Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 09:20 PM EST

PDB ID	:	7KZS
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:

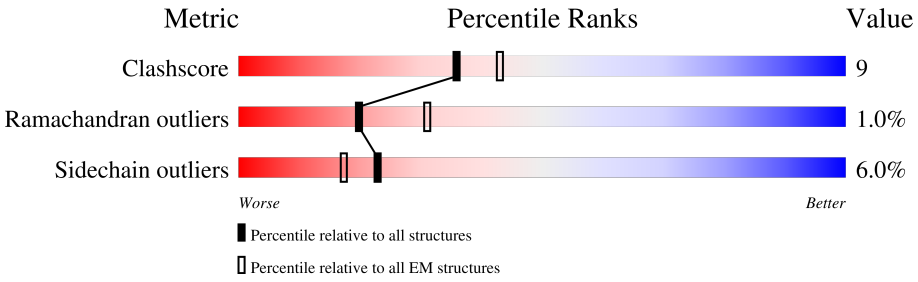
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1477	11% 62% 17% • 20%
1	S	1477	6% 68% 16% • 15%
2	B	884	• 53% 22% • 21%
2	O	884	• 60% 17% • 21%
3	C	583	• 73% 20% • 6%
4	E	555	• 45% 26% • 25%
5	F	399	• 67% 18% 15%
6	G	641	6% 69% 20% • 10%

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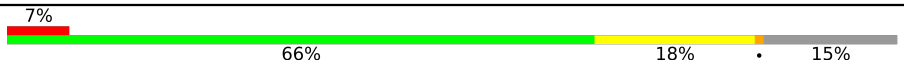
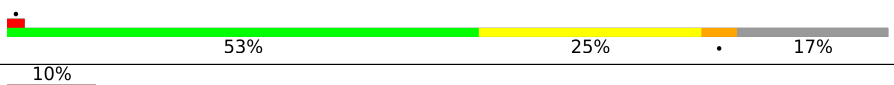
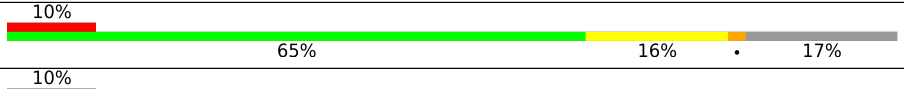
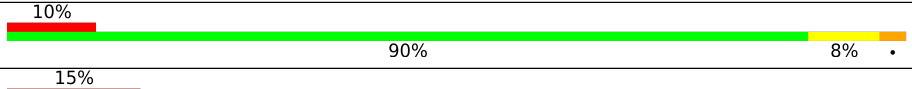
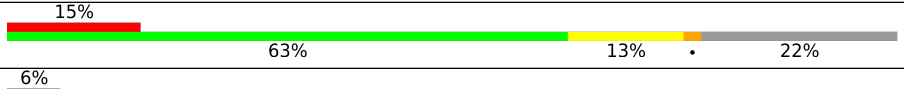
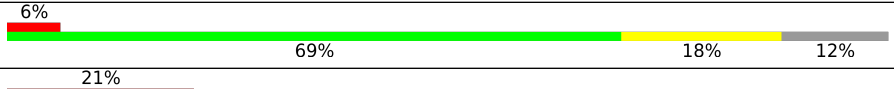
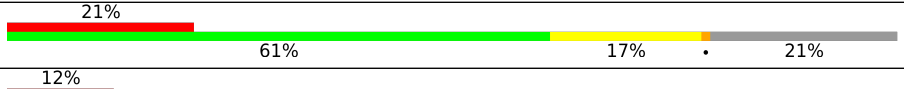
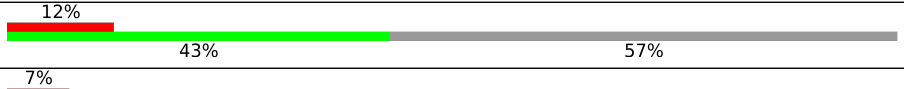
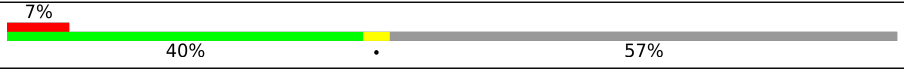
Mol	Chain	Length	Quality of chain
6	H	641	
7	L	394	
7	M	394	
8	P	906	
8	Q	906	
9	W	39	
10	X	197	
11	U	1328	
12	V	1451	
13	Y	58	
14	Z	58	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 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
			Total	C	H	N	O	S		
5	F	340	5466	1730	2740	506	483	7	0	0

There are 25 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 38 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 38 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 50 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	U	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 (three-letter code: ZN) (formula: Zn).

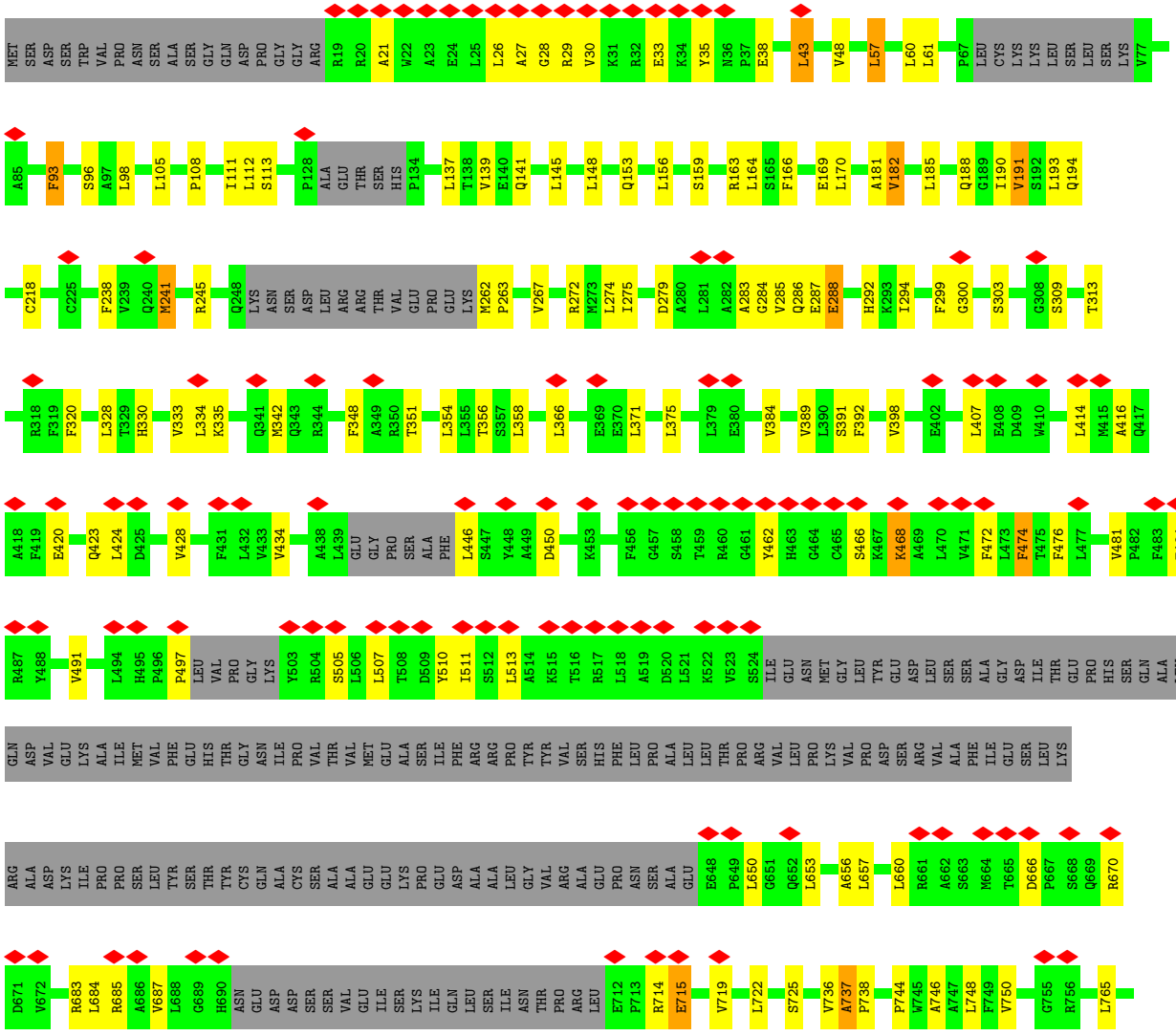
Mol	Chain	Residues	Atoms		AltConf
15	G	1	Total	Zn	0
			1	1	
15	L	2	Total	Zn	0
			2	2	
15	M	2	Total	Zn	0
			2	2	

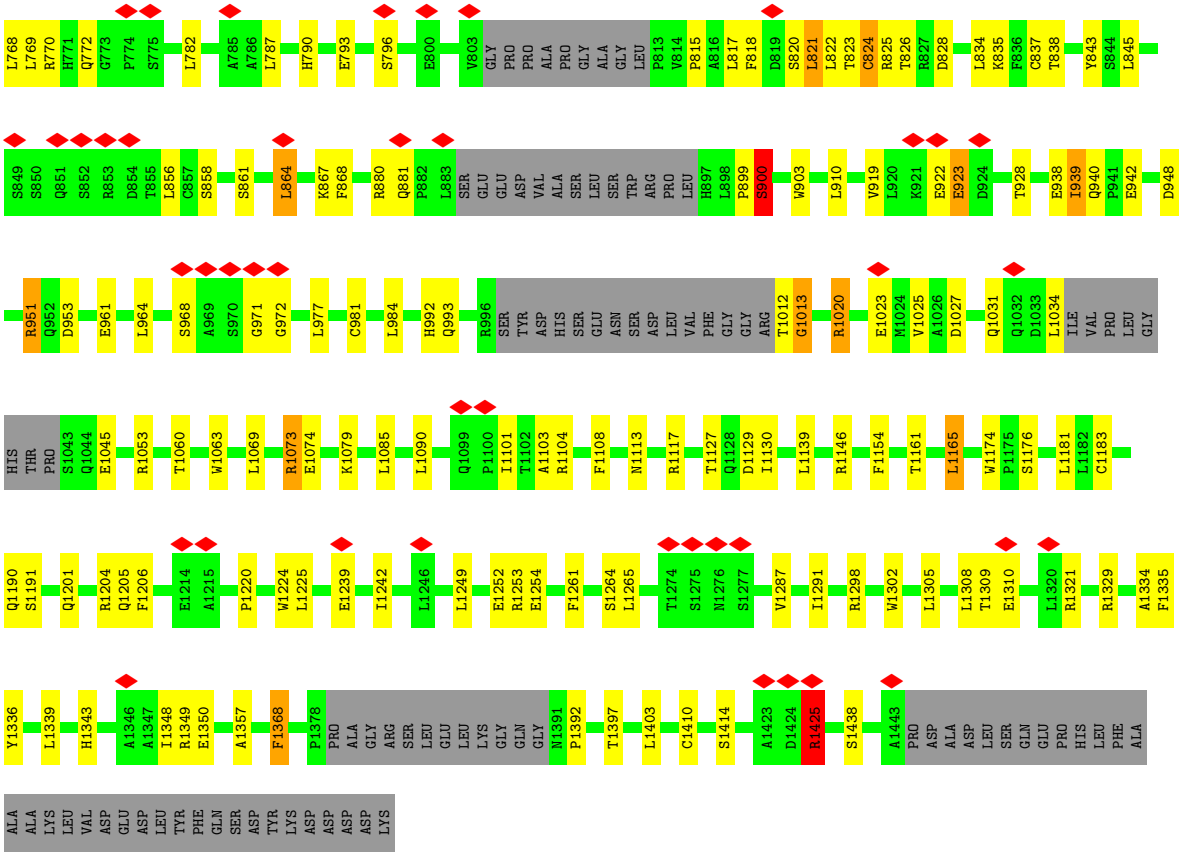
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fanconi anemia group A protein

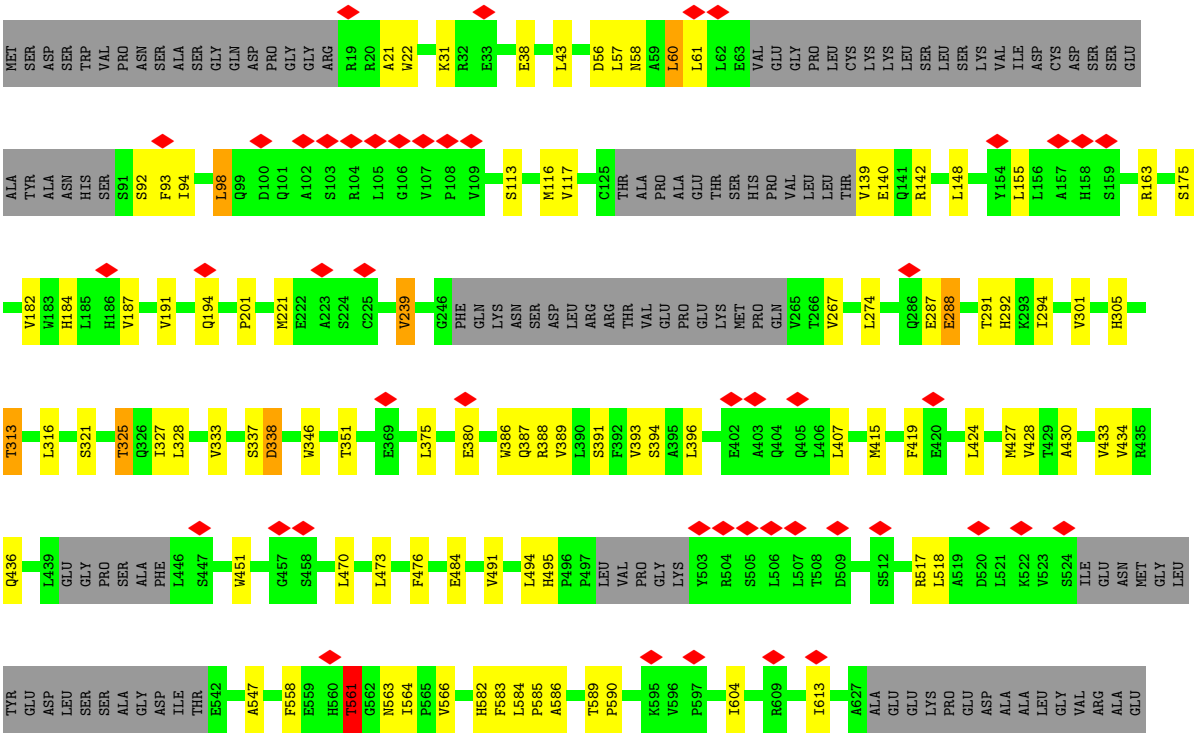
Chain A:

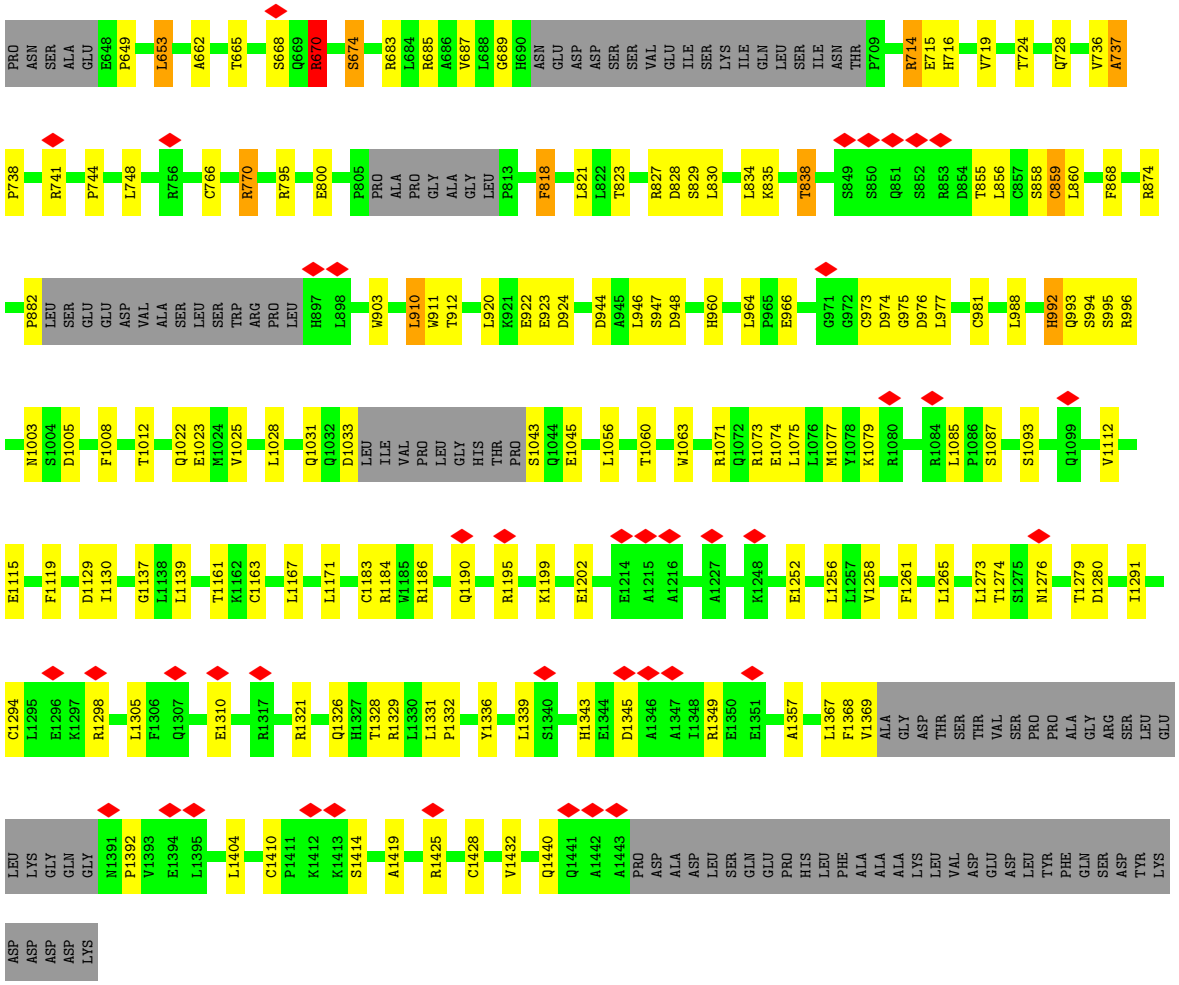




• Molecule 1: Fanconi anemia group A protein

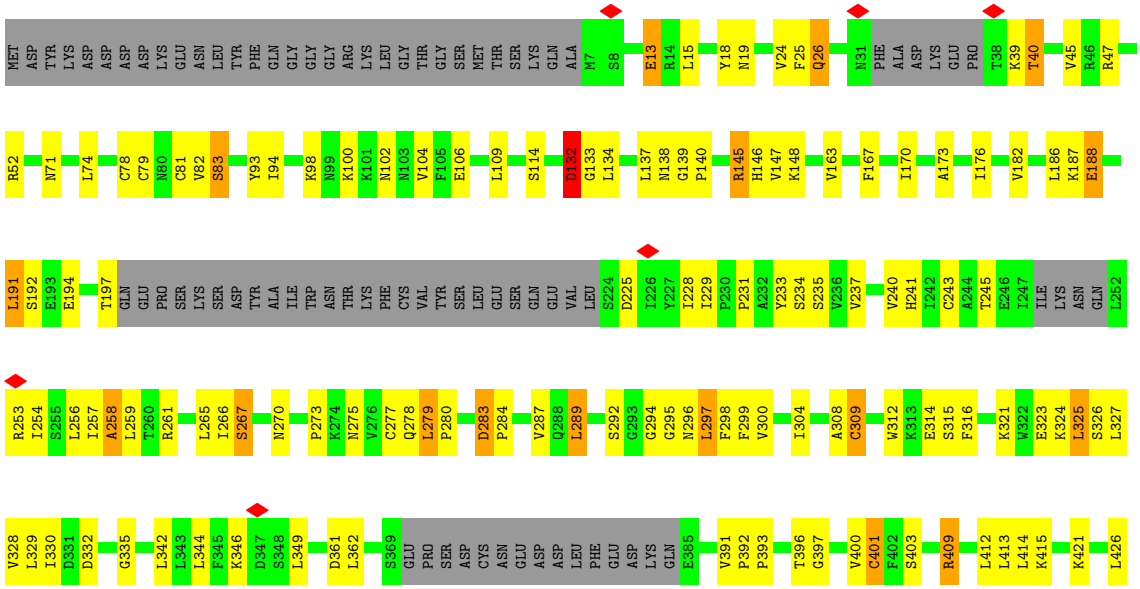
Chain S:

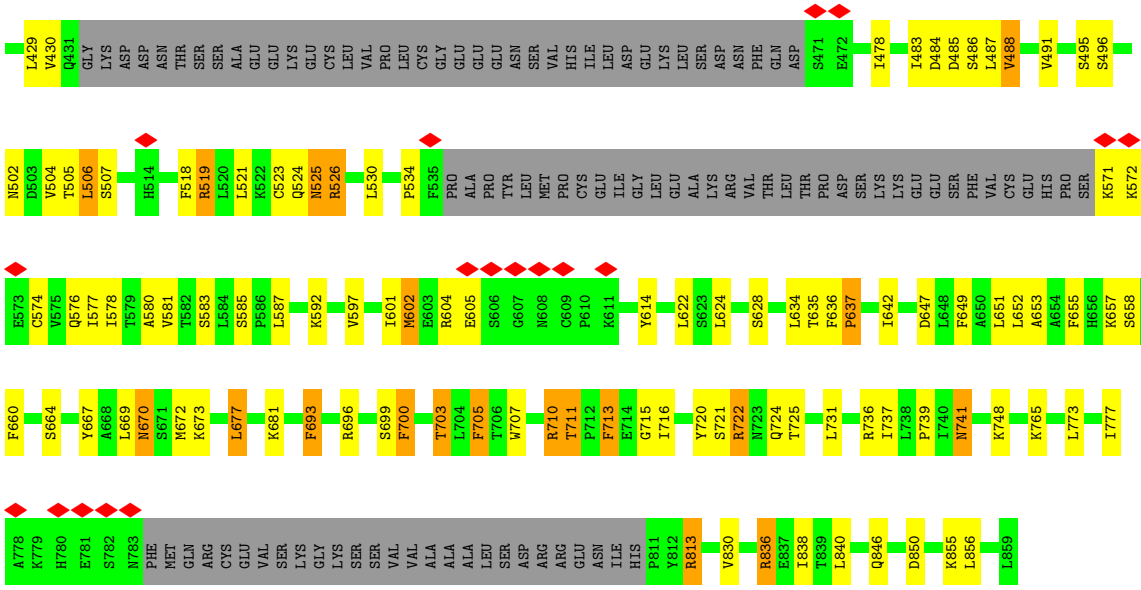




• Molecule 2: Fanconi anemia group B protein

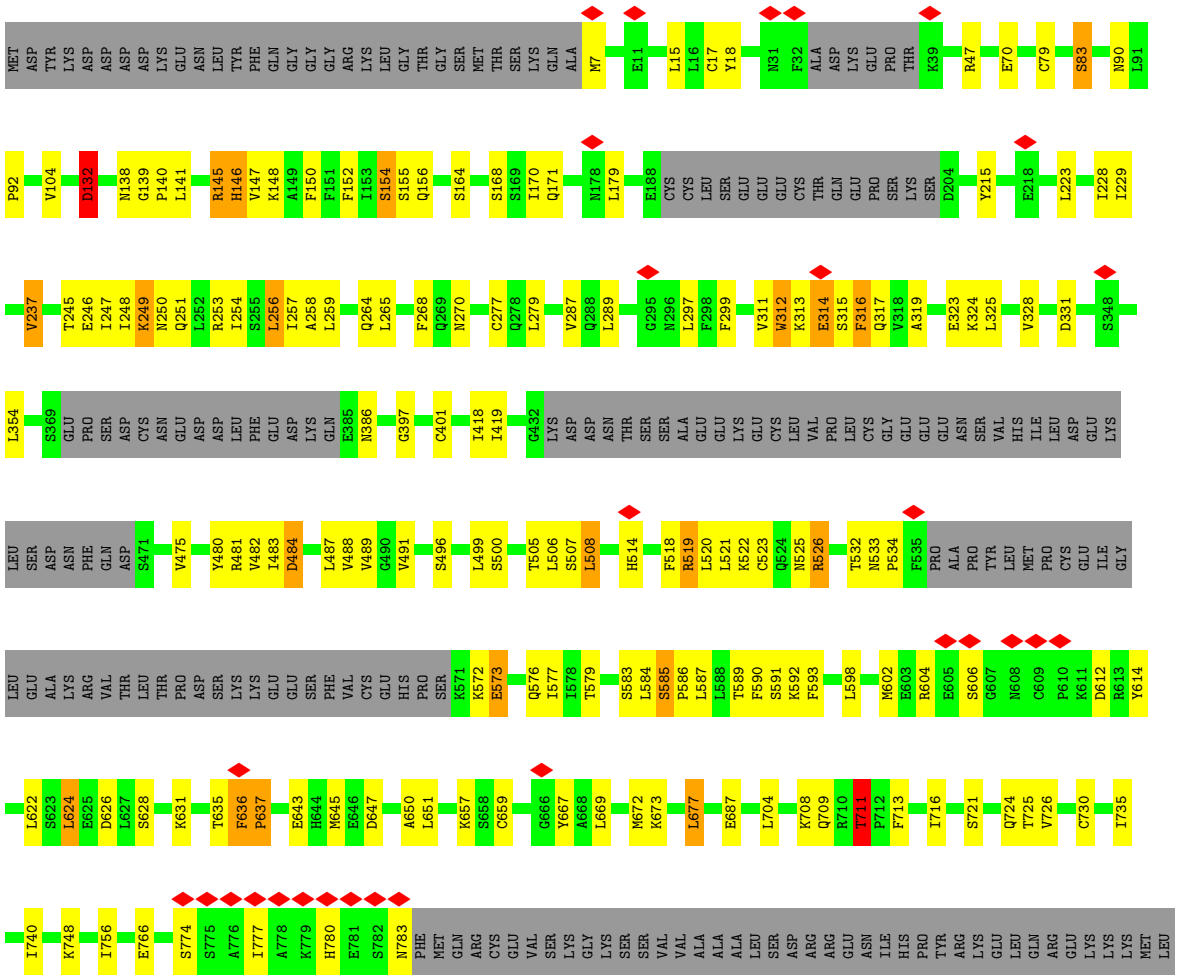
Chain B:





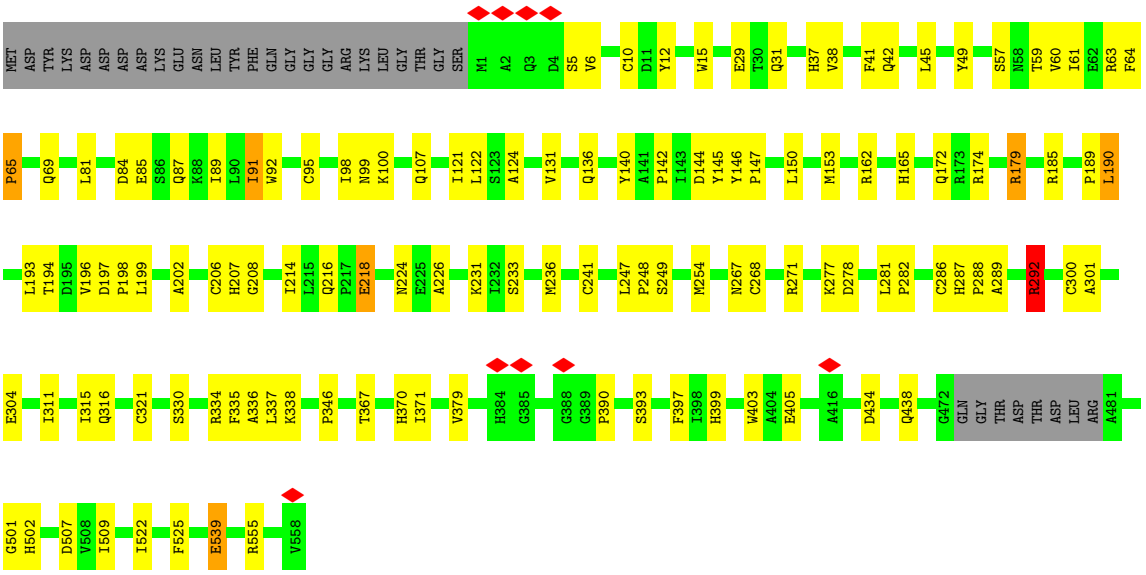
• Molecule 2: Fanconi anemia group B protein

Chain O:



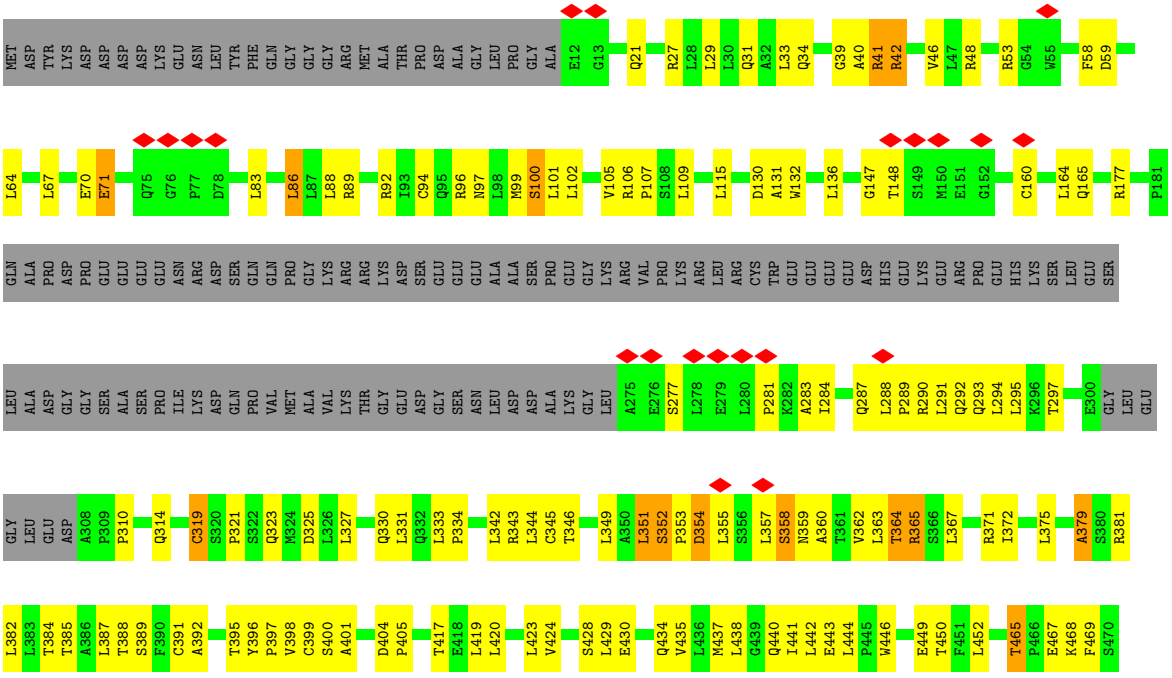
• Molecule 3: Fanconi anemia group C protein

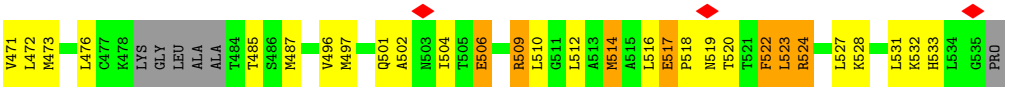
Chain C:



• Molecule 4: Fanconi anemia group E protein

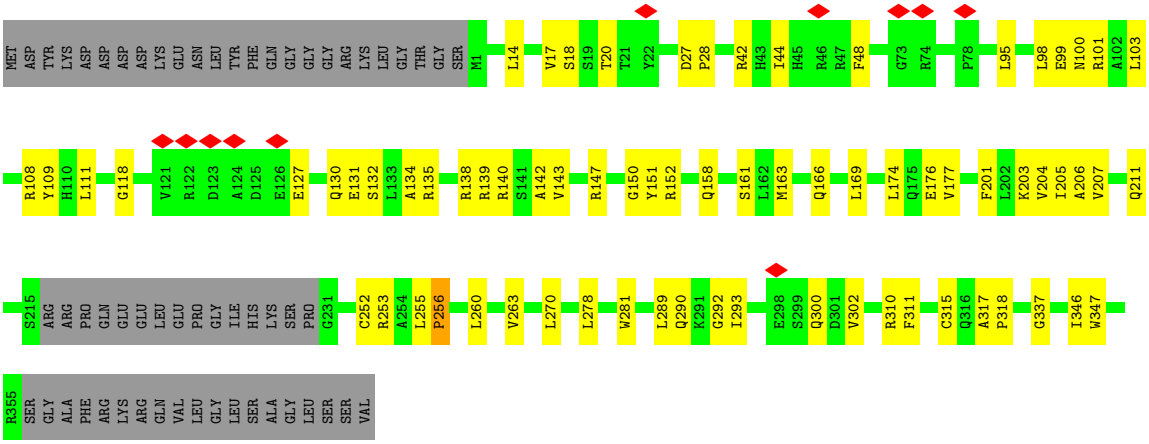
Chain E:





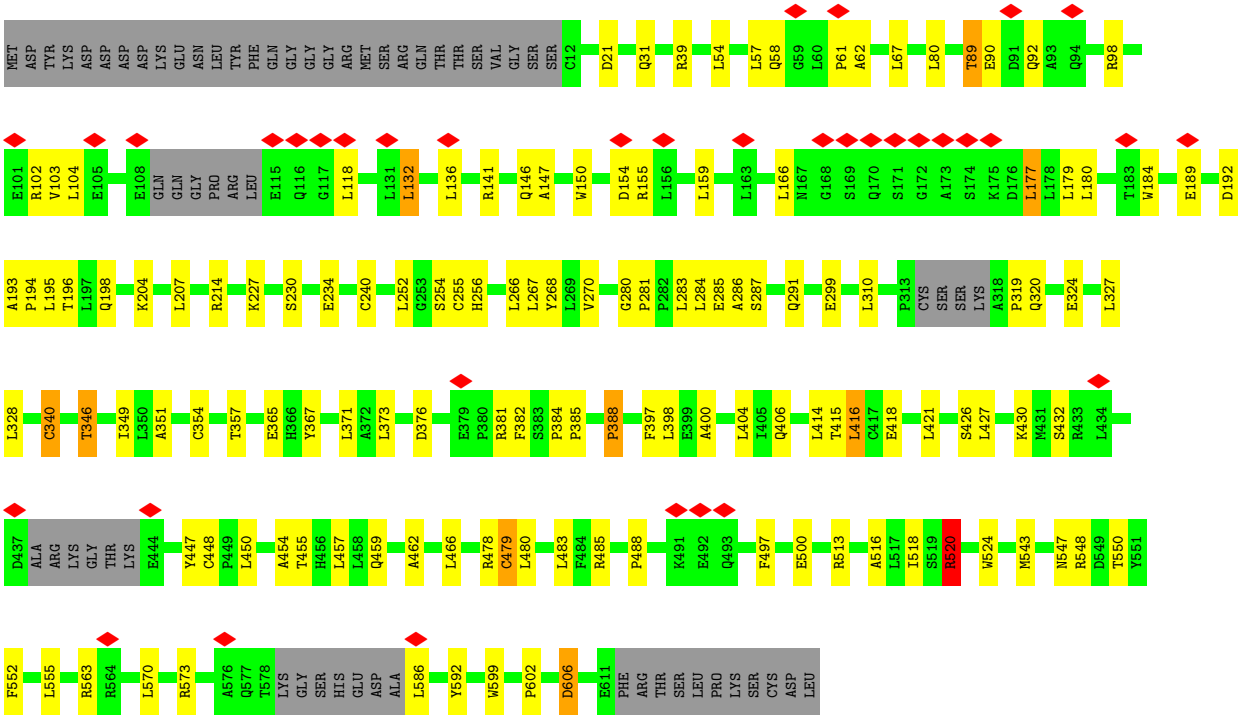
• Molecule 5: Fanconi anemia group F protein

Chain F:



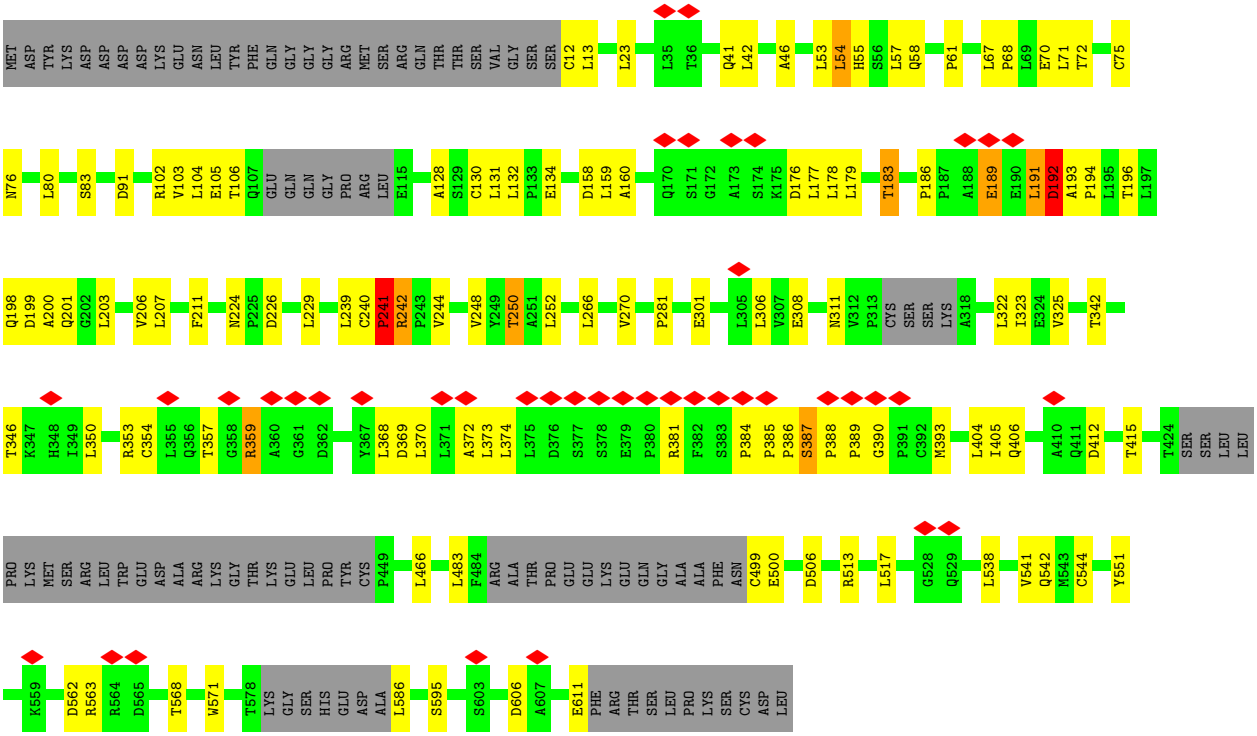
• Molecule 6: Fanconi anemia group G protein

Chain G:



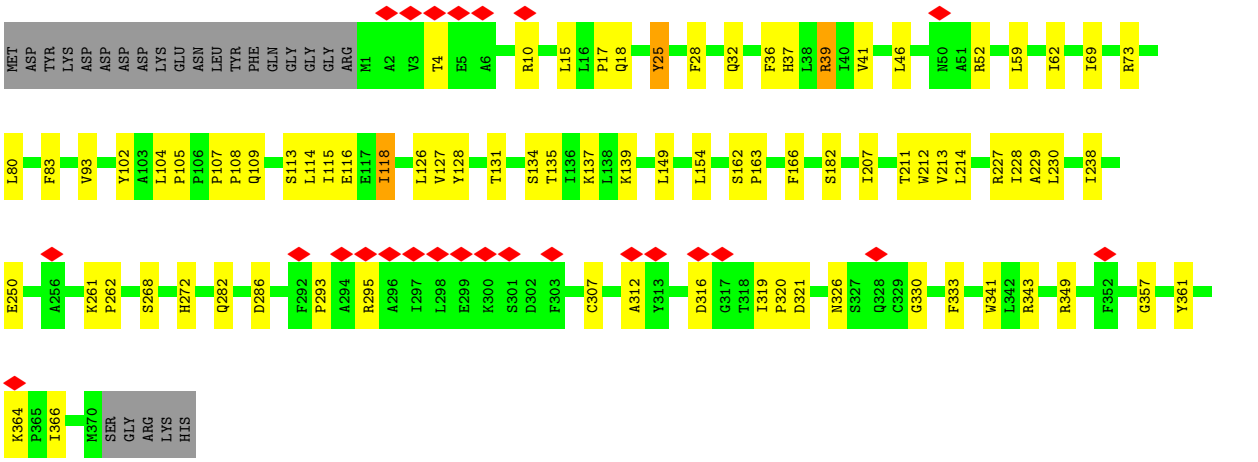
• Molecule 6: Fanconi anemia group G protein

Chain H:



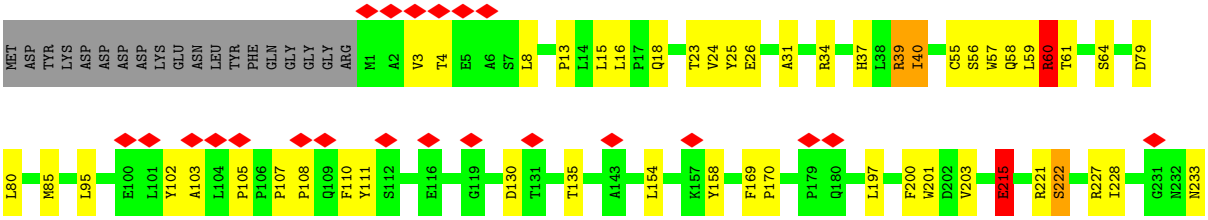
• Molecule 7: E3 ubiquitin-protein ligase FANCL

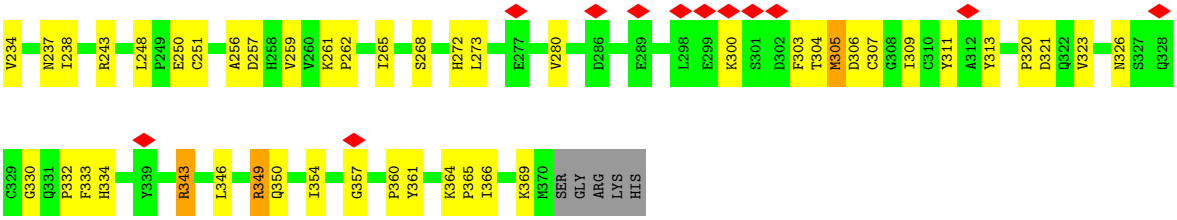
Chain L:



• Molecule 7: E3 ubiquitin-protein ligase FANCL

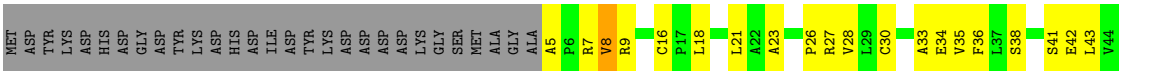
Chain M:

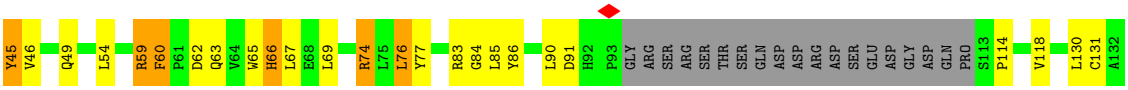


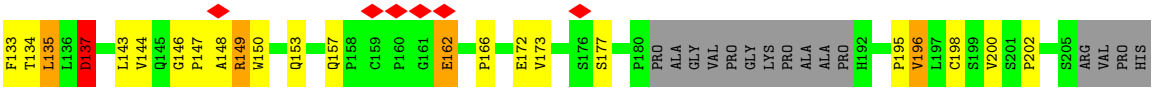


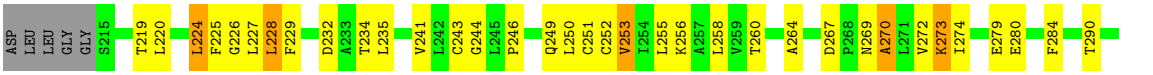
• Molecule 8: Fanconi anemia core complex-associated protein 100

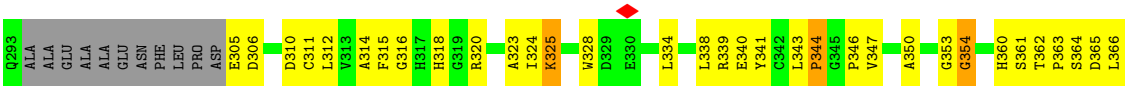
Chain P:

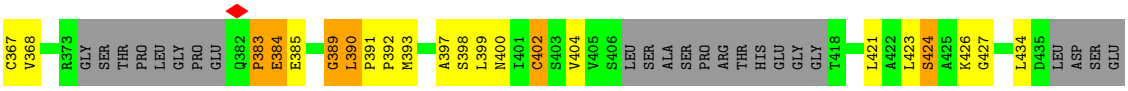


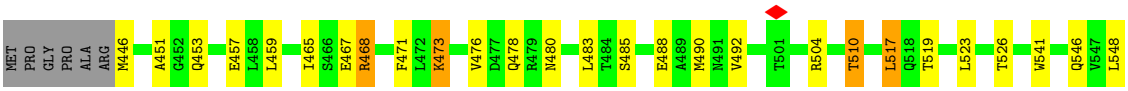


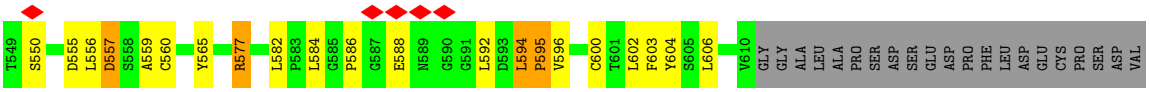


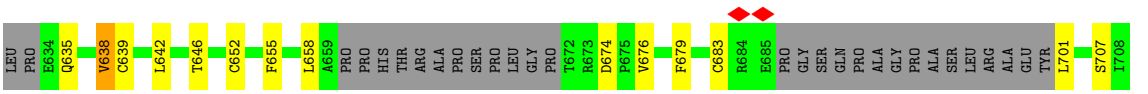


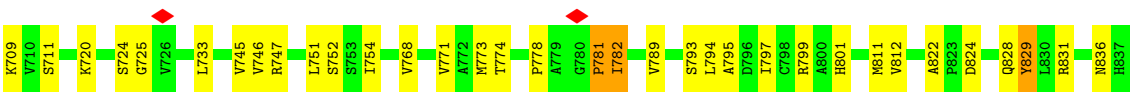


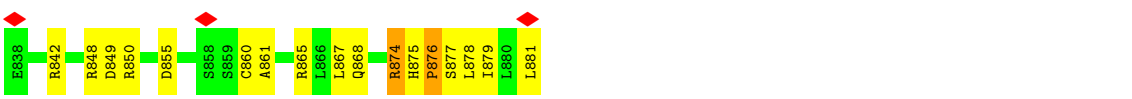






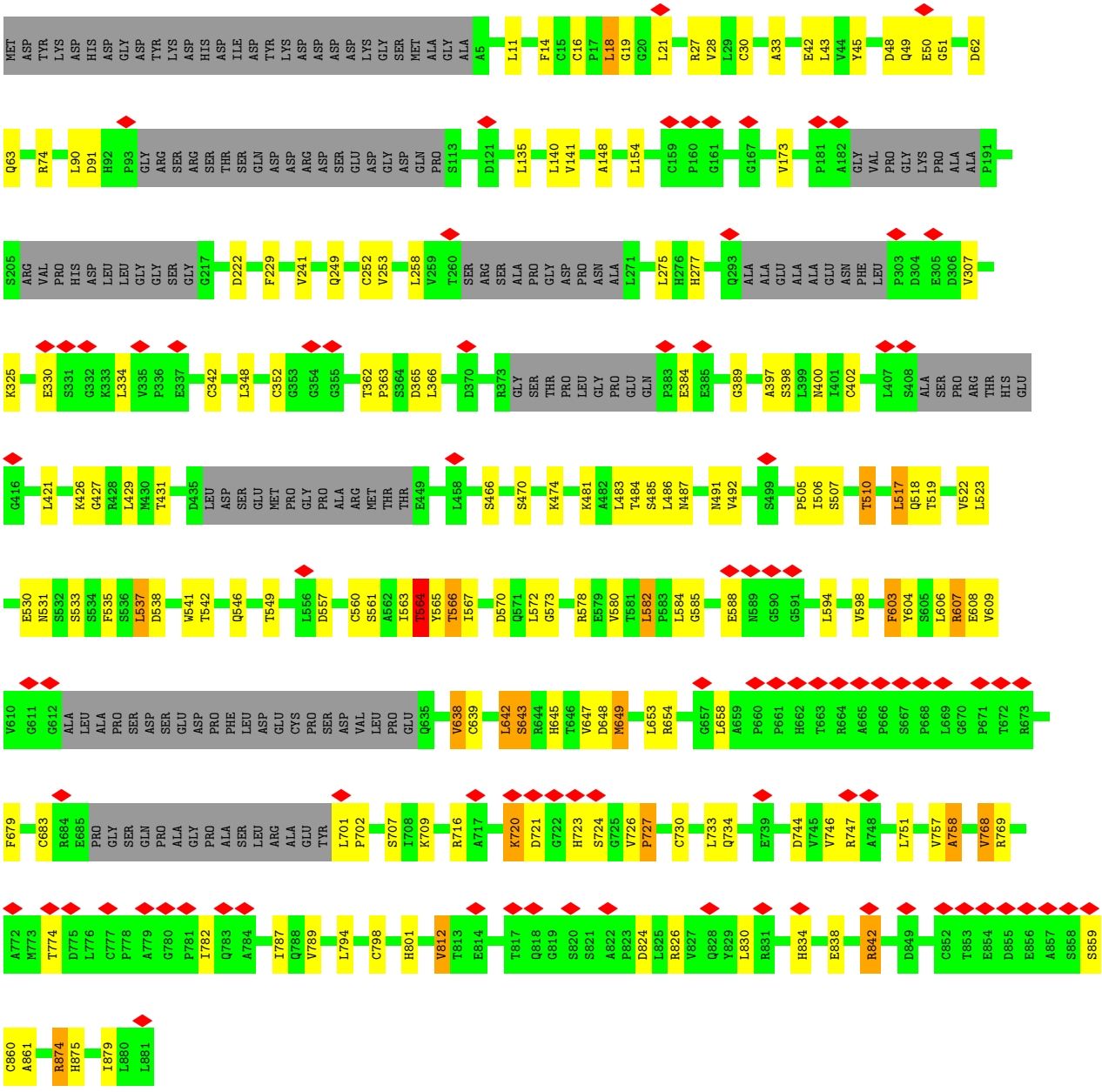






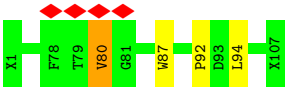
• Molecule 8: Fanconi anemia core complex-associated protein 100

Chain Q:



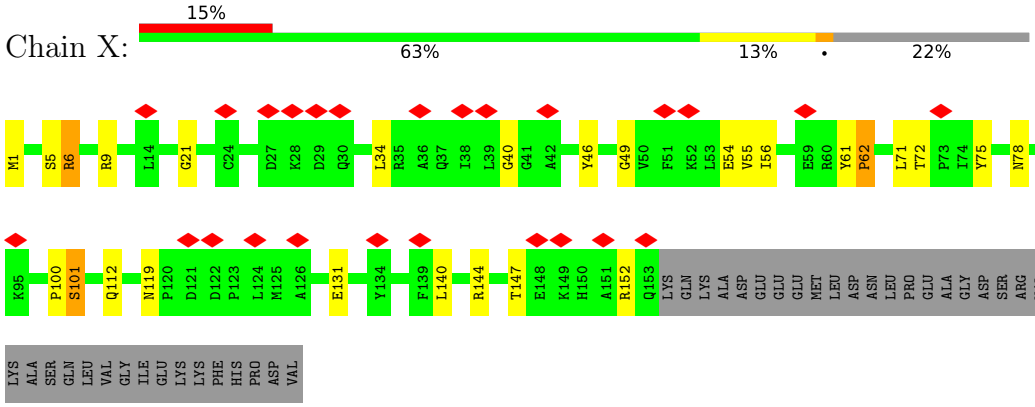
• Molecule 9: Fanconi anemia core complex-associated protein 20

Chain W:



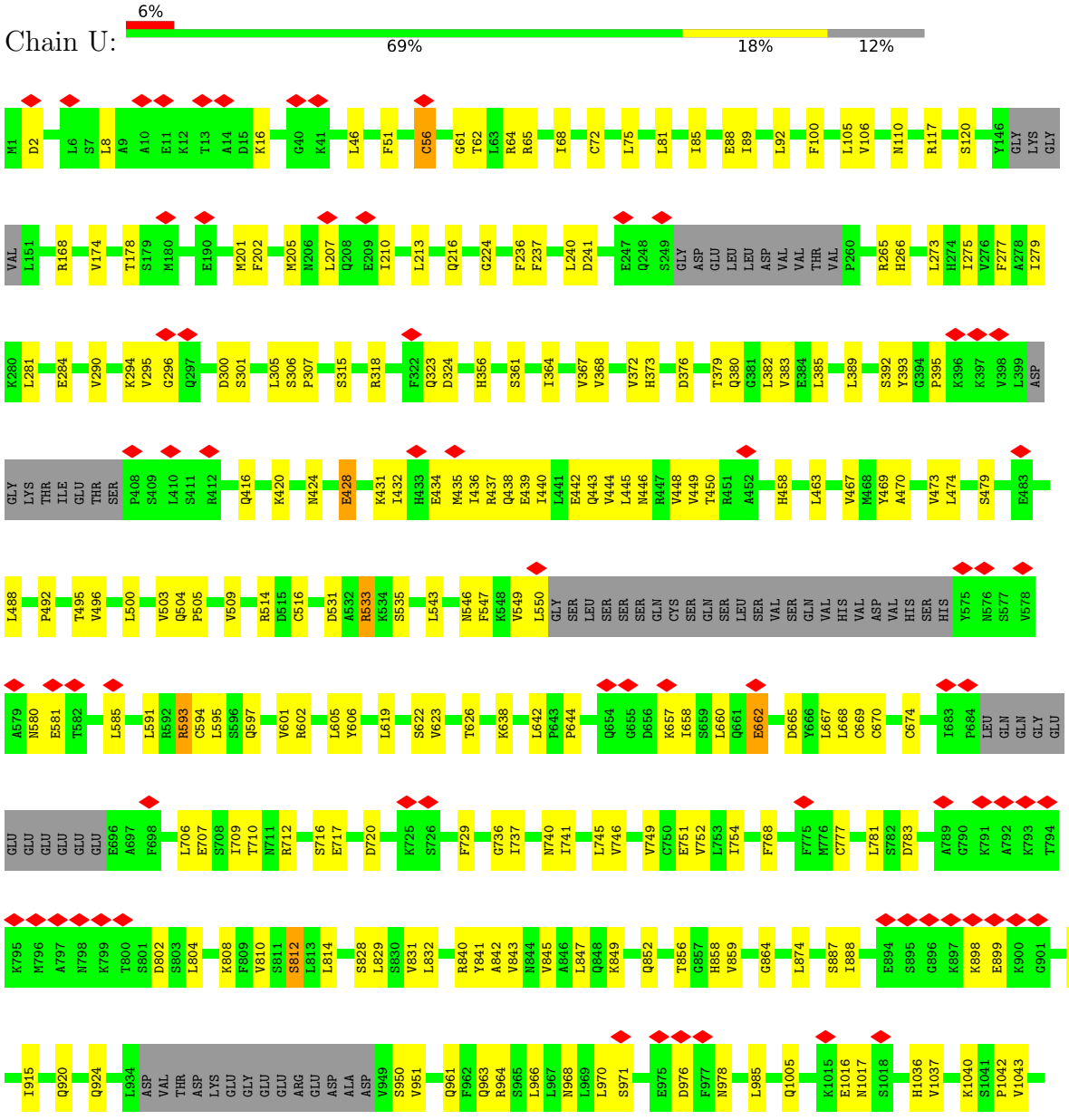
• Molecule 10: Ubiquitin-conjugating enzyme E2 T

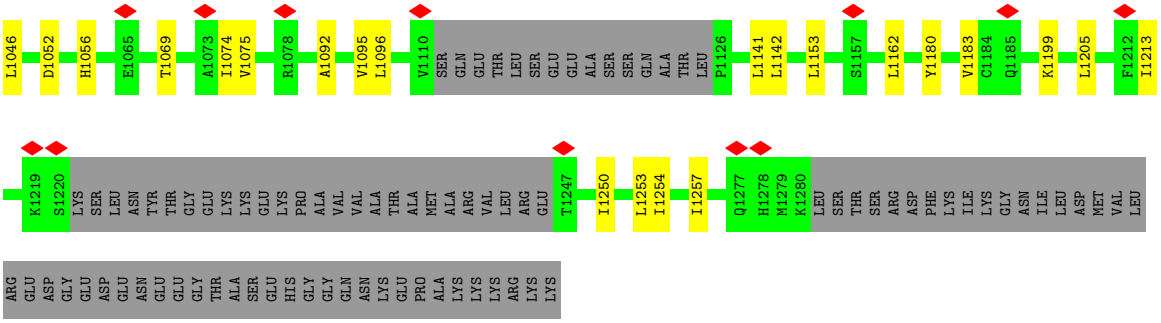
Chain X:



• Molecule 11: Fanconi anemia, complementation group I

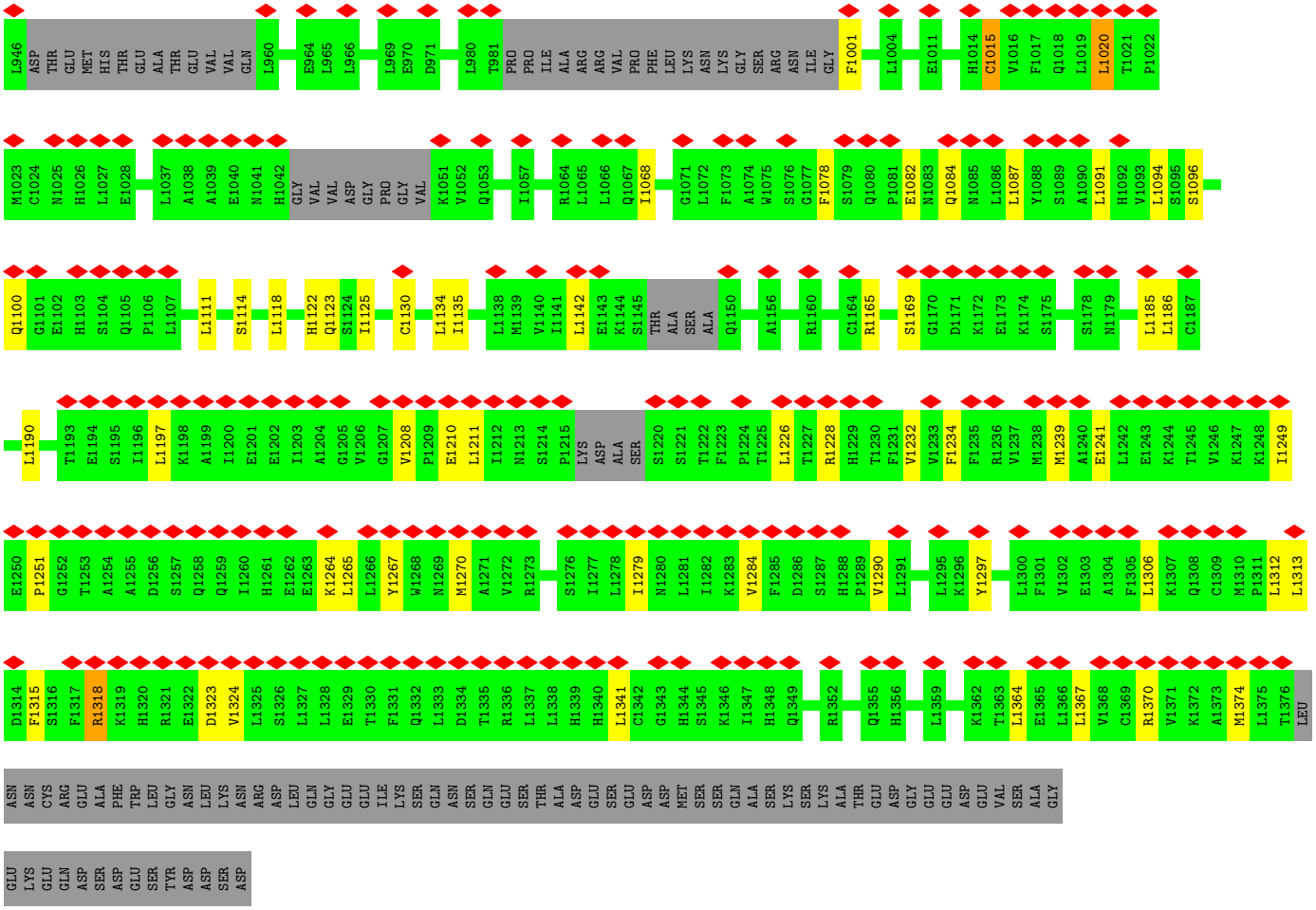
Chain U:





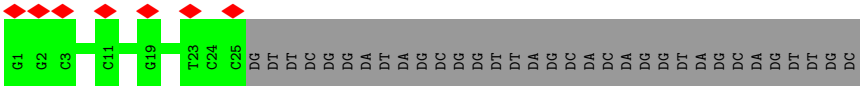
• Molecule 12: Fanconi anemia group D2 protein

Chain V:



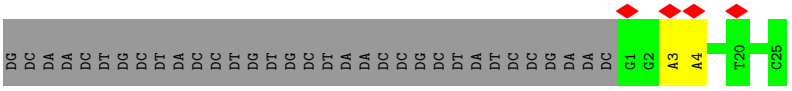
• Molecule 13: DNA (25-MER)

Chain Y:



• Molecule 14: DNA (25-MER)

Chain Z:



4 Experimental information (i)

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 ($e^-/Å^2$)	36.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	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 (Å)	473.088, 473.088, 473.088	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	0/9605	0.97	9/13008 (0.1%)
1	S	0.72	0/10153	0.98	6/13749 (0.0%)
2	B	0.80	2/5707 (0.0%)	1.16	13/7686 (0.2%)
2	O	0.75	1/5701 (0.0%)	1.04	3/7686 (0.0%)
3	C	0.76	0/4497	1.07	4/6103 (0.1%)
4	E	0.83	0/3274	1.22	10/4438 (0.2%)
5	F	0.74	0/2791	1.09	1/3790 (0.0%)
6	G	0.76	0/4568	1.05	3/6215 (0.0%)
6	H	0.72	0/4293	0.98	3/5840 (0.1%)
7	L	0.76	2/3050 (0.1%)	1.04	5/4143 (0.1%)
7	M	0.75	2/3050 (0.1%)	1.03	9/4143 (0.2%)
8	P	0.82	1/5697 (0.0%)	1.23	9/7752 (0.1%)
8	Q	0.73	0/5737	1.04	5/7810 (0.1%)
9	W	0.65	0/202	0.88	0/281
10	X	0.77	0/1267	1.00	1/1722 (0.1%)
11	U	0.73	0/9400	0.98	3/12676 (0.0%)
12	V	0.74	0/9433	0.97	0/12760
13	Y	0.45	0/579	0.89	0/892
14	Z	0.48	0/569	0.96	0/875
All	All	0.75	8/89573 (0.0%)	1.04	84/121569 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	S	0	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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	330	GLY	C-N	-11.74	1.07	1.34
7	M	321	ASP	C-N	-10.48	1.09	1.34
7	M	330	GLY	C-N	-8.72	1.14	1.34
2	B	721	SER	CA-CB	-8.20	1.40	1.52
7	L	321	ASP	C-N	-6.40	1.19	1.34
2	B	583	SER	CA-CB	-5.23	1.45	1.52
2	O	721	SER	CA-CB	-5.18	1.45	1.52
8	P	38	SER	CA-CB	-5.07	1.45	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	321	ASP	O-C-N	-9.79	107.04	122.70
7	M	321	ASP	C-N-CA	9.52	145.50	121.70
8	P	315	PHE	CB-CA-C	-8.47	93.45	110.40
7	M	39	ARG	NE-CZ-NH1	8.28	124.44	120.30
8	Q	727	PRO	N-CD-CG	-7.88	91.38	103.20
8	Q	842	ARG	NE-CZ-NH1	7.53	124.06	120.30
7	M	321	ASP	CA-C-N	7.09	132.80	117.20
8	P	829	TYR	CB-CG-CD1	-7.06	116.77	121.00
3	C	179	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	O	667	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	670	ARG	NE-CZ-NH2	-6.80	116.90	120.30
3	C	292	ARG	CG-CD-NE	-6.79	97.54	111.80
8	P	874	ARG	NE-CZ-NH1	6.77	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	34	GLN	N-CA-CB	-6.73	98.48	110.60
4	E	41	ARG	CG-CD-NE	-6.71	97.71	111.80
6	G	520	ARG	NE-CZ-NH1	6.40	123.50	120.30
8	P	468	ARG	NE-CZ-NH1	6.35	123.48	120.30
7	M	39	ARG	CG-CD-NE	6.32	125.08	111.80
1	S	670	ARG	CG-CD-NE	-6.28	98.62	111.80
1	A	951	ARG	NE-CZ-NH1	6.20	123.40	120.30
4	E	27	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	B	725	THR	N-CA-CB	6.10	121.88	110.30
2	B	47	ARG	CB-CA-C	6.01	122.43	110.40
4	E	343	ARG	CG-CD-NE	5.99	124.38	111.80
7	L	39	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	B	647	ASP	CB-CA-C	5.95	122.31	110.40
4	E	354	ASP	CB-CA-C	5.95	122.29	110.40
7	M	60	ARG	NE-CZ-NH1	5.94	123.27	120.30
8	Q	564	THR	CB-CA-C	-5.91	95.65	111.60
2	O	526	ARG	NE-CZ-NH2	-5.87	117.36	120.30
2	O	667	TYR	CB-CG-CD1	5.87	124.52	121.00
11	U	514	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	C	179	ARG	CG-CD-NE	5.86	124.09	111.80
1	A	1425	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	409	ARG	NE-CZ-NH2	-5.75	117.42	120.30
6	G	376	ASP	CB-CA-C	5.71	121.81	110.40
4	E	365	ARG	CB-CA-C	5.70	121.81	110.40
8	Q	874	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	S	1425	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	B	725	THR	CA-CB-OG1	5.59	120.74	109.00
4	E	27	ARG	NE-CZ-NH1	5.56	123.08	120.30
8	P	310	ASP	CB-CA-C	-5.51	99.38	110.40
7	L	343	ARG	NE-CZ-NH1	5.49	123.05	120.30
7	M	39	ARG	CB-CG-CD	5.47	125.83	111.60
6	G	382	PHE	CB-CA-C	5.44	121.28	110.40
2	B	703	THR	CA-CB-OG1	-5.42	97.62	109.00
1	A	93	PHE	CB-CG-CD2	-5.42	117.01	120.80
2	B	519	ARG	NE-CZ-NH1	5.42	123.01	120.30
8	P	7	ARG	NE-CZ-NH1	5.42	123.01	120.30
5	F	152	ARG	NE-CZ-NH1	5.39	122.99	120.30
7	M	60	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	288	GLU	CB-CA-C	5.34	121.08	110.40
6	H	102	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	S	670	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	714	ARG	NE-CZ-NH2	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	PHE	CB-CG-CD1	5.29	124.50	120.80
6	H	241	PRO	N-CA-C	5.28	125.82	112.10
11	U	533	ARG	NE-CZ-NH1	5.27	122.94	120.30
7	L	349	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	B	741	ASN	CB-CA-C	5.27	120.93	110.40
10	X	6	ARG	NE-CZ-NH1	5.25	122.92	120.30
7	L	10	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	B	519	ARG	CB-CA-C	5.23	120.86	110.40
4	E	533	HIS	CB-CA-C	5.21	120.82	110.40
11	U	437	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	S	1033	ASP	CB-CG-OD2	5.18	122.97	118.30
8	P	874	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	93	PHE	CB-CG-CD1	5.16	124.41	120.80
3	C	91	ILE	CA-CB-CG1	5.15	120.78	111.00
4	E	21	GLN	CB-CA-C	5.13	120.66	110.40
1	A	736	VAL	C-N-CA	5.11	134.49	121.70
7	L	39	ARG	CG-CD-NE	5.11	122.53	111.80
4	E	92	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	B	736	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	B	526	ARG	NE-CZ-NH2	-5.07	117.77	120.30
8	P	797	ILE	CA-CB-CG1	-5.07	101.38	111.00
2	B	836	ARG	NE-CZ-NH1	5.05	122.83	120.30
7	M	60	ARG	CB-CG-CD	5.03	124.69	111.60
1	S	882	PRO	N-CD-CG	-5.03	95.66	103.20
8	P	577	ARG	CB-CA-C	5.02	120.44	110.40
2	B	518	PHE	CB-CG-CD2	-5.02	117.29	120.80
1	S	287	GLU	C-N-CA	5.01	134.24	121.70
8	Q	874	ARG	NE-CZ-NH2	-5.01	117.80	120.30
6	H	189	GLU	CB-CA-C	5.00	120.41	110.40

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
10	X	61	TYR	Mainchain,Peptide
10	X	93	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9402	9487	9431	163	0
1	S	9933	10028	9969	124	0
2	B	5605	5790	5768	143	0
2	O	5594	5759	5740	104	0
3	C	4396	4442	4427	77	0
4	E	3224	3390	3384	110	0
5	F	2726	2740	2729	48	0
6	G	4483	4537	4523	72	0
6	H	4216	4288	4273	84	0
7	L	2974	2977	2970	52	0
7	M	2974	2977	2970	74	0
8	P	5598	5681	5652	173	0
8	Q	5631	5724	5694	96	0
9	W	271	242	196	8	0
10	X	1233	1251	1248	20	0
11	U	9256	9626	9595	148	0
12	V	9258	9475	9422	163	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	87804	88975	88552	1500	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 (1500) 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
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	1.31	0.94
2:O:482:VAL:HG13	2:O:584:LEU:HD11	1.49	0.93
4:E:391:CYS:HG	4:E:398:VAL:HG11	1.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:O:522:LYS:C	2:O:523:CYS:SG	2.59	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
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
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: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
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
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
2:O:522:LYS:O	2:O:523:CYS:SG	2.45	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
1:A:286:GLN:C	1:A:288:GLU:H	1.92	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:L:109:GLN:O	7:L:113:SER:OG	2.05	0.71
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
11:U:751:GLU:CD	11:U:841:TYR:OH	2.29	0.70
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
12:V:432:CYS:HG	12:V:469:CYS:HG	1.34	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:U:395:PRO:HD2	11:U:458:HIS:CE1	2.33	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
4:E:59:ASP:OD1	7:L:166:PHE:CD2	2.53	0.62
4:E:382:LEU:O	4:E:385:THR:OG1	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:E:351:LEU:HD12	4:E:355:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:21:GLY:HA3	10:X:112:GLN:HE22	1.67	0.59
1:A:900:SER:OG	1:A:903:TRP:CD1	2.52	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
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
2:O:164:SER:OG	2:O:215:TYR:OH	2.21	0.58
1:A:28:GLY:C	1:A:30:VAL:H	2.07	0.58
2:B:711:THR:O	2:B:713:PHE:N	2.36	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: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
8:P:311:CYS:SG	8:P:324:ILE:O	2.62	0.57
8:P:679:PHE:C	8:P:679:PHE:CD1	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:P:393:MET:HE1	8:P:434:LEU:HD21	1.86	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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:467:VAL:HG22	11:U:474:LEU:CD1	2.36	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
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
2:O:313:LYS:O	2:O:314:GLU:HB2	2.06	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: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:O:482:VAL:HG13	2:O:584:LEU:CD1	2.30	0.55
4:E:441:ILE:HA	4:E:444:LEU:HD12	1.88	0.55
8:P:74:ARG:HG3	8:P:90:LEU:HB2	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:P:202:PRO:HB3	8:P:225:PHE:CD2	2.42	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: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:G:89:THR:OG1	6:G:90:GLU:N	2.40	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
8:P:392:PRO:C	8:P:393:MET:HG3	2.27	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
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
1:S:988:LEU:HD21	1:S:1077:MET:HE2	1.90	0.54
11:U:440:ILE:O	11:U:444:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
2:B:737:ILE:HG22	2:B:737:ILE:O	2.09	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
3:C:6:VAL:O	3:C:10:CYS:SG	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
8:P:255:LEU:O	8:P:256:LYS:C	2.46	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
4:E:283:ALA:O	4:E:287:GLN:HG3	2.08	0.52
1:S:988:LEU:HD21	1:S:1077:MET:CE	2.40	0.52
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
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:821:LEU:C	1:A:821:LEU:HD23	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:P:30:CYS:SG	8:P:404:VAL:HB	2.50	0.51
1:A:481:VAL:O	1:A:485:SER:OG	2.18	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
2:O:829:LYS:N	8:Q:824:ASP:O	2.43	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
2:B:397:GLY:O	2:B:401:CYS:SG	2.61	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:P:446:MET:HE3	8:P:451:ALA:HB2	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:202:ILE:HG13	12:V:203:ALA:N	2.26	0.51
12:V:210:ASP:O	12:V:213:THR:HG22	2.10	0.51
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:26:PRO:C	8:P:400:ASN:ND2	2.64	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
4:E:473:MET:HE1	4:E:496:VAL:HG11	1.93	0.50
6:H:354:CYS:SG	6:H:359:ARG:HG3	2.50	0.50
8:P:402:CYS:O	8:P:402:CYS:SG	2.61	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
11:U:668:LEU:C	11:U:752:VAL:HG11	2.32	0.50
4:E:467:GLU:O	4:E:471:VAL:HG23	2.10	0.50
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:292:GLN:HE21	4:E:331:LEU:C	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:P:27:ARG:C	8:P:400:ASN:HD21	2.15	0.50
7:M:130:ASP:HB2	7:M:135:THR:HB	1.93	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:486:GLU:O	12:V:490:ASP:CG	2.49	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:O:583:SER:HB3	2:O:586:PRO:HD3	1.93	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:353:GLY:O	8:P:354:GLY:C	2.50	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:939:ILE:O	1:A:1013:GLY:HA2	2.13	0.48
3:C:254:MET:HE1	3:C:281:LEU:HD11	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:922:HIS:HB2	12:V:1001:PHE:CZ	2.49	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:815:PRO:O	1:A:818:PHE:CE1	2.67	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1305:LEU:C	1:A:1308:LEU:HD21	2.35	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
2:B:524:GLN:C	2:B:525:ASN:HD22	2.18	0.47
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:P:366:LEU:HD23	8:P:366:LEU:C	2.35	0.47
8:Q:606:LEU:O	8:Q:609:VAL:N	2.48	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: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
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:192:ASP:CG	6:H:192:ASP:O	2.54	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:143:LEU:C	8:P:143:LEU:HD23	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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
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
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
11:U:380:GLN:CD	11:U:380:GLN:O	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:496:VAL:HG11	11:U:535:SER:HB3	1.97	0.46
4:E:106:ARG:N	4:E:107:PRO:HD2	2.31	0.46
6:G:480:LEU:HD13	6:G:520:ARG:HH11	1.80	0.46
2:O:850:ASP:CG	8:Q:801:HIS:HD1	2.18	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
8:Q:27:ARG:C	8:Q:400:ASN:HD21	2.19	0.46
12:V:609:GLN:O	12:V:613:LEU:HD13	2.15	0.46
2:O:154:SER:OG	2:O:155:SER:O	2.24	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
12:V:364:TRP:C	12:V:364:TRP:CD1	2.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:315:SER:CB	8:P:471:PHE:CE2	3.00	0.45
2:B:602:MET:HE2	8:P:546:GLN:HE21	1.80	0.45
3:C:539:GLU:N	3:C:539:GLU:OE1	2.50	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
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: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
2:O:587:LEU:C	2:O:589:THR:H	2.19	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
12:V:466:ASP:OD1	12:V:466:ASP:C	2.53	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
2:B:82:VAL:O	2:B:83:SER:OG	2.34	0.45
4:E:497:MET:HA	4:E:504:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:176:ASP:OD1	6:H:178:LEU:N	2.49	0.45
2:O:522:LYS:HD2	8:Q:563:ILE:HD13	1.99	0.45
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
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
6:G:592:TYR:CD1	6:G:592:TYR:C	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:VAL:HG22	1:A:476:PHE:CZ	2.51	0.44
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:337:LEU:H	7:L:250:GLU:CD	2.20	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:277:ASP:O	12:V:278:LEU:C	2.56	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:434:ASP:HB3	3:C:438:GLN:HB2	1.99	0.44
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
4:E:522:PHE:C	4:E:523:LEU:HG	2.37	0.44
5:F:14:LEU:HA	5:F:17:VAL:HG22	2.00	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
11:U:968:ASN:HA	11:U:971:SER:HG	1.82	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
1:A:286:GLN:C	1:A:288:GLU:N	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:594:LEU:O	8:P:595:PRO:C	2.55	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: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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	11:U:665:ASP:OD1	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
3:C:287:HIS:ND1	3:C:287:HIS:C	2.72	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: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
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
2:B:298:PHE:HE2	2:B:362:LEU:HB2	1.84	0.43
2:B:710:ARG:O	2:B:711:THR:OG1	2.32	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
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
8:Q:484:THR:OG1	8:Q:485:SER:N	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:P:83:ARG:HD3	8:P:86:TYR:HH	1.82	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:686:LEU:HD13	12:V:811:LYS:HG2	2.01	0.42
2:B:693:PHE:C	2:B:693:PHE:CD1	2.93	0.42
3:C:146:TYR:CB	3:C:147:PRO:HD3	2.50	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:S:346:TRP:CZ3	1:S:386:TRP:HB3	2.55	0.42
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
4:E:41:ARG:O	4:E:42:ARG:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
12:V:391:THR:OG1	12:V:392:ASN:N	2.53	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:P:361:SER:OG	8:P:398:SER:O	2.25	0.41
8:Q:325:LYS:HE2	8:Q:384:GLU:HB3	2.01	0.41
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:768:LEU:O	1:A:772:GLN:C	2.59	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
2:O:590:PHE:C	2:O:592:LYS:H	2.23	0.41
1:S:670:ARG:O	1:S:674:SER:OG	2.38	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
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
8:P:316:GLY:O	8:P:347:VAL:HB	2.21	0.41
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
12:V:534:TYR:CD1	12:V:534:TYR:C	2.93	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
8:Q:707:SER:OG	8:Q:875:HIS:O	2.27	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
3:C:57:SER:C	3:C:59:THR:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:130:ASP:O	4:E:131:ALA:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:249:GLN:HA	8:Q:277:HIS:HA	2.01	0.41
8:Q:567:ILE:O	8:Q:567:ILE:HG22	2.21	0.41
8:Q:642:LEU:O	8:Q:643:SER:C	2.59	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:419:SER:HA	12:V:422:SER:HG	1.85	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
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
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
10:X:75:TYR:OH	10:X:131:GLU:OE1	2.35	0.40
1:A:245:ARG:NH2	1:A:262:MET:HA	2.35	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
4:E:346:THR:H	4:E:346:THR:HG1	1.66	0.40
4:E:472:LEU:HG	4:E:473:MET:HE2	2.04	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:606:TYR:OH	11:U:662:GLU:OE2	2.39	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
6:G:398:LEU:HD12	6:G:592:TYR:CE2	2.57	0.40
6:H:224:ASN:C	6:H:226:ASP:H	2.25	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
2:B:71:ASN:CG	2:B:100:LYS:HG3	2.42	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
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 (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1160/1477 (78%)	1061 (92%)	93 (8%)	6 (0%)	29	68
1	S	1224/1477 (83%)	1115 (91%)	100 (8%)	9 (1%)	22	62
2	B	685/884 (78%)	591 (86%)	78 (11%)	16 (2%)	6	37
2	O	685/884 (78%)	590 (86%)	79 (12%)	16 (2%)	6	37
3	C	546/583 (94%)	475 (87%)	69 (13%)	2 (0%)	34	72
4	E	411/555 (74%)	370 (90%)	39 (10%)	2 (0%)	29	68
5	F	336/399 (84%)	310 (92%)	25 (7%)	1 (0%)	41	76
6	G	567/641 (88%)	510 (90%)	56 (10%)	1 (0%)	47	80
6	H	532/641 (83%)	484 (91%)	42 (8%)	6 (1%)	14	52
7	L	368/394 (93%)	328 (89%)	40 (11%)	0	100	100
7	M	368/394 (93%)	328 (89%)	38 (10%)	2 (0%)	29	68
8	P	726/906 (80%)	616 (85%)	94 (13%)	16 (2%)	6	38
8	Q	732/906 (81%)	636 (87%)	81 (11%)	15 (2%)	7	40
9	W	21/39 (54%)	13 (62%)	7 (33%)	1 (5%)	2	24
10	X	151/197 (77%)	146 (97%)	3 (2%)	2 (1%)	12	48
11	U	1150/1328 (87%)	1053 (92%)	91 (8%)	6 (0%)	29	68
12	V	1131/1451 (78%)	1047 (93%)	78 (7%)	6 (0%)	29	68
All	All	10793/13156 (82%)	9673 (90%)	1013 (9%)	107 (1%)	20	54

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLU
1	A	737	ALA
2	B	132	ASP
2	B	133	GLY
2	B	147	VAL
3	C	84	ASP
4	E	353	PRO
6	H	192	ASP
6	H	241	PRO
6	H	242	ARG
6	H	387	SER

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Mol	Chain	Res	Type
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
1	A	29	ARG
1	A	972	GLY
2	B	138	ASN
6	G	192	ASP
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
7	M	103	ALA
11	U	296	GLY
12	V	414	GLU
1	A	900	SER
2	B	296	ASN
2	B	316	PHE
2	B	325	LEU
2	B	637	PRO
3	C	233	SER
6	H	61	PRO
2	O	132	ASP
2	O	324	LYS

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Mol	Chain	Res	Type
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	B	83	SER
2	B	114	SER
2	B	140	PRO
2	B	713	PHE
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
1	A	26	LEU
2	B	314	GLU
4	E	506	GLU
2	O	70	GLU
2	O	138	ASN
2	O	251	GLN
8	P	822	ALA
12	V	379	VAL
2	B	188	GLU
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

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Mol	Chain	Res	Type
2	B	294	GLY
8	Q	757	VAL
2	B	273	PRO
5	F	337	GLY
8	Q	758	ALA
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1034/1282 (81%)	957 (93%)	77 (7%)	13 40
1	S	1092/1282 (85%)	1018 (93%)	74 (7%)	16 43
2	B	644/810 (80%)	585 (91%)	59 (9%)	9 31
2	O	641/810 (79%)	595 (93%)	46 (7%)	14 41
3	C	480/507 (95%)	459 (96%)	21 (4%)	28 54
4	E	358/467 (77%)	326 (91%)	32 (9%)	9 34
5	F	288/336 (86%)	284 (99%)	4 (1%)	67 80
6	G	483/538 (90%)	444 (92%)	39 (8%)	11 38
6	H	454/538 (84%)	418 (92%)	36 (8%)	12 39
7	L	334/354 (94%)	322 (96%)	12 (4%)	35 60
7	M	334/354 (94%)	316 (95%)	18 (5%)	22 50
8	P	627/749 (84%)	557 (89%)	70 (11%)	6 25
8	Q	630/749 (84%)	584 (93%)	46 (7%)	14 41
9	W	22/22 (100%)	21 (96%)	1 (4%)	27 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	X	136/175 (78%)	132 (97%)	4 (3%)	42 64
11	U	1066/1204 (88%)	1041 (98%)	25 (2%)	50 70
12	V	1065/1324 (80%)	1046 (98%)	19 (2%)	59 76
All	All	9688/11501 (84%)	9105 (94%)	583 (6%)	23 47

All (583) 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	93	PHE
1	A	96	SER
1	A	98	LEU
1	A	113	SER
1	A	145	LEU
1	A	148	LEU
1	A	164	LEU
1	A	169	GLU
1	A	182	VAL
1	A	191	VAL
1	A	241	MET
1	A	272	ARG
1	A	274	LEU
1	A	285	VAL
1	A	313	THR
1	A	333	VAL
1	A	334	LEU
1	A	342	MET
1	A	354	LEU
1	A	371	LEU
1	A	407	LEU
1	A	414	LEU
1	A	423	GLN
1	A	434	VAL
1	A	446	LEU
1	A	450	ASP
1	A	462	TYR
1	A	466	SER
1	A	468	LYS

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Mol	Chain	Res	Type
1	A	491	VAL
1	A	505	SER
1	A	513	LEU
1	A	660	LEU
1	A	666	ASP
1	A	685	ARG
1	A	715	GLU
1	A	782	LEU
1	A	793	GLU
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	948	ASP
1	A	951	ARG
1	A	961	GLU
1	A	964	LEU
1	A	968	SER
1	A	984	LEU
1	A	1020	ARG
1	A	1053	ARG
1	A	1060	THR
1	A	1069	LEU
1	A	1073	ARG
1	A	1146	ARG
1	A	1165	LEU
1	A	1183	CYS
1	A	1190	GLN
1	A	1191	SER
1	A	1309	THR
1	A	1310	GLU
1	A	1368	PHE
1	A	1397	THR
1	A	1403	LEU

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Mol	Chain	Res	Type
1	A	1425	ARG
1	A	1438	SER
2	B	13	GLU
2	B	26	GLN
2	B	40	THR
2	B	81	CYS
2	B	265	LEU
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	297	LEU
2	B	300	VAL
2	B	323	GLU
2	B	349	LEU
2	B	401	CYS
2	B	403	SER
2	B	412	LEU
2	B	486	SER
2	B	488	VAL
2	B	491	VAL
2	B	495	SER
2	B	496	SER
2	B	506	LEU
2	B	507	SER
2	B	519	ARG
2	B	523	CYS
2	B	525	ASN
2	B	571	LYS
2	B	574	CYS
2	B	576	GLN
2	B	585	SER
2	B	592	LYS
2	B	602	MET
2	B	604	ARG
2	B	605	GLU
2	B	622	LEU
2	B	624	LEU
2	B	628	SER
2	B	635	THR

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Mol	Chain	Res	Type
2	B	658	SER
2	B	664	SER
2	B	670	ASN
2	B	677	LEU
2	B	681	LYS
2	B	693	PHE
2	B	699	SER
2	B	700	PHE
2	B	705	PHE
2	B	710	ARG
2	B	716	ILE
2	B	722	ARG
2	B	724	GLN
2	B	741	ASN
2	B	748	LYS
2	B	765	LYS
2	B	813	ARG
2	B	836	ARG
2	B	855	LYS
3	C	12	TYR
3	C	29	GLU
3	C	63	ARG
3	C	65	PRO
3	C	69	GLN
3	C	136	GLN
3	C	144	ASP
3	C	162	ARG
3	C	190	LEU
3	C	194	THR
3	C	207	HIS
3	C	214	ILE
3	C	218	GLU
3	C	236	MET
3	C	241	CYS
3	C	278	ASP
3	C	286	CYS
3	C	292	ARG
3	C	393	SER
3	C	507	ASP
3	C	509	ILE
4	E	42	ARG
4	E	48	ARG

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Mol	Chain	Res	Type
4	E	58	PHE
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	148	THR
4	E	160	CYS
4	E	177	ARG
4	E	293	GLN
4	E	314	GLN
4	E	352	SER
4	E	354	ASP
4	E	357	LEU
4	E	358	SER
4	E	364	THR
4	E	365	ARG
4	E	428	SER
4	E	430	GLU
4	E	443	GLU
4	E	465	THR
4	E	509	ARG
4	E	514	MET
4	E	517	GLU
4	E	519	ASN
4	E	522	PHE
4	E	523	LEU
4	E	524	ARG
4	E	532	LYS
5	F	161	SER
5	F	174	LEU
5	F	270	LEU
5	F	302	VAL
6	G	57	LEU
6	G	80	LEU
6	G	89	THR
6	G	98	ARG
6	G	104	LEU
6	G	118	LEU
6	G	132	LEU
6	G	154	ASP

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Mol	Chain	Res	Type
6	G	155	ARG
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	267	LEU
6	G	327	LEU
6	G	340	CYS
6	G	346	THR
6	G	365	GLU
6	G	371	LEU
6	G	373	LEU
6	G	381	ARG
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	459	GLN
6	G	466	LEU
6	G	478	ARG
6	G	479	CYS
6	G	483	LEU
6	G	520	ARG
6	G	524	TRP
6	G	573	ARG
6	G	606	ASP
6	H	12	CYS
6	H	13	LEU
6	H	41	GLN
6	H	42	LEU
6	H	54	LEU
6	H	91	ASP
6	H	104	LEU
6	H	105	GLU
6	H	130	CYS
6	H	134	GLU
6	H	158	ASP

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Mol	Chain	Res	Type
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	301	GLU
6	H	350	LEU
6	H	359	ARG
6	H	368	LEU
6	H	381	ARG
6	H	393	MET
6	H	404	LEU
6	H	405	ILE
6	H	412	ASP
6	H	466	LEU
6	H	483	LEU
6	H	506	ASP
6	H	562	ASP
6	H	568	THR
6	H	586	LEU
6	H	606	ASP
7	L	4	THR
7	L	25	TYR
7	L	39	ARG
7	L	46	LEU
7	L	116	GLU
7	L	118	ILE
7	L	162	SER
7	L	182	SER
7	L	213	VAL
7	L	227	ARG
7	L	268	SER
7	L	316	ASP
2	O	7	MET
2	O	47	ARG
2	O	104	VAL
2	O	132	ASP
2	O	145	ARG

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Mol	Chain	Res	Type
2	O	168	SER
2	O	171	GLN
2	O	237	VAL
2	O	246	GLU
2	O	256	LEU
2	O	279	LEU
2	O	287	VAL
2	O	315	SER
2	O	317	GLN
2	O	323	GLU
2	O	328	VAL
2	O	386	ASN
2	O	475	VAL
2	O	484	ASP
2	O	491	VAL
2	O	496	SER
2	O	505	THR
2	O	508	LEU
2	O	518	PHE
2	O	519	ARG
2	O	573	GLU
2	O	577	ILE
2	O	579	THR
2	O	585	SER
2	O	602	MET
2	O	606	SER
2	O	612	ASP
2	O	624	LEU
2	O	626	ASP
2	O	628	SER
2	O	631	LYS
2	O	635	THR
2	O	643	GLU
2	O	659	CYS
2	O	677	LEU
2	O	724	GLN
2	O	735	ILE
2	O	740	ILE
2	O	748	LYS
2	O	780	HIS
2	O	783	ASN
8	P	34	GLU

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Mol	Chain	Res	Type
8	P	41	SER
8	P	42	GLU
8	P	45	TYR
8	P	59	ARG
8	P	69	LEU
8	P	74	ARG
8	P	76	LEU
8	P	91	ASP
8	P	131	CYS
8	P	135	LEU
8	P	137	ASP
8	P	149	ARG
8	P	162	GLU
8	P	177	SER
8	P	196	VAL
8	P	198	CYS
8	P	219	THR
8	P	224	LEU
8	P	228	LEU
8	P	232	ASP
8	P	234	THR
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	306	ASP
8	P	325	LYS
8	P	364	SER
8	P	390	LEU
8	P	402	CYS
8	P	424	SER
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	555	ASP

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Mol	Chain	Res	Type
8	P	560	CYS
8	P	577	ARG
8	P	582	LEU
8	P	594	LEU
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	701	LEU
8	P	707	SER
8	P	724	SER
8	P	745	VAL
8	P	747	ARG
8	P	751	LEU
8	P	752	SER
8	P	768	VAL
8	P	774	THR
8	P	789	VAL
8	P	793	SER
8	P	811	MET
8	P	828	GLN
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	222	ASP
8	Q	253	VAL
8	Q	307	VAL
8	Q	334	LEU
8	Q	342	CYS
8	Q	352	CYS
8	Q	362	THR
8	Q	365	ASP
8	Q	470	SER
8	Q	474	LYS
8	Q	481	LYS
8	Q	510	THR

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Mol	Chain	Res	Type
8	Q	517	LEU
8	Q	522	VAL
8	Q	523	LEU
8	Q	542	THR
8	Q	546	GLN
8	Q	560	CYS
8	Q	561	SER
8	Q	564	THR
8	Q	566	THR
8	Q	578	ARG
8	Q	582	LEU
8	Q	598	VAL
8	Q	603	PHE
8	Q	607	ARG
8	Q	638	VAL
8	Q	642	LEU
8	Q	654	ARG
8	Q	658	LEU
8	Q	723	HIS
8	Q	744	ASP
8	Q	747	ARG
8	Q	751	LEU
8	Q	768	VAL
8	Q	769	ARG
8	Q	774	THR
8	Q	782	ILE
8	Q	789	VAL
8	Q	794	LEU
8	Q	812	VAL
8	Q	838	GLU
8	Q	842	ARG
1	S	38	GLU
1	S	43	LEU
1	S	60	LEU
1	S	92	SER
1	S	98	LEU
1	S	142	ARG
1	S	163	ARG
1	S	175	SER
1	S	182	VAL
1	S	191	VAL
1	S	194	GLN

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Mol	Chain	Res	Type
1	S	221	MET
1	S	239	VAL
1	S	267	VAL
1	S	274	LEU
1	S	305	HIS
1	S	313	THR
1	S	325	THR
1	S	333	VAL
1	S	338	ASP
1	S	380	GLU
1	S	491	VAL
1	S	517	ARG
1	S	561	THR
1	S	653	LEU
1	S	670	ARG
1	S	674	SER
1	S	683	ARG
1	S	685	ARG
1	S	714	ARG
1	S	741	ARG
1	S	766	CYS
1	S	770	ARG
1	S	795	ARG
1	S	800	GLU
1	S	818	PHE
1	S	828	ASP
1	S	838	THR
1	S	855	THR
1	S	856	LEU
1	S	858	SER
1	S	859	CYS
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	966	GLU
1	S	973	CYS
1	S	992	HIS
1	S	996	ARG
1	S	1005	ASP

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Mol	Chain	Res	Type
1	S	1012	THR
1	S	1023	GLU
1	S	1031	GLN
1	S	1043	SER
1	S	1045	GLU
1	S	1060	THR
1	S	1093	SER
1	S	1129	ASP
1	S	1139	LEU
1	S	1183	CYS
1	S	1202	GLU
1	S	1265	LEU
1	S	1280	ASP
1	S	1294	CYS
1	S	1310	GLU
1	S	1328	THR
1	S	1339	LEU
1	S	1345	ASP
1	S	1367	LEU
1	S	1369	VAL
1	S	1428	CYS
9	W	94	LEU
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	169	PHE
7	M	222	SER
7	M	243	ARG
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

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Mol	Chain	Res	Type
10	X	72	THR
10	X	101	SER
11	U	56	CYS
11	U	178	THR
11	U	216	GLN
11	U	284	GLU
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	531	ASP
11	U	593	ARG
11	U	657	LYS
11	U	777	CYS
11	U	783	ASP
11	U	812	SER
11	U	852	GLN
11	U	898	LYS
11	U	905	SER
11	U	976	ASP
11	U	1016	GLU
11	U	1199	LYS
12	V	166	ASN
12	V	190	LYS
12	V	221	ASP
12	V	292	MET
12	V	338	SER
12	V	371	THR
12	V	390	SER
12	V	441	SER
12	V	455	SER
12	V	509	MET
12	V	726	SER
12	V	729	CYS
12	V	757	ASP
12	V	828	LYS
12	V	1015	CYS

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Mol	Chain	Res	Type
12	V	1130	CYS
12	V	1208	VAL
12	V	1228	ARG
12	V	1318	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	123	GLN
1	A	993	GLN
1	A	1205	GLN
1	A	1231	HIS
1	A	1417	HIS
2	B	71	ASN
2	B	241	HIS
2	B	270	ASN
2	B	306	ASN
2	B	600	GLN
2	B	656	HIS
2	B	670	ASN
2	B	679	HIS
2	B	780	HIS
3	C	13	GLN
3	C	42	GLN
3	C	58	ASN
3	C	69	GLN
3	C	99	ASN
3	C	107	GLN
3	C	224	ASN
3	C	366	GLN
3	C	382	GLN
3	C	399	HIS
3	C	438	GLN
3	C	441	GLN
3	C	493	ASN
3	C	528	GLN
3	C	534	ASN
3	C	557	GLN
4	E	31	GLN
4	E	292	GLN
4	E	335	GLN

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Mol	Chain	Res	Type
4	E	359	ASN
5	F	130	GLN
5	F	154	ASN
5	F	309	ASN
6	G	31	GLN
6	G	55	HIS
6	G	97	GLN
6	G	320	GLN
6	G	339	HIS
6	G	406	GLN
6	G	498	ASN
6	G	547	ASN
6	G	553	HIS
6	H	26	GLN
6	H	31	GLN
6	H	58	GLN
6	H	320	GLN
6	H	529	GLN
6	H	542	GLN
7	L	18	GLN
7	L	270	ASN
7	L	272	HIS
7	L	282	GLN
2	O	102	ASN
2	O	270	ASN
2	O	512	GLN
2	O	670	ASN
8	P	293	GLN
8	P	318	HIS
8	P	400	ASN
8	P	464	ASN
8	P	546	GLN
8	P	635	GLN
8	P	651	GLN
8	Q	400	ASN
8	Q	491	ASN
8	Q	645	HIS
8	Q	875	HIS
1	S	271	GLN
1	S	286	GLN
1	S	322	HIS
1	S	343	GLN

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Mol	Chain	Res	Type
1	S	352	HIS
1	S	376	GLN
1	S	387	GLN
1	S	436	GLN
1	S	490	GLN
1	S	772	GLN
1	S	869	GLN
1	S	940	GLN
1	S	992	HIS
1	S	993	GLN
1	S	1022	GLN
1	S	1276	ASN
1	S	1307	GLN
1	S	1366	GLN
1	S	1417	HIS
1	S	1440	GLN
7	M	18	GLN
7	M	76	HIS
7	M	244	HIS
7	M	272	HIS
10	X	67	GLN
10	X	112	GLN
10	X	142	ASN
11	U	110	ASN
11	U	206	ASN
11	U	304	ASN
11	U	345	GLN
11	U	373	HIS
11	U	443	GLN
11	U	446	ASN
11	U	465	ASN
11	U	580	ASN
11	U	597	GLN
11	U	618	GLN
11	U	625	GLN
11	U	672	GLN
11	U	851	GLN
11	U	928	GLN
11	U	973	GLN
11	U	978	ASN
11	U	1005	GLN
11	U	1070	ASN

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Mol	Chain	Res	Type
12	V	146	GLN
12	V	166	ASN
12	V	392	ASN
12	V	1083	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

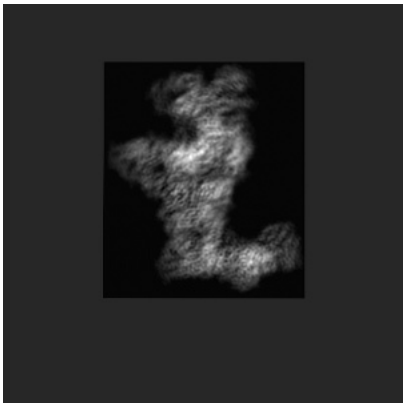
6 Map visualisation

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.

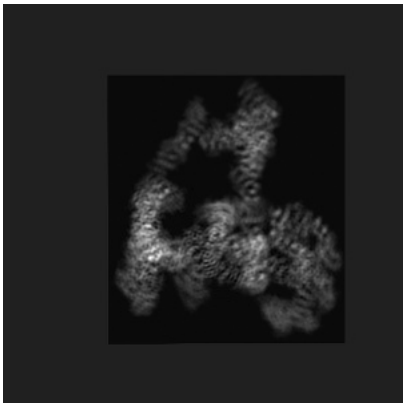
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

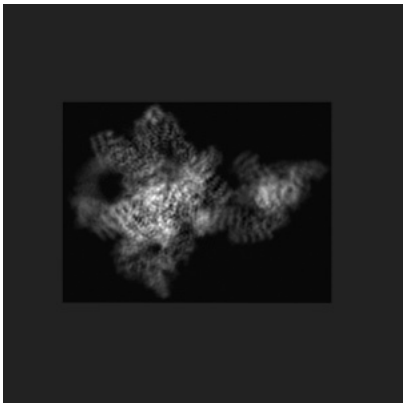
6.1.1 Primary map



X



Y

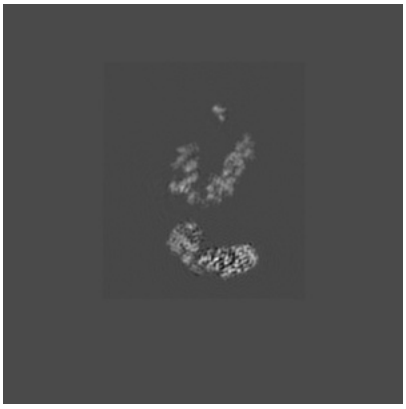


Z

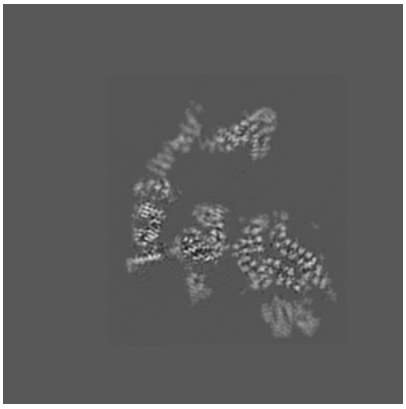
The images above show the map projected in three orthogonal directions.

6.2 Central slices

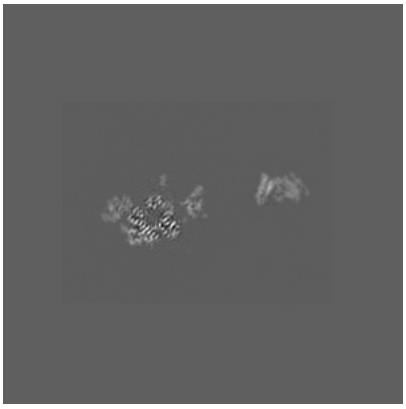
6.2.1 Primary map



X Index: 224



Y Index: 224

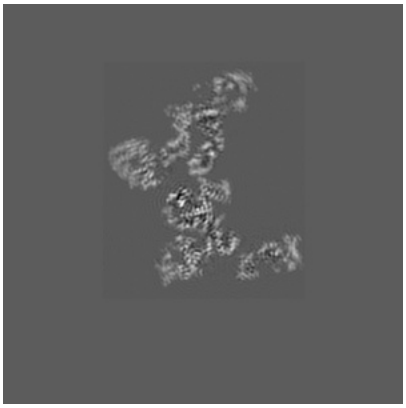


Z Index: 224

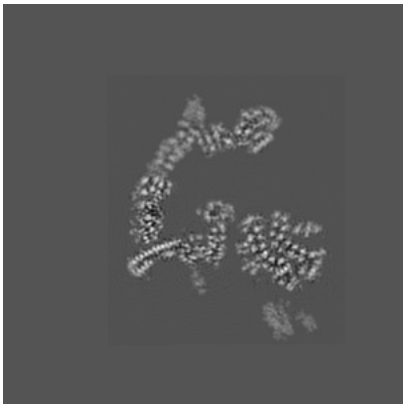
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

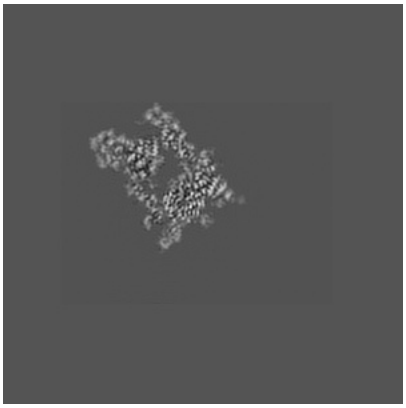
6.3.1 Primary map



X Index: 175



Y Index: 231



Z Index: 161

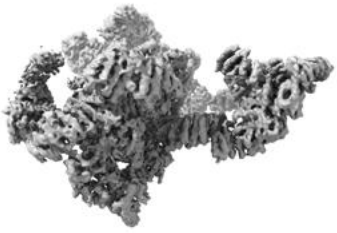
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

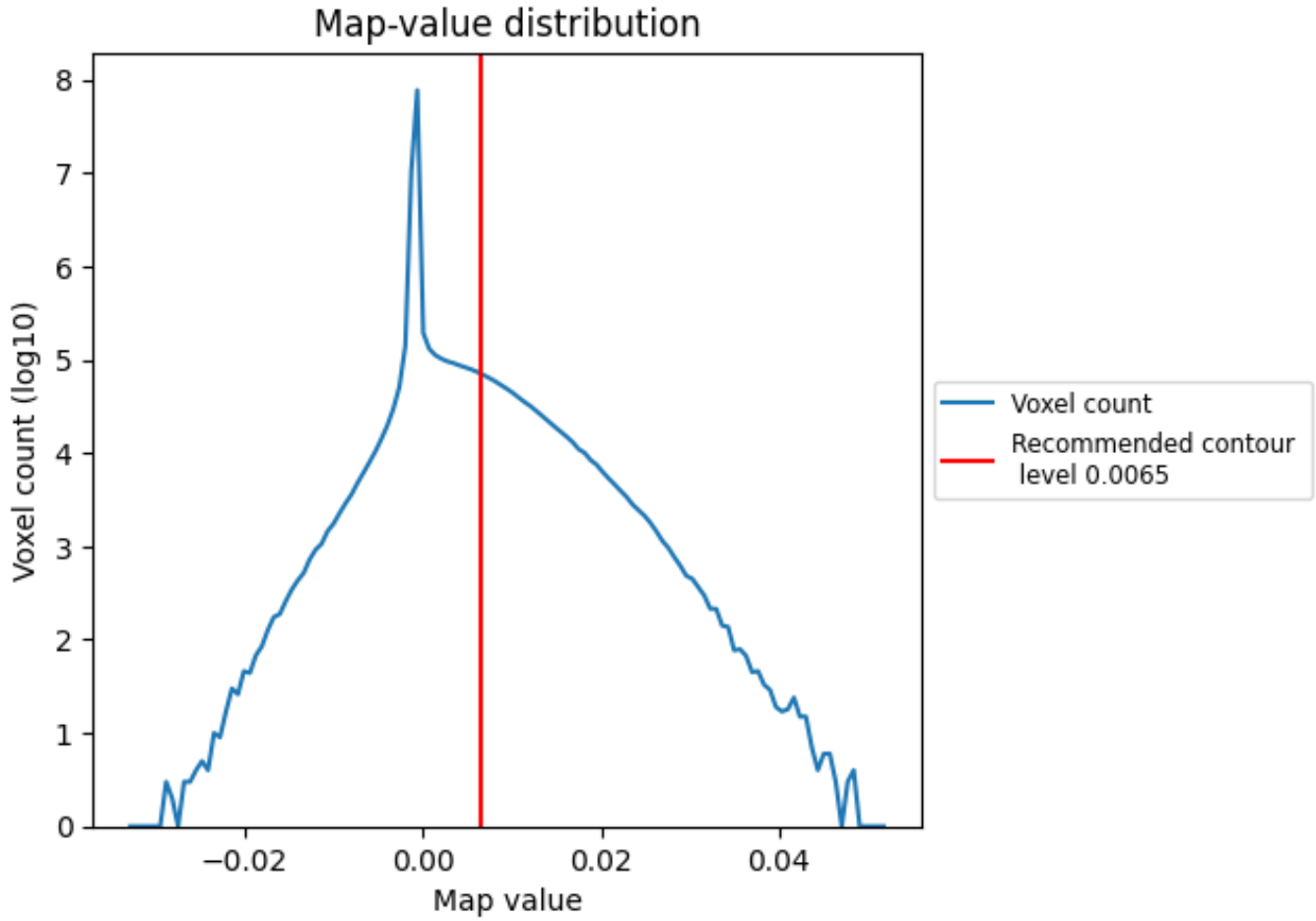
6.5 Mask visualisation (i)

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

7 Map analysis

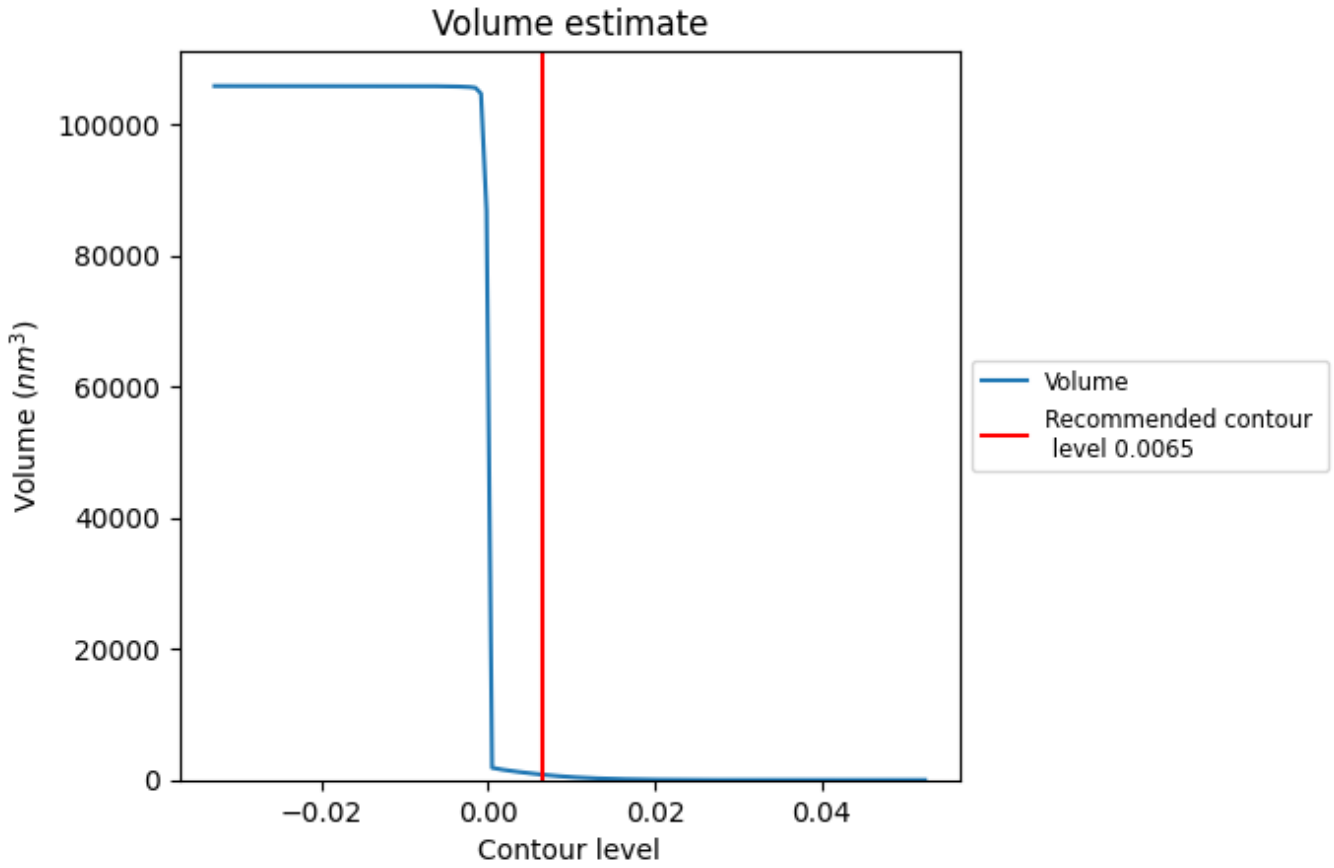
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

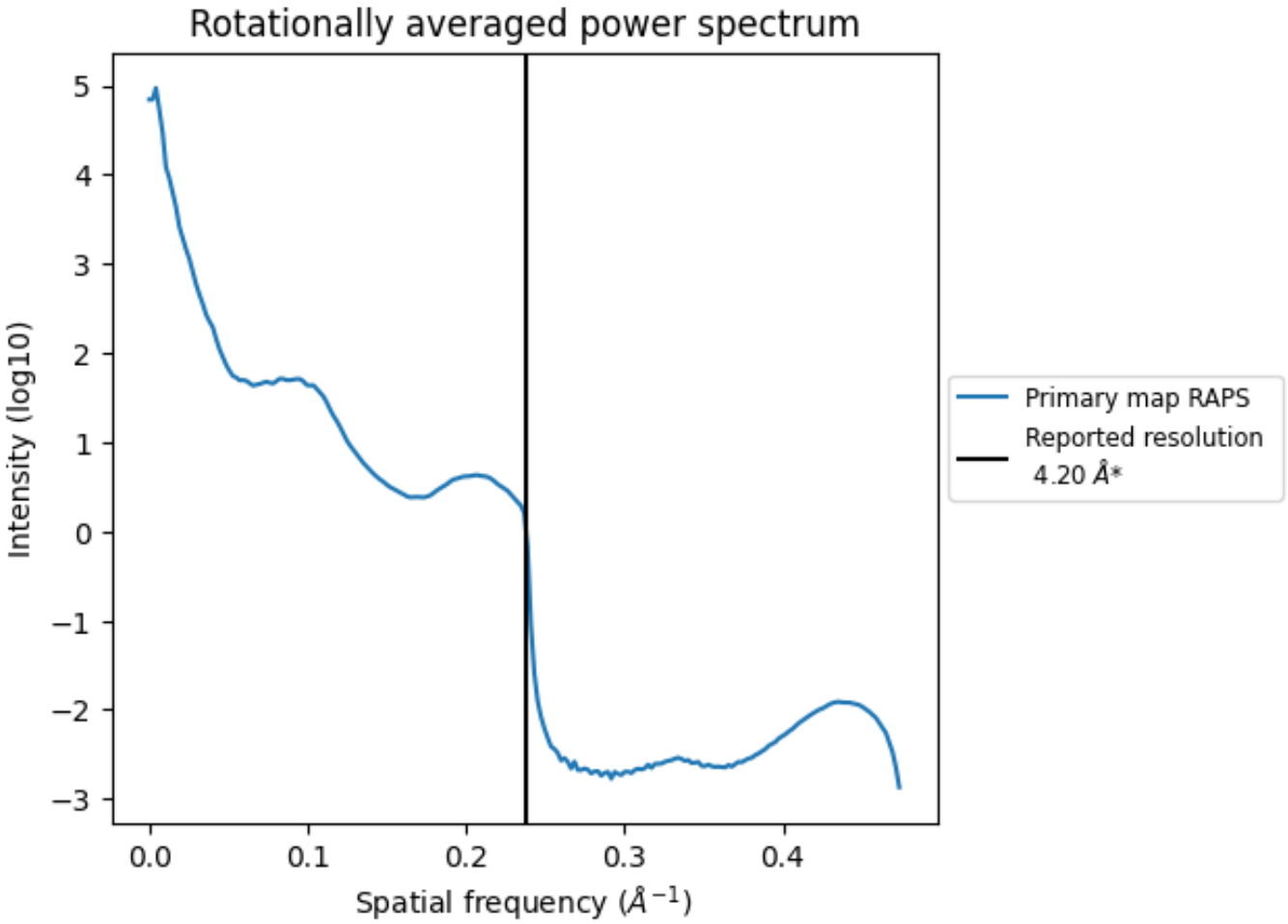
7.2 Volume estimate



The volume at the recommended contour level is 814 nm^3; 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 (i)



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

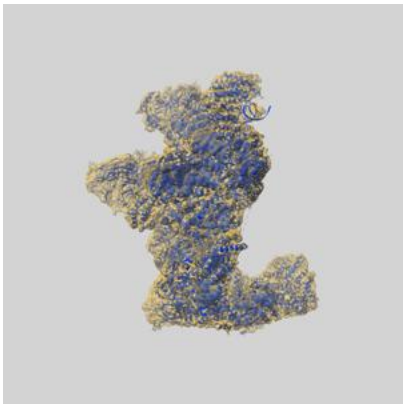
8 Fourier-Shell correlation (i)

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

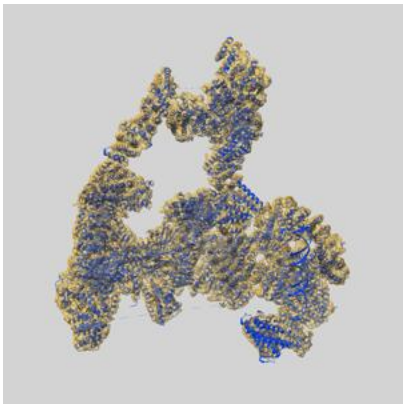
9 Map-model fit

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

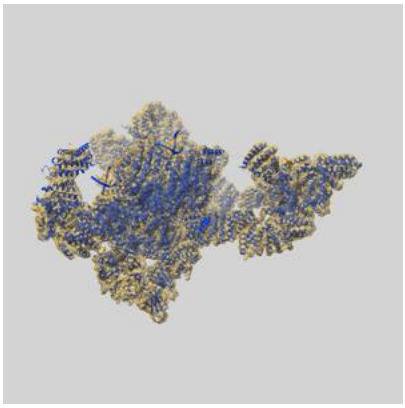
9.1 Map-model overlay



X



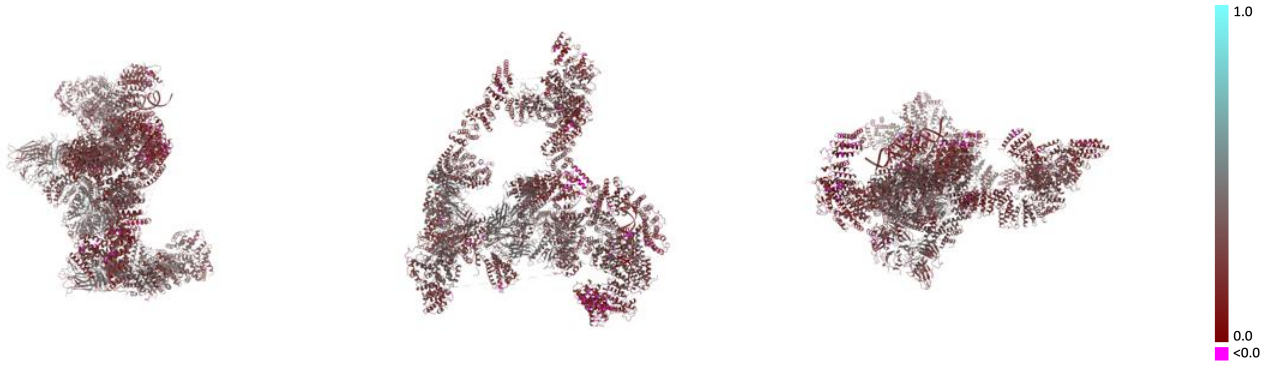
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065 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.

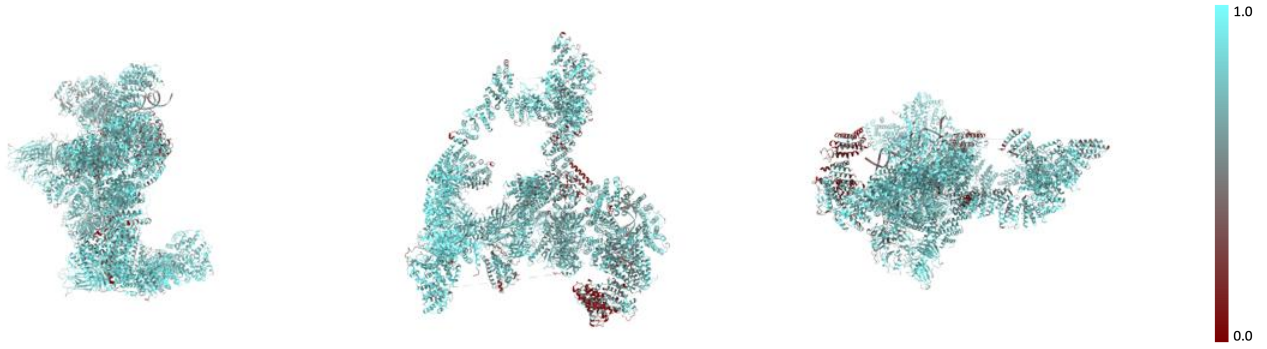
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

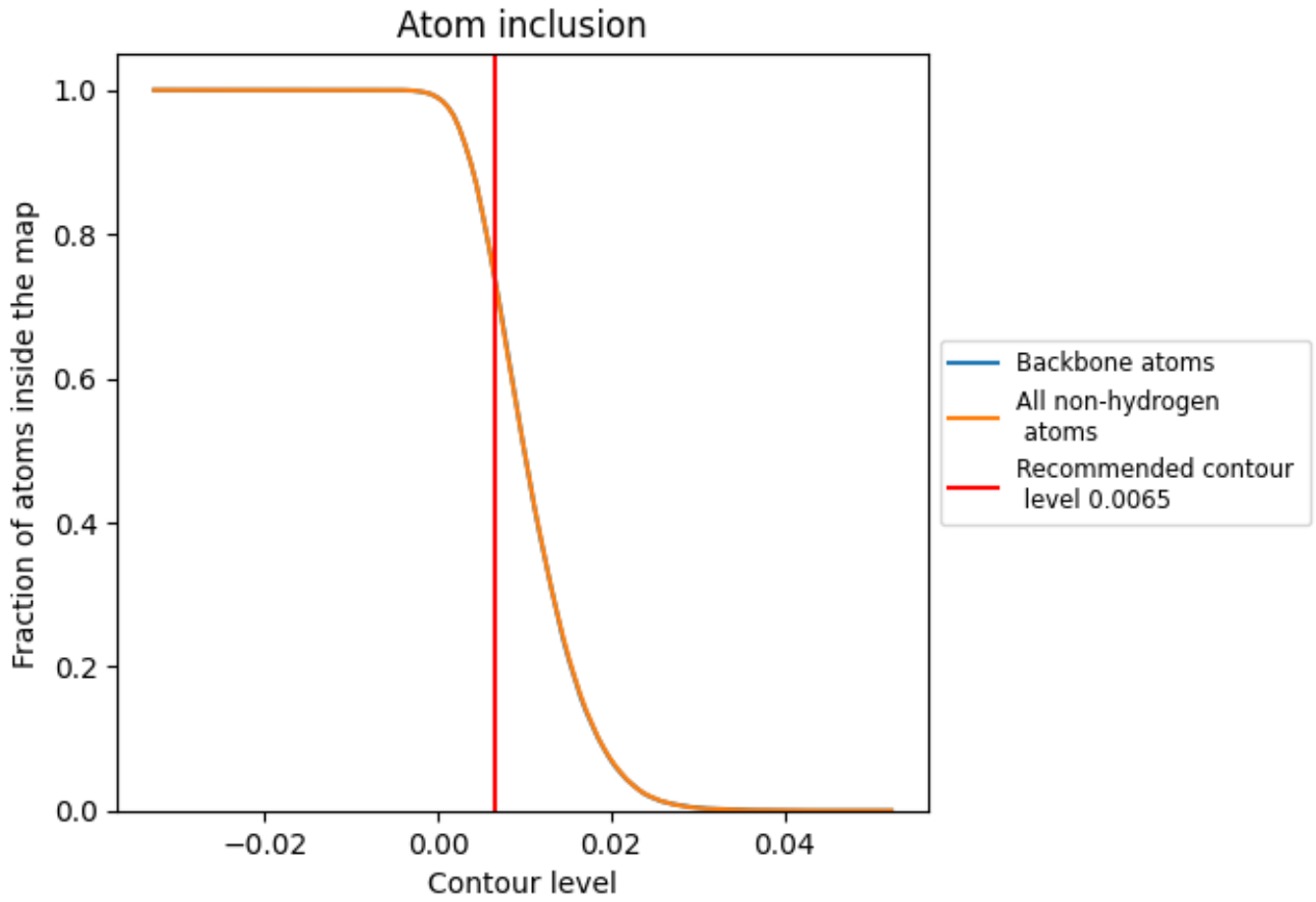
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0065).

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	0.7433	0.3030
A	0.7100	0.2660
B	0.8210	0.3720
C	0.8499	0.3360
E	0.7622	0.3170
F	0.8583	0.3420
G	0.8046	0.3130
H	0.7513	0.2860
L	0.7836	0.3250
M	0.7467	0.3110
O	0.7950	0.3470
P	0.8456	0.4000
Q	0.7230	0.3350
S	0.7549	0.2680
U	0.7377	0.2760
V	0.5945	0.2420
W	0.7546	0.3090
X	0.6211	0.2640
Y	0.5678	0.1830
Z	0.5560	0.1910