



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:39 AM UTC

PDB ID : 7KZS / pdb_00007kzs
EMDB ID : EMD-23088
Title : Structure of the human fanconi anaemia Core-UBE2T-ID-DNA complex in open 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:

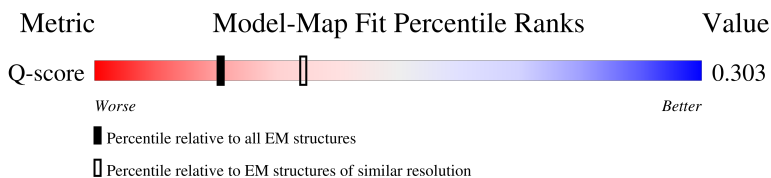
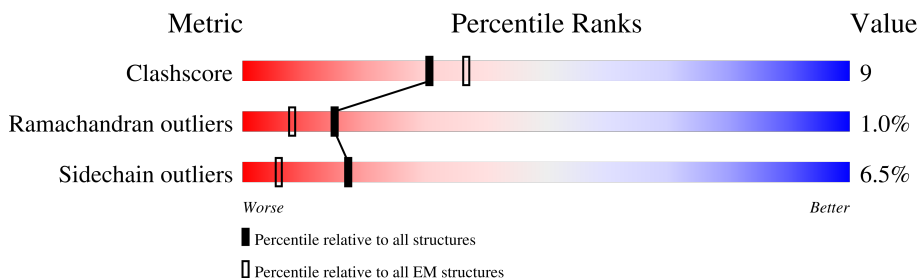
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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.



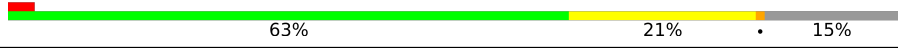
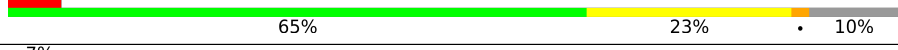
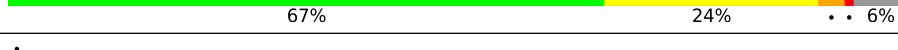
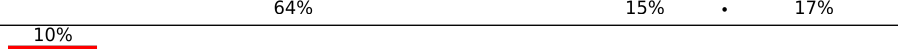
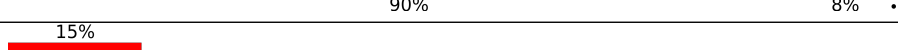
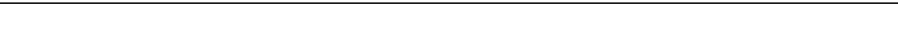
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	11% 60% 18% 20%
1	S	1477	6% 68% 16% 15%
2	B	884	49% 25% 5% 21%
2	O	884	57% 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 176779 atoms, of which 88975 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	1168	Total	C	H	N	O	S	0	0
			18882	5933	9626	1549	1720	54		

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	1153	Total	C	H	N	O	S	0	0
			18733	5970	9475	1527	1709	52		

- Molecule 13 is a DNA chain called DNA (25-MER).

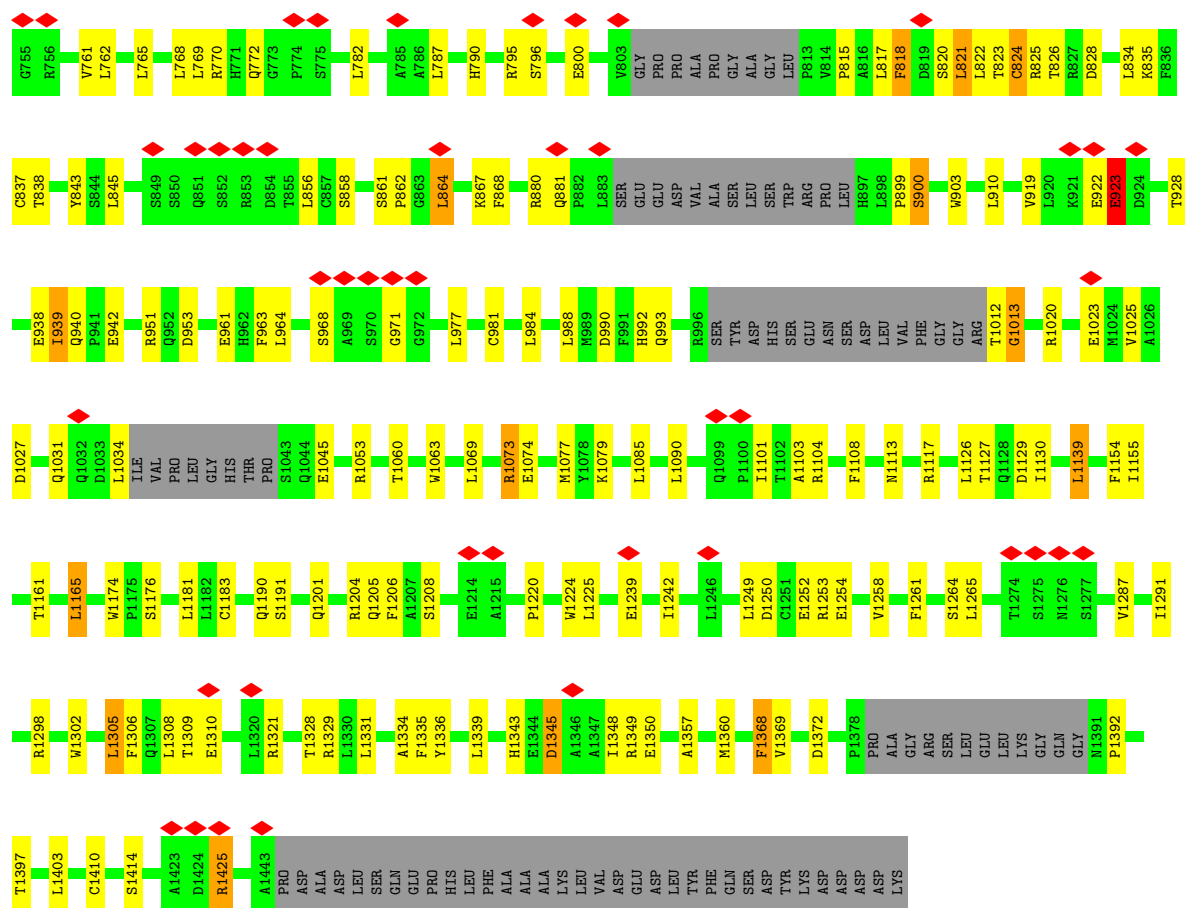
Mol	Chain	Residues	Atoms						AltConf	Trace
13	Y	25	Total	C	H	N	O	P	0	0
			796	243	280	99	149	25		

- Molecule 14 is a DNA chain called DNA (25-MER).

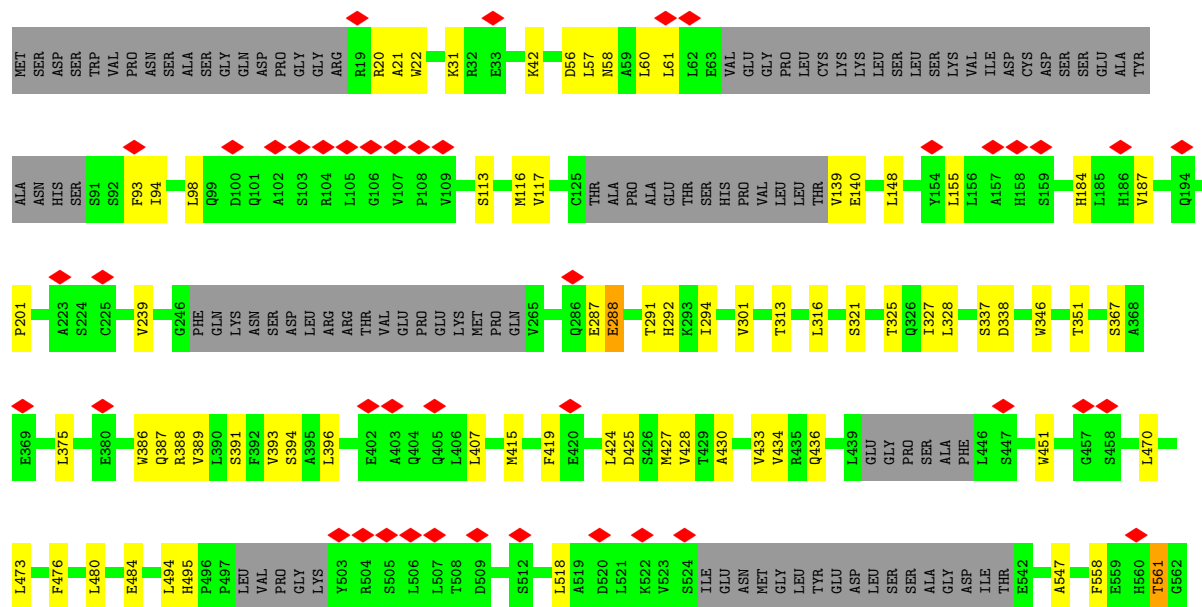
Mol	Chain	Residues	Atoms						AltConf	Trace
14	Z	25	Total	C	H	N	O	P	0	0
			790	241	281	92	151	25		

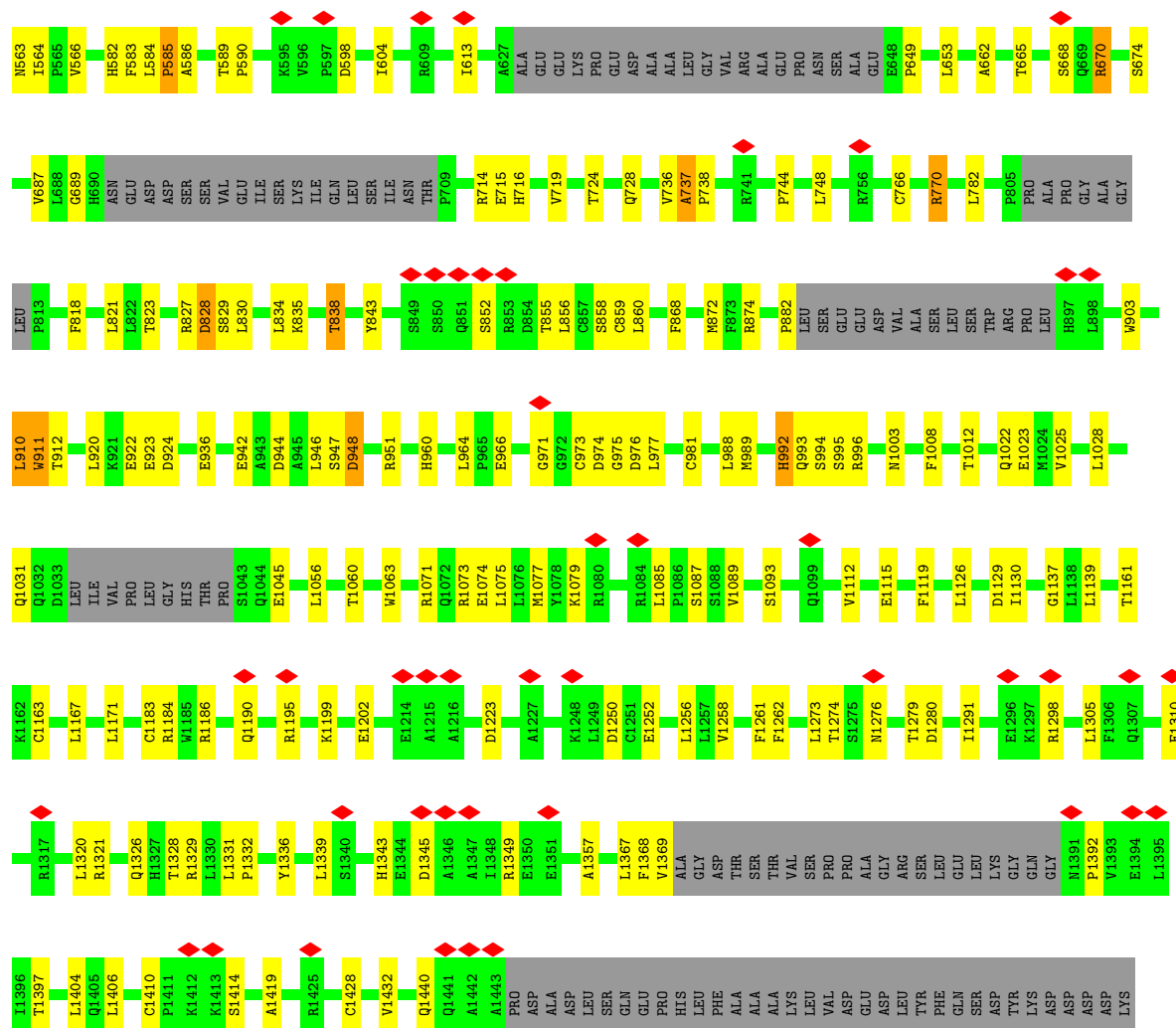
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	

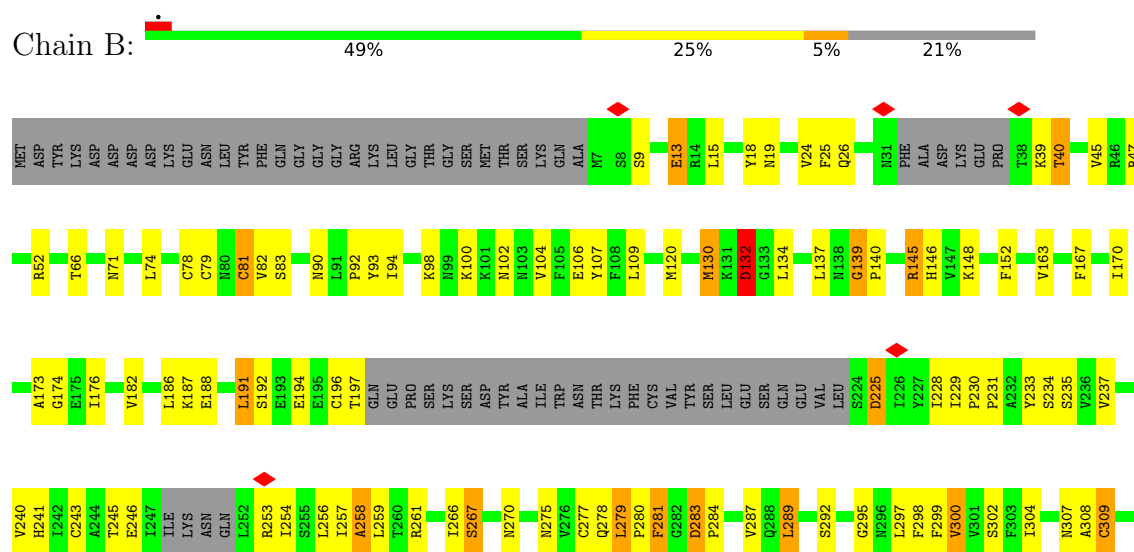


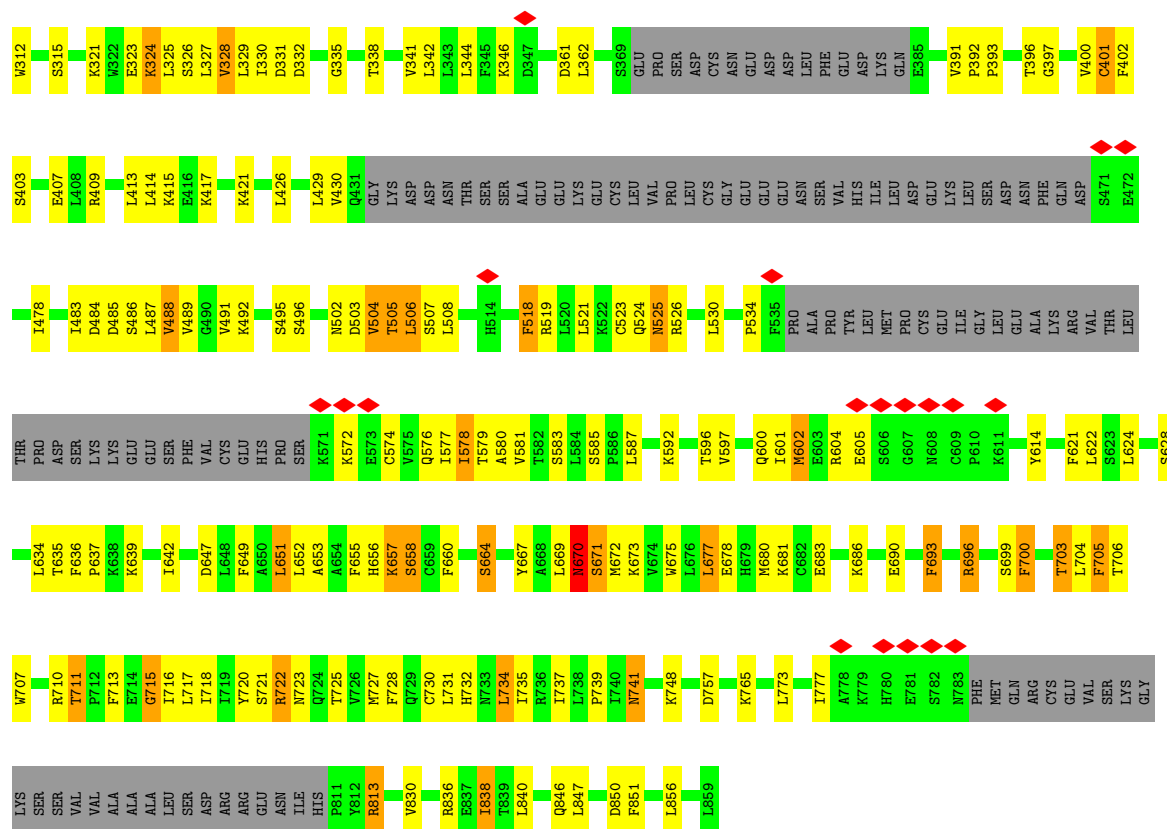
• Molecule 1: Fanconi anemia group A protein



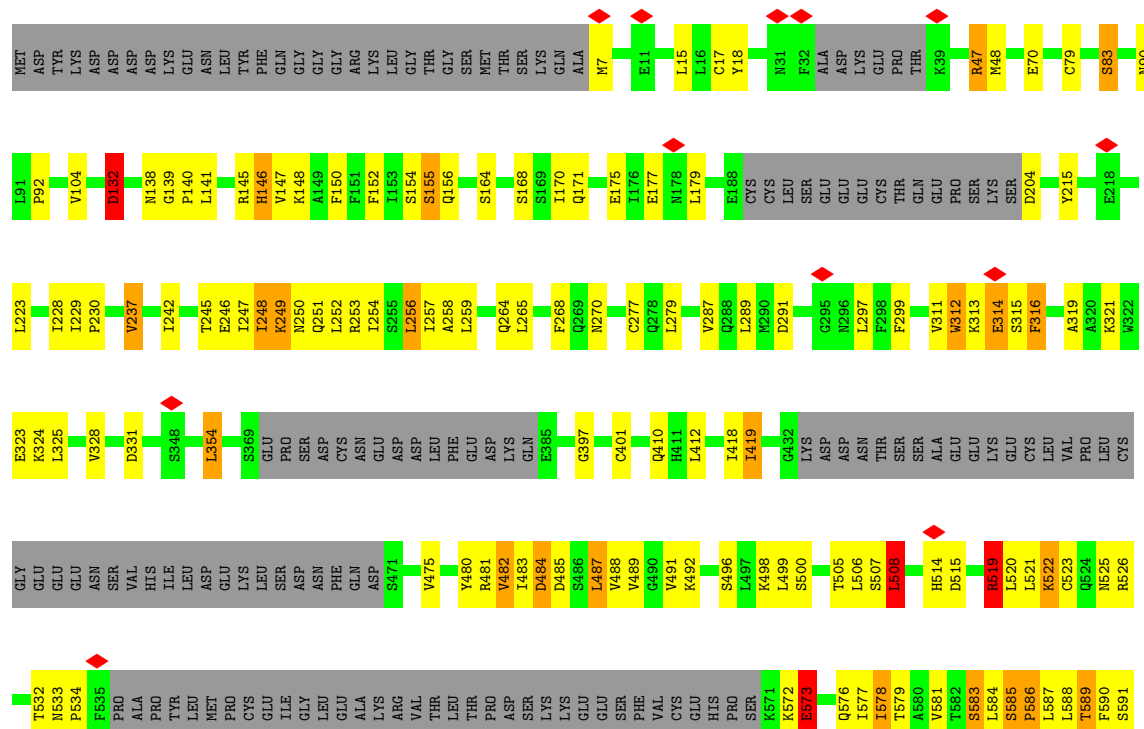


- Molecule 2: Fanconi anemia group B protein

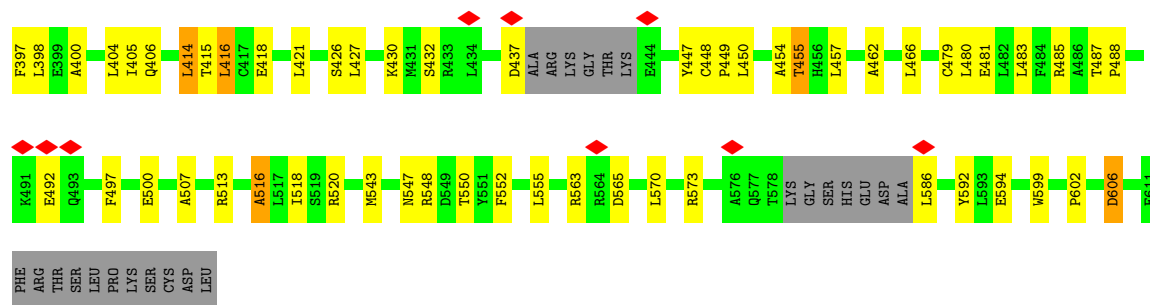




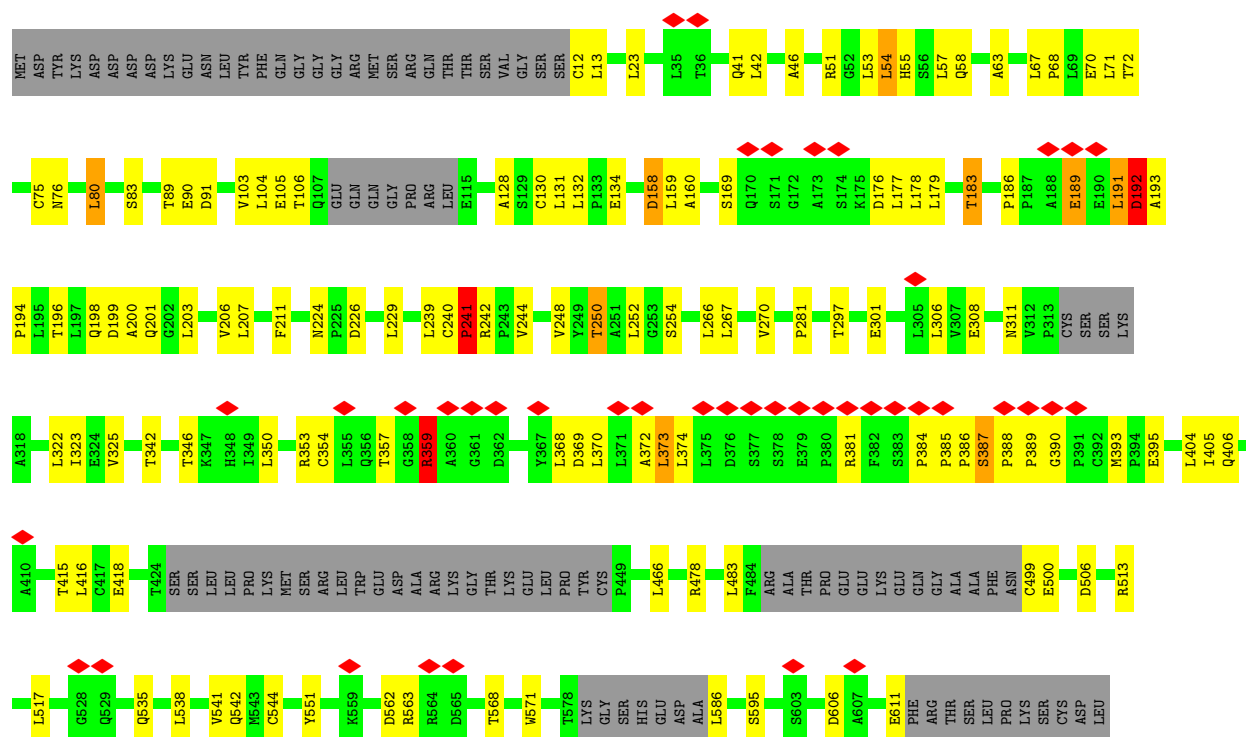
• Molecule 2: Fanconi anemia group B protein



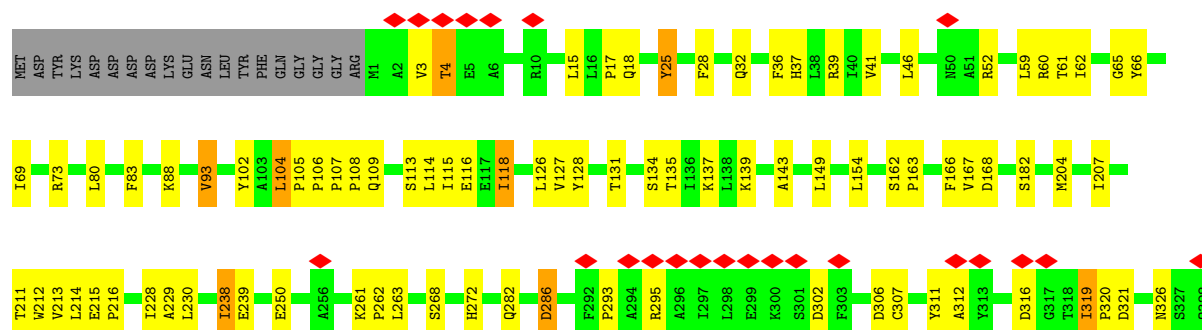




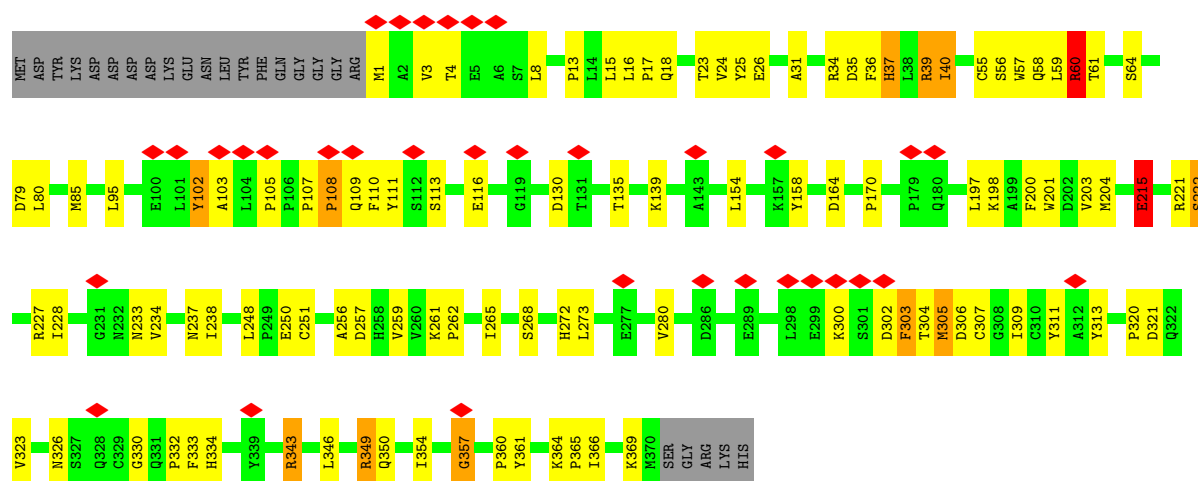
• Molecule 6: Fanconi anemia group G protein



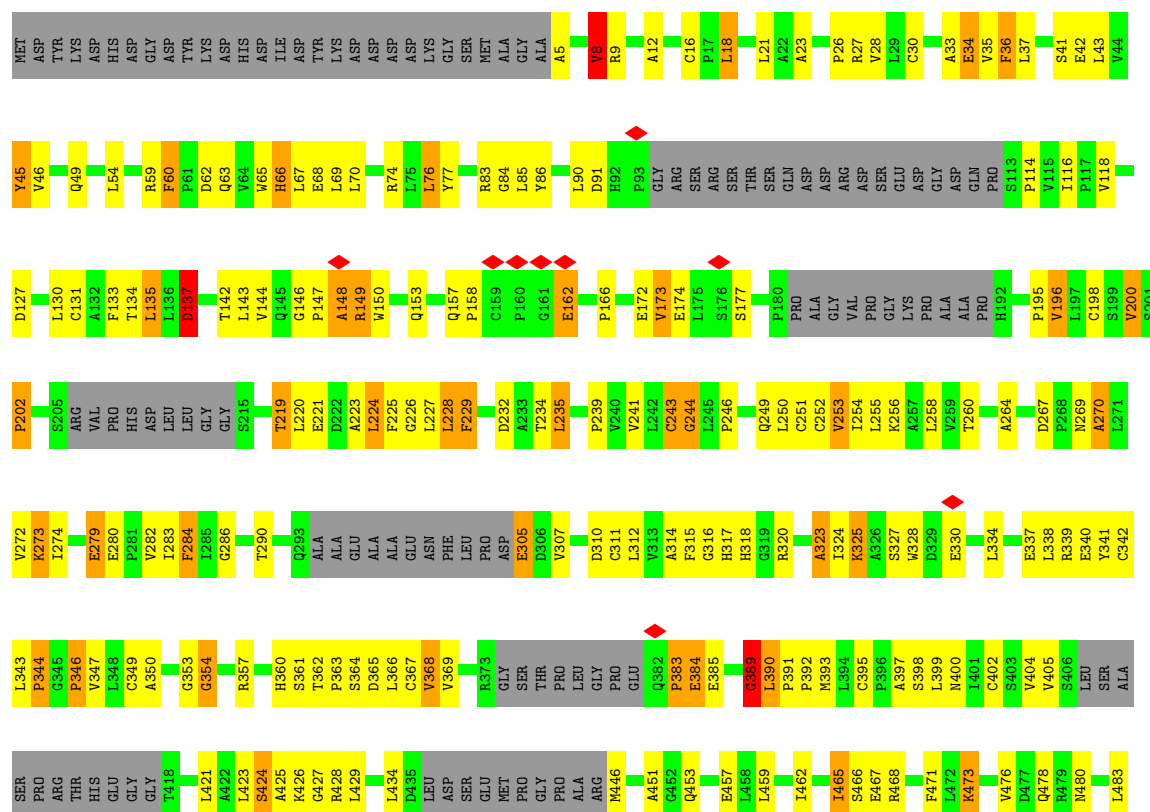
• Molecule 7: E3 ubiquitin-protein ligase FANCL

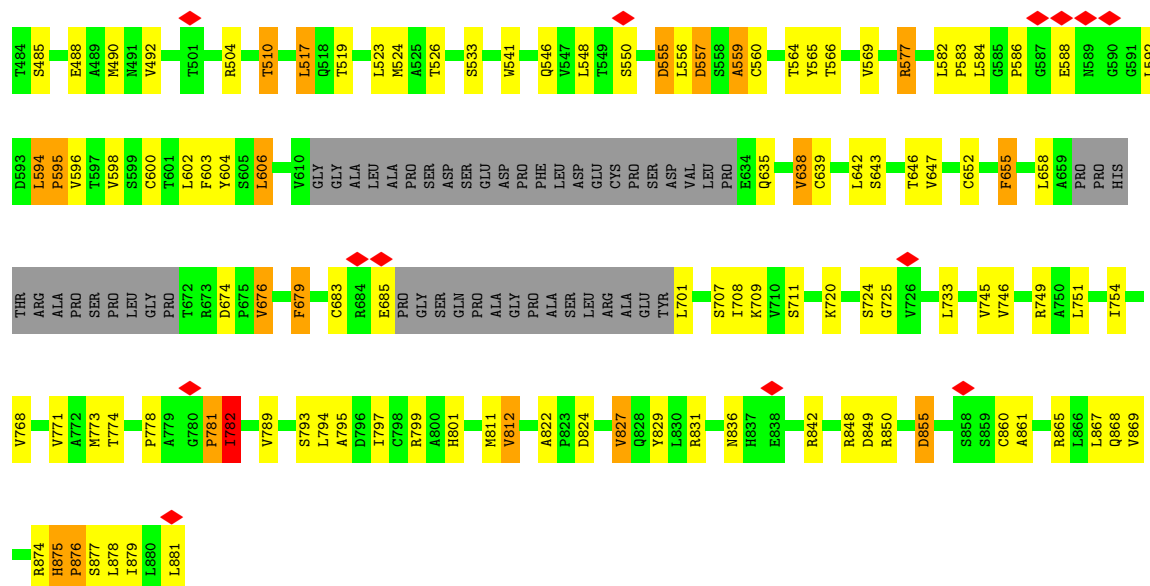


Chain M: 9% 67% 24% 6%

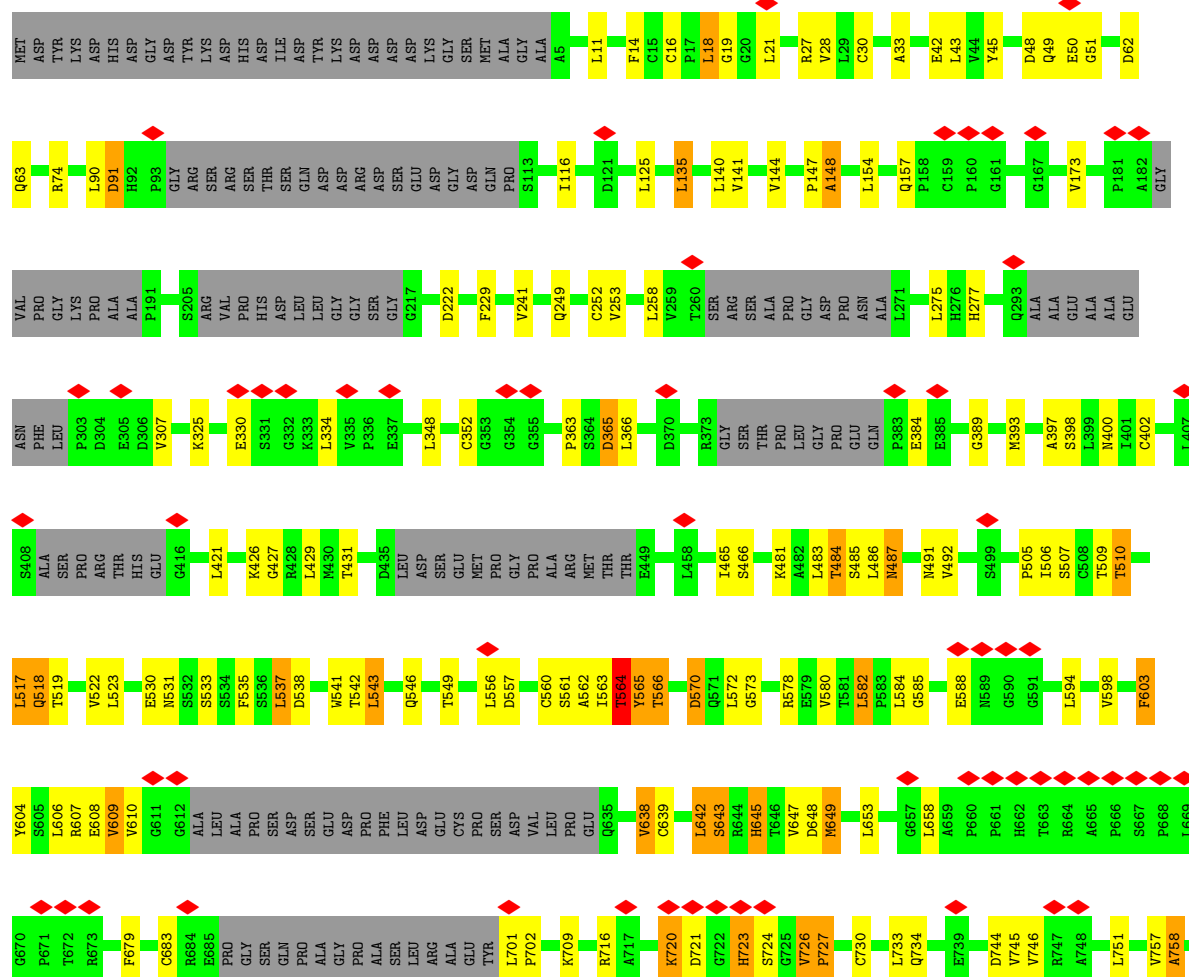


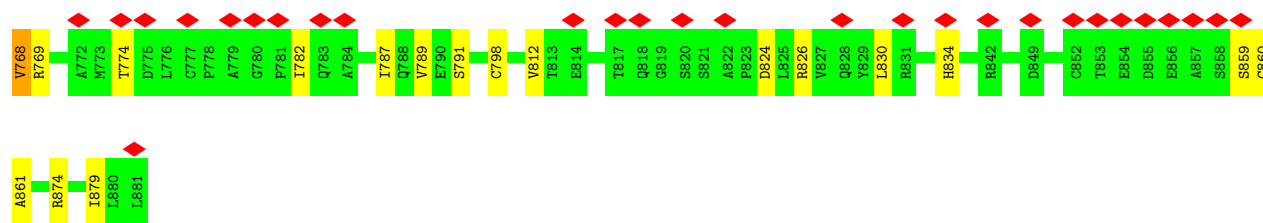
Chain P: 48% 27% 7% 17%



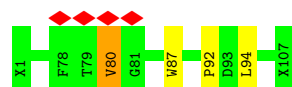
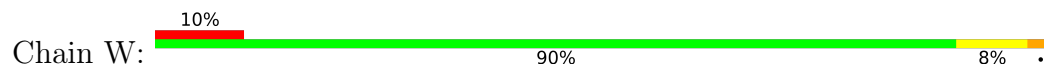


• Molecule 8: Fanconi anemia core complex-associated protein 100

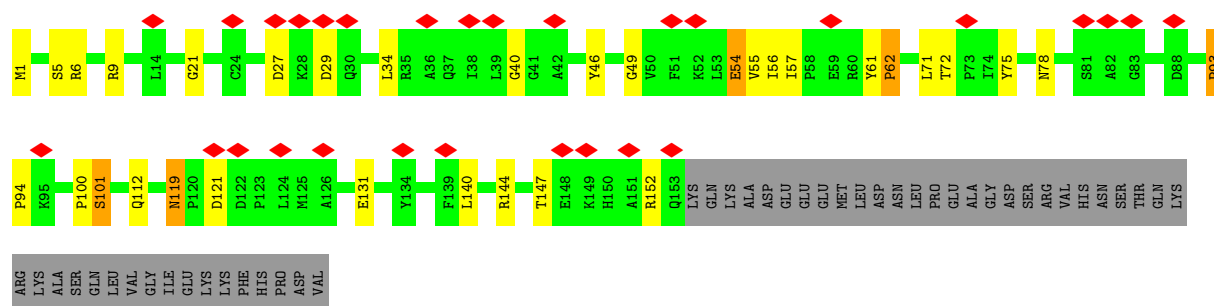




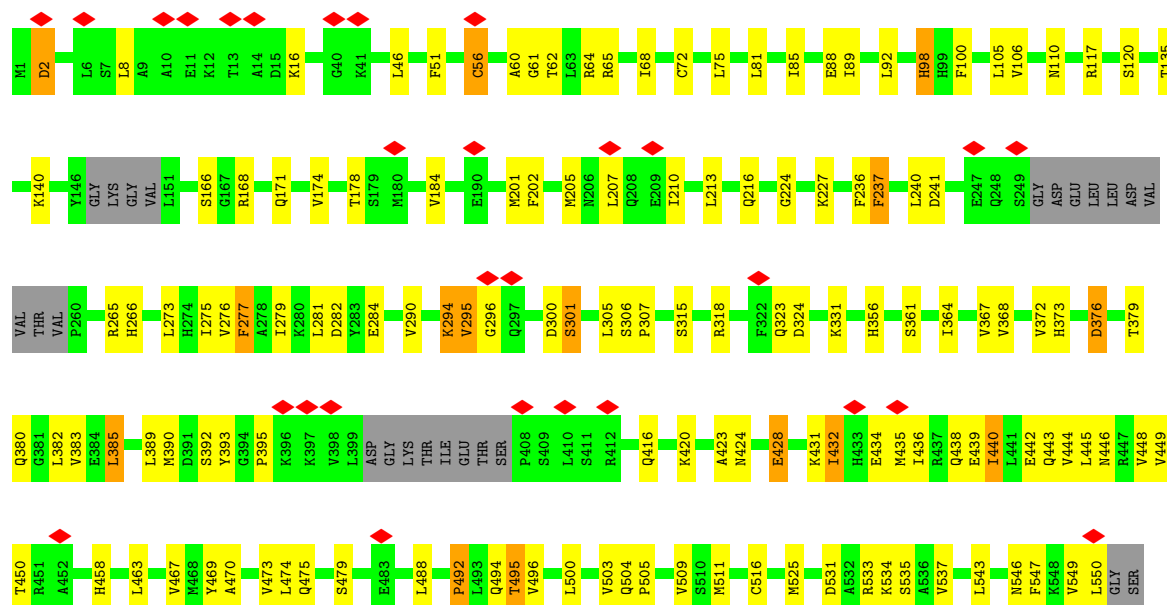
- Molecule 9: Fanconi anemia core complex-associated protein 20

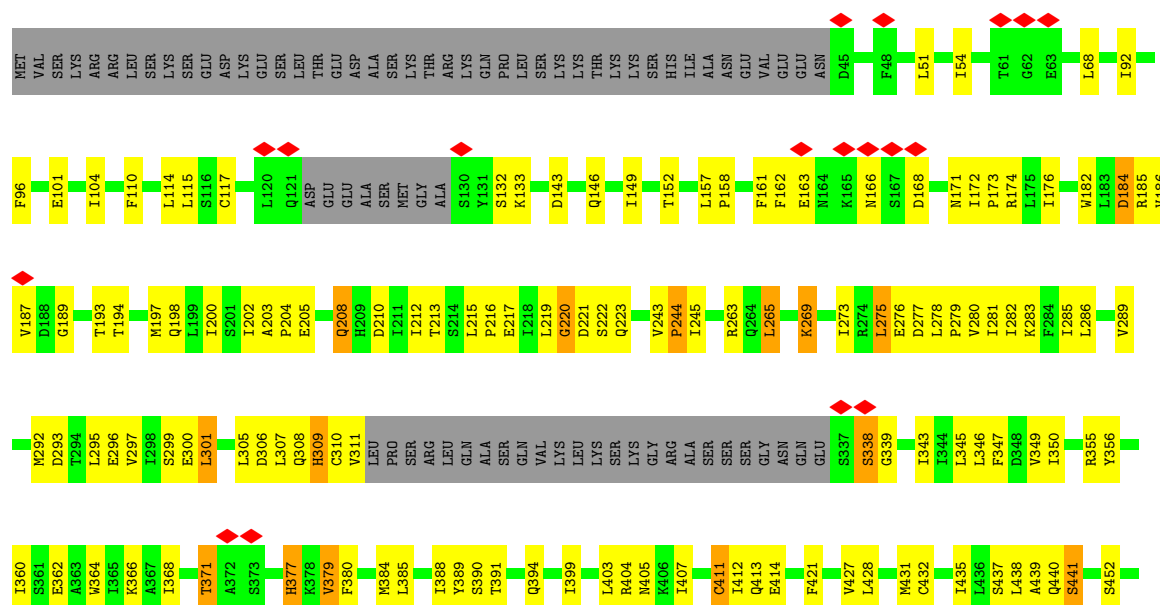


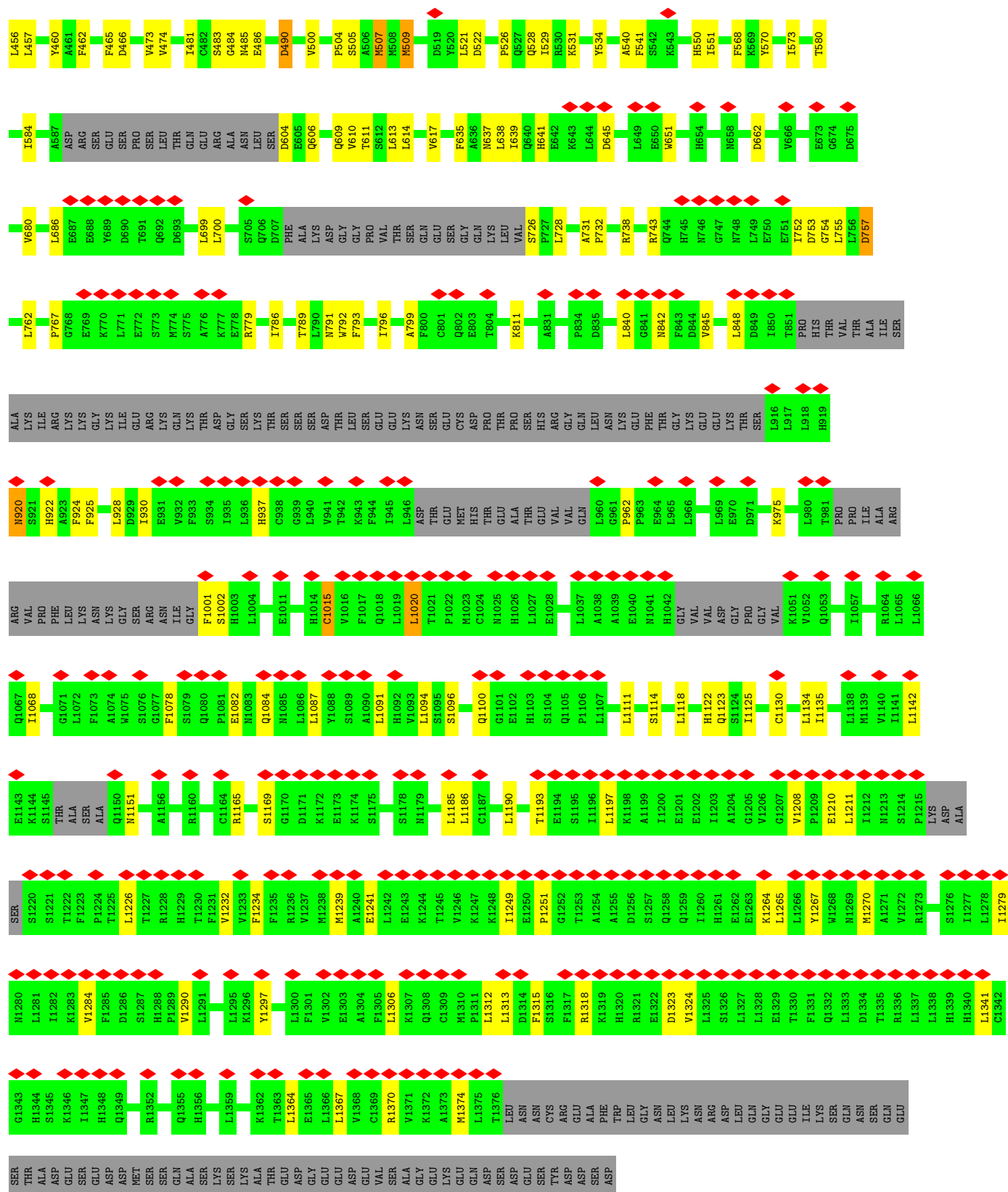
- Molecule 10: Ubiquitin-conjugating enzyme E2 T



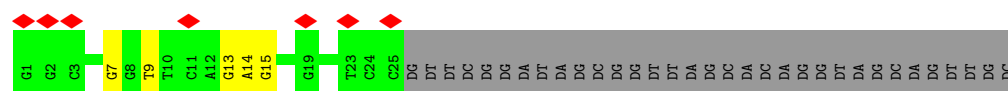
- Molecule 11: Fanconi anemia, complementation group I



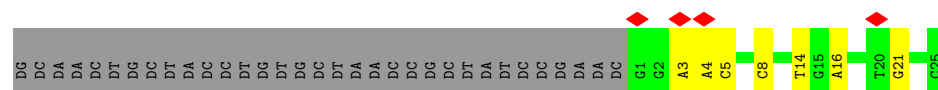




• Molecule 13: DNA (25-MER)



Chain Z:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40749	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	0.052	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0065	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	1.08	0/9605	1.68	28/13008 (0.2%)
1	S	1.08	0/10153	1.71	30/13749 (0.2%)
2	B	1.15	8/5707 (0.1%)	1.66	62/7686 (0.8%)
2	O	1.11	2/5701 (0.0%)	1.56	32/7686 (0.4%)
3	C	1.10	0/4497	1.74	38/6103 (0.6%)
4	E	1.21	1/3274 (0.0%)	1.95	69/4438 (1.6%)
5	F	1.09	0/2791	1.74	18/3790 (0.5%)
6	G	1.11	1/4568 (0.0%)	1.73	35/6215 (0.6%)
6	H	1.06	1/4293 (0.0%)	1.69	13/5840 (0.2%)
7	L	1.10	3/3050 (0.1%)	1.59	26/4143 (0.6%)
7	M	1.10	4/3050 (0.1%)	1.59	18/4143 (0.4%)
8	P	1.18	8/5697 (0.1%)	1.74	71/7752 (0.9%)
8	Q	1.11	3/5737 (0.1%)	1.56	21/7810 (0.3%)
9	W	0.98	0/202	1.34	0/281
10	X	1.16	0/1267	1.65	7/1722 (0.4%)
11	U	1.07	1/9400 (0.0%)	1.73	52/12676 (0.4%)
12	V	1.10	1/9433 (0.0%)	1.72	64/12760 (0.5%)
13	Y	0.38	0/579	1.03	5/892 (0.6%)
14	Z	0.40	0/569	1.16	7/875 (0.8%)
All	All	1.10	33/89573 (0.0%)	1.68	596/121569 (0.5%)

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	6
2	B	0	12
2	O	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3
4	E	0	7
5	F	0	2
6	G	0	5
6	H	0	2
7	L	0	2
7	M	0	1
8	P	0	20
8	Q	0	10
10	X	0	4
11	U	0	4
12	V	0	9
All	All	0	104

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	321	ASP	C-N	-17.19	1.09	1.33
7	L	330	GLY	C-N	-15.67	1.07	1.33
7	M	330	GLY	C-N	-11.51	1.14	1.33
7	L	321	ASP	C-N	-10.34	1.19	1.33
2	B	721	SER	CA-CB	-8.28	1.40	1.53
7	L	357	GLY	C-N	8.01	1.45	1.33
6	H	63	ALA	C-O	6.66	1.32	1.24
2	B	732	HIS	CE1-NE2	6.26	1.38	1.32
6	G	379	GLU	N-CA	6.20	1.51	1.46
8	P	283	ILE	C-O	6.20	1.31	1.24
8	P	286	GLY	C-O	6.12	1.28	1.24
2	B	703	THR	C-O	-5.98	1.15	1.23
8	P	429	LEU	C-O	5.86	1.31	1.24
8	P	282	VAL	C-O	-5.83	1.17	1.24
8	P	116	ILE	N-CA	5.78	1.50	1.45
2	O	487	LEU	C-O	-5.77	1.16	1.23
11	U	432	ILE	N-CA	5.68	1.51	1.46
8	P	647	VAL	C-O	5.55	1.30	1.24
8	Q	116	ILE	N-CA	5.53	1.50	1.45
8	Q	562	ALA	C-O	-5.42	1.19	1.24
7	M	17	PRO	C-O	-5.40	1.17	1.24
8	P	583	PRO	C-O	-5.40	1.17	1.23
12	V	244	PRO	C-O	-5.37	1.17	1.24
2	B	718	ILE	C-O	-5.32	1.18	1.24
4	E	288	LEU	N-CA	5.32	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	588	LEU	C-O	-5.30	1.17	1.24
8	P	243	CYS	C-O	5.27	1.30	1.24
2	B	583	SER	CA-CB	-5.23	1.45	1.53
2	B	657	LYS	C-O	-5.22	1.17	1.23
2	B	664	SER	CA-CB	-5.10	1.46	1.53
2	B	704	LEU	C-O	-5.10	1.18	1.23
8	Q	543	LEU	C-O	-5.03	1.18	1.24
7	M	39	ARG	NE-CZ	5.03	1.38	1.33

All (596) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	321	ASP	CA-C-N	17.54	145.50	120.95
7	M	321	ASP	C-N-CA	17.54	145.50	120.95
7	M	321	ASP	O-C-N	-11.69	107.04	122.59
7	L	168	ASP	CA-CB-CG	9.76	122.36	112.60
3	C	144	ASP	CA-CB-CG	9.56	122.16	112.60
5	F	338	ASP	CA-CB-CG	8.84	121.44	112.60
4	E	432	ASP	CA-CB-CG	8.77	121.37	112.60
13	Y	7	DG	C2'-C3'-O3'	8.65	124.48	111.50
10	X	29	ASP	CA-CB-CG	8.55	121.15	112.60
8	P	12	ALA	CA-C-N	8.34	128.75	121.58
8	P	12	ALA	C-N-CA	8.34	128.75	121.58
1	S	480	LEU	CA-C-N	8.28	125.45	120.24
1	S	480	LEU	C-N-CA	8.28	125.45	120.24
2	B	725	THR	N-CA-CB	8.00	121.88	110.12
6	G	384	PRO	CB-CA-C	-8.00	101.16	110.92
2	B	703	THR	CA-CB-OG1	-7.99	97.62	109.60
14	Z	16	DA	C2'-C3'-O3'	7.93	123.40	111.50
8	P	315	PHE	CB-CA-C	-7.91	93.45	110.45
6	H	158	ASP	CA-CB-CG	7.90	120.50	112.60
8	Q	727	PRO	N-CD-CG	-7.88	91.38	103.20
11	U	611	ASP	CA-CB-CG	7.88	120.48	112.60
2	O	581	VAL	CA-C-O	-7.86	114.65	121.09
4	E	339	LEU	CA-C-N	7.84	128.69	119.98
4	E	339	LEU	C-N-CA	7.84	128.69	119.98
8	Q	723	HIS	CA-CB-CG	7.84	121.64	113.80
6	H	506	ASP	CA-CB-CG	7.80	120.40	112.60
3	C	63	ARG	CA-C-N	7.79	129.33	120.06
3	C	63	ARG	C-N-CA	7.79	129.33	120.06
12	V	309	HIS	CA-C-N	7.79	130.56	120.44
12	V	309	HIS	C-N-CA	7.79	130.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	325	ASP	CA-CB-CG	7.78	120.38	112.60
4	E	354	ASP	CB-CA-C	7.75	122.29	109.89
1	S	948	ASP	CA-CB-CG	7.62	120.22	112.60
7	M	303	PHE	CA-CB-CG	7.61	121.41	113.80
7	M	116	GLU	CB-CG-CD	7.58	125.49	112.60
2	B	735	ILE	CA-C-N	7.54	130.72	120.54
2	B	735	ILE	C-N-CA	7.54	130.72	120.54
2	O	515	ASP	CA-CB-CG	7.54	120.14	112.60
5	F	99	GLU	CB-CG-CD	7.49	125.34	112.60
1	A	480	LEU	CA-C-N	7.44	124.93	120.24
1	A	480	LEU	C-N-CA	7.44	124.93	120.24
6	G	63	ALA	CA-C-N	7.43	126.28	120.33
6	G	63	ALA	C-N-CA	7.43	126.28	120.33
2	B	621	PHE	CA-CB-CG	7.43	121.23	113.80
2	B	725	THR	CA-CB-OG1	7.42	120.74	109.60
2	B	518	PHE	CB-CA-C	-7.42	100.46	112.03
14	Z	14	DT	C2'-C3'-O3'	7.41	122.62	111.50
7	L	167	VAL	CA-C-N	7.38	130.67	120.63
7	L	167	VAL	C-N-CA	7.38	130.67	120.63
4	E	34	GLN	N-CA-CB	-7.38	98.48	110.14
4	E	521	THR	CB-CA-C	7.38	120.79	110.16
8	P	679	PHE	CA-CB-CG	-7.31	106.49	113.80
2	B	92	PRO	CB-CA-C	7.27	120.84	111.46
12	V	300	GLU	CB-CG-CD	7.26	124.95	112.60
8	P	337	GLU	CB-CG-CD	7.24	124.91	112.60
4	E	366	SER	CA-C-N	7.15	130.73	120.79
4	E	366	SER	C-N-CA	7.15	130.73	120.79
2	B	47	ARG	CB-CA-C	7.14	122.43	110.79
6	G	382	PHE	CB-CA-C	7.12	121.28	109.89
1	A	923	GLU	N-CA-C	7.11	119.99	108.34
2	O	721	SER	CA-C-O	-7.10	113.55	121.51
2	B	723	ASN	CA-C-O	-7.10	113.83	121.14
1	A	93	PHE	CA-CB-CG	6.98	120.78	113.80
2	B	174	GLY	CA-C-N	6.97	130.77	120.87
2	B	174	GLY	C-N-CA	6.97	130.77	120.87
6	G	378	SER	CA-C-N	6.95	127.54	119.83
6	G	378	SER	C-N-CA	6.95	127.54	119.83
8	P	127	ASP	CA-CB-CG	6.93	119.53	112.60
4	E	361	THR	CA-C-N	6.93	129.85	120.77
4	E	361	THR	C-N-CA	6.93	129.85	120.77
8	P	390	LEU	O-C-N	-6.93	117.11	121.27
12	V	205	GLU	CB-CG-CD	6.93	124.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	484	THR	CB-CA-C	-6.89	100.06	110.88
1	A	288	GLU	CB-CA-C	6.88	121.08	111.86
8	P	279	GLU	CB-CG-CD	6.85	124.25	112.60
8	P	317	HIS	CA-CB-CG	-6.84	106.96	113.80
6	G	487	THR	CB-CA-C	6.82	117.52	109.47
8	P	244	GLY	CA-C-O	-6.80	115.25	120.76
4	E	91	PRO	CB-CA-C	-6.78	102.71	111.46
2	O	578	ILE	CA-C-O	-6.76	115.23	121.72
8	Q	365	ASP	CA-CB-CG	6.74	119.34	112.60
14	Z	21	DG	C2'-C3'-O3'	6.74	121.61	111.50
8	P	284	PHE	CA-CB-CG	-6.74	107.06	113.80
8	Q	564	THR	CB-CA-C	-6.71	95.65	109.94
8	P	346	PRO	N-CA-CB	6.68	107.71	103.23
8	P	357	ARG	CA-C-N	6.68	131.23	122.95
8	P	357	ARG	C-N-CA	6.68	131.23	122.95
3	C	204	LEU	CA-C-O	-6.67	112.30	119.97
1	S	287	GLU	CA-C-N	6.65	134.24	121.54
1	S	287	GLU	C-N-CA	6.65	134.24	121.54
12	V	168	ASP	CA-CB-CG	6.64	119.25	112.60
14	Z	8	DC	C2'-C3'-O3'	6.61	121.42	111.50
3	C	292	ARG	CG-CD-NE	-6.57	97.54	112.00
8	P	310	ASP	CB-CA-C	-6.55	99.38	110.64
7	L	286	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	510	TYR	CB-CA-C	-6.52	100.64	110.88
11	U	60	ALA	CA-C-N	6.50	127.20	119.98
11	U	60	ALA	C-N-CA	6.50	127.20	119.98
4	E	41	ARG	CG-CD-NE	-6.50	97.71	112.00
6	H	241	PRO	N-CA-C	6.48	125.82	112.47
7	L	143	ALA	CA-C-N	6.48	128.96	120.28
7	L	143	ALA	C-N-CA	6.48	128.96	120.28
8	P	395	CYS	CB-CA-C	6.47	118.98	109.08
4	E	422	CYS	CA-C-O	-6.47	113.69	120.55
2	O	230	PRO	N-CA-C	6.46	118.58	110.70
8	P	239	PRO	CB-CA-C	6.45	119.65	111.39
8	P	327	SER	CA-C-N	6.44	131.30	122.34
8	P	327	SER	C-N-CA	6.44	131.30	122.34
14	Z	5	DC	C2'-C3'-O3'	6.43	121.15	111.50
4	E	287	GLN	CA-C-N	6.42	128.12	120.09
4	E	287	GLN	C-N-CA	6.42	128.12	120.09
8	P	555	ASP	CA-CB-CG	6.40	119.00	112.60
8	Q	565	TYR	CA-C-O	-6.39	113.60	121.78
1	A	1368	PHE	CA-CB-CG	-6.38	107.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1372	ASP	CA-CB-CG	6.38	118.98	112.60
2	B	519	ARG	CB-CA-C	6.37	120.86	110.22
6	G	333	ASP	CA-CB-CG	6.37	118.97	112.60
11	U	440	ILE	CA-C-N	6.36	129.64	120.79
11	U	440	ILE	C-N-CA	6.36	129.64	120.79
2	B	503	ASP	CA-CB-CG	6.36	118.96	112.60
3	C	249	SER	CA-C-O	-6.36	114.15	120.70
2	O	291	ASP	CA-CB-CG	6.34	118.94	112.60
11	U	701	ASP	CA-CB-CG	6.33	118.93	112.60
3	C	136	GLN	CA-C-N	6.32	127.14	119.99
3	C	136	GLN	C-N-CA	6.32	127.14	119.99
4	E	354	ASP	CA-CB-CG	6.32	118.92	112.60
4	E	506	GLU	CA-C-N	6.32	129.07	120.54
4	E	506	GLU	C-N-CA	6.32	129.07	120.54
7	M	39	ARG	CB-CG-CD	6.32	125.83	111.30
7	L	216	PRO	N-CA-CB	6.31	108.35	103.30
1	S	828	ASP	CA-CB-CG	6.31	118.91	112.60
6	G	234	GLU	CB-CG-CD	6.28	123.28	112.60
2	B	92	PRO	N-CA-C	-6.28	101.35	111.14
4	E	361	THR	CB-CA-C	6.27	120.61	110.96
10	X	121	ASP	CA-CB-CG	6.25	118.86	112.60
2	O	492	LYS	CB-CA-C	6.24	119.83	109.53
11	U	282	ASP	CA-CB-CG	6.24	118.84	112.60
11	U	166	SER	CA-C-N	6.24	127.24	120.44
11	U	166	SER	C-N-CA	6.24	127.24	120.44
11	U	1160	ASP	CA-CB-CG	6.24	118.84	112.60
12	V	244	PRO	N-CA-C	-6.22	105.06	113.40
12	V	662	ASP	CA-CB-CG	6.21	118.81	112.60
12	V	309	HIS	CA-CB-CG	6.21	120.01	113.80
4	E	21	GLN	CB-CA-C	6.20	120.66	111.17
2	O	482	VAL	CB-CA-C	6.20	119.81	110.63
4	E	465	THR	N-CA-CB	6.20	119.39	110.03
2	B	686	LYS	CA-C-N	6.20	129.20	120.28
2	B	686	LYS	C-N-CA	6.20	129.20	120.28
12	V	377	HIS	CA-CB-CG	-6.19	107.61	113.80
7	M	108	PRO	N-CA-C	6.18	122.12	113.53
12	V	296	GLU	CB-CG-CD	6.17	123.09	112.60
4	E	130	ASP	CA-CB-CG	6.16	118.76	112.60
3	C	314	THR	CB-CA-C	6.14	120.98	110.79
2	B	741	ASN	CB-CA-C	6.14	120.93	110.56
3	C	251	GLU	CB-CA-C	6.13	120.39	110.96
8	P	428	ARG	CB-CA-C	6.13	120.11	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	389	GLY	CA-C-O	-6.12	115.80	120.76
6	G	481	GLU	CB-CG-CD	6.12	123.00	112.60
1	S	1250	ASP	CA-CB-CG	6.11	118.71	112.60
3	C	91	ILE	CA-CB-CG1	6.11	120.78	110.40
8	P	606	LEU	CA-C-N	6.11	128.78	120.54
8	P	606	LEU	C-N-CA	6.11	128.78	120.54
5	F	306	GLU	CB-CG-CD	6.10	122.97	112.60
1	A	862	PRO	CA-C-N	6.10	126.89	119.99
1	A	862	PRO	C-N-CA	6.10	126.89	119.99
7	L	343	ARG	CA-C-N	6.08	126.69	120.00
7	L	343	ARG	C-N-CA	6.08	126.69	120.00
1	S	670	ARG	CG-CD-NE	-6.08	98.62	112.00
1	A	286	GLN	CB-CA-C	6.06	119.82	109.65
6	G	565	ASP	CA-C-N	6.05	128.30	120.44
6	G	565	ASP	C-N-CA	6.05	128.30	120.44
12	V	490	ASP	CB-CA-C	6.04	120.37	110.88
2	B	718	ILE	CA-C-O	-6.04	114.17	120.27
4	E	365	ARG	CB-CA-C	6.04	121.81	109.67
4	E	44	LEU	CA-C-N	6.03	126.63	119.94
4	E	44	LEU	C-N-CA	6.03	126.63	119.94
12	V	405	ASN	CA-C-N	6.03	128.27	120.44
12	V	405	ASN	C-N-CA	6.03	128.27	120.44
4	E	284	ILE	CA-C-O	-6.01	114.79	121.17
8	P	70	LEU	CA-C-N	6.00	127.22	119.78
8	P	70	LEU	C-N-CA	6.00	127.22	119.78
12	V	217	GLU	CA-C-N	6.00	128.04	120.72
12	V	217	GLU	C-N-CA	6.00	128.04	120.72
2	B	703	THR	CA-C-O	-5.98	115.29	121.87
12	V	962	PRO	N-CA-C	5.98	118.00	110.70
11	U	277	PHE	CA-CB-CG	-5.98	107.82	113.80
4	E	431	PRO	CA-C-N	5.98	129.10	120.79
4	E	431	PRO	C-N-CA	5.98	129.10	120.79
2	B	656	HIS	CA-CB-CG	-5.98	107.82	113.80
12	V	205	GLU	CB-CA-C	5.97	120.26	110.88
8	Q	726	VAL	CA-C-N	5.97	127.31	119.84
8	Q	726	VAL	C-N-CA	5.97	127.31	119.84
12	V	474	VAL	CA-C-N	5.96	126.73	119.99
12	V	474	VAL	C-N-CA	5.96	126.73	119.99
1	S	1406	LEU	CA-C-N	5.96	126.15	120.43
1	S	1406	LEU	C-N-CA	5.96	126.15	120.43
8	Q	603	PHE	CB-CA-C	5.95	118.67	110.34
5	F	197	PRO	N-CA-C	5.95	120.58	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	39	ARG	CG-CD-NE	5.94	125.08	112.00
7	L	4	THR	CB-CA-C	5.94	118.52	111.22
5	F	165	THR	CA-CB-OG1	-5.92	100.72	109.60
4	E	522	PHE	N-CA-C	-5.91	102.90	110.53
5	F	319	PRO	N-CA-C	5.91	117.91	110.70
5	F	242	LEU	CA-C-N	5.89	126.48	119.94
5	F	242	LEU	C-N-CA	5.89	126.48	119.94
8	Q	487	ASN	CA-CB-CG	5.88	118.48	112.60
8	P	577	ARG	CB-CA-C	5.88	120.44	109.86
4	E	530	ALA	CA-C-N	5.88	128.47	120.54
4	E	530	ALA	C-N-CA	5.88	128.47	120.54
6	G	388	PRO	N-CA-C	5.87	117.86	110.70
7	M	35	ASP	CB-CA-C	5.86	119.32	109.48
5	F	298	GLU	CA-C-N	5.85	128.70	120.28
5	F	298	GLU	C-N-CA	5.85	128.70	120.28
2	B	647	ASP	CB-CA-C	5.85	122.31	110.38
11	U	294	LYS	CB-CA-C	5.84	118.57	110.16
2	B	734	LEU	CA-C-O	-5.84	114.30	120.55
6	G	437	ASP	CA-CB-CG	5.83	118.43	112.60
11	U	331	LYS	N-CA-C	-5.83	104.83	111.07
4	E	399	CYS	CA-C-N	5.83	128.09	120.28
4	E	399	CYS	C-N-CA	5.83	128.09	120.28
2	B	579	THR	CB-CA-C	5.82	120.34	109.86
8	P	643	SER	CA-C-N	5.82	130.68	121.72
8	P	643	SER	C-N-CA	5.82	130.68	121.72
7	M	60	ARG	CB-CG-CD	5.82	124.69	111.30
2	B	730	CYS	CA-C-O	-5.82	114.89	121.00
2	O	573	GLU	CB-CA-C	5.81	118.98	110.26
6	G	455	THR	CA-CB-OG1	-5.81	100.88	109.60
3	C	21	VAL	N-CA-CB	5.81	116.95	110.62
4	E	427	GLU	CA-C-N	5.80	129.53	120.82
4	E	427	GLU	C-N-CA	5.80	129.53	120.82
6	G	376	ASP	CB-CA-C	5.80	121.81	110.67
8	P	369	VAL	CA-C-O	-5.80	114.18	120.67
12	V	115	LEU	CA-C-N	5.79	128.93	120.71
12	V	115	LEU	C-N-CA	5.79	128.93	120.71
12	V	507	MET	CA-C-N	5.79	128.31	120.38
12	V	507	MET	C-N-CA	5.79	128.31	120.38
4	E	360	ALA	CA-C-N	5.78	128.28	120.65
4	E	360	ALA	C-N-CA	5.78	128.28	120.65
2	O	589	THR	CA-CB-OG1	-5.78	100.93	109.60
3	C	105	SER	CA-C-N	5.77	126.50	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	105	SER	C-N-CA	5.77	126.50	120.03
6	G	342	THR	CA-CB-OG1	-5.77	100.94	109.60
1	S	971	GLY	CA-C-N	5.76	126.54	120.43
1	S	971	GLY	C-N-CA	5.76	126.54	120.43
8	P	342	CYS	CB-CA-C	5.76	119.41	111.23
6	G	516	ALA	CA-C-O	-5.76	113.59	120.10
12	V	645	ASP	CA-CB-CG	5.76	118.36	112.60
11	U	1218	ASN	CA-CB-CG	5.75	118.35	112.60
2	B	600	GLN	CB-CA-C	5.74	119.88	109.37
2	B	525	ASN	CA-CB-CG	-5.74	106.86	112.60
2	B	728	PHE	CA-C-O	-5.74	114.79	120.70
11	U	836	ASN	CA-C-N	5.74	128.28	120.54
11	U	836	ASN	C-N-CA	5.74	128.28	120.54
4	E	531	LEU	CA-C-N	5.74	128.44	120.29
4	E	531	LEU	C-N-CA	5.74	128.44	120.29
8	Q	727	PRO	N-CA-CB	-5.72	97.24	103.25
11	U	1147	GLU	CA-C-N	5.72	128.22	120.44
11	U	1147	GLU	C-N-CA	5.72	128.22	120.44
7	M	102	TYR	CA-C-N	5.71	132.44	121.54
7	M	102	TYR	C-N-CA	5.71	132.44	121.54
7	L	321	ASP	CA-CB-CG	5.70	118.30	112.60
6	G	326	GLU	CA-C-N	5.70	128.19	120.38
6	G	326	GLU	C-N-CA	5.70	128.19	120.38
11	U	237	PHE	CA-CB-CG	-5.70	108.10	113.80
7	M	36	PHE	CA-CB-CG	5.70	119.50	113.80
2	O	482	VAL	N-CA-CB	-5.69	103.55	111.41
11	U	2	ASP	CA-CB-CG	5.69	118.29	112.60
1	S	598	ASP	CA-CB-CG	5.68	118.28	112.60
12	V	389	TYR	CA-C-N	5.68	128.21	120.54
12	V	389	TYR	C-N-CA	5.68	128.21	120.54
4	E	398	VAL	O-C-N	5.68	127.48	121.91
10	X	57	ILE	CB-CA-C	5.68	116.78	110.71
11	U	475	GLN	N-CA-C	-5.67	106.58	112.93
4	E	467	GLU	CA-C-N	5.67	127.81	120.44
4	E	467	GLU	C-N-CA	5.67	127.81	120.44
2	O	248	ILE	CA-C-O	-5.67	115.84	122.13
11	U	376	ASP	CA-CB-CG	5.66	118.26	112.60
3	C	305	THR	CA-C-O	-5.66	114.97	121.47
2	O	248	ILE	N-CA-C	-5.66	103.82	110.21
4	E	474	GLU	CB-CA-C	5.65	119.83	110.90
8	P	855	ASP	CA-CB-CG	5.65	118.25	112.60
2	B	670	ASN	CB-CA-C	5.65	118.53	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	1076	ASN	CA-C-N	5.64	128.11	120.38
11	U	1076	ASN	C-N-CA	5.64	128.11	120.38
4	E	522	PHE	N-CA-CB	5.64	118.50	110.44
1	S	367	SER	CA-C-N	5.63	127.77	120.44
1	S	367	SER	C-N-CA	5.63	127.77	120.44
5	F	303	PRO	CB-CA-C	-5.63	103.85	111.12
4	E	403	LEU	CA-C-N	5.63	126.08	119.83
4	E	403	LEU	C-N-CA	5.63	126.08	119.83
3	C	316	GLN	CB-CA-C	5.63	119.72	110.88
4	E	343	ARG	CG-CD-NE	5.63	124.38	112.00
11	U	531	ASP	CA-C-N	5.62	127.75	120.44
11	U	531	ASP	C-N-CA	5.62	127.75	120.44
8	Q	726	VAL	CB-CA-C	5.61	116.95	110.89
8	Q	565	TYR	N-CA-C	-5.61	101.89	110.14
3	C	91	ILE	N-CA-CB	5.60	117.10	110.55
4	E	284	ILE	CA-C-N	5.60	127.79	120.28
4	E	284	ILE	C-N-CA	5.60	127.79	120.28
2	B	715	GLY	CA-C-O	-5.59	116.17	121.60
4	E	317	HIS	CA-C-N	5.58	128.79	120.31
4	E	317	HIS	C-N-CA	5.58	128.79	120.31
12	V	275	LEU	CA-C-N	5.58	128.03	120.38
12	V	275	LEU	C-N-CA	5.58	128.03	120.38
1	S	425	ASP	CA-CB-CG	5.58	118.18	112.60
8	P	425	ALA	CA-C-O	-5.55	113.82	120.10
4	E	440	GLN	CB-CA-C	5.55	119.67	110.90
11	U	98	HIS	CA-CB-CG	-5.55	108.25	113.80
3	C	327	GLU	CA-C-N	5.52	127.62	120.44
3	C	327	GLU	C-N-CA	5.52	127.62	120.44
12	V	427	VAL	N-CA-C	-5.52	104.94	110.30
2	O	248	ILE	CA-C-N	5.52	132.09	121.54
2	O	248	ILE	C-N-CA	5.52	132.09	121.54
8	P	466	SER	CA-C-N	5.52	127.94	120.38
8	P	466	SER	C-N-CA	5.52	127.94	120.38
1	A	818	PHE	CA-CB-CG	-5.52	108.28	113.80
1	S	852	SER	CA-C-N	5.52	129.19	121.02
1	S	852	SER	C-N-CA	5.52	129.19	121.02
4	E	493	MET	CA-C-N	5.50	127.60	120.44
4	E	493	MET	C-N-CA	5.50	127.60	120.44
2	O	522	LYS	CA-C-O	-5.50	115.31	121.81
4	E	46	VAL	CB-CA-C	5.50	118.92	111.88
2	O	578	ILE	O-C-N	5.50	127.81	122.69
12	V	504	PRO	CA-C-N	5.50	127.59	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	V	504	PRO	C-N-CA	5.50	127.59	120.44
3	C	179	ARG	CG-CD-NE	5.50	124.09	112.00
2	O	47	ARG	CB-CA-C	5.50	119.09	110.19
2	O	204	ASP	CA-CB-CG	5.50	118.09	112.60
2	O	508	LEU	CA-C-O	-5.49	113.95	120.43
8	P	349	CYS	CA-C-O	-5.49	115.23	120.56
2	B	696	ARG	CB-CG-CD	-5.49	98.67	111.30
8	Q	91	ASP	CA-CB-CG	5.48	118.08	112.60
10	X	27	ASP	CA-CB-CG	5.48	118.08	112.60
8	P	229	PHE	CA-C-O	-5.48	113.22	119.41
11	U	494	GLN	CA-C-N	5.48	127.94	120.54
11	U	494	GLN	C-N-CA	5.48	127.94	120.54
1	S	585	PRO	N-CA-C	5.47	121.74	113.81
4	E	357	LEU	CA-C-N	5.47	127.55	120.44
4	E	357	LEU	C-N-CA	5.47	127.55	120.44
8	P	708	ILE	CA-C-O	-5.47	116.22	121.63
2	B	225	ASP	CA-CB-CG	5.46	118.06	112.60
7	L	319	ILE	N-CA-CB	-5.46	108.06	111.83
6	H	254	SER	CA-C-O	-5.46	115.06	120.90
2	B	407	GLU	CB-CG-CD	5.46	121.88	112.60
6	G	171	SER	CA-C-N	5.44	127.13	120.22
6	G	171	SER	C-N-CA	5.44	127.13	120.22
8	P	827	VAL	CA-C-O	-5.44	115.95	120.80
12	V	388	ILE	CA-C-N	5.44	127.52	120.44
12	V	388	ILE	C-N-CA	5.44	127.52	120.44
3	C	127	PHE	CA-C-N	5.44	131.93	121.54
3	C	127	PHE	C-N-CA	5.44	131.93	121.54
2	O	132	ASP	CA-CB-CG	5.43	118.03	112.60
2	O	519	ARG	CA-C-O	-5.43	114.24	121.46
2	B	196	CYS	CA-C-N	5.41	131.44	121.70
2	B	196	CYS	C-N-CA	5.41	131.44	121.70
2	B	492	LYS	CB-CA-C	5.41	119.06	110.19
1	A	1345	ASP	CA-CB-CG	5.41	118.01	112.60
8	Q	556	LEU	CA-C-N	5.41	131.87	121.54
8	Q	556	LEU	C-N-CA	5.41	131.87	121.54
8	P	254	ILE	CA-C-O	-5.41	114.69	120.85
8	Q	157	GLN	CB-CA-C	5.41	117.14	109.08
2	B	230	PRO	N-CA-C	5.40	115.66	110.47
2	B	671	SER	CA-C-N	5.40	128.30	120.79
2	B	671	SER	C-N-CA	5.40	128.30	120.79
12	V	427	VAL	O-C-N	5.39	127.49	121.94
2	B	300	VAL	CB-CA-C	5.39	118.37	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	323	ALA	CA-C-O	-5.39	114.92	121.28
3	C	435	GLY	CA-C-O	-5.38	117.56	122.24
3	C	436	ARG	CA-C-N	5.38	128.90	120.82
3	C	436	ARG	C-N-CA	5.38	128.90	120.82
7	L	61	THR	N-CA-CB	5.38	118.14	110.06
6	G	594	GLU	CB-CA-C	-5.37	102.21	110.81
10	X	54	GLU	CB-CG-CD	5.37	121.72	112.60
4	E	445	PRO	N-CA-CB	5.36	107.94	103.17
8	P	462	ILE	CA-C-N	5.36	125.93	119.98
8	P	462	ILE	C-N-CA	5.36	125.93	119.98
2	O	321	LYS	CB-CA-C	-5.35	104.19	111.95
7	M	215	GLU	CB-CG-CD	5.35	121.70	112.60
12	V	421	PHE	CA-CB-CG	5.35	119.15	113.80
2	B	678	GLU	CB-CG-CD	5.35	121.69	112.60
8	P	559	ALA	CA-C-N	5.35	130.65	122.95
8	P	559	ALA	C-N-CA	5.35	130.65	122.95
7	L	238	ILE	CA-C-O	-5.34	115.46	120.22
6	G	414	LEU	CA-C-O	-5.34	113.49	120.00
5	F	9	ASP	CA-CB-CG	5.34	117.94	112.60
8	P	219	THR	CB-CA-C	-5.33	100.50	109.72
5	F	320	PRO	N-CA-C	5.33	120.85	113.98
1	S	942	GLU	CB-CG-CD	5.33	121.66	112.60
10	X	93	PRO	N-CA-C	5.33	117.20	110.70
11	U	277	PHE	N-CA-CB	5.33	117.74	110.01
11	U	607	GLU	CA-C-N	5.33	125.86	120.00
11	U	607	GLU	C-N-CA	5.33	125.86	120.00
12	V	920	ASN	CA-CB-CG	5.33	117.92	112.60
5	F	320	PRO	CB-CA-C	-5.32	103.85	111.62
2	O	410	GLN	CA-C-N	5.32	127.67	120.38
2	O	410	GLN	C-N-CA	5.32	127.67	120.38
1	S	1089	VAL	CA-C-N	5.31	127.66	120.65
1	S	1089	VAL	C-N-CA	5.31	127.66	120.65
12	V	1002	SER	CA-C-N	5.31	127.35	120.44
12	V	1002	SER	C-N-CA	5.31	127.35	120.44
8	P	36	PHE	CA-CB-CG	-5.31	108.49	113.80
4	E	443	GLU	CB-CG-CD	5.31	121.63	112.60
8	P	305	GLU	CB-CA-C	5.31	120.19	110.10
1	A	800	GLU	CB-CG-CD	5.31	121.62	112.60
4	E	398	VAL	CA-C-N	5.31	127.34	120.44
4	E	398	VAL	C-N-CA	5.31	127.34	120.44
8	P	797	ILE	CA-CB-CG1	-5.31	101.38	110.40
7	L	302	ASP	CA-CB-CG	5.30	117.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	246	GLU	CB-CG-CD	5.30	121.61	112.60
8	P	655	PHE	CB-CA-C	5.30	115.73	110.33
7	L	306	ASP	CA-C-N	5.30	128.12	120.38
7	L	306	ASP	C-N-CA	5.30	128.12	120.38
2	B	851	PHE	CA-CB-CG	-5.30	108.50	113.80
5	F	205	ILE	N-CA-C	-5.30	104.80	110.36
11	U	376	ASP	CA-C-N	5.29	128.36	120.31
11	U	376	ASP	C-N-CA	5.29	128.36	120.31
2	B	81	CYS	CB-CA-C	-5.29	100.59	109.48
8	P	564	THR	CA-C-N	5.29	130.23	122.77
8	P	564	THR	C-N-CA	5.29	130.23	122.77
2	O	616	VAL	CB-CA-C	5.28	118.40	111.53
7	M	357	GLY	O-C-N	-5.28	116.38	123.67
7	M	302	ASP	CA-CB-CG	5.28	117.88	112.60
12	V	568	PHE	CA-C-N	5.28	127.35	120.28
12	V	568	PHE	C-N-CA	5.28	127.35	120.28
2	B	152	PHE	CA-CB-CG	5.28	119.08	113.80
12	V	208	GLN	O-C-N	5.28	127.50	122.07
6	G	189	GLU	CB-CA-C	5.27	120.13	110.11
8	P	173	VAL	N-CA-CB	-5.27	106.26	112.32
8	P	8	VAL	CA-C-O	-5.27	116.66	121.72
8	P	221	GLU	CB-CG-CD	5.26	121.54	112.60
4	E	533	HIS	CA-CB-CG	5.26	119.06	113.80
6	H	189	GLU	CB-CA-C	5.26	120.41	109.95
12	V	845	VAL	CA-C-O	-5.26	116.12	120.80
2	B	651	LEU	CA-C-O	-5.25	113.93	119.97
8	P	405	VAL	CA-C-N	5.25	131.16	121.70
8	P	405	VAL	C-N-CA	5.25	131.16	121.70
3	C	291	PHE	CB-CA-C	-5.25	102.41	110.81
11	U	1084	VAL	CA-C-N	5.25	127.63	120.54
11	U	1084	VAL	C-N-CA	5.25	127.63	120.54
4	E	506	GLU	CB-CG-CD	5.25	121.52	112.60
2	B	639	LYS	CA-C-N	5.24	125.65	119.83
2	B	639	LYS	C-N-CA	5.24	125.65	119.83
2	B	717	LEU	CA-C-O	-5.24	115.16	120.71
11	U	227	LYS	CA-C-N	5.24	127.25	120.44
11	U	227	LYS	C-N-CA	5.24	127.25	120.44
14	Z	14	DT	C4'-C3'-O3'	-5.24	102.15	110.00
12	V	481	ILE	N-CA-C	-5.23	105.22	110.30
3	C	400	PHE	CA-CB-CG	-5.23	108.57	113.80
4	E	141	ARG	CA-C-O	-5.23	115.33	120.82
5	F	143	VAL	CA-C-O	-5.23	115.31	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	241	PRO	CB-CA-C	-5.22	102.95	111.56
8	Q	509	THR	CA-C-O	-5.22	114.44	120.49
12	V	1151	ASN	CA-C-N	5.22	127.53	120.38
12	V	1151	ASN	C-N-CA	5.22	127.53	120.38
2	O	485	ASP	CB-CA-C	5.22	119.40	110.85
8	P	202	PRO	CB-CA-C	-5.22	102.95	111.56
2	O	155	SER	CA-C-O	-5.21	115.88	121.56
11	U	1061	ASP	CA-CB-CG	5.21	117.81	112.60
12	V	301	LEU	O-C-N	5.21	127.44	122.07
8	P	533	SER	CA-C-N	5.20	127.25	120.28
8	P	533	SER	C-N-CA	5.20	127.25	120.28
1	A	689	GLY	CA-C-O	-5.20	117.79	122.57
1	A	736	VAL	CA-C-N	5.20	134.49	121.80
1	A	736	VAL	C-N-CA	5.20	134.49	121.80
3	C	200	VAL	O-C-N	5.19	127.29	121.94
1	A	78	ILE	CA-C-O	-5.19	116.50	121.63
7	L	321	ASP	CA-C-N	5.18	128.21	120.95
7	L	321	ASP	C-N-CA	5.18	128.21	120.95
2	O	583	SER	CA-C-O	-5.18	115.49	121.19
2	B	402	PHE	CA-CB-CG	-5.18	108.62	113.80
7	L	215	GLU	CB-CG-CD	5.18	121.40	112.60
6	G	211	PHE	CA-CB-CG	-5.17	108.62	113.80
12	V	522	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	9	SER	CA-C-N	5.17	127.72	120.28
2	B	9	SER	C-N-CA	5.17	127.72	120.28
6	H	359	ARG	CA-C-N	5.16	127.45	120.38
6	H	359	ARG	C-N-CA	5.16	127.45	120.38
3	C	191	ILE	CA-C-N	5.16	131.22	122.65
3	C	191	ILE	C-N-CA	5.16	131.22	122.65
12	V	205	GLU	CA-C-N	5.16	127.15	120.44
12	V	205	GLU	C-N-CA	5.16	127.15	120.44
2	B	338	THR	CA-CB-OG1	-5.16	101.86	109.60
12	V	550	HIS	CA-C-N	5.16	127.80	120.53
12	V	550	HIS	C-N-CA	5.16	127.80	120.53
7	L	60	ARG	CA-C-O	-5.15	114.96	120.42
1	S	20	ARG	CA-C-N	5.15	127.18	120.28
1	S	20	ARG	C-N-CA	5.15	127.18	120.28
11	U	385	LEU	CA-C-N	5.15	125.69	119.98
11	U	385	LEU	C-N-CA	5.15	125.69	119.98
12	V	184	ASP	CA-CB-CG	5.15	117.75	112.60
8	P	223	ALA	CA-C-N	5.14	127.13	120.44
8	P	223	ALA	C-N-CA	5.14	127.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	342	PRO	CB-CA-C	-5.14	103.04	111.31
1	S	1223	ASP	CA-C-N	5.14	127.16	120.28
1	S	1223	ASP	C-N-CA	5.14	127.16	120.28
13	Y	13	DG	C2'-C3'-O3'	5.14	119.21	111.50
11	U	1072	PHE	CA-CB-CG	-5.14	108.66	113.80
11	U	1258	GLU	CB-CG-CD	5.14	121.33	112.60
1	A	396	LEU	CA-C-N	5.13	127.22	120.60
1	A	396	LEU	C-N-CA	5.13	127.22	120.60
1	S	936	GLU	CB-CG-CD	5.13	121.33	112.60
8	P	875	HIS	CB-CA-C	5.13	120.28	110.17
7	M	37	HIS	CA-C-O	-5.13	115.97	121.56
6	G	449	PRO	CA-C-O	-5.13	115.61	121.86
12	V	338	SER	CA-C-N	5.12	125.63	119.94
12	V	338	SER	C-N-CA	5.12	125.63	119.94
1	A	990	ASP	CA-CB-CG	5.12	117.72	112.60
1	S	42	LYS	CA-C-N	5.12	127.10	120.44
1	S	42	LYS	C-N-CA	5.12	127.10	120.44
5	F	138	ARG	CA-C-O	-5.12	115.44	121.07
7	L	263	LEU	CA-C-N	5.12	125.62	119.94
7	L	263	LEU	C-N-CA	5.12	125.62	119.94
11	U	184	VAL	N-CA-CB	5.11	114.84	110.08
6	G	143	VAL	CA-C-N	5.11	125.77	119.99
6	G	143	VAL	C-N-CA	5.11	125.77	119.99
6	G	331	PRO	N-CA-C	-5.11	104.47	110.70
6	G	384	PRO	N-CA-C	5.11	116.93	110.70
1	A	136	LEU	CA-C-N	5.11	129.59	121.72
1	A	136	LEU	C-N-CA	5.11	129.59	121.72
8	P	174	GLU	CB-CG-CD	5.11	121.28	112.60
14	Z	14	DT	N1-C1'-C2'	5.11	121.16	113.50
7	L	88	LYS	CB-CA-C	-5.10	102.32	110.79
1	A	1250	ASP	CA-CB-CG	5.10	117.70	112.60
3	C	251	GLU	CB-CG-CD	5.10	121.26	112.60
7	L	93	VAL	O-C-N	5.10	127.46	121.96
2	B	132	ASP	CA-C-N	5.09	131.39	121.41
2	B	132	ASP	C-N-CA	5.09	131.39	121.41
6	G	507	ALA	CA-C-N	5.09	127.11	120.28
6	G	507	ALA	C-N-CA	5.09	127.11	120.28
7	L	239	GLU	CB-CA-C	5.09	118.55	110.19
8	P	317	HIS	CA-C-O	-5.09	115.65	120.90
6	G	361	GLY	O-C-N	5.09	127.07	122.18
3	C	424	TRP	CA-C-N	5.09	127.05	120.44
3	C	424	TRP	C-N-CA	5.09	127.05	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	90	GLU	CB-CG-CD	5.09	121.25	112.60
8	P	869	VAL	CA-C-O	-5.09	115.66	120.95
12	V	265	LEU	CA-C-O	-5.08	115.03	120.42
1	A	923	GLU	CA-C-N	5.08	127.60	120.28
1	A	923	GLU	C-N-CA	5.08	127.60	120.28
3	C	335	PHE	CA-C-O	-5.08	115.26	121.05
11	U	276	VAL	CA-C-O	-5.08	115.42	121.05
12	V	405	ASN	O-C-N	5.08	127.50	122.12
4	E	120	ILE	O-C-N	5.07	127.18	121.90
2	B	757	ASP	CA-CB-CG	5.06	117.66	112.60
7	M	164	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	281	PHE	CA-C-N	5.06	127.62	122.66
2	B	281	PHE	C-N-CA	5.06	127.62	122.66
10	X	119	ASN	CB-CA-C	5.05	115.17	110.17
13	Y	15	DG	C2'-C3'-O3'	5.05	119.08	111.50
12	V	208	GLN	CA-C-N	5.05	127.30	120.38
12	V	208	GLN	C-N-CA	5.05	127.30	120.38
2	O	419	ILE	CA-C-O	-5.05	115.50	120.85
12	V	757	ASP	CA-CB-CG	5.05	117.65	112.60
8	Q	791	SER	CA-C-N	5.04	127.35	120.54
8	Q	791	SER	C-N-CA	5.04	127.35	120.54
12	V	521	LEU	CA-C-N	5.04	127.75	120.38
12	V	521	LEU	C-N-CA	5.04	127.75	120.38
11	U	277	PHE	CB-CA-C	-5.04	102.96	110.88
11	U	636	GLU	CB-CA-C	5.04	115.95	110.15
8	P	368	VAL	CA-C-O	-5.04	115.80	121.75
13	Y	9	DT	N1-C1'-C2'	5.04	121.06	113.50
2	B	338	THR	CB-CA-C	-5.04	100.94	110.16
13	Y	14	DA	C2'-C3'-O3'	5.04	119.05	111.50
5	F	308	HIS	O-C-N	5.03	127.33	122.09
8	P	34	GLU	N-CA-C	-5.03	102.32	110.32
8	Q	726	VAL	N-CA-CB	5.03	114.76	110.08
2	B	331	ASP	N-CA-C	5.03	115.83	107.73
3	C	7	ASP	CA-CB-CG	5.03	117.63	112.60
2	O	586	PRO	CA-C-N	5.03	127.28	120.44
2	O	586	PRO	C-N-CA	5.03	127.28	120.44
11	U	976	ASP	CA-CB-CG	5.03	117.63	112.60
12	V	368	ILE	CA-C-N	5.03	127.33	120.54
12	V	368	ILE	C-N-CA	5.03	127.33	120.54
3	C	34	THR	CA-C-N	5.03	128.36	120.82
3	C	34	THR	C-N-CA	5.03	128.36	120.82
1	S	882	PRO	N-CD-CG	-5.03	95.66	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	577	SER	CA-C-N	5.03	127.53	122.66
11	U	577	SER	C-N-CA	5.03	127.53	122.66
2	B	706	THR	CA-C-O	-5.02	115.23	121.06
4	E	352	SER	N-CA-C	-5.02	104.36	110.13
12	V	217	GLU	CB-CG-CD	5.02	121.14	112.60
6	G	492	GLU	N-CA-C	-5.02	105.47	112.45
2	B	90	ASN	CA-CB-CG	5.02	117.62	112.60
11	U	1052	ASP	CA-CB-CG	5.01	117.61	112.60
6	H	169	SER	CA-C-N	5.01	127.25	120.38
6	H	169	SER	C-N-CA	5.01	127.25	120.38
6	H	51	ARG	CB-CA-C	-5.00	102.96	110.92
1	A	963	PHE	CA-C-N	5.00	125.38	119.83
1	A	963	PHE	C-N-CA	5.00	125.38	119.83
4	E	518	PRO	CA-C-N	5.00	130.92	122.26
4	E	518	PRO	C-N-CA	5.00	130.92	122.26
8	P	158	PRO	CA-C-N	5.00	126.01	120.06
8	P	158	PRO	C-N-CA	5.00	126.01	120.06
8	P	676	VAL	CA-C-O	-5.00	115.07	120.47
11	U	749	VAL	CA-C-O	-5.00	115.87	121.17
6	H	192	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (104) 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	484	GLU	Peptide
1	A	824	CYS	Peptide
1	A	899	PRO	Peptide
1	A	922	GLU	Peptide
1	A	923	GLU	Peptide
2	B	132	ASP	Peptide
2	B	139	GLY	Peptide
2	B	145	ARG	Peptide
2	B	191	LEU	Peptide
2	B	258	ALA	Peptide
2	B	309	CYS	Peptide
2	B	324	LYS	Peptide
2	B	636	PHE	Peptide
2	B	637	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	696	ARG	Peptide
2	B	711	THR	Peptide
2	B	739	PRO	Peptide
3	C	208	GLY	Peptide
3	C	5	SER	Peptide
3	C	539	GLU	Peptide
4	E	147	GLY	Peptide
4	E	277	SER	Peptide
4	E	319	CYS	Peptide
4	E	351	LEU	Peptide
4	E	352	SER	Peptide
4	E	379	ALA	Peptide
4	E	401	ALA	Peptide
5	F	20	THR	Peptide
5	F	256	PRO	Peptide
6	G	132	LEU	Peptide
6	G	388	PRO	Peptide
6	G	500	GLU	Peptide
6	G	563	ARG	Peptide
6	G	61	PRO	Peptide
6	H	132	LEU	Peptide
6	H	563	ARG	Peptide
7	L	135	THR	Peptide
7	L	312	ALA	Peptide
7	M	215	GLU	Peptide
2	O	146	HIS	Peptide
2	O	154	SER	Peptide
2	O	247	ILE	Peptide
2	O	259	LEU	Peptide
2	O	312	TRP	Peptide
2	O	316	PHE	Peptide
2	O	636	PHE	Peptide
2	O	637	PRO	Peptide
2	O	711	THR	Peptide
8	P	146	GLY	Peptide
8	P	162	GLU	Peptide
8	P	270	ALA	Peptide
8	P	273	LYS	Peptide
8	P	314	ALA	Peptide
8	P	344	PRO	Peptide
8	P	383	PRO	Peptide
8	P	389	GLY	Peptide

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Mol	Chain	Res	Type	Group
8	P	397	ALA	Peptide
8	P	427	GLY	Peptide
8	P	504	ARG	Peptide
8	P	556	LEU	Peptide
8	P	584	LEU	Peptide
8	P	588	GLU	Peptide
8	P	60	PHE	Peptide
8	P	635	GLN	Peptide
8	P	720	LYS	Peptide
8	P	725	GLY	Peptide
8	P	781	PRO	Peptide
8	P	8	VAL	Peptide
8	Q	389	GLY	Peptide
8	Q	537	LEU	Peptide
8	Q	549	THR	Peptide
8	Q	584	LEU	Peptide
8	Q	585	GLY	Peptide
8	Q	594	LEU	Peptide
8	Q	647	VAL	Peptide
8	Q	720	LYS	Peptide
8	Q	721	ASP	Peptide
8	Q	724	SER	Peptide
1	S	31	LYS	Peptide
1	S	484	GLU	Peptide
1	S	495	HIS	Peptide
1	S	561	THR	Peptide
1	S	563	ASN	Peptide
1	S	960	HIS	Peptide
11	U	224	GLY	Peptide
11	U	492	PRO	Peptide
11	U	717	GLU	Peptide
11	U	802	ASP	Peptide
12	V	1020	LEU	Peptide
12	V	1169	SER	Peptide
12	V	204	PRO	Peptide
12	V	391	THR	Peptide
12	V	411	CYS	Peptide
12	V	483	SER	Peptide
12	V	485	ASN	Peptide
12	V	541	PHE	Peptide
12	V	842	ASN	Peptide
10	X	152	ARG	Peptide

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Mol	Chain	Res	Type	Group
10	X	61	TYR	Mainchain,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	175	0
1	S	9933	10028	9969	132	0
2	B	5605	5790	5768	155	0
2	O	5594	5759	5740	108	0
3	C	4396	4442	4427	81	0
4	E	3224	3390	3384	116	0
5	F	2726	2740	2729	51	0
6	G	4483	4537	4523	73	0
6	H	4216	4288	4273	84	0
7	L	2974	2977	2971	57	0
7	M	2974	2977	2970	77	0
8	P	5598	5681	5652	179	0
8	Q	5631	5724	5694	96	0
9	W	271	242	196	9	0
10	X	1233	1251	1248	20	0
11	U	9256	9626	9595	157	0
12	V	9258	9475	9422	168	0
13	Y	516	280	280	0	0
14	Z	509	281	281	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	87804	88975	88553	1576	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 9.

All (1576) 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)
8:Q:466:SER:CB	7:M:107:PRO:HB2	1.35	1.55
6:H:342:THR:CG2	6:H:384:PRO:HG3	1.41	1.50
8:Q:466:SER:HB2	7:M:107:PRO:CB	1.59	1.31
6:H:387:SER:OG	6:H:388:PRO:HD3	1.17	1.31
6:H:342:THR:HG21	6:H:384:PRO:CG	1.63	1.27
4:E:391:CYS:SG	4:E:398:VAL:HG11	1.76	1.26
8:Q:466:SER:CB	7:M:107:PRO:CB	2.11	1.23
12:V:146:GLN:NE2	12:V:186:VAL:HA	1.54	1.20
6:H:387:SER:OG	6:H:388:PRO:CD	1.97	1.12
1:A:900:SER:HG	1:A:903:TRP:CD1	1.72	1.05
12:V:146:GLN:HE22	12:V:186:VAL:CA	1.67	1.05
12:V:143:ASP:O	12:V:187:VAL:HG21	1.64	0.97
7:M:361:TYR:CD1	10:X:101:SER:HB3	1.99	0.96
8:Q:466:SER:HB3	7:M:107:PRO:CB	1.90	0.96
2:B:292:SER:OG	2:B:361:ASP:OD1	1.83	0.96
2:B:52:ARG:NH1	8:P:5:ALA:O	1.99	0.95
6:H:387:SER:HG	6:H:388:PRO:HD3	1.22	0.95
4:E:391:CYS:HG	4:E:398:VAL:HG11	1.29	0.94
2:O:482:VAL:HG13	2:O:584:LEU:HD11	1.49	0.93
8:Q:466:SER:HB3	7:M:107:PRO:HB3	1.51	0.92
2:B:362:LEU:O	8:P:468:ARG:NH2	2.04	0.91
12:V:146:GLN:HE22	12:V:186:VAL:HA	0.76	0.90
4:E:391:CYS:SG	4:E:398:VAL:CG1	2.60	0.88
12:V:437:SER:O	12:V:440:GLN:NE2	2.07	0.88
11:U:1213:ILE:HD11	11:U:1253:LEU:HD22	1.52	0.88
6:H:342:THR:CB	6:H:384:PRO:HG3	2.04	0.87
6:H:387:SER:CB	6:H:388:PRO:CD	2.53	0.87
1:A:1410:CYS:SG	1:A:1414:SER:OG	2.31	0.87
2:O:522:LYS:C	2:O:523:CYS:SG	2.59	0.86
7:M:361:TYR:CE1	10:X:101:SER:HA	2.11	0.85
3:C:99:ASN:ND2	3:C:107:GLN:OE1	2.08	0.85
4:E:518:PRO:HB2	4:E:520:THR:HG22	1.58	0.85
2:B:700:PHE:O	2:B:703:THR:OG1	1.94	0.84
4:E:395:THR:O	4:E:399:CYS:SG	2.36	0.84
4:E:64:LEU:HD11	4:E:109:LEU:HD22	1.59	0.84
1:S:494:LEU:HD11	1:S:518:LEU:HD11	1.59	0.84
1:S:737:ALA:HB1	1:S:738:PRO:CD	2.08	0.84
3:C:267:ASN:O	3:C:555:ARG:NH2	2.12	0.83
2:B:667:TYR:HE2	6:H:239:LEU:HD11	1.45	0.82
2:B:660:PHE:CZ	2:B:731:LEU:HD11	2.15	0.81
6:H:342:THR:CG2	6:H:384:PRO:CG	2.36	0.81
6:G:252:LEU:O	6:G:255:CYS:SG	2.38	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:252:CYS:O	5:F:310:ARG:NH1	2.12	0.80
8:P:260:THR:HB	8:P:264:ALA:O	1.81	0.79
8:P:280:GLU:OE1	8:P:318:HIS:HB2	1.83	0.79
1:S:988:LEU:HD21	1:S:1077:MET:HE2	1.65	0.78
5:F:253:ARG:NH2	5:F:300:GLN:O	2.17	0.78
8:P:65:TRP:O	8:P:66:HIS:HB2	1.84	0.78
1:S:351:THR:HG21	1:S:391:SER:HB2	1.65	0.78
1:A:919:VAL:O	1:A:923:GLU:OE2	2.01	0.78
3:C:124:ALA:O	5:F:140:ARG:NH1	2.17	0.77
6:H:103:VAL:O	6:H:106:THR:OG1	2.02	0.77
6:G:141:ARG:NH1	6:G:198:GLN:O	2.17	0.77
1:A:286:GLN:C	1:A:288:GLU:H	1.92	0.77
1:A:1265:LEU:HD11	1:A:1334:ALA:HB1	1.66	0.77
2:O:521:LEU:HD23	2:O:523:CYS:SG	2.23	0.77
2:B:396:THR:O	2:B:400:VAL:HG23	1.85	0.77
11:U:51:PHE:O	11:U:65:ARG:NH2	2.19	0.76
2:O:401:CYS:SG	7:M:107:PRO:HG3	2.25	0.76
11:U:751:GLU:CD	11:U:841:TYR:OH	2.29	0.75
8:P:339:ARG:HB3	8:P:341:TYR:CE1	2.22	0.75
1:A:309:SER:O	8:P:831:ARG:NH2	2.19	0.75
6:H:387:SER:CB	6:H:388:PRO:HD3	2.16	0.75
3:C:92:TRP:HE1	5:F:130:GLN:NE2	1.85	0.75
8:Q:486:LEU:HD12	8:Q:606:LEU:HD11	1.68	0.74
7:L:109:GLN:O	7:L:113:SER:OG	2.05	0.74
3:C:224:ASN:HD22	3:C:249:SER:HB3	1.51	0.73
6:G:214:ARG:NH1	6:G:328:LEU:O	2.21	0.73
8:P:362:THR:HB	8:P:363:PRO:HD2	1.70	0.73
1:S:288:GLU:HB3	1:S:292:HIS:HB2	1.69	0.73
1:S:288:GLU:CB	1:S:292:HIS:HB2	2.18	0.73
1:A:818:PHE:CZ	1:A:861:SER:OG	2.41	0.73
6:G:346:THR:O	6:G:349:ILE:N	2.21	0.73
2:B:667:TYR:CE2	6:H:239:LEU:HD11	2.22	0.73
12:V:208:GLN:O	12:V:212:ILE:HG22	1.88	0.73
2:B:132:ASP:OD2	2:B:145:ARG:NH1	2.22	0.72
8:P:320:ARG:NH2	8:P:340:GLU:OE1	2.22	0.72
6:G:141:ARG:NH1	6:G:196:THR:OG1	2.23	0.72
6:H:342:THR:HG21	6:H:384:PRO:HG3	0.73	0.72
11:U:470:ALA:O	11:U:473:VAL:HG22	1.90	0.72
2:O:522:LYS:O	2:O:523:CYS:SG	2.45	0.72
1:S:1025:VAL:HG21	1:S:1085:LEU:HD13	1.71	0.72
6:G:513:ARG:HD3	6:G:543:MET:SD	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:PRO:HA	3:C:145:TYR:HE1	1.55	0.71
8:P:594:LEU:O	8:P:596:VAL:N	2.23	0.71
1:S:920:LEU:O	1:S:923:GLU:OE1	2.08	0.71
4:E:283:ALA:O	4:E:287:GLN:CG	2.39	0.71
4:E:342:LEU:O	4:E:346:THR:N	2.21	0.70
2:B:602:MET:SD	2:B:602:MET:N	2.64	0.70
11:U:379:THR:HA	11:U:382:LEU:HD12	1.73	0.70
1:A:992:HIS:O	1:A:1073:ARG:NH2	2.25	0.70
2:B:430:VAL:HG21	8:P:638:VAL:HG12	1.74	0.70
4:E:53:ARG:NH1	7:L:361:TYR:O	2.24	0.70
8:P:362:THR:OG1	8:P:365:ASP:OD1	2.10	0.69
3:C:142:PRO:HA	3:C:145:TYR:CE1	2.26	0.69
6:G:252:LEU:HA	6:G:255:CYS:SG	2.33	0.69
6:H:306:LEU:HD22	6:H:346:THR:HG21	1.72	0.69
6:H:386:PRO:HB3	6:H:390:GLY:HA3	1.75	0.69
1:A:1425:ARG:HH11	1:A:1425:ARG:HB2	1.57	0.69
4:E:509:ARG:HA	4:E:512:LEU:HD12	1.74	0.69
2:O:245:THR:HG22	2:O:254:ILE:HG22	1.73	0.69
10:X:5:SER:O	10:X:9:ARG:NH1	2.26	0.69
8:P:284:PHE:CG	8:P:350:ALA:HB3	2.29	0.68
12:V:146:GLN:NE2	12:V:187:VAL:H	1.92	0.68
2:B:478:ILE:HD11	2:B:597:VAL:HG21	1.73	0.68
1:S:1336:TYR:OH	1:S:1357:ALA:O	2.11	0.68
8:P:523:LEU:HD23	8:P:592:LEU:HD11	1.75	0.68
12:V:1315:PHE:O	12:V:1318:ARG:NH1	2.27	0.68
7:M:354:ILE:HG12	7:M:369:LYS:HG2	1.74	0.67
2:O:520:LEU:HD11	8:Q:565:TYR:HB3	1.75	0.67
3:C:202:ALA:O	3:C:206:CYS:SG	2.52	0.67
8:P:150:TRP:HZ3	8:P:195:PRO:HG3	1.60	0.67
1:S:1161:THR:O	1:S:1321:ARG:NH2	2.27	0.67
1:S:993:GLN:HE22	1:S:1074:GLU:HB2	1.60	0.67
2:O:179:LEU:HD22	2:O:223:LEU:HD11	1.76	0.67
12:V:345:LEU:O	12:V:349:VAL:HG23	1.95	0.67
6:H:72:THR:O	6:H:76:ASN:ND2	2.28	0.67
6:H:58:GLN:OE1	6:H:70:GLU:OE2	2.13	0.66
3:C:122:LEU:O	5:F:140:ARG:NE	2.28	0.66
8:Q:229:PHE:HE1	8:Q:252:CYS:HG	1.41	0.66
2:B:280:PRO:HD2	2:B:309:CYS:SG	2.36	0.66
3:C:31:GLN:OE1	3:C:185:ARG:NH1	2.29	0.66
1:S:407:LEU:HD11	1:S:433:VAL:CG1	2.25	0.66
1:A:1176:SER:HA	1:S:964:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:670:CYS:O	11:U:674:CYS:SG	2.54	0.66
1:A:474:PHE:HD2	1:A:510:TYR:CG	2.13	0.66
1:S:375:LEU:HD11	1:S:396:LEU:HD11	1.77	0.66
11:U:543:LEU:HB3	11:U:550:LEU:HD21	1.78	0.66
11:U:450:THR:HG21	12:V:356:TYR:HA	1.78	0.66
3:C:224:ASN:HD22	3:C:249:SER:CB	2.09	0.65
1:S:1276:ASN:O	1:S:1279:THR:OG1	2.10	0.65
2:B:534:PRO:HA	2:B:572:LYS:HE2	1.78	0.65
8:P:35:VAL:HG21	8:P:421:LEU:HD22	1.78	0.65
1:S:737:ALA:HB1	1:S:738:PRO:HD3	1.77	0.65
1:S:1326:GLN:OE1	1:S:1329:ARG:NH2	2.29	0.65
2:B:667:TYR:HE2	6:H:239:LEU:CD1	2.09	0.65
2:B:850:ASP:OD2	8:P:801:HIS:ND1	2.30	0.65
7:M:303:PHE:CZ	7:M:305:MET:HB3	2.32	0.65
2:O:155:SER:O	2:O:156:GLN:HB3	1.96	0.65
4:E:70:GLU:HB3	4:E:83:LEU:HD22	1.79	0.65
6:G:147:ALA:HB1	6:G:159:LEU:HD11	1.77	0.65
8:P:253:VAL:HG23	8:P:272:VAL:HA	1.79	0.65
8:Q:491:ASN:HB3	8:Q:535:PHE:CE1	2.32	0.65
8:P:220:LEU:HD13	8:P:224:LEU:CD2	2.27	0.64
2:O:521:LEU:O	2:O:523:CYS:SG	2.55	0.64
8:P:850:ARG:HG2	8:P:855:ASP:HB2	1.78	0.64
12:V:308:GLN:HG3	12:V:309:HIS:CD2	2.32	0.64
2:B:233:TYR:O	2:B:237:VAL:HG23	1.97	0.64
5:F:163:MET:HB3	5:F:207:VAL:HG21	1.79	0.64
2:O:146:HIS:O	2:O:148:LYS:N	2.31	0.64
7:M:107:PRO:HD2	7:M:108:PRO:HD3	1.79	0.64
1:A:822:LEU:HD23	1:A:823:THR:N	2.12	0.64
1:S:1410:CYS:SG	1:S:1414:SER:OG	2.56	0.64
1:A:656:ALA:HB3	1:A:683:ARG:NH2	2.13	0.64
4:E:294:LEU:O	4:E:297:THR:OG1	2.06	0.64
7:L:357:GLY:O	7:L:366:ILE:HG22	1.98	0.64
1:A:818:PHE:HA	1:A:821:LEU:HB3	1.78	0.63
1:S:737:ALA:HB1	1:S:738:PRO:HD2	1.79	0.63
12:V:273:ILE:HG21	12:V:281:ILE:CD1	2.28	0.63
2:B:667:TYR:CE2	6:H:239:LEU:CD1	2.82	0.63
3:C:95:CYS:O	3:C:98:ILE:HG22	1.98	0.63
1:S:834:LEU:O	1:S:838:THR:OG1	2.17	0.63
1:A:1113:ASN:O	1:A:1117:ARG:NE	2.31	0.63
2:B:146:HIS:O	2:B:148:LYS:N	2.31	0.63
11:U:622:SER:O	11:U:626:THR:OG1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:395:PRO:HD2	11:U:458:HIS:CE1	2.33	0.63
1:A:28:GLY:C	1:A:30:VAL:H	2.07	0.63
8:Q:563:ILE:CG2	8:Q:565:TYR:CE1	2.82	0.63
2:B:415:LYS:HG2	7:L:28:PHE:CZ	2.34	0.63
8:P:324:ILE:HG12	8:P:338:LEU:HD23	1.80	0.63
3:C:304:GLU:HG3	4:E:165:GLN:HA	1.81	0.63
6:G:240:CYS:O	6:G:240:CYS:SG	2.56	0.63
1:A:880:ARG:NH1	1:A:953:ASP:OD1	2.31	0.63
1:S:1063:TRP:CH2	1:S:1329:ARG:NH2	2.67	0.63
8:P:343:LEU:HB3	8:P:344:PRO:HD2	1.81	0.62
1:A:1045:GLU:OE2	1:A:1104:ARG:N	2.31	0.62
8:P:655:PHE:CE2	8:P:754:ILE:HD12	2.34	0.62
1:A:474:PHE:CD2	1:A:510:TYR:CD2	2.86	0.62
2:B:526:ARG:HD2	2:B:653:ALA:HA	1.81	0.62
4:E:96:ARG:O	4:E:100:SER:OG	2.18	0.62
7:M:58:GLN:O	7:M:61:THR:OG1	2.18	0.62
2:B:325:LEU:HA	2:B:344:LEU:O	1.98	0.62
8:P:679:PHE:C	8:P:679:PHE:CD1	2.76	0.62
4:E:59:ASP:OD1	7:L:166:PHE:CD2	2.53	0.62
5:F:203:LYS:O	5:F:206:ALA:HB3	1.99	0.62
6:G:547:ASN:HD22	6:G:550:THR:HG23	1.64	0.62
11:U:364:ILE:O	11:U:367:VAL:HB	1.99	0.62
12:V:197:MET:HA	12:V:200:ILE:HG22	1.81	0.62
11:U:858:HIS:HB2	11:U:864:GLY:O	2.00	0.62
4:E:291:LEU:O	4:E:295:LEU:HG	1.98	0.62
5:F:201:PHE:CE2	5:F:205:ILE:HD11	2.34	0.62
1:A:1161:THR:O	1:A:1321:ARG:NH2	2.33	0.62
3:C:367:THR:HG21	3:C:403:TRP:CZ3	2.34	0.62
4:E:382:LEU:O	4:E:385:THR:OG1	2.16	0.62
8:Q:563:ILE:HG21	8:Q:565:TYR:CE1	2.35	0.61
1:A:815:PRO:HA	1:A:818:PHE:HE1	1.64	0.61
6:H:240:CYS:O	6:H:242:ARG:N	2.33	0.61
11:U:856:THR:OG1	11:U:858:HIS:O	2.18	0.61
12:V:792:TRP:CE2	12:V:796:ILE:HD11	2.36	0.61
1:S:547:ALA:HB1	1:S:582:HIS:HA	1.83	0.61
1:S:1075:LEU:HD12	1:S:1119:PHE:HD2	1.64	0.61
12:V:146:GLN:NE2	12:V:186:VAL:CA	2.43	0.61
8:P:312:LEU:O	8:P:323:ALA:HA	2.01	0.61
4:E:506:GLU:O	4:E:510:LEU:HG	1.99	0.61
8:P:389:GLY:HA2	8:P:390:LEU:HD23	1.80	0.61
11:U:241:ASP:OD1	11:U:265:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:438:GLN:O	11:U:442:GLU:HG2	2.01	0.61
4:E:283:ALA:O	4:E:287:GLN:HG2	1.99	0.61
2:B:231:PRO:O	2:B:234:SER:OG	2.13	0.61
8:Q:538:ASP:O	8:Q:570:ASP:O	2.18	0.61
2:O:480:TYR:HE2	2:O:622:LEU:HD13	1.66	0.61
11:U:295:VAL:HG13	11:U:301:SER:HA	1.83	0.61
12:V:343:ILE:O	12:V:346:LEU:HB3	2.01	0.61
11:U:668:LEU:HB3	11:U:752:VAL:HG11	1.83	0.60
5:F:18:SER:O	5:F:100:ASN:ND2	2.34	0.60
1:A:35:TYR:CE2	6:H:311:ASN:HB2	2.36	0.60
1:A:744:PRO:O	1:A:748:LEU:HG	2.02	0.60
6:H:513:ARG:O	6:H:517:LEU:HG	2.02	0.60
7:L:115:ILE:CD1	8:P:459:LEU:HD11	2.32	0.60
1:S:1258:VAL:HG13	1:S:1305:LEU:HD21	1.82	0.60
7:M:261:LYS:HB2	7:M:262:PRO:HD3	1.84	0.60
8:P:83:ARG:HD3	8:P:86:TYR:OH	2.01	0.60
8:Q:565:TYR:O	8:Q:566:THR:HG22	2.02	0.60
1:S:737:ALA:CB	1:S:738:PRO:CD	2.80	0.60
5:F:132:SER:O	5:F:135:ARG:HG2	2.00	0.60
6:G:513:ARG:CD	6:G:543:MET:SD	2.90	0.60
8:P:360:HIS:CE1	8:P:367:CYS:HB2	2.37	0.60
11:U:434:GLU:OE1	11:U:434:GLU:N	2.33	0.60
1:A:835:LYS:HZ3	1:A:903:TRP:CD1	2.20	0.59
4:E:351:LEU:HD12	4:E:355:LEU:HD11	1.84	0.59
4:E:473:MET:HE1	4:E:496:VAL:HG11	1.84	0.59
1:S:424:LEU:O	1:S:428:VAL:HG23	2.02	0.59
1:A:790:HIS:HE2	1:A:843:TYR:HH	1.49	0.59
8:P:399:LEU:O	8:P:423:LEU:O	2.20	0.59
7:M:303:PHE:CE1	7:M:305:MET:HB3	2.38	0.59
12:V:263:ARG:NH1	12:V:293:ASP:OD2	2.35	0.59
8:Q:48:ASP:O	8:Q:51:GLY:O	2.20	0.59
1:A:1265:LEU:HD11	1:A:1334:ALA:CB	2.32	0.59
8:P:510:THR:HA	8:P:526:THR:O	2.02	0.59
1:A:474:PHE:CD2	1:A:510:TYR:CG	2.90	0.59
12:V:275:LEU:O	12:V:279:PRO:HD3	2.02	0.59
12:V:371:THR:O	12:V:377:HIS:NE2	2.34	0.59
3:C:301:ALA:HB1	3:C:311:ILE:HD13	1.83	0.59
10:X:21:GLY:HA3	10:X:112:GLN:HE22	1.67	0.59
1:S:1419:ALA:HB2	1:S:1440:GLN:HE22	1.68	0.59
8:P:290:THR:OG1	8:P:325:LYS:NZ	2.30	0.59
11:U:768:PHE:CD1	11:U:832:LEU:HD11	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD21	1:A:105:LEU:HD11	1.85	0.59
12:V:171:ASN:HD21	12:V:174:ARG:CZ	2.15	0.58
2:B:289:LEU:O	2:B:330:ILE:HG21	2.02	0.58
6:H:342:THR:CB	6:H:384:PRO:CG	2.78	0.58
8:P:392:PRO:C	8:P:393:MET:HG3	2.27	0.58
2:O:164:SER:OG	2:O:215:TYR:OH	2.21	0.58
2:B:711:THR:O	2:B:713:PHE:N	2.36	0.58
3:C:254:MET:HE2	3:C:281:LEU:HD11	1.85	0.58
4:E:516:LEU:HD13	4:E:527:LEU:HB3	1.85	0.58
7:L:105:PRO:O	7:L:107:PRO:HD3	2.03	0.58
1:S:428:VAL:HG22	1:S:476:PHE:CE1	2.39	0.58
1:A:139:VAL:O	1:A:141:GLN:N	2.33	0.58
1:A:185:LEU:HD12	1:A:191:VAL:HG22	1.85	0.58
1:A:1336:TYR:OH	1:A:1357:ALA:O	2.21	0.58
11:U:75:LEU:HD12	11:U:81:LEU:HD11	1.84	0.58
12:V:273:ILE:HD13	12:V:281:ILE:HD13	1.86	0.58
5:F:98:LEU:O	5:F:101:ARG:NH2	2.37	0.58
1:S:430:ALA:O	1:S:434:VAL:HG23	2.03	0.58
12:V:428:LEU:HD23	12:V:431:MET:SD	2.43	0.58
1:A:835:LYS:HE2	1:A:903:TRP:CE2	2.39	0.58
1:A:977:LEU:O	1:A:981:CYS:SG	2.61	0.58
1:S:687:VAL:O	1:S:714:ARG:NH1	2.37	0.58
2:B:658:SER:OG	2:B:727:MET:HE2	2.02	0.58
2:O:651:LEU:HD13	2:O:704:LEU:HD11	1.85	0.58
8:Q:43:LEU:HB3	8:Q:45:TYR:CE1	2.39	0.58
1:S:649:PRO:O	1:S:653:LEU:HD12	2.04	0.58
7:M:55:CYS:SG	7:M:59:LEU:HD23	2.44	0.58
1:A:428:VAL:HG22	1:A:476:PHE:CE1	2.39	0.57
3:C:38:VAL:O	3:C:41:PHE:HB3	2.04	0.57
8:P:153:GLN:NE2	8:P:172:GLU:OE1	2.37	0.57
11:U:840:ARG:NH2	11:U:899:GLU:OE2	2.37	0.57
6:G:497:PHE:CE1	8:P:273:LYS:HB2	2.39	0.57
2:O:248:ILE:O	2:O:249:LYS:O	2.22	0.57
2:O:526:ARG:HH22	2:O:657:LYS:HB2	1.69	0.57
1:A:737:ALA:HB3	1:A:738:PRO:HD3	1.85	0.57
6:G:497:PHE:HB2	8:P:229:PHE:O	2.04	0.57
2:O:482:VAL:CG1	2:O:584:LEU:HD11	2.31	0.57
12:V:101:GLU:HA	12:V:104:ILE:HG12	1.87	0.57
1:A:657:LEU:HD23	1:A:725:SER:HB3	1.86	0.57
2:O:766:GLU:OE2	8:Q:874:ARG:NH2	2.36	0.57
1:A:1117:ARG:HB2	1:A:1165:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:ILE:CD1	2:B:237:VAL:HG21	2.35	0.57
2:O:257:ILE:HD11	2:O:299:PHE:CZ	2.40	0.57
1:A:750:VAL:HG21	1:A:790:HIS:HB3	1.87	0.57
3:C:224:ASN:ND2	3:C:249:SER:HB3	2.18	0.57
1:A:1201:GLN:HE21	1:A:1205:GLN:HE21	1.53	0.57
2:B:397:GLY:O	2:B:401:CYS:SG	2.61	0.57
8:P:255:LEU:O	8:P:256:LYS:C	2.46	0.57
1:S:994:SER:OG	1:S:995:SER:N	2.38	0.57
1:A:299:PHE:CD1	1:A:358:LEU:HD13	2.40	0.57
1:A:715:GLU:O	1:A:719:VAL:HG12	2.05	0.57
8:Q:466:SER:HB2	7:M:107:PRO:HB2	0.63	0.57
8:Q:505:PRO:HB3	8:Q:533:SER:HB3	1.87	0.57
2:B:18:TYR:CE1	2:B:19:ASN:OD1	2.58	0.56
6:H:206:VAL:HG13	6:H:325:VAL:HG22	1.85	0.56
11:U:488:LEU:HD21	11:U:500:LEU:HD11	1.87	0.56
1:A:821:LEU:C	1:A:821:LEU:HD23	2.30	0.56
8:P:130:LEU:CA	8:P:144:VAL:HG23	2.36	0.56
8:Q:570:ASP:OD1	8:Q:570:ASP:N	2.37	0.56
11:U:751:GLU:HA	11:U:754:ILE:HD12	1.87	0.56
2:B:79:CYS:HB3	2:B:94:ILE:HD12	1.86	0.56
4:E:396:TYR:CZ	4:E:400:SER:HB3	2.40	0.56
6:H:406:GLN:OE1	6:H:595:SER:OG	2.22	0.56
8:P:27:ARG:N	8:P:400:ASN:ND2	2.52	0.56
1:S:415:MET:HE2	1:S:419:PHE:HE2	1.71	0.56
7:M:107:PRO:CD	7:M:108:PRO:HD3	2.34	0.56
12:V:1122:HIS:O	12:V:1165:ARG:NH1	2.38	0.56
1:A:746:ALA:O	1:A:750:VAL:HG23	2.04	0.56
6:G:291:GLN:NE2	6:G:299:GLU:OE2	2.38	0.56
8:Q:11:LEU:HD11	8:Q:429:LEU:HD22	1.88	0.56
1:A:153:GLN:HG3	1:A:190:ILE:HD11	1.88	0.56
3:C:330:SER:HB2	3:C:334:ARG:HD2	1.87	0.56
2:O:520:LEU:HD21	8:Q:565:TYR:HD2	1.70	0.56
2:O:419:ILE:HG13	8:Q:483:LEU:HD12	1.87	0.56
8:P:674:ASP:OD1	8:P:676:VAL:N	2.38	0.56
6:G:268:TYR:CE1	1:S:93:PHE:CE2	2.94	0.56
6:G:552:PHE:CE2	6:G:602:PRO:HG3	2.40	0.56
8:P:311:CYS:SG	8:P:324:ILE:O	2.62	0.56
8:Q:580:VAL:HG12	8:Q:582:LEU:CD2	2.36	0.56
7:M:361:TYR:CE1	10:X:101:SER:CA	2.87	0.56
8:P:344:PRO:HD3	8:P:390:LEU:HD11	1.88	0.56
11:U:467:VAL:HG22	11:U:474:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:PHE:HB3	1:A:1360:MET:HE1	1.88	0.56
2:B:705:PHE:CD1	2:B:705:PHE:N	2.74	0.56
5:F:201:PHE:CD2	5:F:205:ILE:HD11	2.40	0.56
2:O:277:CYS:HB2	2:O:316:PHE:HB3	1.87	0.56
8:P:228:LEU:CD1	8:P:312:LEU:HD22	2.35	0.56
8:P:393:MET:CE	8:P:434:LEU:HD21	2.35	0.56
11:U:533:ARG:HD2	11:U:597:GLN:HE22	1.69	0.56
1:A:1025:VAL:HG21	1:A:1085:LEU:HD13	1.88	0.56
4:E:379:ALA:HB2	4:E:419:LEU:HD11	1.86	0.56
12:V:1265:LEU:HD13	12:V:1323:ASP:HB3	1.87	0.56
1:A:351:THR:HG21	1:A:391:SER:CB	2.36	0.55
3:C:6:VAL:O	3:C:10:CYS:SG	2.59	0.55
5:F:289:LEU:HD13	6:G:480:LEU:HD22	1.88	0.55
5:F:346:ILE:HG23	5:F:347:TRP:CD2	2.42	0.55
8:Q:537:LEU:HD12	8:Q:572:LEU:HD23	1.88	0.55
12:V:265:LEU:O	12:V:269:LYS:HG2	2.05	0.55
12:V:347:PHE:HA	12:V:350:ILE:HD12	1.87	0.55
12:V:1094:LEU:HD23	12:V:1114:SER:HB3	1.87	0.55
1:A:30:VAL:HG22	6:H:369:ASP:HA	1.89	0.55
2:O:840:LEU:HD21	8:Q:812:VAL:CG1	2.36	0.55
8:P:26:PRO:C	8:P:400:ASN:ND2	2.64	0.55
8:Q:16:CYS:SG	8:Q:426:LYS:O	2.63	0.55
3:C:370:HIS:CE1	7:L:272:HIS:HA	2.41	0.55
6:G:447:TYR:HE1	6:G:488:PRO:O	1.89	0.55
1:S:1368:PHE:CZ	1:S:1392:PRO:CB	2.90	0.55
11:U:174:VAL:HG21	11:U:201:MET:HG2	1.89	0.55
11:U:202:PHE:CE1	11:U:210:ILE:HG23	2.41	0.55
12:V:639:ILE:O	12:V:743:ARG:NH2	2.40	0.55
2:B:675:TRP:CZ2	2:B:680:MET:HE3	2.41	0.55
2:O:482:VAL:HG13	2:O:584:LEU:CD1	2.30	0.55
4:E:292:GLN:HE21	4:E:331:LEU:C	2.14	0.55
4:E:441:ILE:HA	4:E:444:LEU:HD12	1.88	0.55
2:O:313:LYS:O	2:O:314:GLU:HB2	2.06	0.55
8:P:74:ARG:HG3	8:P:90:LEU:HB2	1.88	0.55
11:U:668:LEU:C	11:U:752:VAL:HG11	2.32	0.55
7:L:228:ILE:HD12	7:L:238:ILE:HD12	1.89	0.55
2:O:481:ARG:NE	2:O:647:ASP:OD1	2.40	0.55
1:S:1112:VAL:HG11	1:S:1163:CYS:SG	2.47	0.55
1:A:818:PHE:HZ	1:A:861:SER:OG	1.83	0.55
1:A:845:LEU:HD23	1:A:856:LEU:HD11	1.88	0.55
2:B:521:LEU:CD1	2:B:587:LEU:HD21	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:486:GLU:O	12:V:490:ASP:CG	2.49	0.55
1:A:30:VAL:HG12	6:H:373:LEU:HD12	1.88	0.55
2:B:722:ARG:HG3	2:B:722:ARG:O	2.05	0.55
3:C:60:VAL:HG23	3:C:64:PHE:CE1	2.42	0.55
5:F:292:GLY:HA3	6:G:485:ARG:HD2	1.88	0.55
7:L:36:PHE:HB3	7:L:59:LEU:HD13	1.88	0.55
11:U:591:LEU:HA	11:U:594:CYS:SG	2.46	0.55
4:E:384:THR:O	4:E:388:THR:HG23	2.07	0.54
5:F:317:ALA:HB1	5:F:318:PRO:CD	2.37	0.54
6:H:193:ALA:HB1	6:H:194:PRO:HD2	1.88	0.54
4:E:359:ASN:O	4:E:363:LEU:HD23	2.07	0.54
4:E:528:LYS:HA	4:E:531:LEU:HD23	1.89	0.54
7:L:311:TYR:OH	7:L:361:TYR:OH	2.26	0.54
8:P:202:PRO:HB3	8:P:225:PHE:CD2	2.42	0.54
8:P:393:MET:HE1	8:P:434:LEU:HD21	1.89	0.54
1:A:181:ALA:O	1:A:185:LEU:HD23	2.07	0.54
2:B:257:ILE:HD11	2:B:299:PHE:CE1	2.42	0.54
7:L:41:VAL:HB	7:L:52:ARG:HB2	1.90	0.54
8:P:228:LEU:HD11	8:P:312:LEU:HD22	1.89	0.54
2:B:651:LEU:HD22	2:B:655:PHE:CZ	2.42	0.54
1:S:1368:PHE:CZ	1:S:1392:PRO:HB3	2.43	0.54
2:B:315:SER:HB3	8:P:471:PHE:CZ	2.43	0.54
2:B:485:ASP:OD1	2:O:725:THR:HG23	2.07	0.54
3:C:140:TYR:CE2	5:F:169:LEU:HD22	2.41	0.54
2:O:245:THR:OG1	8:Q:18:LEU:HD12	2.08	0.54
8:P:27:ARG:C	8:P:400:ASN:HD21	2.15	0.54
8:P:137:ASP:OD1	8:P:137:ASP:N	2.40	0.54
8:P:523:LEU:HD21	8:P:652:CYS:SG	2.48	0.54
2:B:79:CYS:HB3	2:B:94:ILE:CD1	2.38	0.54
4:E:391:CYS:O	4:E:395:THR:HA	2.07	0.54
6:H:179:LEU:O	6:H:183:THR:OG1	2.23	0.54
7:L:230:LEU:HA	7:L:293:PRO:CD	2.38	0.54
11:U:364:ILE:O	11:U:368:VAL:HG23	2.06	0.54
12:V:172:ILE:HG22	12:V:176:ILE:HD11	1.90	0.54
7:M:8:LEU:HD21	7:M:25:TYR:HE2	1.73	0.54
12:V:462:PHE:HB2	12:V:473:VAL:HG11	1.89	0.54
2:B:277:CYS:SG	2:B:278:GLN:N	2.81	0.54
8:P:368:VAL:O	8:P:391:PRO:HD2	2.08	0.54
12:V:289:VAL:HG12	12:V:297:VAL:HG11	1.90	0.54
3:C:92:TRP:HE1	5:F:130:GLN:HE22	1.54	0.54
1:S:818:PHE:HA	1:S:821:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1063:TRP:CZ3	1:S:1329:ARG:NH2	2.76	0.54
1:A:153:GLN:NE2	1:A:188:GLN:O	2.41	0.54
2:B:298:PHE:HE1	2:B:312:TRP:CD1	2.24	0.54
6:H:499:CYS:SG	6:H:500:GLU:N	2.81	0.54
2:O:756:ILE:HD13	8:Q:859:SER:HB3	1.90	0.54
8:P:353:GLY:O	8:P:354:GLY:C	2.50	0.54
11:U:440:ILE:O	11:U:444:VAL:HG23	2.07	0.54
2:O:257:ILE:CD1	2:O:299:PHE:CE1	2.91	0.53
1:A:474:PHE:CE2	1:A:510:TYR:CD2	2.96	0.53
1:A:1252:GLU:O	1:A:1298:ARG:NH2	2.41	0.53
4:E:399:CYS:O	4:E:440:GLN:NE2	2.41	0.53
7:M:8:LEU:HD21	7:M:25:TYR:CE2	2.43	0.53
12:V:1251:PRO:HA	12:V:1312:LEU:HD21	1.89	0.53
6:G:89:THR:OG1	6:G:90:GLU:N	2.40	0.53
11:U:849:LYS:O	11:U:859:VAL:HG12	2.08	0.53
1:A:1302:TRP:O	1:A:1305:LEU:HG	2.08	0.53
4:E:40:ALA:N	4:E:97:ASN:OD1	2.41	0.53
5:F:176:GLU:HG3	5:F:177:VAL:N	2.23	0.53
8:P:733:LEU:HD22	8:P:746:VAL:HG11	1.90	0.53
1:S:665:THR:HA	9:W:80:VAL:HG22	1.89	0.53
1:S:1079:LYS:HG3	1:S:1130:ILE:HD11	1.89	0.53
11:U:658:ILE:HG23	11:U:737:ILE:HG21	1.90	0.53
12:V:220:GLY:H	12:V:223:GLN:HE22	1.54	0.53
1:A:194:GLN:HG3	1:A:241:MET:SD	2.48	0.53
1:A:815:PRO:HA	1:A:818:PHE:CE1	2.41	0.53
2:B:240:VAL:CG1	2:B:256:LEU:HD11	2.39	0.53
2:B:602:MET:CE	8:P:546:GLN:HE21	2.21	0.53
3:C:61:ILE:HA	3:C:64:PHE:HB2	1.89	0.53
6:H:71:LEU:O	6:H:75:CYS:SG	2.62	0.53
7:L:320:PRO:HA	7:L:333:PHE:O	2.09	0.53
7:M:109:GLN:O	7:M:113:SER:OG	2.25	0.53
12:V:526:PRO:HA	12:V:529:ILE:HD12	1.89	0.53
2:B:74:LEU:CD2	2:B:98:LYS:HD3	2.38	0.53
4:E:29:LEU:HA	4:E:46:VAL:HG11	1.89	0.53
1:S:974:ASP:O	1:S:976:ASP:N	2.42	0.53
7:M:197:LEU:O	7:M:200:PHE:N	2.42	0.53
12:V:280:VAL:O	12:V:283:LYS:HB3	2.09	0.53
4:E:396:TYR:O	4:E:400:SER:N	2.24	0.53
8:P:361:SER:OG	8:P:398:SER:O	2.25	0.53
7:M:365:PRO:HG3	11:U:266:HIS:CE1	2.43	0.53
11:U:874:LEU:HD22	11:U:915:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:3:DA:H2''	14:Z:4:DA:C8	2.44	0.53
2:B:657:LYS:HD2	2:B:720:TYR:CE1	2.44	0.53
3:C:179:ARG:HG2	5:F:150:GLY:HA2	1.91	0.53
6:G:320:GLN:NE2	6:G:324:GLU:OE2	2.42	0.53
7:L:214:LEU:HD13	7:L:229:ALA:HB2	1.90	0.53
1:A:684:LEU:HD11	1:A:722:LEU:HD21	1.90	0.53
2:B:737:ILE:HG22	2:B:737:ILE:O	2.09	0.53
6:G:406:GLN:HG2	6:G:599:TRP:CE3	2.44	0.53
1:A:1063:TRP:CZ2	1:A:1329:ARG:NH1	2.77	0.53
2:B:421:LYS:HG3	7:L:18:GLN:HE21	1.73	0.53
2:O:401:CYS:SG	7:M:107:PRO:CG	2.97	0.53
2:O:830:VAL:HG22	8:Q:826:ARG:HG3	1.91	0.53
12:V:930:ILE:HG21	12:V:1015:CYS:SG	2.49	0.53
6:H:203:LEU:HD21	6:H:323:ILE:HD12	1.89	0.52
2:O:514:HIS:ND1	2:O:593:PHE:HA	2.24	0.52
8:P:398:SER:HA	8:P:424:SER:HA	1.92	0.52
8:Q:487:ASN:ND2	7:M:13:PRO:O	2.34	0.52
7:M:154:LEU:HD23	7:M:158:TYR:CD1	2.43	0.52
7:M:228:ILE:HD12	7:M:238:ILE:HD12	1.90	0.52
7:M:357:GLY:O	7:M:366:ILE:HG22	2.08	0.52
1:A:57:LEU:HD12	1:A:112:LEU:HD23	1.90	0.52
2:B:680:MET:HE1	2:B:700:PHE:CE2	2.44	0.52
4:E:438:LEU:O	4:E:442:LEU:HG	2.09	0.52
5:F:311:PHE:O	5:F:315:CYS:SG	2.56	0.52
1:S:1079:LYS:CG	1:S:1130:ILE:HD11	2.40	0.52
7:M:215:GLU:OE1	7:M:227:ARG:NH1	2.43	0.52
11:U:98:HIS:O	11:U:140:LYS:NZ	2.35	0.52
12:V:920:ASN:HA	12:V:924:PHE:HB2	1.90	0.52
4:E:345:CYS:O	4:E:349:LEU:HG	2.09	0.52
4:E:396:TYR:HA	4:E:399:CYS:HB2	1.91	0.52
1:S:977:LEU:O	1:S:981:CYS:SG	2.59	0.52
11:U:707:GLU:O	11:U:710:THR:OG1	2.23	0.52
11:U:729:PHE:HA	11:U:736:GLY:O	2.09	0.52
12:V:385:LEU:HD22	12:V:399:ILE:HG23	1.90	0.52
1:A:35:TYR:CE2	6:H:308:GLU:O	2.63	0.52
4:E:33:LEU:HD23	4:E:39:GLY:O	2.09	0.52
4:E:522:PHE:HA	4:E:524:ARG:HH21	1.73	0.52
11:U:450:THR:HG21	12:V:356:TYR:CA	2.39	0.52
2:B:295:GLY:O	2:B:297:LEU:N	2.42	0.52
2:B:524:GLN:C	2:B:525:ASN:HD22	2.18	0.52
4:E:283:ALA:O	4:E:287:GLN:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:533:ARG:CD	11:U:597:GLN:HE22	2.21	0.52
1:A:928:THR:HG23	1:A:971:GLY:HA3	1.91	0.52
2:B:235:SER:O	2:B:261:ARG:NH1	2.42	0.52
3:C:254:MET:HE3	3:C:294:VAL:HG13	1.92	0.52
4:E:407:LEU:O	4:E:447:LYS:NZ	2.39	0.52
8:P:67:LEU:HD22	8:P:76:LEU:HD21	1.92	0.52
8:Q:563:ILE:HG22	8:Q:565:TYR:CE1	2.45	0.52
1:S:715:GLU:O	1:S:719:VAL:HG13	2.09	0.52
1:A:900:SER:OG	1:A:903:TRP:CD1	2.52	0.52
2:B:642:ILE:HD11	2:B:693:PHE:CE2	2.45	0.52
3:C:371:ILE:HG21	3:C:397:PHE:CE1	2.44	0.52
4:E:83:LEU:HD21	7:L:93:VAL:HG21	1.91	0.52
8:P:366:LEU:HD23	8:P:366:LEU:C	2.35	0.52
8:Q:768:VAL:HG12	8:Q:787:ILE:HG12	1.91	0.52
11:U:295:VAL:HG23	11:U:305:LEU:HD13	1.92	0.52
12:V:219:LEU:HD22	12:V:223:GLN:HE21	1.73	0.52
4:E:514:MET:O	4:E:517:GLU:HB2	2.09	0.52
6:G:266:LEU:O	6:G:270:VAL:HG23	2.10	0.52
2:O:265:LEU:HD22	2:O:311:VAL:HG21	1.90	0.52
8:P:446:MET:CE	8:P:451:ALA:HB2	2.40	0.52
12:V:1020:LEU:HD13	12:V:1068:ILE:HG21	1.91	0.52
1:A:328:LEU:HD23	1:A:389:VAL:HG22	1.92	0.51
1:A:1305:LEU:C	1:A:1308:LEU:HD21	2.35	0.51
8:P:30:CYS:SG	8:P:404:VAL:HB	2.50	0.51
5:F:147:ARG:O	5:F:151:TYR:HB3	2.10	0.51
6:H:186:PRO:HG2	6:H:201:GLN:HG2	1.91	0.51
6:H:192:ASP:CG	6:H:192:ASP:O	2.54	0.51
2:O:829:LYS:N	8:Q:824:ASP:O	2.43	0.51
8:P:143:LEU:C	8:P:143:LEU:HD23	2.35	0.51
7:M:23:THR:HG23	7:M:24:VAL:HG23	1.91	0.51
12:V:1232:VAL:HG22	12:V:1290:VAL:CG2	2.40	0.51
1:A:1261:PHE:HB2	1:A:1291:ILE:HG21	1.91	0.51
5:F:290:GLN:O	6:G:485:ARG:NH2	2.42	0.51
8:P:157:GLN:O	8:P:157:GLN:HG2	2.09	0.51
1:S:117:VAL:HG13	1:S:148:LEU:HD21	1.91	0.51
7:M:79:ASP:OD1	7:M:80:LEU:N	2.43	0.51
12:V:243:VAL:HG13	12:V:244:PRO:HD3	1.92	0.51
8:Q:229:PHE:HE1	8:Q:252:CYS:SG	2.32	0.51
7:M:311:TYR:O	10:X:9:ARG:NE	2.44	0.51
11:U:729:PHE:O	11:U:740:ASN:ND2	2.40	0.51
12:V:210:ASP:O	12:V:213:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:TRP:CZ3	1:A:1225:LEU:HD13	2.45	0.51
2:B:602:MET:CE	8:P:546:GLN:NE2	2.74	0.51
8:P:733:LEU:CD2	8:P:746:VAL:HG11	2.41	0.51
8:Q:510:THR:O	8:Q:510:THR:OG1	2.28	0.51
1:S:288:GLU:HB2	1:S:292:HIS:HB2	1.90	0.51
1:S:1167:LEU:O	1:S:1171:LEU:HG	2.10	0.51
11:U:1079:THR:O	11:U:1083:THR:OG1	2.27	0.51
12:V:1135:ILE:HG21	12:V:1185:LEU:HD13	1.90	0.51
1:S:57:LEU:HD13	1:S:98:LEU:HD22	1.91	0.51
1:A:30:VAL:HG21	6:H:372:ALA:HB3	1.91	0.51
1:A:163:ARG:N	8:P:849:ASP:OD2	2.44	0.51
4:E:514:MET:SD	4:E:514:MET:N	2.84	0.51
4:E:528:LYS:O	4:E:531:LEU:HB3	2.11	0.51
2:O:228:ILE:HG22	2:O:229:ILE:H	1.75	0.51
1:S:835:LYS:HG2	1:S:903:TRP:CE3	2.46	0.51
11:U:380:GLN:CD	11:U:380:GLN:O	2.54	0.51
3:C:288:PRO:O	3:C:292:ARG:HG2	2.11	0.51
3:C:335:PHE:HZ	4:E:40:ALA:HB1	1.76	0.51
4:E:429:LEU:HD21	4:E:437:MET:HG3	1.92	0.51
6:H:544:CYS:O	6:H:544:CYS:SG	2.68	0.51
2:O:289:LEU:HD21	2:O:297:LEU:HD23	1.93	0.51
8:P:523:LEU:CD2	8:P:652:CYS:SG	2.99	0.51
11:U:887:SER:OG	11:U:888:ILE:N	2.44	0.51
11:U:1017:ASN:O	11:U:1074:ILE:HG12	2.11	0.51
5:F:15:LEU:O	5:F:18:SER:OG	2.27	0.51
2:O:669:LEU:HD11	2:O:672:MET:HG2	1.93	0.51
11:U:382:LEU:O	11:U:385:LEU:HB3	2.11	0.51
1:A:300:GLY:O	1:A:303:SER:OG	2.21	0.51
4:E:524:ARG:O	4:E:527:LEU:HB2	2.11	0.51
8:P:74:ARG:HD2	8:P:90:LEU:HD12	1.92	0.51
8:P:473:LYS:O	8:P:476:VAL:HB	2.11	0.51
8:Q:14:PHE:N	8:Q:427:GLY:O	2.40	0.51
8:Q:716:ARG:O	8:Q:720:LYS:HG3	2.11	0.51
11:U:75:LEU:CD1	11:U:81:LEU:HD11	2.41	0.51
11:U:467:VAL:HG22	11:U:474:LEU:HD11	1.92	0.51
11:U:808:LYS:O	11:U:812:SER:OG	2.29	0.51
6:H:354:CYS:SG	6:H:359:ARG:HG3	2.50	0.50
1:S:393:VAL:HA	1:S:396:LEU:HD12	1.93	0.50
1:S:566:VAL:HG13	1:S:1273:LEU:HG	1.93	0.50
4:E:467:GLU:O	4:E:471:VAL:HG23	2.10	0.50
8:Q:27:ARG:C	8:Q:400:ASN:HD21	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:642:LEU:O	11:U:644:PRO:HD3	2.10	0.50
12:V:157:LEU:N	12:V:158:PRO:HD2	2.26	0.50
12:V:1125:ILE:HD11	12:V:1134:LEU:HD13	1.93	0.50
1:A:770:ARG:NH1	1:A:820:SER:O	2.44	0.50
2:B:521:LEU:HD11	2:B:587:LEU:HD21	1.93	0.50
8:Q:709:LYS:HB2	8:Q:879:ILE:HG22	1.93	0.50
2:B:39:LYS:HG3	2:B:40:THR:O	2.11	0.50
2:B:245:THR:HB	8:P:18:LEU:HD11	1.93	0.50
3:C:92:TRP:NE1	5:F:118:GLY:HA2	2.26	0.50
4:E:487:MET:HE3	4:E:487:MET:O	2.11	0.50
6:H:387:SER:CB	6:H:388:PRO:HD2	2.41	0.50
7:L:127:VAL:HG22	7:L:137:LYS:O	2.11	0.50
11:U:277:PHE:O	11:U:281:LEU:HG	2.11	0.50
12:V:1210:GLU:N	12:V:1210:GLU:OE1	2.44	0.50
4:E:404:ASP:HB2	4:E:405:PRO:HD3	1.93	0.50
6:G:21:ASP:OD1	6:G:195:LEU:HD12	2.11	0.50
2:O:675:TRP:CZ2	2:O:680:MET:HE3	2.47	0.50
7:M:130:ASP:HB2	7:M:135:THR:HB	1.93	0.50
12:V:202:ILE:HG13	12:V:203:ALA:N	2.26	0.50
1:A:288:GLU:HA	1:A:292:HIS:HB3	1.94	0.50
4:E:472:LEU:O	4:E:476:LEU:N	2.41	0.50
6:H:80:LEU:O	6:H:83:SER:OG	2.26	0.50
8:P:16:CYS:O	8:P:16:CYS:SG	2.69	0.50
8:P:27:ARG:CA	8:P:400:ASN:HD21	2.24	0.50
8:P:86:TYR:CD1	8:P:86:TYR:N	2.80	0.50
11:U:660:LEU:HD12	11:U:741:ILE:HG23	1.93	0.50
12:V:184:ASP:O	12:V:185:ARG:HG3	2.12	0.50
12:V:1094:LEU:HD21	12:V:1118:LEU:HD12	1.94	0.50
3:C:153:MET:SD	5:F:143:VAL:HG13	2.51	0.50
3:C:281:LEU:HB2	3:C:282:PRO:HD3	1.92	0.50
4:E:397:PRO:HA	4:E:400:SER:OG	2.11	0.50
6:G:159:LEU:HD23	6:G:177:LEU:HD12	1.94	0.50
6:H:388:PRO:HD2	6:H:389:PRO:HD3	1.92	0.50
2:O:139:GLY:O	2:O:141:LEU:N	2.45	0.50
2:O:533:ASN:O	2:O:572:LYS:NZ	2.36	0.50
7:M:105:PRO:HB3	7:M:110:PHE:CD2	2.47	0.50
11:U:1037:VAL:HA	11:U:1040:LYS:O	2.11	0.50
1:A:822:LEU:HD12	1:A:867:LYS:CE	2.42	0.50
2:B:521:LEU:O	8:P:565:TYR:HA	2.12	0.50
8:Q:28:VAL:HG23	8:Q:400:ASN:HD21	1.77	0.50
1:S:328:LEU:HD22	1:S:389:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:1213:ILE:HG23	11:U:1250:ILE:CG2	2.42	0.50
12:V:1306:LEU:HD21	12:V:1367:LEU:HB3	1.93	0.50
1:A:33:GLU:O	6:H:311:ASN:ND2	2.45	0.50
2:B:107:TYR:CE1	2:B:130:MET:HE3	2.47	0.50
2:B:534:PRO:HA	2:B:572:LYS:CE	2.41	0.50
2:B:614:TYR:OH	8:P:638:VAL:HA	2.12	0.50
8:P:771:VAL:HG12	8:P:773:MET:SD	2.52	0.50
1:S:56:ASP:OD1	1:S:58:ASN:N	2.42	0.50
10:X:40:GLY:N	10:X:49:GLY:O	2.45	0.50
12:V:466:ASP:OD1	12:V:466:ASP:C	2.53	0.50
2:B:137:LEU:HD11	2:B:173:ALA:HB1	1.93	0.49
8:Q:679:PHE:CZ	8:Q:683:CYS:SG	3.03	0.49
12:V:146:GLN:NE2	12:V:187:VAL:N	2.58	0.49
1:A:653:LEU:O	1:A:657:LEU:HD13	2.12	0.49
2:B:240:VAL:HG11	2:B:256:LEU:HD11	1.94	0.49
2:B:577:ILE:CD1	2:B:649:PHE:CD1	2.95	0.49
6:H:342:THR:HB	6:H:384:PRO:CG	2.42	0.49
8:Q:135:LEU:HD12	8:Q:140:LEU:HD12	1.95	0.49
8:Q:492:VAL:CG2	8:Q:535:PHE:HB3	2.42	0.49
12:V:295:LEU:O	12:V:299:SER:OG	2.29	0.49
2:B:342:LEU:HG	2:B:344:LEU:CD2	2.42	0.49
4:E:465:THR:OG1	4:E:467:GLU:HB3	2.12	0.49
6:G:400:ALA:O	6:G:404:LEU:HG	2.13	0.49
2:O:256:LEU:HD23	2:O:268:PHE:HB2	1.93	0.49
11:U:424:ASN:O	11:U:428:GLU:HG2	2.11	0.49
11:U:662:GLU:OE2	11:U:667:LEU:HD22	2.12	0.49
11:U:745:LEU:O	11:U:749:VAL:HG23	2.13	0.49
12:V:364:TRP:C	12:V:364:TRP:CD1	2.90	0.49
1:A:424:LEU:HD23	1:A:476:PHE:HB2	1.95	0.49
1:A:1368:PHE:CE2	1:A:1392:PRO:HB2	2.47	0.49
2:B:259:LEU:CD1	2:B:284:PRO:HB2	2.42	0.49
6:G:592:TYR:CD1	6:G:592:TYR:C	2.90	0.49
2:O:583:SER:HB3	2:O:586:PRO:HD3	1.93	0.49
2:O:587:LEU:C	2:O:589:THR:H	2.19	0.49
8:Q:33:ALA:O	8:Q:49:GLN:HB2	2.13	0.49
7:M:25:TYR:HB2	7:M:40:ILE:HG23	1.92	0.49
10:X:46:TYR:OH	10:X:75:TYR:O	2.18	0.49
12:V:189:GLY:O	12:V:193:THR:OG1	2.28	0.49
1:A:159:SER:OG	8:P:848:ARG:NH2	2.45	0.49
6:G:54:LEU:HD23	6:G:58:GLN:HG3	1.93	0.49
6:H:191:LEU:HD12	6:H:192:ASP:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:557:ASP:OD1	8:P:557:ASP:N	2.45	0.49
1:S:668:SER:O	1:S:670:ARG:NH1	2.44	0.49
11:U:1056:HIS:CE1	11:U:1069:THR:HG22	2.48	0.49
12:V:277:ASP:O	12:V:278:LEU:C	2.56	0.49
12:V:611:THR:HG22	12:V:651:TRP:CD2	2.47	0.49
6:G:351:ALA:HB1	6:G:367:TYR:CE2	2.48	0.49
8:Q:252:CYS:SG	8:Q:275:LEU:HD11	2.53	0.49
8:Q:510:THR:O	8:Q:645:HIS:CD2	2.65	0.49
10:X:6:ARG:NH1	10:X:100:PRO:O	2.46	0.49
11:U:117:ARG:O	11:U:168:ARG:NH2	2.43	0.49
11:U:324:ASP:N	11:U:324:ASP:OD1	2.44	0.49
1:A:288:GLU:HA	1:A:292:HIS:CB	2.42	0.49
2:B:707:TRP:CH2	2:B:715:GLY:HA3	2.47	0.49
6:G:136:LEU:HD23	6:G:136:LEU:H	1.77	0.49
6:G:518:ILE:HD11	6:G:550:THR:HG22	1.95	0.49
7:L:126:LEU:HD11	7:L:128:TYR:O	2.12	0.49
8:P:224:LEU:O	8:P:227:LEU:HB3	2.13	0.49
12:V:505:SER:O	12:V:509:MET:HE2	2.13	0.49
1:A:286:GLN:C	1:A:288:GLU:N	2.64	0.49
2:B:675:TRP:HZ2	2:B:680:MET:HE3	1.78	0.49
5:F:95:LEU:O	5:F:99:GLU:HG2	2.12	0.49
2:O:585:SER:N	2:O:586:PRO:CD	2.75	0.49
8:P:829:TYR:OH	8:P:879:ILE:CD1	2.60	0.49
11:U:207:LEU:HD23	11:U:210:ILE:HD12	1.95	0.49
8:Q:604:TYR:O	8:Q:638:VAL:HG23	2.12	0.49
1:S:470:LEU:O	1:S:473:LEU:HB2	2.13	0.49
11:U:549:VAL:HG23	11:U:580:ASN:ND2	2.28	0.49
12:V:301:LEU:HD11	12:V:305:LEU:HD12	1.94	0.49
12:V:1190:LEU:HB3	12:V:1241:GLU:HG2	1.95	0.49
3:C:64:PHE:N	3:C:65:PRO:HD2	2.28	0.49
3:C:337:LEU:H	7:L:250:GLU:CD	2.20	0.49
4:E:83:LEU:HD11	7:L:93:VAL:CG2	2.43	0.49
4:E:101:LEU:O	4:E:105:VAL:HG22	2.12	0.49
4:E:387:LEU:HD12	4:E:391:CYS:SG	2.53	0.49
4:E:522:PHE:C	4:E:523:LEU:HG	2.37	0.49
11:U:746:VAL:HG11	11:U:781:LEU:HD11	1.95	0.49
12:V:310:CYS:SG	12:V:311:VAL:N	2.86	0.49
12:V:411:CYS:HB2	12:V:412:ILE:HG13	1.93	0.49
1:A:1368:PHE:HE2	1:A:1392:PRO:HB2	1.78	0.48
2:B:850:ASP:OD1	8:P:874:ARG:NH1	2.44	0.48
4:E:469:PHE:O	4:E:473:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:237:VAL:CG1	2:O:258:ALA:HB1	2.43	0.48
1:S:770:ARG:NH1	1:S:821:LEU:O	2.43	0.48
7:M:234:VAL:HG11	7:M:259:VAL:HG11	1.94	0.48
7:M:261:LYS:CB	7:M:262:PRO:HD3	2.43	0.48
4:E:102:LEU:HA	4:E:105:VAL:HG22	1.96	0.48
5:F:42:ARG:NH2	5:F:127:GLU:O	2.46	0.48
2:O:18:TYR:CE2	2:O:92:PRO:HD3	2.48	0.48
8:P:480:ASN:HA	8:P:483:LEU:HD12	1.94	0.48
8:P:603:PHE:HA	8:P:638:VAL:O	2.14	0.48
8:Q:701:LEU:HG	8:Q:702:PRO:HD2	1.94	0.48
1:S:1368:PHE:CZ	1:S:1392:PRO:HB2	2.48	0.48
11:U:8:LEU:HD22	11:U:16:LYS:HB3	1.95	0.48
2:B:506:LEU:N	2:B:525:ASN:OD1	2.45	0.48
3:C:42:GLN:HE22	3:C:85:GLU:H	1.61	0.48
8:P:594:LEU:O	8:P:595:PRO:C	2.55	0.48
1:S:823:THR:HG23	1:S:829:SER:HB2	1.95	0.48
4:E:391:CYS:O	4:E:395:THR:CA	2.61	0.48
8:P:517:LEU:O	8:P:519:THR:N	2.46	0.48
8:Q:505:PRO:CB	8:Q:533:SER:HB3	2.44	0.48
8:Q:726:VAL:HA	8:Q:727:PRO:HD2	1.62	0.48
1:S:337:SER:HB2	1:S:428:VAL:HG11	1.95	0.48
10:X:49:GLY:HA3	10:X:147:THR:HG23	1.95	0.48
11:U:275:ILE:HG22	11:U:279:ILE:HD11	1.95	0.48
11:U:597:GLN:O	11:U:602:ARG:NH2	2.45	0.48
12:V:243:VAL:CG1	12:V:244:PRO:HD3	2.43	0.48
12:V:1364:LEU:HD23	12:V:1367:LEU:HD21	1.95	0.48
6:G:62:ALA:CB	6:G:102:ARG:HD2	2.42	0.48
6:G:89:THR:N	6:G:92:GLN:OE1	2.41	0.48
6:G:374:LEU:HD13	6:G:393:MET:HE1	1.96	0.48
6:H:193:ALA:HB1	6:H:194:PRO:CD	2.43	0.48
6:H:342:THR:HG21	6:H:384:PRO:CD	2.37	0.48
8:P:709:LYS:HB2	8:P:879:ILE:HG22	1.96	0.48
12:V:275:LEU:O	12:V:279:PRO:CD	2.62	0.48
12:V:282:ILE:HA	12:V:285:ILE:HD12	1.96	0.48
12:V:452:SER:O	12:V:456:LEU:HD23	2.13	0.48
2:B:308:ALA:HB3	2:B:325:LEU:HD13	1.95	0.48
3:C:289:ALA:HB1	4:E:132:TRP:HZ3	1.78	0.48
6:G:255:CYS:SG	6:G:256:HIS:N	2.87	0.48
6:H:23:LEU:HD22	6:H:46:ALA:HA	1.94	0.48
8:P:27:ARG:N	8:P:400:ASN:HD21	2.10	0.48
1:A:263:PRO:O	1:A:267:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:HD23	1:A:725:SER:CB	2.43	0.48
4:E:388:THR:O	4:E:392:ALA:N	2.47	0.48
7:L:134:SER:O	7:L:154:LEU:HD12	2.13	0.48
12:V:435:ILE:O	12:V:438:LEU:HB3	2.14	0.48
1:A:415:MET:HE3	1:A:419:PHE:CE2	2.49	0.48
1:A:939:ILE:O	1:A:1013:GLY:HA2	2.13	0.48
3:C:337:LEU:N	7:L:250:GLU:OE1	2.46	0.48
6:G:479:CYS:SG	6:G:516:ALA:CB	3.01	0.48
6:H:538:LEU:O	6:H:542:GLN:NE2	2.46	0.48
7:L:114:LEU:O	7:L:118:ILE:HD12	2.13	0.48
2:O:229:ILE:CG2	2:O:256:LEU:HD21	2.42	0.48
2:O:774:SER:HB3	8:Q:834:HIS:HB2	1.95	0.48
8:P:711:SER:HA	8:P:782:ILE:HG21	1.95	0.48
1:S:239:VAL:HG11	1:S:301:VAL:HG22	1.95	0.48
11:U:920:GLN:O	11:U:924:GLN:NE2	2.46	0.48
11:U:1052:ASP:O	11:U:1056:HIS:ND1	2.47	0.48
12:V:1279:ILE:HG23	12:V:1341:LEU:HD11	1.96	0.48
4:E:64:LEU:HA	4:E:67:LEU:HD12	1.95	0.48
4:E:429:LEU:HD21	4:E:437:MET:CG	2.44	0.48
4:E:434:GLN:O	4:E:437:MET:HB2	2.13	0.48
6:G:147:ALA:CB	6:G:159:LEU:HD11	2.43	0.48
7:L:311:TYR:HH	7:L:361:TYR:HH	1.55	0.48
2:O:593:PHE:CE1	2:O:622:LEU:HB3	2.48	0.48
1:S:394:SER:HB3	1:S:436:GLN:HE21	1.77	0.48
1:S:558:PHE:O	1:S:561:THR:O	2.32	0.48
1:S:724:THR:HG22	9:W:87:TRP:CH2	2.49	0.48
12:V:922:HIS:HB2	12:V:1001:PHE:CZ	2.49	0.48
1:A:988:LEU:HD23	1:A:1077:MET:HE3	1.96	0.48
2:B:856:LEU:HD23	8:P:867:LEU:HD11	1.96	0.48
3:C:315:ILE:CG2	3:C:399:HIS:HA	2.44	0.48
4:E:288:LEU:HD21	4:E:330:GLN:OE1	2.12	0.48
6:H:177:LEU:HB2	6:H:211:PHE:CE2	2.49	0.48
8:Q:733:LEU:HD22	8:Q:746:VAL:HG11	1.95	0.48
1:S:346:TRP:HE1	1:S:387:GLN:HE21	1.61	0.48
11:U:85:ILE:O	11:U:89:ILE:HG12	2.14	0.48
1:A:753:MET:HE3	1:A:761:VAL:HG21	1.96	0.47
1:A:815:PRO:O	1:A:818:PHE:CE1	2.67	0.47
3:C:287:HIS:ND1	3:C:287:HIS:C	2.72	0.47
8:P:311:CYS:HG	8:P:324:ILE:C	2.21	0.47
8:Q:537:LEU:HD22	8:Q:541:TRP:CD2	2.49	0.47
12:V:613:LEU:O	12:V:617:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG21	1:A:391:SER:HB2	1.96	0.47
2:B:280:PRO:HG2	2:B:321:LYS:HD3	1.95	0.47
2:B:283:ASP:HB3	2:B:304:ILE:HD12	1.96	0.47
2:B:488:VAL:HG12	2:B:581:VAL:HG22	1.95	0.47
4:E:59:ASP:OD1	7:L:166:PHE:HD2	1.97	0.47
6:G:31:GLN:NE2	6:G:320:GLN:OE1	2.45	0.47
6:G:415:THR:HG21	1:S:21:ALA:HB3	1.96	0.47
2:O:17:CYS:SG	2:O:331:ASP:HB2	2.55	0.47
2:O:711:THR:O	2:O:713:PHE:N	2.47	0.47
8:P:196:VAL:O	8:P:244:GLY:N	2.43	0.47
11:U:833:ARG:HA	11:U:839:MET:HE3	1.94	0.47
12:V:68:LEU:HD11	12:V:117:CYS:CB	2.44	0.47
1:A:822:LEU:HD12	1:A:867:LYS:NZ	2.29	0.47
2:B:700:PHE:N	2:B:700:PHE:CD1	2.82	0.47
3:C:196:VAL:O	3:C:199:LEU:N	2.47	0.47
2:O:170:ILE:HG22	2:O:170:ILE:O	2.14	0.47
2:O:523:CYS:O	2:O:525:ASN:ND2	2.47	0.47
8:Q:580:VAL:HG12	8:Q:582:LEU:HD23	1.96	0.47
8:Q:730:CYS:O	8:Q:734:GLN:HG2	2.14	0.47
10:X:54:GLU:HB2	10:X:71:LEU:HD21	1.97	0.47
11:U:619:LEU:O	11:U:623:VAL:HG23	2.14	0.47
11:U:993:SER:HB3	11:U:1006:MET:HE2	1.96	0.47
4:E:449:GLU:HA	4:E:452:LEU:HD12	1.96	0.47
6:G:146:GLN:NE2	6:G:150:TRP:CD2	2.83	0.47
6:G:397:PHE:CZ	8:P:235:LEU:HD22	2.50	0.47
2:O:237:VAL:HG11	2:O:258:ALA:HB1	1.96	0.47
8:P:390:LEU:HG	8:P:390:LEU:O	2.14	0.47
1:S:321:SER:O	1:S:325:THR:OG1	2.31	0.47
11:U:61:GLY:HA2	11:U:64:ARG:HD2	1.95	0.47
11:U:804:LEU:N	11:U:804:LEU:HD12	2.30	0.47
12:V:362:GLU:O	12:V:366:LYS:HG2	2.14	0.47
2:B:530:LEU:HD12	2:B:649:PHE:HE1	1.78	0.47
3:C:336:ALA:HA	7:L:250:GLU:OE2	2.13	0.47
6:G:227:LYS:O	6:G:230:SER:OG	2.32	0.47
7:M:57:TRP:CZ3	7:M:60:ARG:HD3	2.49	0.47
11:U:1153:LEU:HD11	11:U:1162:LEU:HD22	1.96	0.47
4:E:417:THR:HA	4:E:420:LEU:HD12	1.95	0.47
6:H:229:LEU:HD23	6:H:252:LEU:HD23	1.97	0.47
8:P:586:PRO:HD3	8:P:592:LEU:HD12	1.95	0.47
8:P:778:PRO:HD3	8:P:824:ASP:O	2.15	0.47
11:U:237:PHE:CD1	11:U:240:LEU:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:ILE:HG22	3:C:122:LEU:HD22	1.97	0.47
6:H:388:PRO:CD	6:H:389:PRO:HD3	2.45	0.47
7:L:307:CYS:O	7:L:333:PHE:HA	2.14	0.47
2:O:488:VAL:HG11	2:O:650:ALA:HA	1.97	0.47
8:Q:606:LEU:O	8:Q:609:VAL:N	2.48	0.47
1:S:728:GLN:HE21	9:W:87:TRP:CG	2.31	0.47
1:S:1252:GLU:O	1:S:1298:ARG:NH2	2.47	0.47
7:M:31:ALA:O	7:M:34:ARG:HB2	2.14	0.47
7:M:227:ARG:HA	7:M:237:ASN:HA	1.97	0.47
7:M:268:SER:HB2	11:U:469:TYR:O	2.14	0.47
11:U:593:ARG:NE	12:V:182:TRP:HE3	2.13	0.47
12:V:212:ILE:HD11	12:V:245:ILE:HG12	1.97	0.47
2:B:298:PHE:CE1	2:B:312:TRP:CD1	3.03	0.47
2:B:693:PHE:C	2:B:693:PHE:CD1	2.93	0.47
2:B:703:THR:HG22	2:B:705:PHE:CE1	2.50	0.47
3:C:45:LEU:HB3	3:C:89:ILE:HG21	1.97	0.47
4:E:389:SER:O	4:E:392:ALA:HB3	2.14	0.47
6:G:427:LEU:HD21	8:P:226:GLY:CA	2.45	0.47
6:H:387:SER:HB3	6:H:388:PRO:CD	2.43	0.47
8:P:794:LEU:CD2	8:P:867:LEU:HD23	2.45	0.47
1:S:744:PRO:O	1:S:748:LEU:HG	2.15	0.47
7:M:95:LEU:HD22	7:M:102:TYR:OH	2.15	0.47
11:U:463:LEU:O	11:U:467:VAL:HG23	2.14	0.47
11:U:534:LYS:O	11:U:604:MET:HE1	2.14	0.47
1:A:1287:VAL:O	1:A:1291:ILE:HG12	2.15	0.47
3:C:197:ASP:N	3:C:198:PRO:CD	2.78	0.47
6:H:266:LEU:O	6:H:270:VAL:HG23	2.14	0.47
7:L:62:ILE:HG12	7:L:102:TYR:OH	2.15	0.47
8:P:173:VAL:HG23	8:P:258:LEU:HD11	1.96	0.47
7:M:349:ARG:NE	11:U:273:LEU:HD11	2.29	0.47
11:U:593:ARG:NE	12:V:182:TRP:CE3	2.83	0.47
3:C:193:LEU:HD22	5:F:138:ARG:HB3	1.97	0.47
4:E:41:ARG:O	4:E:42:ARG:C	2.57	0.47
7:L:104:LEU:HD12	7:L:104:LEU:HA	1.73	0.47
2:O:141:LEU:HD11	2:O:152:PHE:HB2	1.97	0.47
2:O:522:LYS:C	2:O:523:CYS:HG	1.98	0.47
2:O:590:PHE:C	2:O:592:LYS:H	2.23	0.47
8:P:384:GLU:O	8:P:385:GLU:HG3	2.15	0.47
12:V:276:GLU:O	12:V:279:PRO:HD2	2.15	0.47
2:B:673:LYS:O	2:B:677:LEU:HD22	2.16	0.46
2:O:145:ARG:HG3	2:O:150:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:61:LEU:CD1	1:S:116:MET:HB3	2.45	0.46
11:U:174:VAL:HG11	11:U:201:MET:HG2	1.96	0.46
11:U:390:MET:HE3	11:U:423:ALA:N	2.30	0.46
11:U:750:CYS:SG	11:U:777:CYS:SG	3.13	0.46
12:V:307:LEU:HD11	12:V:380:PHE:CD2	2.51	0.46
8:P:133:PHE:O	8:P:133:PHE:CG	2.67	0.46
11:U:669:CYS:SG	11:U:804:LEU:O	2.73	0.46
11:U:1043:VAL:HA	11:U:1046:LEU:HD12	1.97	0.46
12:V:403:LEU:O	12:V:407:ILE:HG12	2.15	0.46
1:A:650:LEU:HD21	1:A:687:VAL:HG21	1.96	0.46
1:A:818:PHE:HZ	1:A:861:SER:CB	2.29	0.46
1:A:835:LYS:HZ3	1:A:903:TRP:CG	2.32	0.46
2:B:504:VAL:HG21	2:B:578:ILE:HD13	1.97	0.46
3:C:247:LEU:N	3:C:248:PRO:CD	2.79	0.46
4:E:391:CYS:C	4:E:426:MET:HE1	2.40	0.46
6:G:454:ALA:O	6:G:457:LEU:HB3	2.16	0.46
6:H:160:ALA:HB2	6:H:177:LEU:HD21	1.96	0.46
8:P:36:PHE:CD1	8:P:46:VAL:HG22	2.51	0.46
1:S:993:GLN:NE2	1:S:1074:GLU:HB2	2.30	0.46
12:V:728:LEU:HG	12:V:840:LEU:HD11	1.97	0.46
2:B:505:THR:HG22	8:P:548:LEU:HD21	1.98	0.46
8:P:346:PRO:HG2	8:P:363:PRO:HD3	1.97	0.46
1:S:327:ILE:O	1:S:388:ARG:NH1	2.49	0.46
1:S:728:GLN:NE2	9:W:87:TRP:CD2	2.83	0.46
11:U:966:LEU:O	11:U:970:LEU:HG	2.16	0.46
1:A:768:LEU:O	1:A:772:GLN:C	2.59	0.46
8:P:711:SER:OG	8:P:782:ILE:HD13	2.15	0.46
1:S:291:THR:HA	1:S:294:ILE:HD12	1.97	0.46
12:V:132:SER:OG	12:V:133:LYS:N	2.48	0.46
12:V:275:LEU:O	12:V:278:LEU:HB3	2.15	0.46
12:V:526:PRO:HG2	12:V:848:LEU:HD22	1.96	0.46
1:A:48:VAL:HG13	6:H:270:VAL:HG13	1.98	0.46
1:A:166:PHE:CE2	1:A:170:LEU:HD11	2.50	0.46
2:B:722:ARG:O	2:B:722:ARG:CG	2.63	0.46
6:H:198:GLN:HG3	6:H:322:LEU:HD11	1.97	0.46
8:P:850:ARG:CG	8:P:855:ASP:HB2	2.44	0.46
8:Q:348:LEU:HD11	8:Q:363:PRO:HD3	1.98	0.46
11:U:496:VAL:HG11	11:U:535:SER:HB3	1.97	0.46
12:V:534:TYR:CD1	12:V:534:TYR:C	2.93	0.46
1:A:415:MET:HE3	1:A:419:PHE:HE2	1.81	0.46
4:E:106:ARG:N	4:E:107:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:487:MET:HE2	12:V:202:ILE:HG21	1.98	0.46
6:G:480:LEU:HD13	6:G:520:ARG:HH11	1.80	0.46
8:P:77:TYR:HB3	8:P:85:LEU:HD21	1.97	0.46
1:A:108:PRO:HG2	1:A:111:ILE:HD12	1.97	0.46
1:A:1335:PHE:CE2	1:A:1339:LEU:HD12	2.50	0.46
2:B:705:PHE:N	2:B:705:PHE:HD1	2.14	0.46
8:P:196:VAL:O	8:P:243:CYS:HA	2.16	0.46
8:P:860:CYS:SG	8:P:861:ALA:N	2.89	0.46
1:S:113:SER:HB2	1:S:155:LEU:HD13	1.97	0.46
1:S:184:HIS:HA	1:S:187:VAL:HG12	1.96	0.46
12:V:306:ASP:HB2	12:V:308:GLN:HG2	1.97	0.46
2:B:167:PHE:HA	2:B:186:LEU:HD11	1.98	0.46
2:B:526:ARG:NH2	2:B:655:PHE:O	2.49	0.46
3:C:379:VAL:HG13	3:C:390:PRO:HB3	1.97	0.46
7:L:326:ASN:HD22	7:L:364:LYS:HG3	1.80	0.46
8:P:137:ASP:O	8:P:157:GLN:NE2	2.49	0.46
12:V:609:GLN:O	12:V:613:LEU:HD13	2.15	0.46
1:A:900:SER:HG	1:A:903:TRP:CG	2.28	0.46
8:Q:563:ILE:HG22	8:Q:564:THR:N	2.30	0.46
11:U:1036:HIS:CE1	11:U:1042:PRO:HA	2.51	0.46
11:U:1052:ASP:HB3	11:U:1075:VAL:HG11	1.97	0.46
4:E:465:THR:OG1	4:E:468:LYS:HG3	2.16	0.45
6:H:55:HIS:O	2:O:264:GLN:NE2	2.49	0.45
2:O:83:SER:HA	2:O:90:ASN:HA	1.96	0.45
8:P:130:LEU:HA	8:P:144:VAL:HG23	1.97	0.45
1:S:586:ALA:O	1:S:604:ILE:HD11	2.16	0.45
1:S:993:GLN:HE22	1:S:1074:GLU:CB	2.27	0.45
11:U:504:GLN:N	11:U:505:PRO:CD	2.79	0.45
11:U:525:MET:HE1	11:U:537:VAL:HG23	1.98	0.45
12:V:680:VAL:HG22	12:V:700:LEU:HD23	1.98	0.45
2:B:102:ASN:HB3	2:B:104:VAL:HB	1.97	0.45
2:B:308:ALA:HB3	2:B:325:LEU:CD1	2.47	0.45
3:C:57:SER:C	3:C:59:THR:H	2.23	0.45
3:C:190:LEU:HD13	3:C:196:VAL:HG21	1.98	0.45
6:H:387:SER:HB3	6:H:388:PRO:HD2	1.98	0.45
2:O:669:LEU:O	2:O:709:GLN:NE2	2.49	0.45
8:P:23:ALA:HA	8:P:399:LEU:HD12	1.98	0.45
8:Q:506:ILE:HD13	8:Q:531:ASN:HA	1.97	0.45
1:S:868:PHE:CZ	1:S:910:LEU:HD22	2.52	0.45
1:S:1022:GLN:HA	1:S:1085:LEU:HD22	1.97	0.45
1:A:845:LEU:HD23	1:A:856:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:SER:CB	8:P:471:PHE:CE2	3.00	0.45
3:C:539:GLU:N	3:C:539:GLU:OE1	2.50	0.45
4:E:130:ASP:O	4:E:131:ALA:C	2.58	0.45
4:E:371:ARG:O	4:E:375:LEU:HG	2.16	0.45
4:E:391:CYS:SG	4:E:423:LEU:CD2	3.04	0.45
2:O:489:VAL:HG21	2:O:508:LEU:HD21	1.98	0.45
8:P:220:LEU:HD13	8:P:224:LEU:HD22	1.96	0.45
8:P:362:THR:HB	8:P:363:PRO:CD	2.44	0.45
8:Q:642:LEU:O	8:Q:643:SER:C	2.59	0.45
1:S:1331:LEU:N	1:S:1332:PRO:HD2	2.31	0.45
12:V:540:ALA:HA	12:V:551:ILE:HD11	1.97	0.45
1:A:1079:LYS:HG3	1:A:1130:ILE:HD13	1.98	0.45
1:A:1239:GLU:HA	1:A:1242:ILE:HD12	1.97	0.45
2:B:266:ILE:HG22	2:B:267:SER:O	2.16	0.45
3:C:287:HIS:ND1	3:C:288:PRO:HD2	2.31	0.45
3:C:405:GLU:N	3:C:405:GLU:OE1	2.50	0.45
7:L:107:PRO:N	7:L:108:PRO:CD	2.79	0.45
8:P:251:CYS:SG	8:P:274:ILE:HD13	2.57	0.45
8:Q:173:VAL:CG2	8:Q:258:LEU:HD13	2.47	0.45
1:S:566:VAL:CG2	1:S:1274:THR:HG23	2.46	0.45
1:S:1025:VAL:HG21	1:S:1085:LEU:CD1	2.42	0.45
7:M:170:PRO:HB3	7:M:222:SER:O	2.17	0.45
12:V:364:TRP:CZ2	12:V:380:PHE:CE1	3.05	0.45
1:A:835:LYS:HE2	1:A:903:TRP:CZ2	2.52	0.45
2:B:71:ASN:CG	2:B:100:LYS:HG3	2.42	0.45
2:B:414:LEU:HD21	7:L:37:HIS:HB2	1.97	0.45
4:E:435:VAL:HA	4:E:438:LEU:HB3	1.98	0.45
4:E:501:GLN:HG3	4:E:502:ALA:N	2.31	0.45
6:G:388:PRO:CG	8:P:270:ALA:HB1	2.47	0.45
2:O:15:LEU:O	2:O:79:CYS:SG	2.74	0.45
8:P:8:VAL:CG1	8:P:9:ARG:N	2.79	0.45
7:M:307:CYS:SG	7:M:334:HIS:N	2.89	0.45
11:U:8:LEU:HD22	11:U:16:LYS:CB	2.46	0.45
11:U:88:GLU:O	11:U:92:LEU:HD23	2.16	0.45
11:U:1213:ILE:HG23	11:U:1250:ILE:HG21	1.97	0.45
1:A:218:CYS:HB3	1:A:294:ILE:HA	1.99	0.45
1:A:424:LEU:O	1:A:428:VAL:HG23	2.16	0.45
4:E:497:MET:HA	4:E:504:ILE:CD1	2.47	0.45
6:H:176:ASP:OD1	6:H:178:LEU:N	2.49	0.45
6:H:224:ASN:C	6:H:226:ASP:H	2.25	0.45
2:O:522:LYS:HD2	8:Q:563:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:861:ALA:O	8:P:865:ARG:HB2	2.16	0.45
7:M:203:VAL:CG1	7:M:280:VAL:HG21	2.47	0.45
11:U:202:PHE:CE1	11:U:213:LEU:HD23	2.52	0.45
11:U:295:VAL:O	11:U:300:ASP:O	2.35	0.45
11:U:392:SER:HB2	11:U:393:TYR:CD2	2.51	0.45
11:U:814:LEU:HD21	11:U:842:ALA:HB1	1.99	0.45
11:U:843:VAL:O	11:U:847:LEU:HD13	2.16	0.45
1:A:765:LEU:HD11	1:A:787:LEU:HD21	1.99	0.45
5:F:103:LEU:HD21	5:F:111:LEU:HD22	1.99	0.45
7:L:69:ILE:O	7:L:73:ARG:HG2	2.17	0.45
8:Q:733:LEU:CD2	8:Q:746:VAL:HG11	2.46	0.45
12:V:394:GLN:OE1	12:V:394:GLN:N	2.50	0.45
1:A:824:CYS:SG	1:A:825:ARG:N	2.89	0.45
2:B:78:CYS:SG	2:B:134:LEU:HD21	2.57	0.45
6:H:370:LEU:HD11	6:H:374:LEU:HD11	1.99	0.45
2:O:519:ARG:HG3	2:O:520:LEU:O	2.17	0.45
8:P:27:ARG:CA	8:P:400:ASN:ND2	2.80	0.45
8:P:130:LEU:N	8:P:144:VAL:HG23	2.31	0.45
8:P:795:ALA:HB1	8:P:799:ARG:NH2	2.32	0.45
8:Q:42:GLU:OE1	8:Q:62:ASP:N	2.50	0.45
1:A:35:TYR:HE2	6:H:308:GLU:O	2.00	0.45
1:A:335:LYS:O	1:A:335:LYS:HD3	2.16	0.45
2:B:328:VAL:O	2:B:329:LEU:HD23	2.17	0.45
2:B:526:ARG:NH1	8:P:559:ALA:O	2.50	0.45
2:B:669:LEU:HD11	2:B:672:MET:HG2	1.99	0.45
5:F:207:VAL:O	5:F:211:GLN:NE2	2.33	0.45
6:H:353:ARG:O	6:H:357:THR:OG1	2.30	0.45
2:O:726:VAL:O	2:O:730:CYS:SG	2.57	0.45
2:O:756:ILE:HD13	8:Q:859:SER:CB	2.47	0.45
1:S:989:MET:HE1	1:S:1077:MET:CG	2.47	0.45
7:M:326:ASN:HD22	7:M:364:LYS:HG3	1.80	0.45
11:U:706:LEU:O	11:U:710:THR:HG23	2.16	0.45
12:V:306:ASP:HB2	12:V:308:GLN:CG	2.47	0.45
12:V:439:ALA:HA	12:V:457:LEU:HD12	1.98	0.45
3:C:316:GLN:NE2	3:C:405:GLU:OE2	2.50	0.45
7:L:204:MET:HA	7:L:204:MET:HE2	1.99	0.45
8:P:33:ALA:O	8:P:49:GLN:HB2	2.17	0.45
8:P:134:THR:OG1	8:P:135:LEU:N	2.49	0.45
8:Q:28:VAL:HG23	8:Q:400:ASN:ND2	2.32	0.45
11:U:716:SER:HA	11:U:720:ASP:OD2	2.17	0.45
1:A:428:VAL:HG22	1:A:476:PHE:CZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:GLN:O	1:A:1034:LEU:HB3	2.18	0.44
2:B:426:LEU:O	2:B:429:LEU:HB3	2.16	0.44
2:B:660:PHE:CE1	2:B:731:LEU:HD11	2.52	0.44
3:C:338:LYS:HB3	3:C:346:PRO:HG3	1.98	0.44
4:E:344:LEU:HD23	4:E:367:LEU:HD21	1.99	0.44
4:E:391:CYS:SG	4:E:423:LEU:HD21	2.57	0.44
6:H:250:THR:HG21	6:H:281:PRO:HB2	1.99	0.44
8:Q:492:VAL:HG22	8:Q:535:PHE:CB	2.47	0.44
10:X:34:LEU:HB2	10:X:55:VAL:HB	1.99	0.44
11:U:100:PHE:CD2	11:U:105:LEU:HD21	2.52	0.44
11:U:828:SER:O	11:U:831:VAL:HG22	2.16	0.44
12:V:580:THR:O	12:V:584:ILE:HG12	2.18	0.44
12:V:699:LEU:HD22	12:V:762:LEU:HD21	1.99	0.44
12:V:1082:GLU:OE2	12:V:1082:GLU:N	2.51	0.44
1:A:1174:TRP:HB3	1:A:1204:ARG:NH1	2.31	0.44
2:B:170:ILE:HG23	2:B:170:ILE:O	2.18	0.44
4:E:358:SER:O	4:E:362:VAL:HG23	2.17	0.44
6:G:39:ARG:NH2	6:G:319:PRO:O	2.50	0.44
6:H:241:PRO:O	6:H:242:ARG:HB3	2.17	0.44
2:O:397:GLY:HA3	7:M:111:TYR:CE2	2.53	0.44
2:O:500:SER:O	2:O:604:ARG:NH1	2.50	0.44
2:O:651:LEU:CD1	2:O:704:LEU:HD11	2.47	0.44
1:S:872:MET:HE2	1:S:911:TRP:CD1	2.52	0.44
11:U:593:ARG:CZ	12:V:182:TRP:HE3	2.29	0.44
11:U:1180:TYR:HA	11:U:1183:VAL:HG12	1.98	0.44
11:U:1254:ILE:HA	11:U:1257:ILE:HG22	1.99	0.44
1:A:1264:SER:HB2	1:A:1287:VAL:CG1	2.47	0.44
2:B:25:PHE:CD1	2:B:45:VAL:HG22	2.53	0.44
2:B:670:ASN:ND2	2:B:670:ASN:N	2.65	0.44
4:E:294:LEU:HD13	4:E:310:PRO:CG	2.47	0.44
5:F:139:ARG:O	5:F:142:ALA:HB3	2.18	0.44
6:G:497:PHE:CZ	8:P:273:LYS:HB2	2.53	0.44
8:Q:564:THR:O	8:Q:564:THR:OG1	2.29	0.44
1:S:662:ALA:O	1:S:665:THR:HG23	2.18	0.44
12:V:360:ILE:O	12:V:364:TRP:HB2	2.16	0.44
12:V:635:PHE:O	12:V:638:LEU:HB3	2.17	0.44
1:A:320:PHE:CB	1:A:366:LEU:HD11	2.47	0.44
1:A:942:GLU:OE1	1:A:1012:THR:HG23	2.17	0.44
1:A:1201:GLN:HE21	1:A:1205:GLN:NE2	2.15	0.44
3:C:100:LYS:HE2	5:F:109:TYR:CD1	2.52	0.44
3:C:434:ASP:HB3	3:C:438:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:281:PRO:HD3	4:E:323:GLN:HB3	2.00	0.44
5:F:293:ILE:O	5:F:293:ILE:HG13	2.17	0.44
8:P:84:GLY:O	8:P:130:LEU:HD21	2.17	0.44
8:Q:860:CYS:SG	8:Q:861:ALA:N	2.89	0.44
11:U:385:LEU:O	11:U:389:LEU:HD12	2.17	0.44
12:V:786:ILE:HA	12:V:789:THR:HG22	1.99	0.44
12:V:791:ASN:OD1	12:V:925:PHE:HA	2.18	0.44
12:V:922:HIS:HB2	12:V:1001:PHE:CE2	2.53	0.44
2:B:245:THR:HG23	2:B:254:ILE:HG22	2.00	0.44
2:O:481:ARG:HD2	2:O:647:ASP:OD1	2.18	0.44
2:O:520:LEU:HD21	8:Q:565:TYR:CD2	2.50	0.44
8:P:453:GLN:O	8:P:457:GLU:HG3	2.17	0.44
8:P:541:TRP:CE2	8:P:604:TYR:HD2	2.36	0.44
1:S:1404:LEU:HD21	1:S:1432:VAL:HG22	1.99	0.44
11:U:496:VAL:HG12	11:U:500:LEU:HD12	1.99	0.44
11:U:829:LEU:HD23	11:U:832:LEU:HD12	1.99	0.44
12:V:452:SER:O	12:V:456:LEU:CD2	2.65	0.44
12:V:752:ILE:O	12:V:755:LEU:N	2.38	0.44
1:A:286:GLN:HB3	1:A:288:GLU:HG3	2.00	0.44
2:B:241:HIS:CE1	2:B:243:CYS:SG	3.10	0.44
2:B:773:LEU:HA	2:B:838:ILE:HG21	1.99	0.44
4:E:321:PRO:O	4:E:325:ASP:N	2.48	0.44
4:E:522:PHE:CD1	4:E:522:PHE:N	2.83	0.44
5:F:14:LEU:HA	5:F:17:VAL:HG22	2.00	0.44
7:L:106:PRO:C	7:L:108:PRO:HD2	2.43	0.44
1:S:716:HIS:NE2	9:W:92:PRO:HG3	2.33	0.44
7:M:309:ILE:O	10:X:62:PRO:HG3	2.18	0.44
11:U:638:LYS:O	11:U:712:ARG:NH2	2.51	0.44
12:V:792:TRP:NE1	12:V:796:ILE:HD11	2.32	0.44
12:V:1186:LEU:HD11	12:V:1234:PHE:CE1	2.53	0.44
2:B:15:LEU:CD2	2:B:24:VAL:HG22	2.48	0.44
3:C:172:GLN:O	3:C:174:ARG:HG2	2.18	0.44
8:P:200:VAL:HG13	8:P:220:LEU:HG	1.98	0.44
11:U:449:VAL:HG21	12:V:356:TYR:HE2	1.83	0.44
11:U:961:GLN:HG2	11:U:964:ARG:HH22	1.82	0.44
1:A:61:LEU:CD2	1:A:105:LEU:HD11	2.46	0.44
2:B:245:THR:CB	8:P:18:LEU:HD11	2.47	0.44
4:E:86:LEU:O	4:E:89:ARG:HB3	2.18	0.44
4:E:316:LEU:O	4:E:324:MET:HE1	2.17	0.44
6:G:252:LEU:HD13	6:G:268:TYR:CE1	2.53	0.44
2:O:673:LYS:O	2:O:677:LEU:HD22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:850:ASP:O	8:Q:798:CYS:HB3	2.18	0.44
8:P:794:LEU:HD23	8:P:867:LEU:HD23	1.99	0.44
1:S:736:VAL:HG21	9:W:80:VAL:HG21	2.00	0.44
11:U:315:SER:O	11:U:318:ARG:HG2	2.18	0.44
12:V:413:GLN:OE1	12:V:413:GLN:N	2.51	0.44
2:O:499:LEU:HD12	2:O:576:GLN:HG2	1.98	0.44
8:P:35:VAL:HG21	8:P:421:LEU:CD2	2.45	0.44
8:P:37:LEU:C	8:P:37:LEU:HD23	2.43	0.44
8:Q:507:SER:OG	8:Q:530:GLU:HB2	2.18	0.44
1:S:1075:LEU:HD11	1:S:1115:GLU:HB3	1.99	0.44
7:M:256:ALA:HB3	7:M:259:VAL:HG23	1.99	0.44
11:U:72:CYS:HA	11:U:75:LEU:HG	1.98	0.44
12:V:500:VAL:HG12	12:V:507:MET:HG2	1.99	0.44
2:B:228:ILE:HG22	2:B:229:ILE:H	1.83	0.43
2:B:846:GLN:HG3	8:P:878:LEU:HD11	2.00	0.43
3:C:268:CYS:SG	3:C:271:ARG:HG2	2.58	0.43
4:E:31:GLN:HB3	7:L:341:TRP:CH2	2.53	0.43
5:F:260:LEU:O	5:F:263:VAL:HB	2.18	0.43
8:P:147:PRO:O	8:P:149:ARG:N	2.50	0.43
8:P:362:THR:CB	8:P:363:PRO:HD2	2.45	0.43
8:P:471:PHE:CD1	8:P:471:PHE:C	2.95	0.43
8:Q:421:LEU:HD23	8:Q:431:THR:HG22	2.00	0.43
7:M:256:ALA:HB3	7:M:259:VAL:CG2	2.48	0.43
11:U:1037:VAL:HG22	11:U:1042:PRO:HB3	2.00	0.43
12:V:146:GLN:HB3	12:V:187:VAL:CG2	2.47	0.43
12:V:604:ASP:N	12:V:606:GLN:OE1	2.51	0.43
1:A:818:PHE:CZ	1:A:861:SER:CB	3.00	0.43
1:A:1020:ARG:NH1	1:A:1023:GLU:OE1	2.51	0.43
1:A:1206:PHE:CD1	1:A:1206:PHE:C	2.96	0.43
2:B:192:SER:HB2	2:B:194:GLU:OE1	2.17	0.43
2:B:308:ALA:N	2:B:325:LEU:HD12	2.33	0.43
2:B:487:LEU:O	2:B:581:VAL:HA	2.18	0.43
3:C:131:VAL:HG22	5:F:166:GLN:OE1	2.17	0.43
6:G:283:LEU:O	6:G:286:ALA:HB3	2.18	0.43
8:Q:517:LEU:O	8:Q:519:THR:N	2.51	0.43
1:S:1343:HIS:HE2	1:S:1349:ARG:HG3	1.82	0.43
7:M:16:LEU:O	7:M:18:GLN:OE1	2.36	0.43
7:M:300:LYS:HB3	7:M:303:PHE:CD1	2.53	0.43
7:M:311:TYR:HB3	10:X:9:ARG:CD	2.47	0.43
11:U:446:ASN:HD21	12:V:355:ARG:HD2	1.83	0.43
12:V:531:LYS:O	12:V:534:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ALA:O	1:A:420:GLU:HG3	2.18	0.43
2:B:120:MET:HE3	2:B:120:MET:HB2	1.94	0.43
2:B:176:ILE:HD12	2:B:182:VAL:HG21	2.00	0.43
2:B:840:LEU:HD21	8:P:812:VAL:HG11	2.00	0.43
3:C:522:ILE:O	3:C:525:PHE:HB3	2.17	0.43
6:G:427:LEU:HD21	8:P:226:GLY:HA3	1.99	0.43
7:L:80:LEU:O	7:L:83:PHE:HB3	2.18	0.43
7:L:261:LYS:HB3	7:L:262:PRO:HD3	2.00	0.43
8:P:344:PRO:CD	8:P:390:LEU:HD11	2.47	0.43
8:Q:366:LEU:HD12	8:Q:398:SER:OG	2.18	0.43
1:A:27:ALA:HB3	6:H:372:ALA:CB	2.48	0.43
1:A:35:TYR:CD2	6:H:311:ASN:HB2	2.52	0.43
1:A:507:LEU:O	1:A:511:ILE:HG12	2.17	0.43
1:A:1206:PHE:CD2	1:A:1220:PRO:HD3	2.53	0.43
2:B:391:VAL:HB	2:B:392:PRO:HD3	1.99	0.43
2:B:846:GLN:OE1	8:P:877:SER:OG	2.30	0.43
4:E:372:ILE:HA	4:E:375:LEU:HD12	2.00	0.43
5:F:278:LEU:HA	5:F:281:TRP:HB2	2.01	0.43
6:G:354:CYS:O	6:G:357:THR:OG1	2.35	0.43
6:H:186:PRO:HB3	6:H:200:ALA:HB3	2.00	0.43
7:L:357:GLY:O	7:L:366:ILE:CG2	2.64	0.43
11:U:416:GLN:O	11:U:420:LYS:HB2	2.18	0.43
11:U:431:LYS:HB2	11:U:432:ILE:HG23	2.00	0.43
12:V:149:ILE:O	12:V:152:THR:OG1	2.31	0.43
12:V:184:ASP:C	12:V:185:ARG:HG3	2.43	0.43
12:V:731:ALA:HB3	12:V:732:PRO:CD	2.48	0.43
7:L:212:TRP:CD1	7:L:295:ARG:HD3	2.54	0.43
1:S:770:ARG:HD2	1:S:770:ARG:HA	1.86	0.43
12:V:110:PHE:CE2	12:V:114:LEU:HD11	2.54	0.43
12:V:570:TYR:HA	12:V:573:ILE:HD12	1.99	0.43
1:A:835:LYS:HB2	1:A:903:TRP:CZ3	2.53	0.43
1:A:1139:LEU:HD23	1:A:1181:LEU:HD22	1.99	0.43
2:B:259:LEU:HD12	2:B:284:PRO:HB2	2.00	0.43
2:B:426:LEU:CD1	8:P:606:LEU:HD21	2.49	0.43
3:C:150:LEU:CD2	5:F:139:ARG:HG2	2.49	0.43
6:G:555:LEU:HD21	6:G:570:LEU:HB2	2.00	0.43
6:H:186:PRO:HB3	6:H:200:ALA:CB	2.48	0.43
6:H:388:PRO:N	6:H:389:PRO:CD	2.81	0.43
7:L:32:GLN:HG2	7:L:32:GLN:O	2.18	0.43
8:P:28:VAL:HA	8:P:36:PHE:O	2.18	0.43
7:M:256:ALA:HA	7:M:323:VAL:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:272:HIS:CE1	7:M:273:LEU:HD21	2.53	0.43
11:U:546:ASN:O	11:U:547:PHE:CD1	2.71	0.43
12:V:285:ILE:O	12:V:289:VAL:HG13	2.19	0.43
12:V:1078:PHE:HB3	12:V:1087:LEU:HD11	1.99	0.43
1:A:824:CYS:HB2	1:A:938:GLU:HB3	2.01	0.43
2:B:187:LYS:HG2	2:B:229:ILE:HD11	2.01	0.43
8:P:328:TRP:HA	8:P:334:LEU:HA	2.01	0.43
1:S:1087:SER:O	1:S:1137:GLY:HA3	2.19	0.43
7:M:201:TRP:CH2	7:M:221:ARG:HB3	2.54	0.43
12:V:379:VAL:O	12:V:380:PHE:C	2.61	0.43
1:A:497:PRO:HB3	1:A:511:ILE:HD11	2.01	0.43
2:B:484:ASP:N	2:B:484:ASP:OD1	2.52	0.43
3:C:226:ALA:HA	3:C:231:LYS:HE3	2.00	0.43
4:E:290:ARG:O	4:E:294:LEU:HG	2.19	0.43
4:E:485:THR:HG23	4:E:520:THR:OG1	2.19	0.43
6:G:547:ASN:ND2	6:G:550:THR:HG23	2.30	0.43
7:M:248:LEU:HD22	11:U:509:VAL:HG23	1.99	0.43
11:U:665:ASP:OD1	11:U:665:ASP:N	2.52	0.43
11:U:706:LEU:HA	11:U:709:ILE:HD12	2.00	0.43
12:V:1091:LEU:CD2	12:V:1111:LEU:HD12	2.49	0.43
4:E:424:VAL:HA	4:E:429:LEU:HD22	2.00	0.43
4:E:446:TRP:CD1	4:E:450:THR:HG21	2.53	0.43
6:G:430:LYS:NZ	8:P:328:TRP:HB2	2.34	0.43
8:P:83:ARG:CD	8:P:86:TYR:OH	2.67	0.43
8:Q:154:LEU:HD22	8:Q:258:LEU:HD23	2.01	0.43
1:S:313:THR:HA	1:S:316:LEU:HB3	2.00	0.43
1:S:583:PHE:CE1	1:S:613:ILE:HG12	2.54	0.43
1:S:988:LEU:HD21	1:S:1077:MET:CE	2.40	0.43
1:S:992:HIS:CD2	1:S:1073:ARG:NH2	2.87	0.43
11:U:950:SER:OG	11:U:951:VAL:N	2.52	0.43
12:V:432:CYS:SG	12:V:465:PHE:CD2	3.12	0.43
12:V:928:LEU:O	12:V:975:LYS:NZ	2.45	0.43
1:A:279:ASP:O	1:A:283:ALA:HB3	2.19	0.43
1:A:328:LEU:CD2	1:A:389:VAL:HG22	2.49	0.43
1:A:818:PHE:CD2	1:A:818:PHE:C	2.97	0.43
2:B:298:PHE:HE2	2:B:362:LEU:HB2	1.84	0.43
2:B:602:MET:HE1	8:P:546:GLN:NE2	2.33	0.43
2:B:710:ARG:O	2:B:711:THR:OG1	2.32	0.43
4:E:395:THR:C	4:E:399:CYS:HG	2.17	0.43
5:F:278:LEU:HD23	5:F:281:TRP:CE3	2.53	0.43
6:G:586:LEU:N	6:G:586:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:312:TRP:CD1	2:O:319:ALA:HB2	2.54	0.43
8:P:602:LEU:HD21	8:P:642:LEU:CD1	2.49	0.43
8:P:655:PHE:CE2	8:P:754:ILE:CD1	3.02	0.43
1:S:1252:GLU:HB3	1:S:1256:LEU:HD23	2.01	0.43
7:M:233:ASN:HD21	7:M:332:PRO:HG3	1.84	0.43
10:X:140:LEU:O	10:X:144:ARG:HB2	2.19	0.43
11:U:392:SER:HB2	11:U:393:TYR:CE2	2.54	0.43
6:G:416:LEU:HD13	1:S:22:TRP:CH2	2.54	0.42
6:H:67:LEU:HD11	6:H:106:THR:HG21	2.01	0.42
2:O:583:SER:HB3	2:O:586:PRO:CD	2.49	0.42
8:P:311:CYS:HA	8:P:324:ILE:O	2.18	0.42
1:S:415:MET:SD	1:S:451:TRP:HZ2	2.41	0.42
12:V:456:LEU:HD12	12:V:460:TYR:CE2	2.54	0.42
1:A:940:GLN:HA	1:A:1013:GLY:HA2	2.01	0.42
1:A:1127:THR:HG22	1:A:1129:ASP:H	1.85	0.42
2:B:329:LEU:HD12	2:B:342:LEU:HD23	2.01	0.42
4:E:333:LEU:N	4:E:334:PRO:CD	2.82	0.42
7:L:154:LEU:HD23	7:L:163:PRO:HB3	2.00	0.42
7:L:207:ILE:O	7:L:211:THR:OG1	2.28	0.42
2:O:483:ILE:HG22	2:O:484:ASP:H	1.84	0.42
1:S:351:THR:CG2	1:S:391:SER:HB2	2.40	0.42
1:S:992:HIS:O	1:S:1073:ARG:NH2	2.52	0.42
11:U:500:LEU:HA	11:U:503:VAL:HG12	2.01	0.42
11:U:768:PHE:CE1	11:U:832:LEU:HD11	2.55	0.42
1:A:28:GLY:O	1:A:30:VAL:N	2.44	0.42
1:A:1139:LEU:CD2	1:A:1181:LEU:HD22	2.49	0.42
2:B:93:TYR:HB2	2:B:109:LEU:HD11	2.00	0.42
2:B:307:ASN:C	2:B:325:LEU:HD12	2.43	0.42
3:C:371:ILE:HG21	3:C:397:PHE:HE1	1.82	0.42
4:E:487:MET:SD	12:V:202:ILE:HG21	2.59	0.42
4:E:517:GLU:CB	4:E:518:PRO:CD	2.98	0.42
6:H:244:VAL:O	6:H:248:VAL:HG23	2.19	0.42
2:O:590:PHE:C	2:O:592:LYS:N	2.76	0.42
8:Q:147:PRO:O	8:Q:148:ALA:C	2.61	0.42
8:Q:484:THR:OG1	8:Q:485:SER:N	2.52	0.42
8:Q:648:ASP:O	8:Q:649:MET:HB2	2.19	0.42
1:S:1008:PHE:O	1:S:1008:PHE:CG	2.73	0.42
11:U:2:ASP:HB2	11:U:46:LEU:HD21	2.01	0.42
12:V:339:GLY:C	12:V:343:ILE:HD12	2.44	0.42
12:V:686:LEU:HD13	12:V:811:LYS:HG2	2.01	0.42
3:C:146:TYR:CB	3:C:147:PRO:HD3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:193:ALA:HB1	6:G:194:PRO:HD2	2.02	0.42
6:H:67:LEU:HB2	6:H:68:PRO:HD3	2.02	0.42
7:L:139:LYS:HA	7:L:149:LEU:HD23	2.01	0.42
2:O:766:GLU:N	2:O:845:VAL:HG11	2.34	0.42
8:Q:653:LEU:HD23	8:Q:758:ALA:HA	2.01	0.42
1:S:665:THR:CA	9:W:80:VAL:HG22	2.48	0.42
1:S:874:ARG:O	1:S:946:LEU:HD11	2.18	0.42
11:U:106:VAL:O	11:U:110:ASN:ND2	2.52	0.42
12:V:194:THR:O	12:V:198:GLN:NE2	2.52	0.42
12:V:198:GLN:O	12:V:202:ILE:HG23	2.19	0.42
12:V:1239:MET:SD	12:V:1297:TYR:HB2	2.60	0.42
2:B:279:LEU:HA	2:B:280:PRO:HD3	1.92	0.42
2:B:409:ARG:O	2:B:413:LEU:HG	2.19	0.42
4:E:381:ARG:HH21	12:V:309:HIS:HB2	1.85	0.42
6:G:67:LEU:HD21	6:G:103:VAL:HA	2.00	0.42
6:G:414:LEU:HD21	6:G:462:ALA:HB3	2.01	0.42
7:L:25:TYR:CD1	7:L:25:TYR:N	2.88	0.42
8:P:60:PHE:N	8:P:60:PHE:CD1	2.86	0.42
8:P:267:ASP:OD1	8:P:269:ASN:ND2	2.51	0.42
8:P:341:TYR:N	8:P:341:TYR:CD1	2.86	0.42
1:A:818:PHE:HA	1:A:821:LEU:HD13	2.00	0.42
1:A:1103:ALA:O	1:A:1104:ARG:HB2	2.20	0.42
2:B:401:CYS:HB2	8:P:465:ILE:HG21	2.01	0.42
2:B:652:LEU:CD2	2:B:720:TYR:CE2	3.02	0.42
2:O:488:VAL:HG12	2:O:488:VAL:O	2.19	0.42
2:O:614:TYR:CG	8:Q:639:CYS:HB3	2.54	0.42
8:Q:466:SER:CA	7:M:107:PRO:HB2	2.32	0.42
12:V:286:LEU:HA	12:V:289:VAL:HG22	2.02	0.42
12:V:404:ARG:NH2	12:V:441:SER:OG	2.53	0.42
12:V:490:ASP:OD1	12:V:528:GLN:NE2	2.52	0.42
12:V:1313:LEU:HD13	12:V:1324:VAL:HB	2.02	0.42
2:B:281:PHE:CD2	2:B:307:ASN:CG	2.98	0.42
2:B:502:ASN:HB3	2:B:601:ILE:HG23	2.00	0.42
4:E:71:GLU:OE1	4:E:71:GLU:HA	2.20	0.42
5:F:317:ALA:HB1	5:F:318:PRO:HD2	2.02	0.42
6:G:447:TYR:CE1	6:G:488:PRO:O	2.71	0.42
7:L:36:PHE:CB	7:L:59:LEU:HD13	2.48	0.42
8:P:60:PHE:CE1	8:P:118:VAL:HG21	2.55	0.42
8:P:133:PHE:CD2	8:P:133:PHE:C	2.95	0.42
1:S:346:TRP:CZ3	1:S:386:TRP:HB3	2.55	0.42
1:S:558:PHE:O	1:S:561:THR:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1195:ARG:O	1:S:1199:LYS:HG3	2.20	0.42
1:S:1261:PHE:HB2	1:S:1291:ILE:HG21	2.01	0.42
7:M:107:PRO:N	7:M:108:PRO:CD	2.82	0.42
11:U:383:VAL:HG21	11:U:436:ILE:HG21	2.00	0.42
12:V:157:LEU:N	12:V:158:PRO:CD	2.82	0.42
12:V:793:PHE:HA	12:V:796:ILE:HD12	2.01	0.42
1:A:1090:LEU:HD22	1:A:1108:PHE:CE1	2.55	0.42
1:A:1368:PHE:CZ	1:A:1392:PRO:HG2	2.54	0.42
5:F:158:GLN:HA	5:F:207:VAL:HG13	2.01	0.42
7:L:282:GLN:NE2	7:L:286:ASP:OD2	2.53	0.42
2:O:506:LEU:HD23	2:O:507:SER:O	2.19	0.42
2:O:514:HIS:CE1	2:O:593:PHE:HA	2.54	0.42
2:O:534:PRO:HA	2:O:572:LYS:HD2	2.00	0.42
2:O:598:LEU:HD22	8:Q:603:PHE:CD2	2.54	0.42
1:S:1262:PHE:CD1	1:S:1262:PHE:C	2.98	0.42
7:M:306:ASP:OD1	7:M:313:TYR:HB2	2.19	0.42
12:V:1096:SER:O	12:V:1100:GLN:NE2	2.53	0.42
1:A:137:LEU:O	1:A:137:LEU:HD12	2.20	0.42
1:A:1027:ASP:OD2	1:S:1184:ARG:NH2	2.51	0.42
3:C:196:VAL:O	3:C:199:LEU:HB3	2.20	0.42
4:E:395:THR:C	4:E:399:CYS:SG	3.02	0.42
5:F:345:SER:O	5:F:348:THR:OG1	2.36	0.42
12:V:1226:LEU:HD21	12:V:1234:PHE:CE2	2.55	0.42
12:V:1249:ILE:HD11	12:V:1267:TYR:HE2	1.84	0.42
1:A:769:LEU:HD13	1:A:821:LEU:HD11	2.02	0.42
1:A:1305:LEU:HA	1:A:1308:LEU:HD21	2.02	0.42
4:E:360:ALA:O	4:E:364:THR:OG1	2.38	0.42
7:L:319:ILE:HG23	7:L:320:PRO:HD2	2.02	0.42
2:O:624:LEU:HD12	2:O:624:LEU:HA	1.80	0.42
2:O:658:SER:OG	2:O:727:MET:HE2	2.19	0.42
8:P:83:ARG:HD3	8:P:86:TYR:HH	1.83	0.42
7:M:361:TYR:CD1	10:X:101:SER:CB	2.89	0.42
11:U:581:GLU:O	11:U:585:LEU:HG	2.20	0.42
12:V:273:ILE:HG21	12:V:281:ILE:HD13	2.01	0.42
1:A:1101:ILE:HG21	1:A:1154:PHE:CE2	2.55	0.41
1:A:1220:PRO:O	1:A:1253:ARG:NH2	2.53	0.41
1:A:1343:HIS:CE1	1:A:1348:ILE:HB	2.55	0.41
5:F:27:ASP:HB2	5:F:28:PRO:HD2	2.01	0.41
6:G:254:SER:HA	6:G:285:GLU:OE2	2.20	0.41
7:L:17:PRO:O	8:P:490:MET:SD	2.78	0.41
8:Q:325:LYS:HE2	8:Q:384:GLU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:60:LEU:HD22	1:S:94:ILE:HG23	2.02	0.41
1:S:584:LEU:HB2	1:S:585:PRO:CD	2.50	0.41
1:S:736:VAL:CG2	9:W:80:VAL:HG21	2.50	0.41
11:U:372:VAL:HG13	11:U:373:HIS:CD2	2.55	0.41
12:V:307:LEU:HD12	12:V:380:PHE:HA	2.01	0.41
2:B:188:GLU:O	2:B:225:ASP:HB2	2.20	0.41
2:B:602:MET:HE2	8:P:546:GLN:HE21	1.85	0.41
3:C:277:LYS:HG3	3:C:321:CYS:SG	2.61	0.41
3:C:501:GLY:O	3:C:502:HIS:ND1	2.52	0.41
5:F:203:LYS:O	5:F:207:VAL:HG23	2.20	0.41
6:G:62:ALA:HB2	6:G:102:ARG:HD2	2.01	0.41
6:G:310:LEU:HD21	6:G:340:CYS:SG	2.60	0.41
8:Q:531:ASN:ND2	8:Q:573:GLY:O	2.53	0.41
1:S:977:LEU:HB2	1:S:1028:LEU:HD21	2.02	0.41
11:U:210:ILE:HD13	11:U:236:PHE:CE2	2.55	0.41
12:V:171:ASN:HD21	12:V:174:ARG:NE	2.17	0.41
12:V:215:LEU:N	12:V:216:PRO:CD	2.83	0.41
1:A:156:LEU:O	8:P:848:ARG:NH2	2.53	0.41
1:A:348:PHE:CZ	1:A:356:THR:CG2	3.03	0.41
1:A:868:PHE:CZ	1:A:910:LEU:HD23	2.55	0.41
3:C:216:GLN:HB3	3:C:218:GLU:OE2	2.21	0.41
4:E:294:LEU:HD13	4:E:310:PRO:HG3	2.02	0.41
6:G:146:GLN:NE2	6:G:146:GLN:O	2.53	0.41
1:S:670:ARG:O	1:S:674:SER:OG	2.38	0.41
7:M:204:MET:HE3	7:M:204:MET:HB2	1.93	0.41
10:X:78:ASN:ND2	10:X:119:ASN:O	2.39	0.41
11:U:810:VAL:HG21	11:U:845:VAL:CG1	2.51	0.41
12:V:101:GLU:HA	12:V:104:ILE:CG1	2.49	0.41
12:V:1111:LEU:HD23	12:V:1142:LEU:HD23	2.02	0.41
1:A:21:ALA:HA	6:H:415:THR:CG2	2.51	0.41
1:A:398:VAL:HG11	2:B:813:ARG:NH1	2.35	0.41
2:B:15:LEU:HB2	2:B:327:LEU:CD1	2.50	0.41
3:C:278:ASP:C	3:C:279:SER:O	2.62	0.41
6:G:280:GLY:N	6:G:281:PRO:CD	2.83	0.41
6:G:284:LEU:O	6:G:287:SER:OG	2.22	0.41
6:H:541:VAL:HG13	6:H:551:TYR:CZ	2.55	0.41
6:H:571:TRP:HH2	6:H:611:GLU:N	2.18	0.41
2:O:481:ARG:CD	2:O:647:ASP:OD1	2.68	0.41
2:O:483:ILE:O	2:O:484:ASP:C	2.62	0.41
8:P:316:GLY:O	8:P:347:VAL:HB	2.21	0.41
8:P:392:PRO:C	8:P:393:MET:CG	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:594:LEU:O	8:P:596:VAL:HG12	2.20	0.41
1:S:139:VAL:HG12	1:S:140:GLU:N	2.36	0.41
1:S:665:THR:HA	9:W:80:VAL:HA	2.02	0.41
1:S:859:CYS:SG	1:S:860:LEU:N	2.94	0.41
1:S:988:LEU:CD2	1:S:1077:MET:HE2	2.45	0.41
11:U:492:PRO:O	11:U:495:THR:OG1	2.38	0.41
1:A:993:GLN:HE22	1:A:1074:GLU:CG	2.33	0.41
2:B:237:VAL:HG13	2:B:258:ALA:HB1	2.02	0.41
2:B:324:LYS:O	2:B:325:LEU:C	2.63	0.41
2:B:483:ILE:HD13	2:B:634:LEU:HD12	2.02	0.41
2:B:777:ILE:HG23	2:B:830:VAL:HG13	2.03	0.41
3:C:254:MET:HB3	3:C:297:MET:HE1	2.02	0.41
4:E:524:ARG:O	4:E:528:LYS:N	2.36	0.41
5:F:44:ILE:HG23	5:F:48:PHE:CZ	2.55	0.41
8:P:45:TYR:CD1	8:P:45:TYR:N	2.88	0.41
8:P:711:SER:HB2	8:P:881:LEU:HD23	2.02	0.41
7:M:251:CYS:O	7:M:251:CYS:SG	2.78	0.41
11:U:928:GLN:HE22	11:U:950:SER:C	2.29	0.41
12:V:172:ILE:N	12:V:173:PRO:CD	2.84	0.41
12:V:1264:LYS:HE3	12:V:1312:LEU:HD22	2.02	0.41
1:A:1249:LEU:HD12	1:A:1252:GLU:HB2	2.02	0.41
2:B:191:LEU:HD23	2:B:197:THR:N	2.35	0.41
3:C:42:GLN:NE2	3:C:85:GLU:H	2.19	0.41
3:C:87:GLN:O	3:C:91:ILE:HG12	2.20	0.41
8:Q:874:ARG:HA	8:Q:874:ARG:HE	1.86	0.41
7:M:265:ILE:CD1	11:U:469:TYR:OH	2.67	0.41
7:M:309:ILE:HD11	7:M:360:PRO:HG2	2.02	0.41
7:M:343:ARG:HH12	7:M:350:GLN:HE22	1.68	0.41
11:U:290:VAL:O	11:U:294:LYS:N	2.54	0.41
12:V:51:LEU:HD23	12:V:54:ILE:HD11	2.01	0.41
12:V:146:GLN:CD	12:V:187:VAL:H	2.28	0.41
12:V:1197:LEU:HD13	12:V:1270:MET:HG3	2.02	0.41
12:V:1211:LEU:HD13	12:V:1284:VAL:HG21	2.02	0.41
1:A:182:VAL:O	1:A:185:LEU:HB2	2.20	0.41
1:A:468:LYS:O	1:A:472:PHE:HD2	2.03	0.41
3:C:186:VAL:HG13	5:F:145:MET:HE3	2.02	0.41
6:H:53:LEU:O	6:H:57:LEU:HG	2.20	0.41
2:O:132:ASP:OD1	2:O:132:ASP:N	2.53	0.41
2:O:265:LEU:CD2	2:O:311:VAL:HG21	2.51	0.41
2:O:532:THR:HB	2:O:573:GLU:HG2	2.03	0.41
2:O:614:TYR:CD1	8:Q:639:CYS:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:147:PRO:O	8:P:148:ALA:C	2.63	0.41
8:Q:141:VAL:HG21	8:Q:241:VAL:HG21	2.03	0.41
8:Q:565:TYR:N	8:Q:565:TYR:CD1	2.89	0.41
1:S:827:ARG:HA	1:S:830:LEU:HD12	2.01	0.41
7:M:15:LEU:HD23	7:M:26:GLU:O	2.20	0.41
12:V:184:ASP:O	12:V:185:ARG:CG	2.69	0.41
12:V:637:ASN:O	12:V:641:HIS:ND1	2.46	0.41
12:V:752:ILE:O	12:V:754:GLY:N	2.53	0.41
1:A:27:ALA:HB3	6:H:372:ALA:HB2	2.02	0.41
1:A:286:GLN:O	1:A:288:GLU:N	2.48	0.41
2:B:82:VAL:O	2:B:83:SER:OG	2.34	0.41
6:H:128:ALA:HA	6:H:131:LEU:HD13	2.03	0.41
6:H:191:LEU:O	6:H:193:ALA:N	2.53	0.41
6:H:196:THR:OG1	6:H:198:GLN:O	2.19	0.41
2:O:253:ARG:HG3	2:O:270:ASN:HD22	1.86	0.41
2:O:591:SER:HA	2:O:624:LEU:HD22	2.03	0.41
8:P:368:VAL:HG12	8:P:391:PRO:HG2	2.01	0.41
8:P:488:GLU:O	8:P:492:VAL:HG23	2.21	0.41
8:Q:74:ARG:HD2	8:Q:90:LEU:HD12	2.02	0.41
1:S:328:LEU:HD22	1:S:389:VAL:CG2	2.51	0.41
1:S:1079:LYS:HG3	1:S:1130:ILE:CD1	2.51	0.41
7:M:365:PRO:CB	11:U:266:HIS:CE1	3.04	0.41
11:U:275:ILE:O	11:U:279:ILE:HG13	2.20	0.41
11:U:1092:ALA:O	11:U:1096:LEU:HG	2.21	0.41
1:A:43:LEU:HD11	6:H:308:GLU:CB	2.50	0.41
2:B:13:GLU:HB3	2:B:26:GLN:HG3	2.03	0.41
2:B:330:ILE:N	2:B:330:ILE:HD12	2.36	0.41
2:B:332:ASP:OD1	2:B:335:GLY:N	2.43	0.41
2:B:393:PRO:HA	7:L:131:THR:HA	2.02	0.41
2:B:524:GLN:O	2:B:580:ALA:HA	2.21	0.41
3:C:15:TRP:HZ3	3:C:37:HIS:HB3	1.86	0.41
3:C:81:LEU:HD21	3:C:121:ILE:HG23	2.03	0.41
3:C:300:CYS:HB2	4:E:164:LEU:CD2	2.51	0.41
4:E:472:LEU:O	4:E:476:LEU:CB	2.69	0.41
5:F:204:VAL:O	5:F:207:VAL:N	2.54	0.41
5:F:255:LEU:HB3	5:F:256:PRO:HD2	2.03	0.41
6:G:421:LEU:HG	6:G:455:THR:HG21	2.02	0.41
2:O:155:SER:O	2:O:156:GLN:CB	2.67	0.41
2:O:487:LEU:HB2	2:O:584:LEU:CD2	2.51	0.41
2:O:774:SER:CB	8:Q:834:HIS:HB2	2.51	0.41
8:P:43:LEU:HD13	8:P:59:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:54:LEU:HD11	8:P:114:PRO:HB2	2.01	0.41
8:P:253:VAL:HG23	8:P:272:VAL:CA	2.49	0.41
8:Q:30:CYS:SG	8:Q:402:CYS:SG	3.08	0.41
8:Q:537:LEU:HD22	8:Q:541:TRP:CE2	2.56	0.41
1:S:589:THR:N	1:S:590:PRO:CD	2.84	0.41
7:M:311:TYR:OH	7:M:361:TYR:OH	2.34	0.41
7:M:361:TYR:CE1	10:X:101:SER:HB3	2.51	0.41
10:X:54:GLU:HB2	10:X:71:LEU:HD11	2.03	0.41
11:U:56:CYS:SG	11:U:62:THR:HG22	2.61	0.41
11:U:65:ARG:HA	11:U:68:ILE:HG22	2.02	0.41
11:U:202:PHE:HA	11:U:205:MET:SD	2.60	0.41
11:U:488:LEU:HD11	11:U:496:VAL:HG13	2.02	0.41
11:U:1142:LEU:HD11	11:U:1205:LEU:HD22	2.03	0.41
12:V:1078:PHE:O	12:V:1084:GLN:NE2	2.54	0.41
1:A:1343:HIS:HE2	1:A:1349:ARG:HG3	1.86	0.41
2:B:139:GLY:O	2:B:140:PRO:C	2.64	0.41
3:C:189:PRO:HG2	3:C:190:LEU:HG	2.03	0.41
4:E:99:MET:HB2	4:E:136:LEU:HD13	2.03	0.41
4:E:288:LEU:N	4:E:289:PRO:HD2	2.36	0.41
5:F:131:GLU:O	5:F:134:ALA:HB3	2.21	0.41
6:G:384:PRO:HB2	6:G:385:PRO:HD2	2.03	0.41
7:L:212:TRP:CE2	7:L:214:LEU:HD12	2.56	0.41
8:P:21:LEU:HD12	8:P:423:LEU:HD21	2.02	0.41
8:P:253:VAL:HG23	8:P:272:VAL:HG23	2.02	0.41
8:P:360:HIS:ND1	8:P:367:CYS:O	2.54	0.41
8:P:446:MET:HE1	8:P:451:ALA:HB2	2.03	0.41
8:Q:249:GLN:HA	8:Q:277:HIS:HA	2.01	0.41
1:S:419:PHE:CE1	1:S:427:MET:SD	3.13	0.41
1:S:737:ALA:CB	1:S:738:PRO:HD2	2.48	0.41
11:U:439:GLU:O	11:U:443:GLN:NE2	2.54	0.41
11:U:445:LEU:O	11:U:448:VAL:HB	2.21	0.41
11:U:1095:VAL:HG11	11:U:1141:LEU:HD11	2.03	0.41
12:V:1370:ARG:O	12:V:1374:MET:HG2	2.21	0.41
1:A:193:LEU:HD11	1:A:238:PHE:CE1	2.56	0.40
1:A:375:LEU:HD11	1:A:392:PHE:HE1	1.86	0.40
1:A:651:GLY:O	1:A:654:THR:OG1	2.35	0.40
2:B:253:ARG:HE	2:B:270:ASN:HD22	1.68	0.40
3:C:49:TYR:CE1	3:C:92:TRP:HB3	2.57	0.40
3:C:165:HIS:CE1	3:C:206:CYS:HA	2.55	0.40
3:C:370:HIS:ND1	7:L:272:HIS:HA	2.36	0.40
4:E:319:CYS:SG	4:E:327:LEU:HD22	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:346:THR:H	4:E:346:THR:HG1	1.66	0.40
6:H:388:PRO:HD2	6:H:389:PRO:CD	2.51	0.40
7:L:15:LEU:HD23	7:L:15:LEU:HA	1.95	0.40
2:O:522:LYS:HG2	2:O:523:CYS:N	2.37	0.40
8:P:829:TYR:OH	8:P:879:ILE:HD13	2.21	0.40
8:P:875:HIS:HB3	8:P:876:PRO:HD3	2.03	0.40
7:M:197:LEU:O	7:M:198:LYS:C	2.64	0.40
10:X:75:TYR:OH	10:X:131:GLU:OE1	2.35	0.40
11:U:511:MET:HE3	11:U:511:MET:HB3	2.02	0.40
1:A:245:ARG:NH2	1:A:262:MET:HA	2.35	0.40
1:A:1305:LEU:C	1:A:1308:LEU:CD2	2.94	0.40
1:A:1425:ARG:HB2	1:A:1425:ARG:NH1	2.32	0.40
2:B:98:LYS:HB3	2:B:106:GLU:HB2	2.02	0.40
2:B:163:VAL:HG13	2:B:191:LEU:HD11	2.03	0.40
2:B:326:SER:OG	2:B:346:LYS:HA	2.21	0.40
2:B:700:PHE:N	2:B:700:PHE:HD1	2.20	0.40
4:E:83:LEU:HD21	7:L:93:VAL:CG2	2.51	0.40
4:E:284:ILE:CG2	4:E:327:LEU:HD13	2.51	0.40
2:O:418:ILE:HD11	7:M:37:HIS:NE2	2.36	0.40
2:O:645:MET:SD	2:O:687:GLU:HG3	2.61	0.40
1:S:843:TYR:CD1	1:S:843:TYR:C	2.99	0.40
7:M:15:LEU:HD23	7:M:15:LEU:HA	1.95	0.40
12:V:92:ILE:O	12:V:96:PHE:HB2	2.21	0.40
2:B:601:ILE:C	2:B:602:MET:SD	3.05	0.40
4:E:429:LEU:O	4:E:434:GLN:NE2	2.40	0.40
5:F:108:ARG:O	5:F:111:LEU:HB3	2.21	0.40
2:O:634:LEU:HD21	2:O:647:ASP:CG	2.46	0.40
8:Q:517:LEU:O	8:Q:518:GLN:C	2.64	0.40
1:S:1056:LEU:O	1:S:1071:ARG:NH2	2.53	0.40
1:S:1075:LEU:HD12	1:S:1119:PHE:CD2	2.50	0.40
7:M:55:CYS:HB3	7:M:59:LEU:HB3	2.02	0.40
7:M:320:PRO:HA	7:M:333:PHE:O	2.21	0.40
11:U:237:PHE:HA	11:U:240:LEU:HD12	2.03	0.40
11:U:601:VAL:O	11:U:605:LEU:HD23	2.22	0.40
11:U:966:LEU:HA	11:U:985:LEU:HD13	2.03	0.40
1:A:275:ILE:HG23	1:A:330:HIS:CE1	2.56	0.40
1:A:384:VAL:HG13	1:A:389:VAL:HG21	2.03	0.40
1:A:822:LEU:HD12	1:A:867:LYS:HE2	2.04	0.40
1:A:837:CYS:HA	1:A:864:LEU:HD21	2.02	0.40
2:B:421:LYS:CG	7:L:18:GLN:HE21	2.34	0.40
6:G:184:TRP:O	6:G:204:LYS:NZ	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:398:LEU:HD12	6:G:592:TYR:CE2	2.57	0.40
2:O:229:ILE:HG23	2:O:256:LEU:HD21	2.03	0.40
2:O:708:LYS:HB2	2:O:716:ILE:HG22	2.02	0.40
1:S:874:ARG:NH2	1:S:944:ASP:OD1	2.55	0.40
11:U:595:LEU:HA	11:U:602:ARG:HG2	2.04	0.40
11:U:963:GLN:HE22	11:U:1005:GLN:HE22	1.69	0.40
12:V:161:PHE:HB3	12:V:162:PHE:CE1	2.56	0.40
12:V:222:SER:OG	12:V:223:GLN:OE1	2.33	0.40
12:V:738:ARG:HD2	12:V:799:ALA:HA	2.04	0.40
12:V:1123:GLN:O	12:V:1165:ARG:NH2	2.54	0.40
1:A:1254:GLU:OE1	1:A:1254:GLU:HA	2.22	0.40
6:G:548:ARG:NH2	6:G:606:ASP:OD1	2.54	0.40
6:H:54:LEU:O	6:H:58:GLN:HG2	2.22	0.40
7:L:65:GLY:C	7:L:66:TYR:CD1	2.99	0.40
2:O:777:ILE:HD13	8:Q:830:LEU:HD13	2.04	0.40
1:S:1186:ARG:O	1:S:1190:GLN:NE2	2.46	0.40
12:V:610:VAL:O	12:V:614:LEU:HG	2.21	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	S	1224/1477 (83%)	1115 (91%)	100 (8%)	9 (1%)	18	54
2	B	74/884 (8%)	72 (97%)	2 (3%)	0	100	100
2	O	685/884 (78%)	590 (86%)	79 (12%)	16 (2%)	5	29
3	C	546/583 (94%)	475 (87%)	69 (13%)	2 (0%)	30	66
4	E	121/555 (22%)	111 (92%)	10 (8%)	0	100	100
6	H	248/641 (39%)	224 (90%)	22 (9%)	2 (1%)	16	52
7	L	368/394 (93%)	328 (89%)	40 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	368/394 (93%)	328 (89%)	38 (10%)	2 (0%)	24	62
8	P	726/906 (80%)	616 (85%)	94 (13%)	16 (2%)	5	29
8	Q	732/906 (81%)	636 (87%)	81 (11%)	15 (2%)	6	32
9	W	21/39 (54%)	13 (62%)	7 (33%)	1 (5%)	2	17
10	X	151/197 (77%)	146 (97%)	3 (2%)	2 (1%)	9	41
11	U	1150/1328 (87%)	1053 (92%)	91 (8%)	6 (0%)	24	62
12	V	1131/1451 (78%)	1047 (93%)	78 (7%)	6 (0%)	24	62
All	All	7545/10639 (71%)	6754 (90%)	714 (10%)	77 (1%)	15	47

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	84	ASP
6	H	387	SER
2	O	83	SER
2	O	147	VAL
2	O	249	LYS
8	P	66	HIS
8	P	148	ALA
8	P	550	SER
8	P	781	PRO
8	Q	557	ASP
8	Q	643	SER
8	Q	649	MET
1	S	288	GLU
1	S	947	SER
1	S	975	GLY
2	O	314	GLU
2	O	637	PRO
8	P	63	GLN
8	P	354	GLY
8	P	782	ILE
8	Q	50	GLU
8	Q	148	ALA
8	Q	397	ALA
8	Q	607	ARG
1	S	338	ASP
1	S	689	GLY
1	S	737	ALA
9	W	80	VAL

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Mol	Chain	Res	Type
7	M	103	ALA
11	U	296	GLY
12	V	414	GLU
3	C	233	SER
2	O	132	ASP
2	O	324	LYS
2	O	325	LEU
2	O	354	LEU
8	P	137	ASP
8	P	557	ASP
8	Q	518	GLN
8	Q	588	GLU
11	U	356	HIS
11	U	978	ASN
12	V	753	ASP
12	V	767	PRO
2	O	140	PRO
2	O	250	ASN
8	P	426	LYS
8	P	595	PRO
8	Q	63	GLN
8	Q	330	GLU
1	S	564	ILE
1	S	1003	ASN
11	U	120	SER
11	U	376	ASP
2	O	70	GLU
2	O	138	ASN
2	O	251	GLN
8	P	822	ALA
12	V	379	VAL
6	H	385	PRO
2	O	636	PHE
8	P	62	ASP
8	P	383	PRO
8	P	384	GLU
8	Q	19	GLY
8	Q	608	GLU
10	X	62	PRO
12	V	220	GLY
8	Q	757	VAL
8	Q	758	ALA

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Mol	Chain	Res	Type
10	X	94	PRO
12	V	484	GLY
7	M	215	GLU
1	S	201	PRO
11	U	662	GLU
2	O	711	THR
8	P	166	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%)	951 (92%)	83 (8%)	11	32
1	S	565/1282 (44%)	525 (93%)	40 (7%)	13	36
2	B	644/810 (80%)	577 (90%)	67 (10%)	7	23
2	O	641/810 (79%)	590 (92%)	51 (8%)	11	32
3	C	480/507 (95%)	460 (96%)	20 (4%)	26	49
4	E	358/467 (77%)	324 (90%)	34 (10%)	8	26
5	F	288/336 (86%)	282 (98%)	6 (2%)	47	65
6	G	483/538 (90%)	444 (92%)	39 (8%)	11	32
6	H	454/538 (84%)	410 (90%)	44 (10%)	8	26
7	L	334/354 (94%)	321 (96%)	13 (4%)	28	50
7	M	334/354 (94%)	316 (95%)	18 (5%)	20	43
8	P	627/749 (84%)	547 (87%)	80 (13%)	4	18
8	Q	564/749 (75%)	519 (92%)	45 (8%)	11	32
9	W	22/22 (100%)	21 (96%)	1 (4%)	24	47
10	X	136/175 (78%)	132 (97%)	4 (3%)	37	58
11	U	1066/1204 (88%)	1040 (98%)	26 (2%)	43	63
12	V	1065/1324 (80%)	1046 (98%)	19 (2%)	51	66
All	All	9095/11501 (79%)	8505 (94%)	590 (6%)	17	38

All (590) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	43	LEU
1	A	57	LEU
1	A	60	LEU
1	A	78	ILE
1	A	96	SER
1	A	98	LEU
1	A	148	LEU
1	A	149	LEU
1	A	169	GLU
1	A	182	VAL
1	A	191	VAL
1	A	239	VAL
1	A	241	MET
1	A	274	LEU
1	A	285	VAL
1	A	313	THR
1	A	325	THR
1	A	333	VAL
1	A	334	LEU
1	A	342	MET
1	A	354	LEU
1	A	371	LEU
1	A	377	GLU
1	A	383	GLU
1	A	407	LEU
1	A	414	LEU
1	A	425	ASP
1	A	434	VAL
1	A	446	LEU
1	A	450	ASP
1	A	462	TYR
1	A	466	SER
1	A	468	LYS
1	A	491	VAL
1	A	505	SER
1	A	513	LEU
1	A	666	ASP
1	A	685	ARG
1	A	715	GLU
1	A	762	LEU
1	A	782	LEU

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Mol	Chain	Res	Type
1	A	795	ARG
1	A	796	SER
1	A	817	LEU
1	A	821	LEU
1	A	826	THR
1	A	828	ASP
1	A	834	LEU
1	A	838	THR
1	A	858	SER
1	A	864	LEU
1	A	881	GLN
1	A	900	SER
1	A	939	ILE
1	A	951	ARG
1	A	961	GLU
1	A	964	LEU
1	A	968	SER
1	A	984	LEU
1	A	1053	ARG
1	A	1060	THR
1	A	1069	LEU
1	A	1073	ARG
1	A	1126	LEU
1	A	1139	LEU
1	A	1155	ILE
1	A	1165	LEU
1	A	1183	CYS
1	A	1190	GLN
1	A	1191	SER
1	A	1208	SER
1	A	1258	VAL
1	A	1305	LEU
1	A	1309	THR
1	A	1310	GLU
1	A	1328	THR
1	A	1331	LEU
1	A	1345	ASP
1	A	1369	VAL
1	A	1397	THR
1	A	1403	LEU
1	A	1425	ARG
2	B	13	GLU

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Mol	Chain	Res	Type
2	B	40	THR
2	B	66	THR
2	B	81	CYS
2	B	130	MET
2	B	267	SER
2	B	275	ASN
2	B	279	LEU
2	B	283	ASP
2	B	287	VAL
2	B	289	LEU
2	B	300	VAL
2	B	302	SER
2	B	323	GLU
2	B	328	VAL
2	B	341	VAL
2	B	401	CYS
2	B	403	SER
2	B	417	LYS
2	B	486	SER
2	B	488	VAL
2	B	489	VAL
2	B	491	VAL
2	B	495	SER
2	B	496	SER
2	B	504	VAL
2	B	505	THR
2	B	506	LEU
2	B	507	SER
2	B	508	LEU
2	B	518	PHE
2	B	523	CYS
2	B	574	CYS
2	B	576	GLN
2	B	578	ILE
2	B	585	SER
2	B	592	LYS
2	B	596	THR
2	B	602	MET
2	B	604	ARG
2	B	605	GLU
2	B	622	LEU
2	B	624	LEU

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Mol	Chain	Res	Type
2	B	628	SER
2	B	635	THR
2	B	658	SER
2	B	664	SER
2	B	670	ASN
2	B	671	SER
2	B	677	LEU
2	B	681	LYS
2	B	683	GLU
2	B	690	GLU
2	B	693	PHE
2	B	699	SER
2	B	700	PHE
2	B	705	PHE
2	B	716	ILE
2	B	722	ARG
2	B	734	LEU
2	B	741	ASN
2	B	748	LYS
2	B	765	LYS
2	B	813	ARG
2	B	836	ARG
2	B	838	ILE
2	B	847	LEU
3	C	19	LEU
3	C	65	PRO
3	C	136	GLN
3	C	144	ASP
3	C	162	ARG
3	C	190	LEU
3	C	194	THR
3	C	200	VAL
3	C	207	HIS
3	C	214	ILE
3	C	218	GLU
3	C	223	VAL
3	C	236	MET
3	C	241	CYS
3	C	245	ARG
3	C	278	ASP
3	C	286	CYS
3	C	312	ILE

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Mol	Chain	Res	Type
3	C	393	SER
3	C	509	ILE
4	E	23	GLU
4	E	42	ARG
4	E	48	ARG
4	E	71	GLU
4	E	86	LEU
4	E	88	LEU
4	E	94	CYS
4	E	100	SER
4	E	115	LEU
4	E	123	GLN
4	E	148	THR
4	E	160	CYS
4	E	276	GLU
4	E	284	ILE
4	E	314	GLN
4	E	338	ASP
4	E	352	SER
4	E	354	ASP
4	E	357	LEU
4	E	358	SER
4	E	364	THR
4	E	428	SER
4	E	430	GLU
4	E	443	GLU
4	E	448	GLU
4	E	465	THR
4	E	467	GLU
4	E	509	ARG
4	E	514	MET
4	E	517	GLU
4	E	522	PHE
4	E	523	LEU
4	E	524	ARG
4	E	532	LYS
5	F	136	LEU
5	F	161	SER
5	F	171	LEU
5	F	174	LEU
5	F	270	LEU
5	F	302	VAL

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Mol	Chain	Res	Type
6	G	13	LEU
6	G	57	LEU
6	G	74	THR
6	G	80	LEU
6	G	89	THR
6	G	104	LEU
6	G	118	LEU
6	G	149	LEU
6	G	156	LEU
6	G	161	LEU
6	G	166	LEU
6	G	177	LEU
6	G	179	LEU
6	G	180	LEU
6	G	189	GLU
6	G	207	LEU
6	G	234	GLU
6	G	250	THR
6	G	259	MET
6	G	267	LEU
6	G	327	LEU
6	G	340	CYS
6	G	346	THR
6	G	365	GLU
6	G	368	LEU
6	G	371	LEU
6	G	373	LEU
6	G	381	ARG
6	G	405	ILE
6	G	416	LEU
6	G	418	GLU
6	G	426	SER
6	G	432	SER
6	G	448	CYS
6	G	450	LEU
6	G	466	LEU
6	G	483	LEU
6	G	573	ARG
6	G	606	ASP
6	H	12	CYS
6	H	13	LEU
6	H	41	GLN

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Mol	Chain	Res	Type
6	H	42	LEU
6	H	54	LEU
6	H	80	LEU
6	H	89	THR
6	H	91	ASP
6	H	104	LEU
6	H	105	GLU
6	H	130	CYS
6	H	134	GLU
6	H	158	ASP
6	H	159	LEU
6	H	183	THR
6	H	189	GLU
6	H	191	LEU
6	H	192	ASP
6	H	199	ASP
6	H	207	LEU
6	H	241	PRO
6	H	250	THR
6	H	267	LEU
6	H	297	THR
6	H	301	GLU
6	H	350	LEU
6	H	359	ARG
6	H	368	LEU
6	H	373	LEU
6	H	381	ARG
6	H	393	MET
6	H	395	GLU
6	H	404	LEU
6	H	405	ILE
6	H	416	LEU
6	H	418	GLU
6	H	466	LEU
6	H	478	ARG
6	H	483	LEU
6	H	535	GLN
6	H	562	ASP
6	H	568	THR
6	H	586	LEU
6	H	606	ASP
7	L	3	VAL

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Mol	Chain	Res	Type
7	L	4	THR
7	L	25	TYR
7	L	39	ARG
7	L	46	LEU
7	L	104	LEU
7	L	116	GLU
7	L	118	ILE
7	L	162	SER
7	L	182	SER
7	L	213	VAL
7	L	268	SER
7	L	316	ASP
2	O	7	MET
2	O	47	ARG
2	O	48	MET
2	O	104	VAL
2	O	132	ASP
2	O	168	SER
2	O	171	GLN
2	O	175	GLU
2	O	177	GLU
2	O	237	VAL
2	O	242	ILE
2	O	246	GLU
2	O	252	LEU
2	O	256	LEU
2	O	279	LEU
2	O	287	VAL
2	O	315	SER
2	O	323	GLU
2	O	328	VAL
2	O	354	LEU
2	O	412	LEU
2	O	475	VAL
2	O	484	ASP
2	O	491	VAL
2	O	496	SER
2	O	498	LYS
2	O	505	THR
2	O	508	LEU
2	O	519	ARG
2	O	573	GLU

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Mol	Chain	Res	Type
2	O	577	ILE
2	O	578	ILE
2	O	579	THR
2	O	585	SER
2	O	606	SER
2	O	611	LYS
2	O	612	ASP
2	O	624	LEU
2	O	628	SER
2	O	635	THR
2	O	643	GLU
2	O	659	CYS
2	O	677	LEU
2	O	703	THR
2	O	724	GLN
2	O	727	MET
2	O	735	ILE
2	O	740	ILE
2	O	741	ASN
2	O	780	HIS
2	O	783	ASN
8	P	18	LEU
8	P	34	GLU
8	P	41	SER
8	P	42	GLU
8	P	45	TYR
8	P	68	GLU
8	P	69	LEU
8	P	76	LEU
8	P	91	ASP
8	P	131	CYS
8	P	135	LEU
8	P	137	ASP
8	P	142	THR
8	P	149	ARG
8	P	162	GLU
8	P	177	SER
8	P	196	VAL
8	P	198	CYS
8	P	200	VAL
8	P	219	THR
8	P	224	LEU

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Mol	Chain	Res	Type
8	P	228	LEU
8	P	232	ASP
8	P	234	THR
8	P	235	LEU
8	P	241	VAL
8	P	246	PRO
8	P	249	GLN
8	P	250	LEU
8	P	252	CYS
8	P	253	VAL
8	P	279	GLU
8	P	305	GLU
8	P	307	VAL
8	P	325	LYS
8	P	330	GLU
8	P	364	SER
8	P	402	CYS
8	P	424	SER
8	P	465	ILE
8	P	467	GLU
8	P	473	LYS
8	P	478	GLN
8	P	485	SER
8	P	510	THR
8	P	517	LEU
8	P	524	MET
8	P	555	ASP
8	P	560	CYS
8	P	566	THR
8	P	569	VAL
8	P	577	ARG
8	P	582	LEU
8	P	594	LEU
8	P	598	VAL
8	P	600	CYS
8	P	638	VAL
8	P	639	CYS
8	P	646	THR
8	P	658	LEU
8	P	683	CYS
8	P	685	GLU
8	P	701	LEU

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Mol	Chain	Res	Type
8	P	707	SER
8	P	724	SER
8	P	745	VAL
8	P	749	ARG
8	P	751	LEU
8	P	768	VAL
8	P	774	THR
8	P	782	ILE
8	P	789	VAL
8	P	793	SER
8	P	811	MET
8	P	812	VAL
8	P	827	VAL
8	P	836	ASN
8	P	842	ARG
8	P	868	GLN
8	P	876	PRO
8	Q	18	LEU
8	Q	21	LEU
8	Q	91	ASP
8	Q	125	LEU
8	Q	135	LEU
8	Q	144	VAL
8	Q	222	ASP
8	Q	253	VAL
8	Q	307	VAL
8	Q	334	LEU
8	Q	352	CYS
8	Q	365	ASP
8	Q	393	MET
8	Q	465	ILE
8	Q	481	LYS
8	Q	510	THR
8	Q	517	LEU
8	Q	522	VAL
8	Q	523	LEU
8	Q	542	THR
8	Q	543	LEU
8	Q	546	GLN
8	Q	560	CYS
8	Q	561	SER
8	Q	564	THR

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Mol	Chain	Res	Type
8	Q	566	THR
8	Q	570	ASP
8	Q	578	ARG
8	Q	582	LEU
8	Q	598	VAL
8	Q	609	VAL
8	Q	610	VAL
8	Q	638	VAL
8	Q	642	LEU
8	Q	645	HIS
8	Q	658	LEU
8	Q	723	HIS
8	Q	744	ASP
8	Q	745	VAL
8	Q	751	LEU
8	Q	768	VAL
8	Q	769	ARG
8	Q	774	THR
8	Q	782	ILE
8	Q	789	VAL
1	S	766	CYS
1	S	770	ARG
1	S	782	LEU
1	S	828	ASP
1	S	838	THR
1	S	855	THR
1	S	856	LEU
1	S	858	SER
1	S	910	LEU
1	S	911	TRP
1	S	912	THR
1	S	922	GLU
1	S	924	ASP
1	S	948	ASP
1	S	951	ARG
1	S	966	GLU
1	S	973	CYS
1	S	992	HIS
1	S	996	ARG
1	S	1012	THR
1	S	1023	GLU
1	S	1031	GLN

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Mol	Chain	Res	Type
1	S	1045	GLU
1	S	1060	THR
1	S	1093	SER
1	S	1126	LEU
1	S	1129	ASP
1	S	1139	LEU
1	S	1183	CYS
1	S	1202	GLU
1	S	1280	ASP
1	S	1310	GLU
1	S	1320	LEU
1	S	1328	THR
1	S	1339	LEU
1	S	1345	ASP
1	S	1367	LEU
1	S	1369	VAL
1	S	1397	THR
1	S	1428	CYS
9	W	94	LEU
7	M	1	MET
7	M	3	VAL
7	M	4	THR
7	M	39	ARG
7	M	40	ILE
7	M	56	SER
7	M	60	ARG
7	M	64	SER
7	M	85	MET
7	M	139	LYS
7	M	222	SER
7	M	250	GLU
7	M	257	ASP
7	M	304	THR
7	M	305	MET
7	M	343	ARG
7	M	346	LEU
7	M	349	ARG
10	X	1	MET
10	X	56	ILE
10	X	72	THR
10	X	101	SER
11	U	56	CYS

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Mol	Chain	Res	Type
11	U	135	THR
11	U	171	GLN
11	U	178	THR
11	U	216	GLN
11	U	284	GLU
11	U	295	VAL
11	U	301	SER
11	U	306	SER
11	U	307	PRO
11	U	323	GLN
11	U	361	SER
11	U	428	GLU
11	U	435	MET
11	U	479	SER
11	U	495	THR
11	U	516	CYS
11	U	593	ARG
11	U	626	THR
11	U	631	LEU
11	U	777	CYS
11	U	783	ASP
11	U	812	SER
11	U	905	SER
11	U	1016	GLU
11	U	1135	ILE
12	V	163	GLU
12	V	166	ASN
12	V	221	ASP
12	V	269	LYS
12	V	292	MET
12	V	338	SER
12	V	371	THR
12	V	384	MET
12	V	390	SER
12	V	441	SER
12	V	509	MET
12	V	726	SER
12	V	757	ASP
12	V	779	ARG
12	V	937	HIS
12	V	1015	CYS
12	V	1130	CYS

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Mol	Chain	Res	Type
12	V	1193	THR
12	V	1208	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	88	ASN
1	A	123	GLN
1	A	851	GLN
1	A	881	GLN
1	A	913	HIS
1	A	993	GLN
1	A	1046	HIS
1	A	1128	GLN
1	A	1205	GLN
1	A	1231	HIS
1	A	1307	GLN
1	A	1417	HIS
2	B	71	ASN
2	B	138	ASN
2	B	178	ASN
2	B	241	HIS
2	B	263	ASN
2	B	270	ASN
2	B	306	ASN
2	B	473	GLN
2	B	512	GLN
2	B	600	GLN
2	B	656	HIS
2	B	670	ASN
2	B	729	GLN
2	B	753	ASN
2	B	780	HIS
2	B	827	ASN
3	C	13	GLN
3	C	42	GLN
3	C	58	ASN
3	C	69	GLN
3	C	111	ASN
3	C	224	ASN
3	C	283	GLN

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Mol	Chain	Res	Type
3	C	366	GLN
3	C	382	GLN
3	C	399	HIS
3	C	438	GLN
3	C	441	GLN
3	C	465	GLN
3	C	485	GLN
3	C	528	GLN
3	C	557	GLN
4	E	31	GLN
4	E	287	GLN
4	E	335	GLN
4	E	359	ASN
5	F	7	HIS
5	F	68	GLN
5	F	130	GLN
5	F	244	ASN
5	F	308	HIS
6	G	31	GLN
6	G	32	ASN
6	G	55	HIS
6	G	58	GLN
6	G	97	GLN
6	G	116	GLN
6	G	320	GLN
6	G	339	HIS
6	G	343	GLN
6	G	348	HIS
6	G	406	GLN
6	G	498	ASN
6	G	529	GLN
6	G	542	GLN
6	G	547	ASN
6	G	553	HIS
6	H	20	ASN
6	H	58	GLN
6	H	215	GLN
6	H	261	ASN
6	H	348	HIS
6	H	529	GLN
6	H	542	GLN
7	L	18	GLN

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Mol	Chain	Res	Type
7	L	258	HIS
7	L	270	ASN
7	L	282	GLN
7	L	322	GLN
7	L	328	GLN
7	L	331	GLN
2	O	44	HIS
2	O	71	ASN
2	O	102	ASN
2	O	270	ASN
2	O	512	GLN
2	O	533	ASN
2	O	661	GLN
2	O	670	ASN
8	P	293	GLN
8	P	308	HIS
8	P	318	HIS
8	P	400	ASN
8	P	464	ASN
8	P	635	GLN
8	P	765	HIS
8	P	868	GLN
8	P	875	HIS
8	Q	308	HIS
8	Q	317	HIS
8	Q	360	HIS
8	Q	491	ASN
8	Q	645	HIS
8	Q	651	GLN
1	S	851	GLN
1	S	869	GLN
1	S	940	GLN
1	S	956	GLN
1	S	992	HIS
1	S	993	GLN
1	S	1022	GLN
1	S	1201	GLN
1	S	1307	GLN
1	S	1366	GLN
1	S	1417	HIS
1	S	1440	GLN
7	M	18	GLN

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Mol	Chain	Res	Type
7	M	32	GLN
7	M	76	HIS
7	M	99	GLN
7	M	232	ASN
7	M	233	ASN
7	M	272	HIS
7	M	283	ASN
7	M	328	GLN
7	M	331	GLN
10	X	26	GLN
10	X	67	GLN
10	X	112	GLN
11	U	18	GLN
11	U	123	ASN
11	U	206	ASN
11	U	345	GLN
11	U	373	HIS
11	U	438	GLN
11	U	443	GLN
11	U	528	ASN
11	U	580	ASN
11	U	597	GLN
11	U	625	GLN
11	U	672	GLN
11	U	826	GLN
11	U	851	GLN
11	U	858	HIS
11	U	872	GLN
11	U	924	GLN
11	U	928	GLN
11	U	958	GLN
11	U	961	GLN
11	U	963	GLN
11	U	978	ASN
11	U	1030	ASN
11	U	1070	ASN
11	U	1109	GLN
11	U	1127	ASN
11	U	1182	GLN
12	V	67	GLN
12	V	146	GLN
12	V	171	ASN

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Mol	Chain	Res	Type
12	V	392	ASN
12	V	545	ASN
12	V	623	GLN
12	V	658	ASN
12	V	974	GLN
12	V	1005	GLN
12	V	1018	GLN
12	V	1032	ASN
12	V	1041	ASN
12	V	1083	ASN
12	V	1176	ASN
12	V	1192	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2
7	M	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	9:UNK	C	73:GLU	N	37.33
1	W	95:TRP	C	101:UNK	N	7.01
1	L	321:ASP	C	322:GLN	N	1.19
1	M	330:GLY	C	331:GLN	N	1.14
1	M	321:ASP	C	322:GLN	N	1.09
1	L	330:GLY	C	331:GLN	N	1.07

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23088. These allow visual inspection of the internal detail of the map and identification of artifacts.

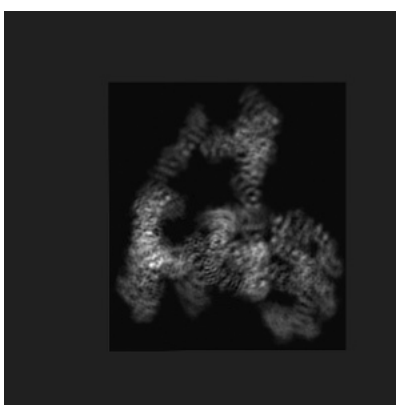
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

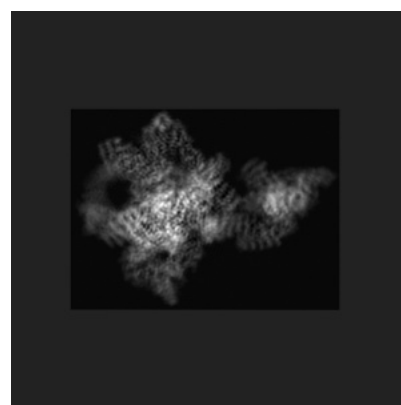
6.1.1 Primary map



X



Y



Z

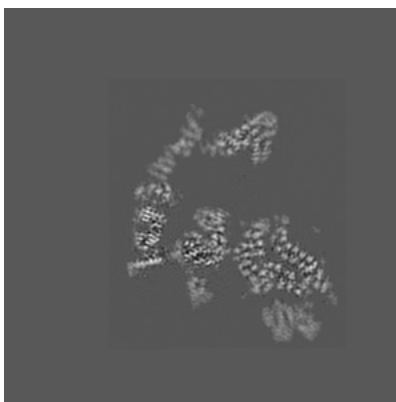
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

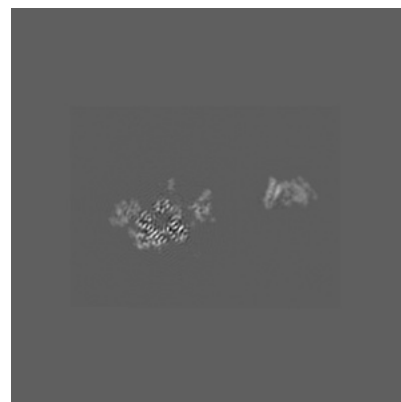
6.2.1 Primary map



X Index: 224



Y Index: 224

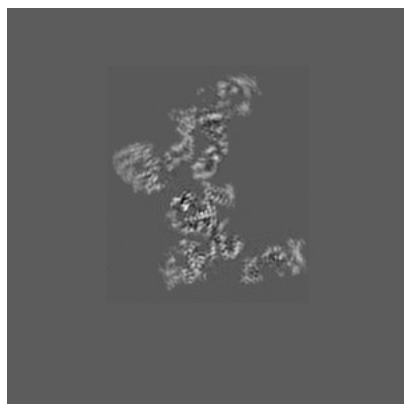


Z Index: 224

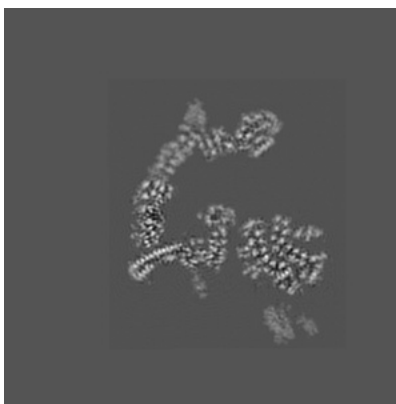
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

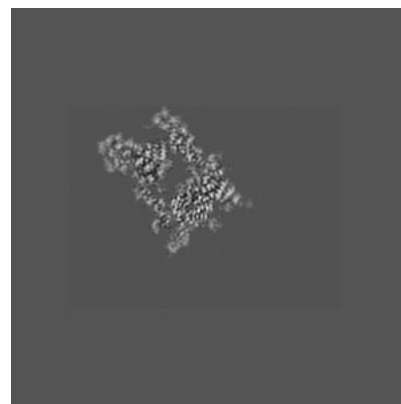
6.3.1 Primary map



X Index: 175



Y Index: 231



Z Index: 161

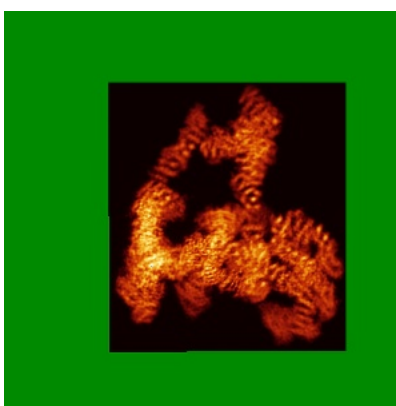
The images above show the largest variance slices of the map in three orthogonal directions.

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

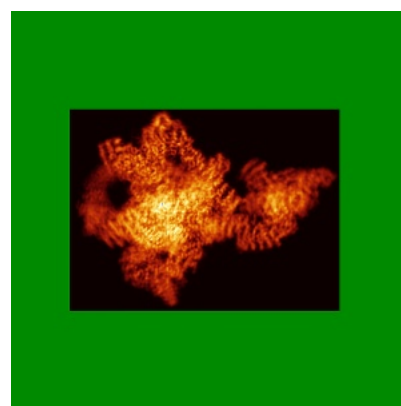
6.4.1 Primary map



X



Y

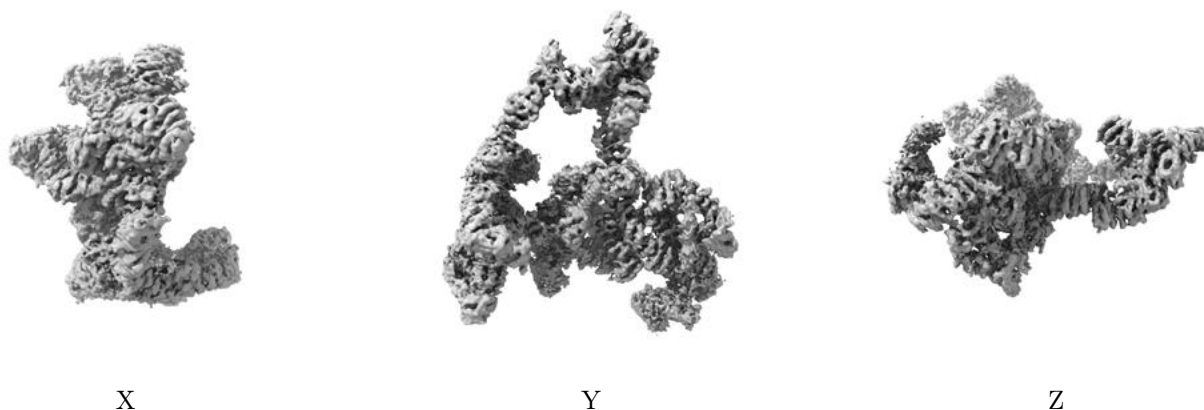


Z

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 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

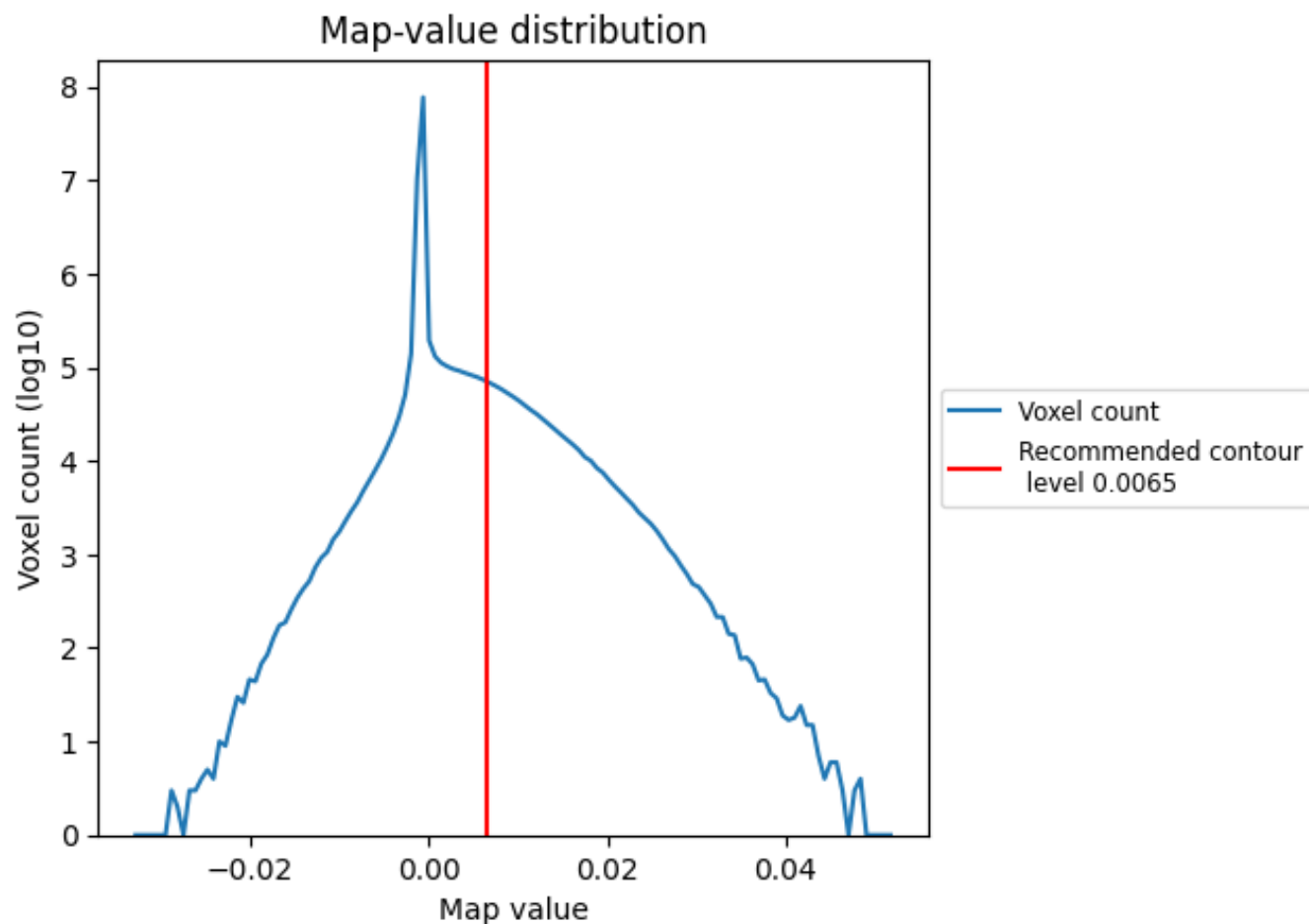
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

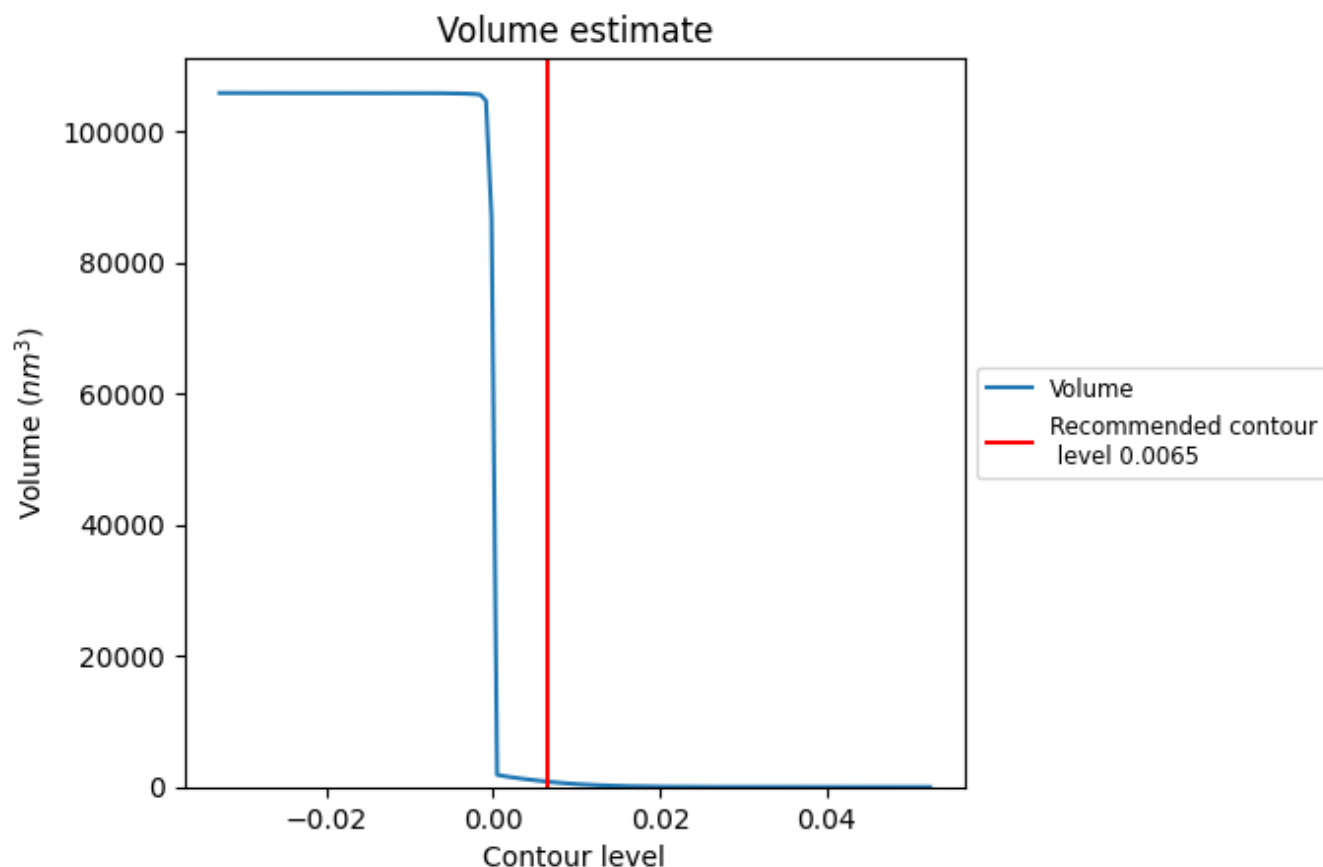
This section contains the results of statistical analysis of the map.

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.

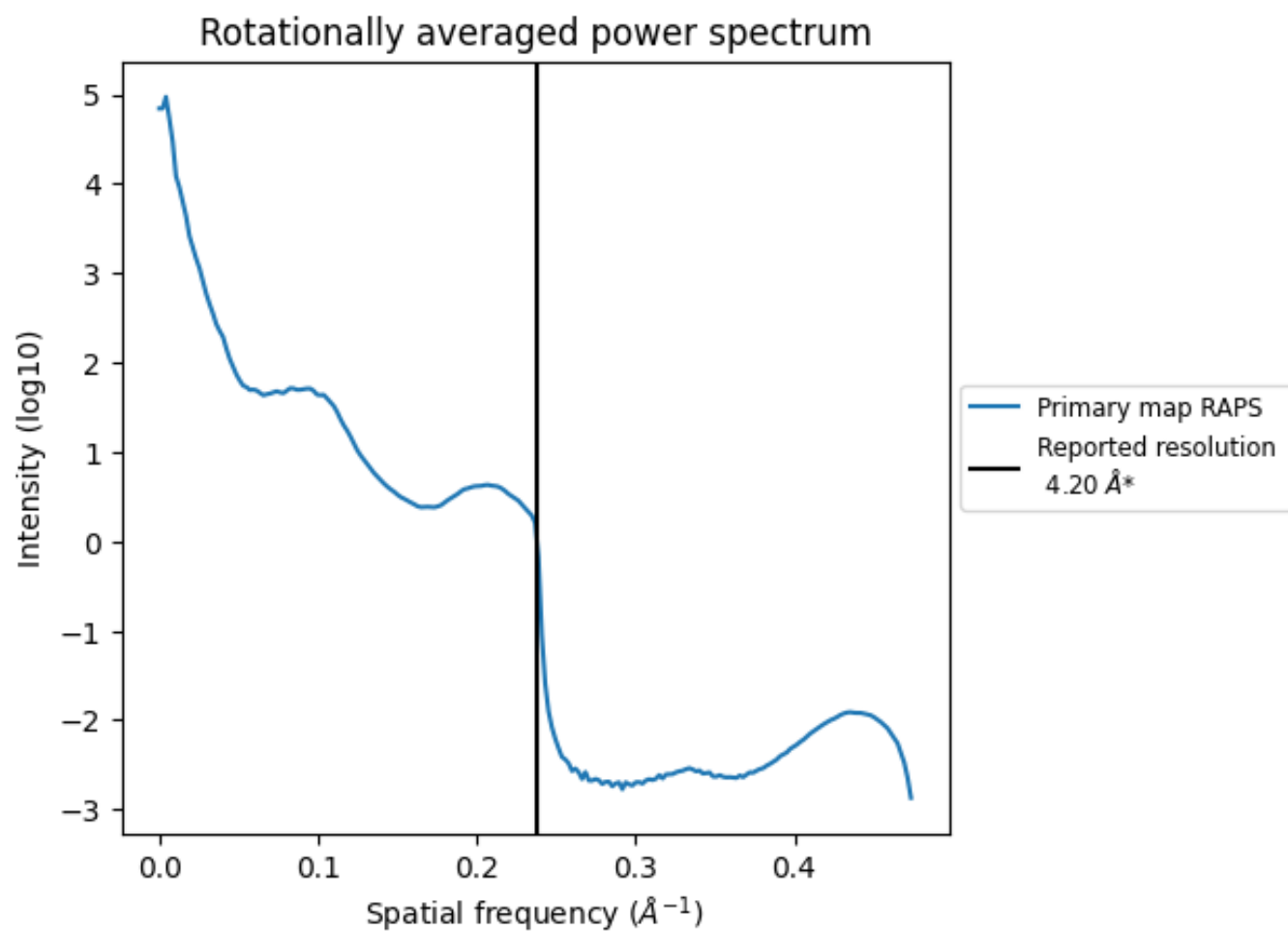
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 814 nm³; this corresponds to an approximate mass of 736 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

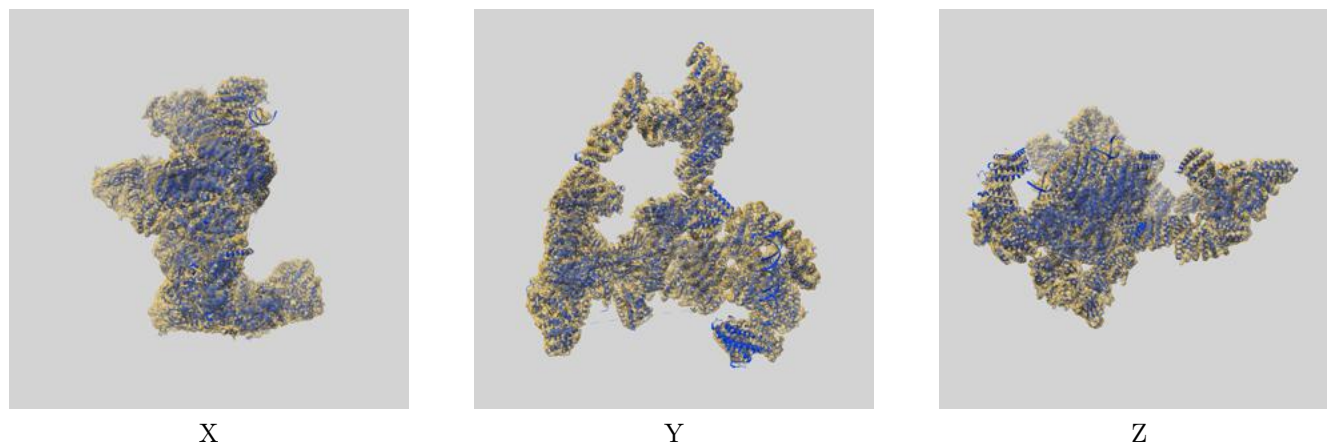
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

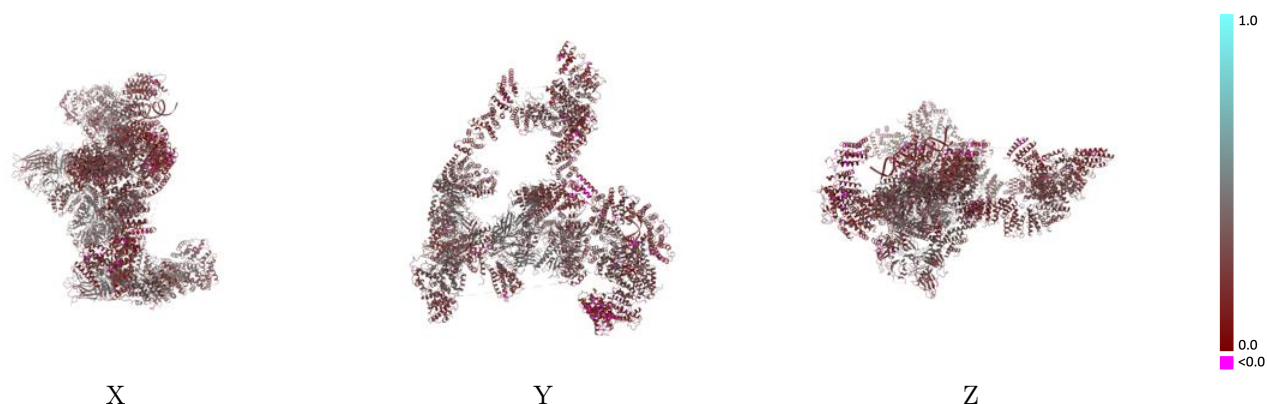
This section contains information regarding the fit between EMDB map EMD-23088 and PDB model 7KZS. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



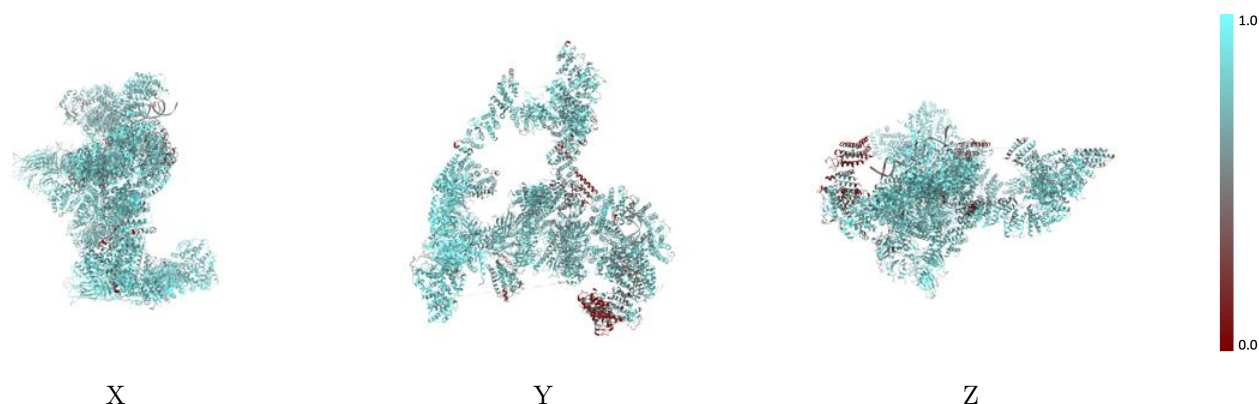
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



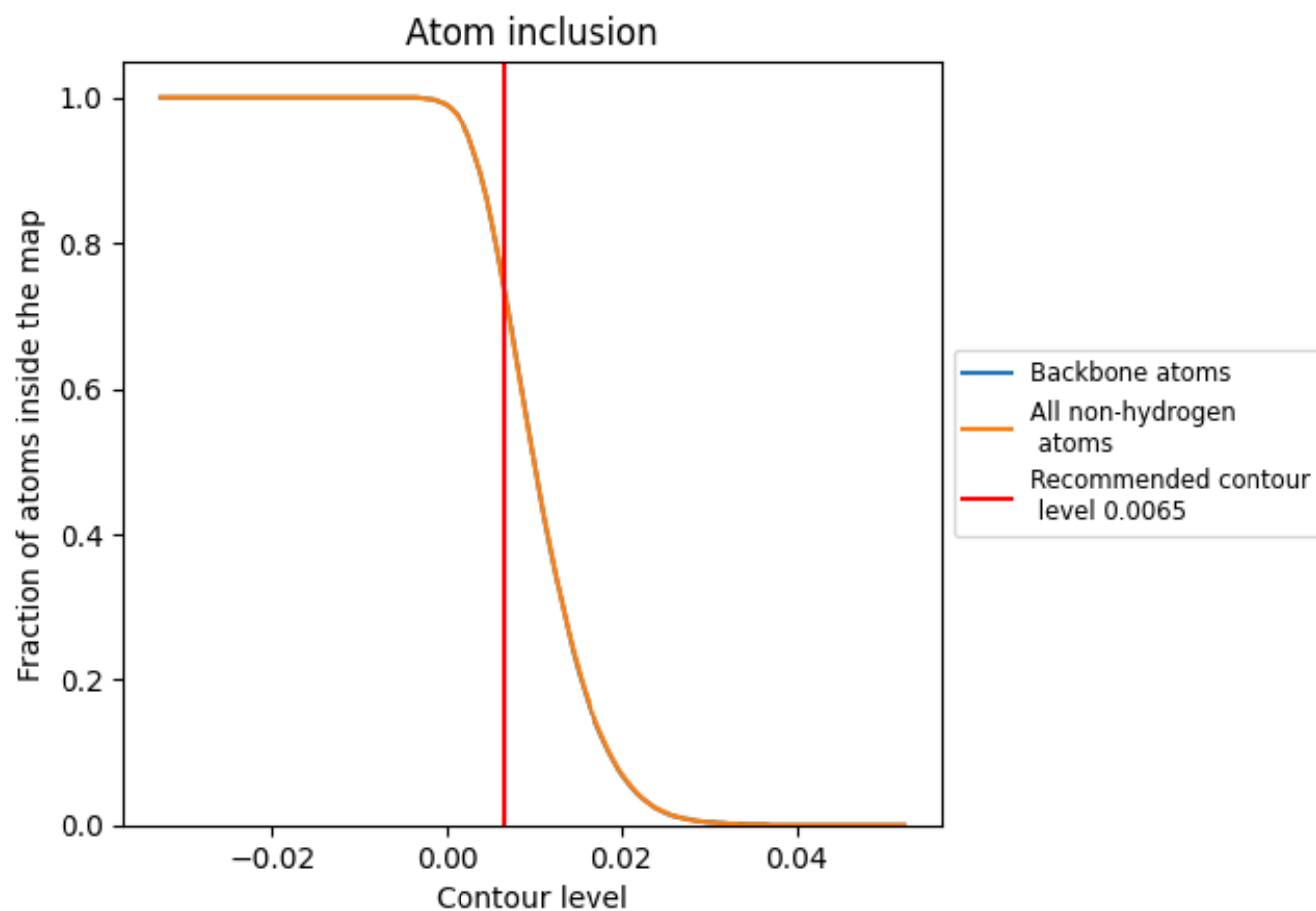
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.3030
A	 0.7100	 0.2660
B	 0.8210	 0.3720
C	 0.8500	 0.3360
E	 0.7620	 0.3170
F	 0.8580	 0.3420
G	 0.8050	 0.3130
H	 0.7510	 0.2860
L	 0.7840	 0.3250
M	 0.7470	 0.3110
O	 0.7950	 0.3470
P	 0.8460	 0.4000
Q	 0.7230	 0.3350
S	 0.7550	 0.2680
U	 0.7380	 0.2760
V	 0.5950	 0.2420
W	 0.7550	 0.3090
X	 0.6210	 0.2640
Y	 0.5680	 0.1830
Z	 0.5560	 0.1910

