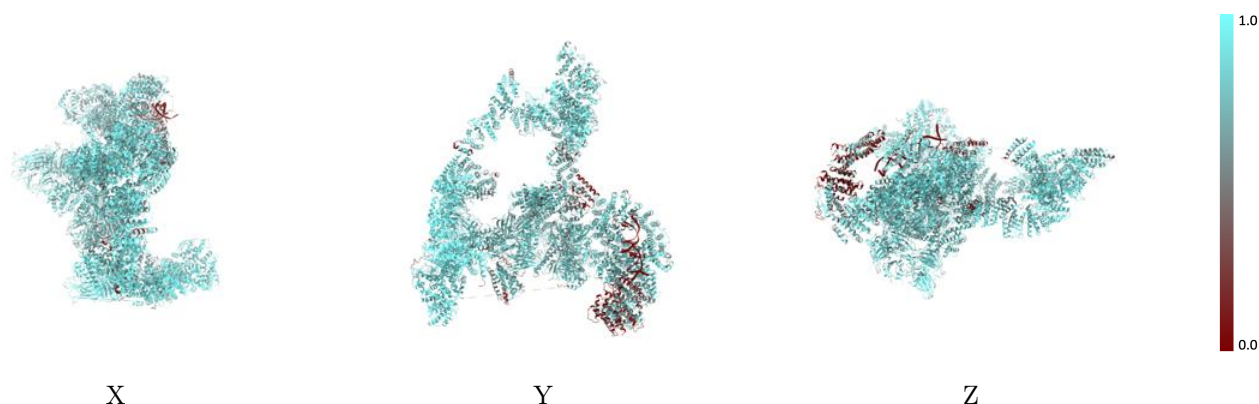
The images above show the 3D surface view of the map at the recommended contour level 0.0055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



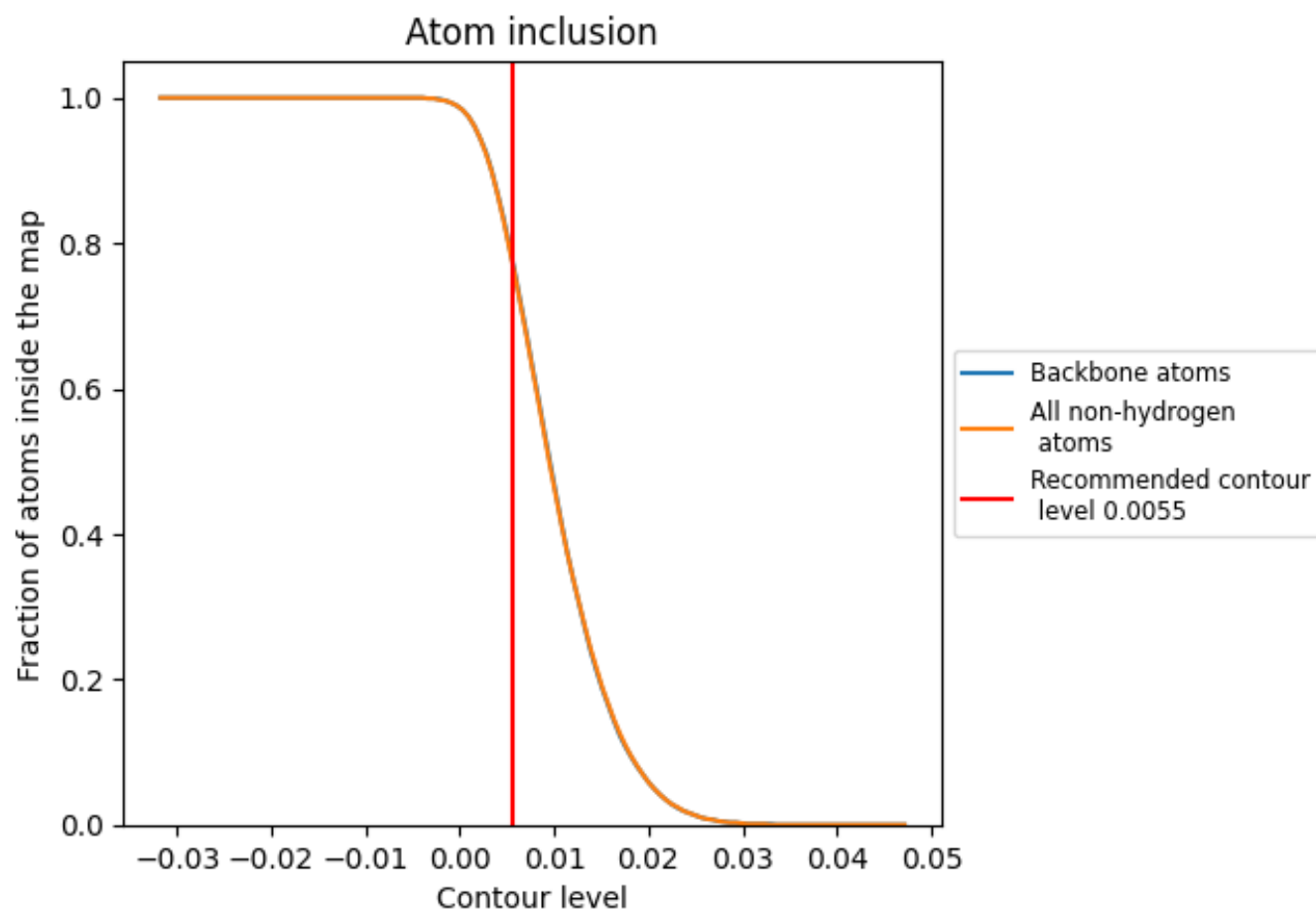
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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	 0.7790	 0.2970
A	 0.7670	 0.2690
B	 0.8550	 0.3580
C	 0.8920	 0.3400
E	 0.8170	 0.3290
F	 0.9120	 0.3520
G	 0.8480	 0.3220
H	 0.7910	 0.2560
L	 0.8280	 0.3290
M	 0.7940	 0.3110
O	 0.8070	 0.2790
P	 0.8730	 0.3790
Q	 0.7620	 0.2880
S	 0.8310	 0.2840
U	 0.7700	 0.2940
V	 0.5890	 0.2340
W	 0.8180	 0.3330
X	 0.8150	 0.2820
Y	 0.0720	 0.1240
Z	 0.1150	 0.1350

