



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:03 AM UTC

PDB ID : 7KZR / pdb_00007kzr
EMDB ID : EMD-23087
Title : Structure of the human Fanconi Anaemia Core-UBE2T-ID complex
Authors : Wang, S.L.; Pavletich, N.P.
Deposited on : 2020-12-10
Resolution : 4.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

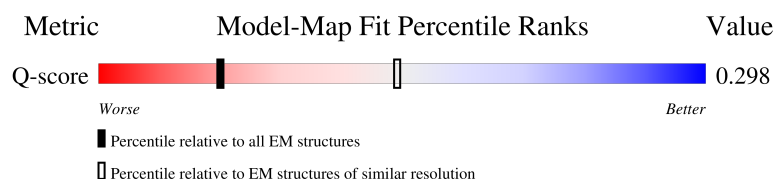
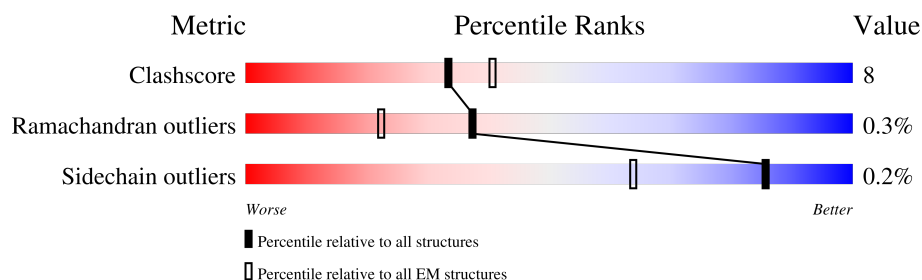
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 Å.

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



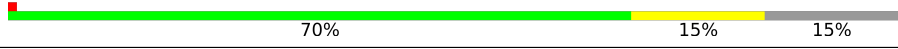
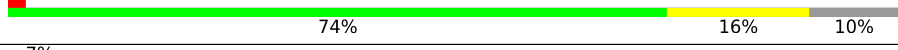
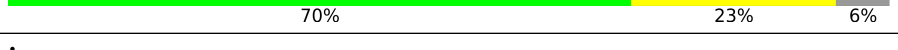
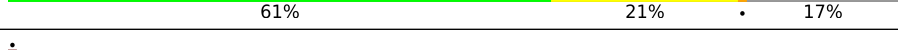
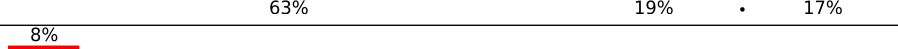
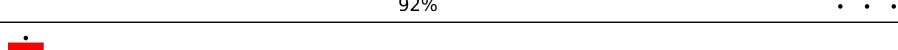
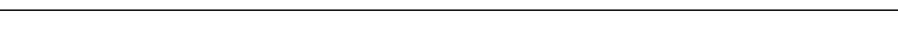
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	1477	
1	S	1477	
2	B	884	
2	O	884	

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Mol	Chain	Length	Quality of chain
3	C	583	
4	E	555	
5	F	399	
6	G	641	
6	H	641	
7	L	394	
7	M	394	
8	P	906	
8	Q	906	
9	W	39	
10	U	1328	
11	V	1451	
12	X	197	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 175108 atoms, of which 88363 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fanconi anemia group A protein.

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

There are 44 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 50 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 25 discrepancies between the modelled and reference sequences:

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

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

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

There are 19 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 25 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 38 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 38 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 50 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 10 is a protein called Fanconi anemia, complementation group I.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	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 11 is a protein called Fanconi anemia group D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	V	1153	Total	C	H	N	O	S	0	0
			18733	5970	9475	1527	1709	52		

- Molecule 12 is a protein called Ubiquitin-conjugating enzyme E2 T.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	X	153	Total	C	H	N	O	S	0	0
			2399	772	1200	205	215	7		

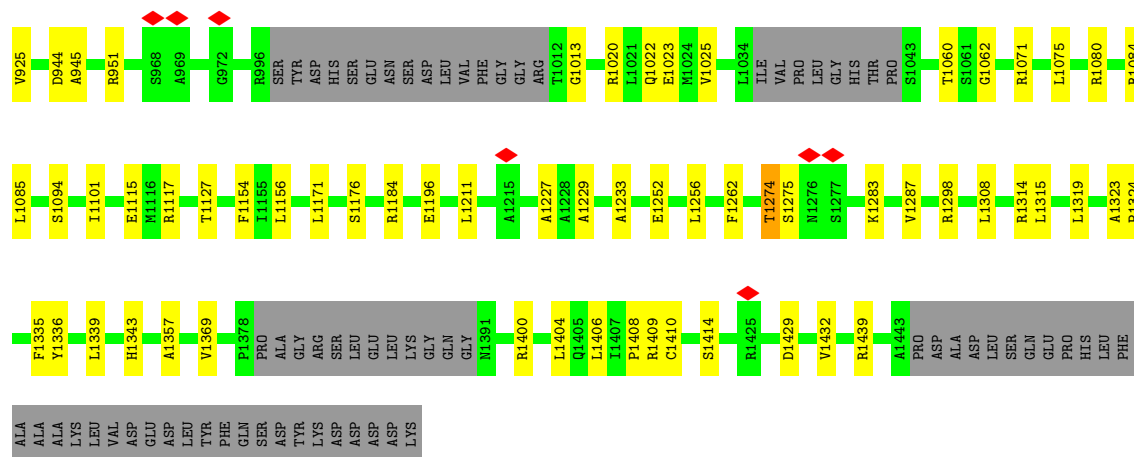
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	G	1	Total	Zn	0
			1	1	

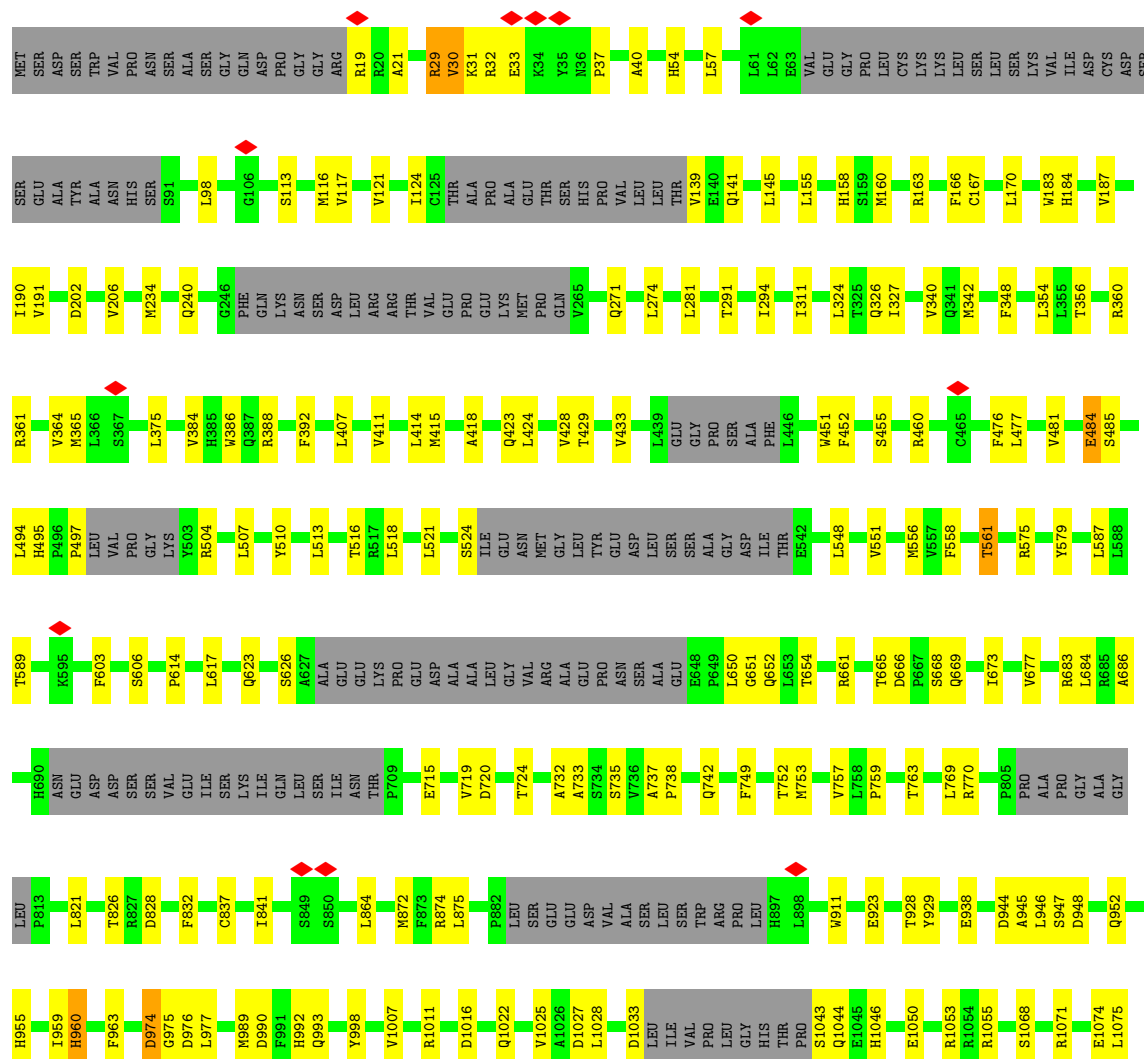
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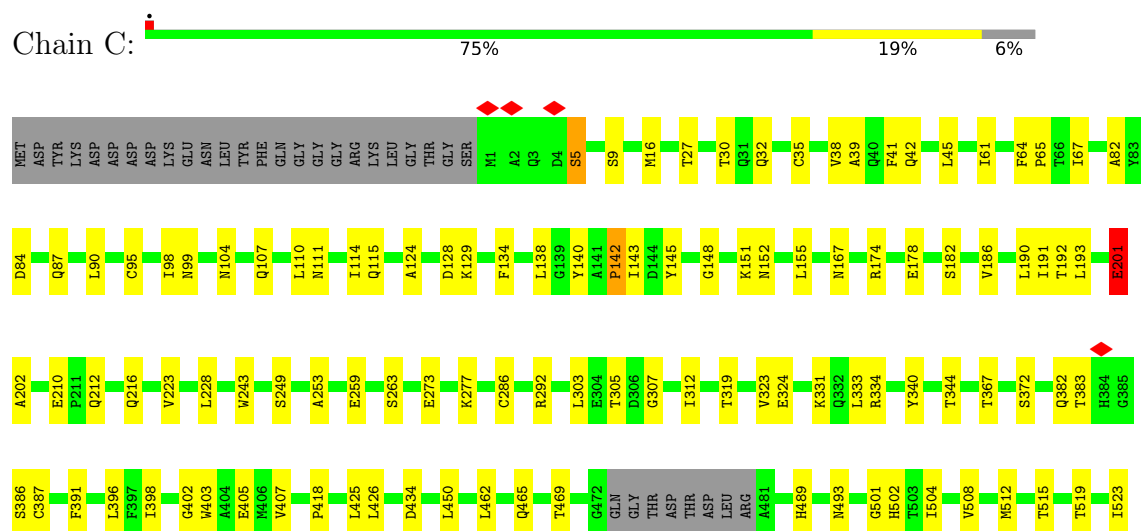
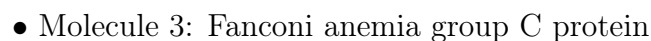
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Mol	Chain	Residues	Atoms		AltConf
13	L	2	Total 2	Zn 2	0
13	M	2	Total 2	Zn 2	0



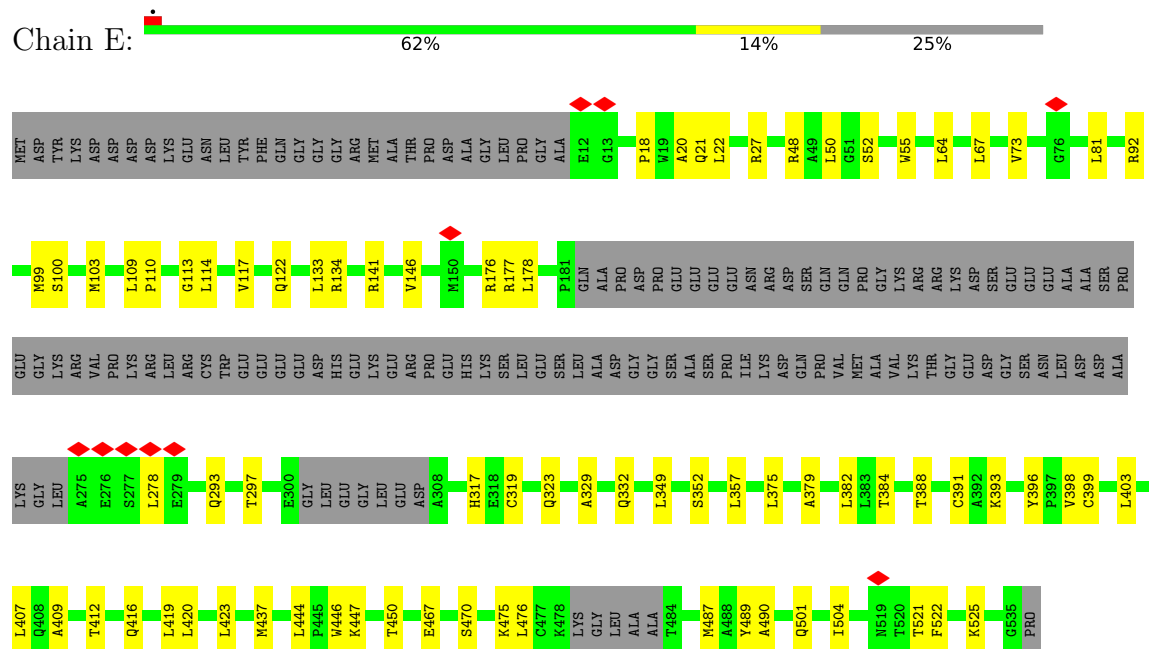
• Molecule 1: Fanconi anemia group A protein



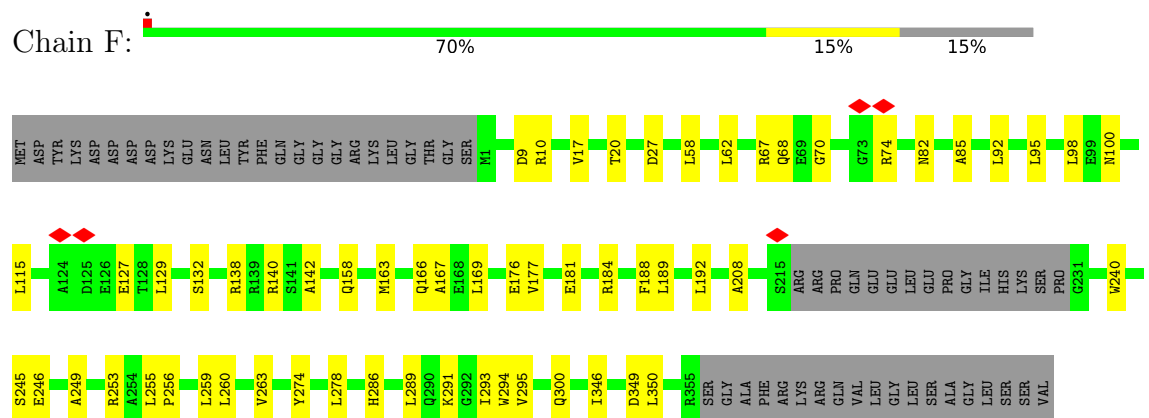




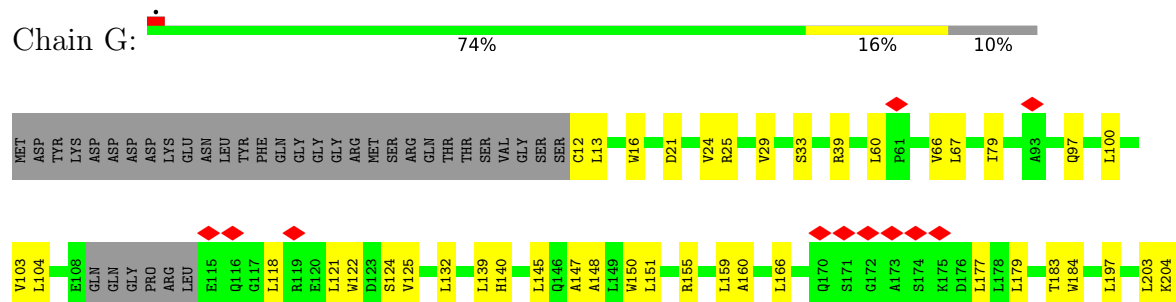
• Molecule 4: Fanconi anemia group E protein

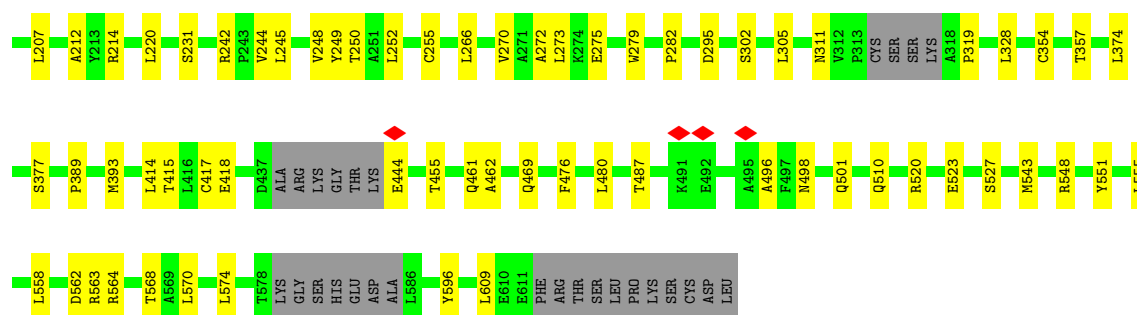


• Molecule 5: Fanconi anemia group F protein

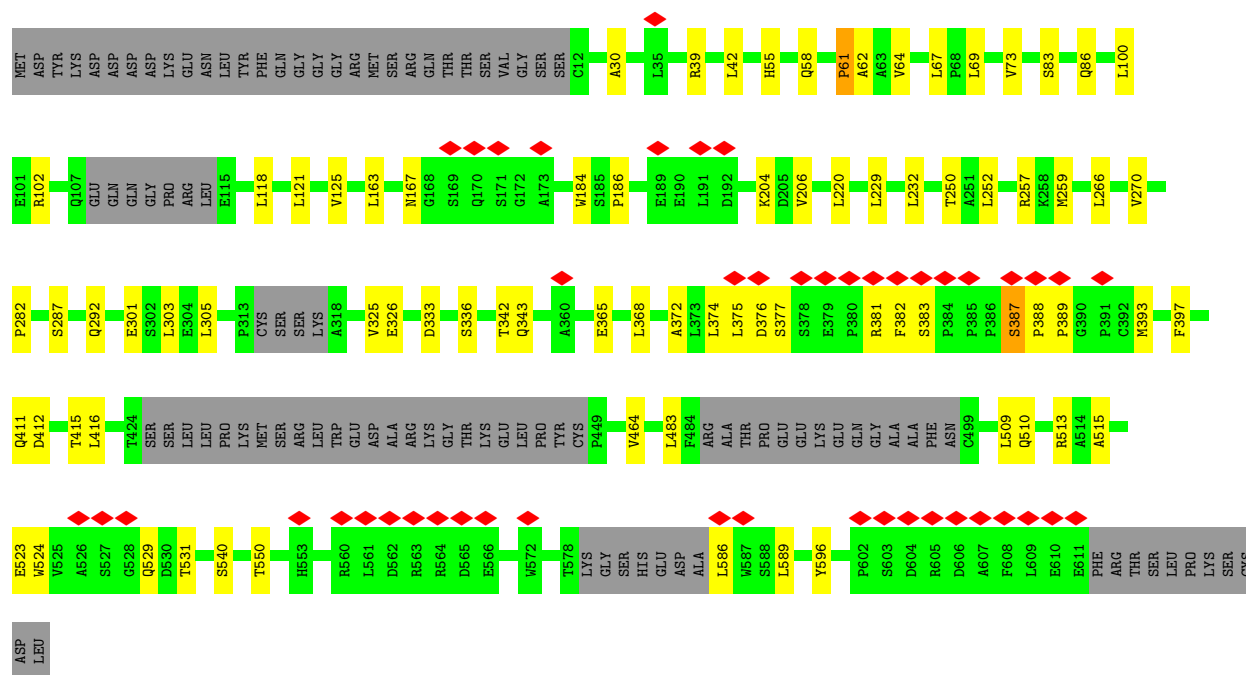
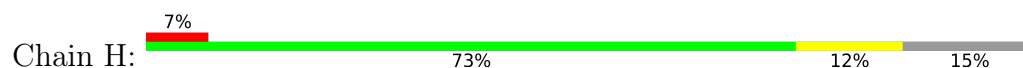


• Molecule 6: Fanconi anemia group G protein

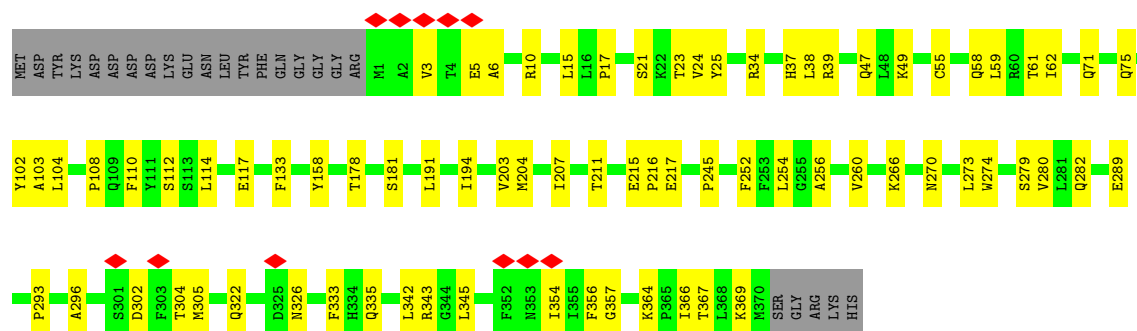
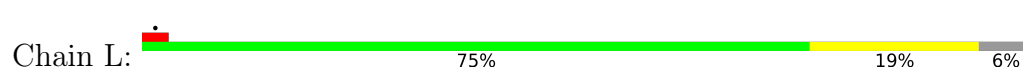




• Molecule 6: Fanconi anemia group G protein



• Molecule 7: E3 ubiquitin-protein ligase FANCL



• Molecule 7: E3 ubiquitin-protein ligase FANCL

Frequency	Percentage
Daily	70%
Weekly	23%
Monthly	6%



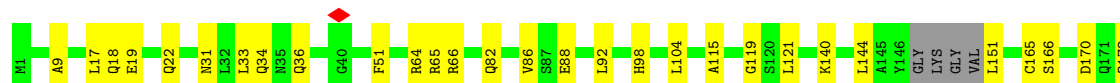
Frequency	Percentage
Daily	61%
Weekly	21%
Monthly	17%
Other	1%



Chain Q:



Chain U: 72% 16% 12%





LYS	GLN	LYS	ALA	ASP	GLU	GLU	MET	LEU	ASP	ASN	LEU	PRO	GLU	ALA	GLY	ASP	SER	ARG	VAL	HIS	ASN	SER	THR	GLN	LYS	ARG	LYS	ALA	SER	SER	GLN	LEU	VAL	GLY	ILE	GLU	LYS	PHE	HIS	PRO	ASP	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114249	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	480.40384, 480.40384, 480.40384	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07233, 1.07233, 1.07233	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	0.70	2/9605 (0.0%)	0.88	1/13008 (0.0%)
1	S	0.70	0/10153	0.88	1/13749 (0.0%)
2	B	1.06	19/5707 (0.3%)	1.07	5/7686 (0.1%)
2	O	0.79	4/5701 (0.1%)	0.92	2/7686 (0.0%)
3	C	0.67	1/4497 (0.0%)	0.88	2/6103 (0.0%)
4	E	0.67	1/3274 (0.0%)	1.02	0/4438
5	F	0.60	0/2791	0.83	0/3790
6	G	0.65	0/4568	0.83	0/6215
6	H	0.65	0/4293	0.87	0/5840
7	L	0.68	0/3050	0.82	0/4143
7	M	0.73	1/3050 (0.0%)	0.96	0/4143
8	P	1.00	10/5697 (0.2%)	1.06	6/7752 (0.1%)
8	Q	0.74	0/5737	0.91	2/7810 (0.0%)
9	W	0.54	0/202	0.77	0/281
10	U	0.61	0/9400	0.90	3/12676 (0.0%)
11	V	0.72	0/9433	1.07	2/12760 (0.0%)
12	X	0.57	0/1233	0.71	0/1683
All	All	0.74	38/88391 (0.0%)	0.93	24/119763 (0.0%)

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	4
1	S	0	8
2	B	0	11
2	O	0	12
3	C	0	1
4	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	2
6	H	0	1
7	L	0	1
7	M	0	2
8	P	0	7
8	Q	0	14
9	W	0	2
10	U	0	1
12	X	0	2
All	All	0	70

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	656	HIS	CE1-NE2	14.99	1.47	1.32
2	B	656	HIS	CG-ND1	11.70	1.51	1.38
2	B	704	LEU	C-O	-9.50	1.11	1.23
2	B	717	LEU	C-O	-9.32	1.12	1.23
2	O	591	SER	CA-CB	-8.74	1.42	1.53
2	B	719	ILE	C-O	-7.78	1.15	1.24
7	M	357	GLY	C-N	-7.48	1.22	1.33
3	C	201	GLU	CD-OE2	7.04	1.38	1.25
2	B	623	SER	C-O	-6.63	1.18	1.24
2	B	652	LEU	C-O	-6.45	1.15	1.24
2	B	705	PHE	C-O	-6.39	1.15	1.24
2	B	529	LYS	C-O	-6.33	1.16	1.24
2	B	489	VAL	CA-CB	-5.94	1.46	1.54
2	B	710	ARG	NE-CZ	5.93	1.39	1.33
8	P	569	VAL	C-O	5.93	1.29	1.24
8	P	766	LEU	C-O	-5.82	1.16	1.23
2	B	583	SER	CA-CB	-5.79	1.45	1.53
8	P	602	LEU	C-O	-5.78	1.16	1.23
2	O	585	SER	CA-CB	-5.68	1.46	1.53
1	A	1176	SER	CA-CB	-5.64	1.44	1.53
2	O	590	PHE	C-O	-5.60	1.17	1.24
8	P	558	SER	C-O	5.58	1.31	1.24
2	B	616	VAL	CA-C	-5.56	1.45	1.52
2	B	719	ILE	CA-CB	-5.49	1.47	1.54
4	E	100	SER	CA-CB	-5.39	1.44	1.53
8	P	545	ILE	C-O	-5.30	1.18	1.24
2	B	579	THR	C-O	5.28	1.30	1.23
8	P	583	PRO	C-O	-5.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	723	ASN	C-O	5.22	1.30	1.24
8	P	581	THR	C-O	5.19	1.30	1.23
2	B	667	TYR	C-O	-5.18	1.17	1.23
8	P	523	LEU	C-O	-5.12	1.17	1.23
2	B	576	GLN	CA-C	-5.12	1.47	1.53
1	A	1127	THR	C-O	5.08	1.29	1.23
2	B	581	VAL	CA-C	-5.07	1.46	1.52
2	O	508	LEU	C-O	-5.03	1.17	1.23
8	P	647	VAL	CA-C	-5.02	1.46	1.52
8	P	635	GLN	C-O	5.01	1.29	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	564	THR	OG1-CB-CG2	8.37	126.04	109.30
8	P	594	LEU	O-C-N	-7.42	115.33	121.12
8	P	84	GLY	N-CA-C	6.71	116.32	110.21
8	P	542	THR	CA-CB-OG1	-6.45	99.92	109.60
2	B	525	ASN	CB-CA-C	-6.39	98.66	109.72
8	Q	569	VAL	N-CA-CB	-6.31	104.47	111.66
10	U	440	ILE	N-CA-C	-6.07	104.59	110.42
10	U	209	GLU	CA-C-N	6.06	124.06	120.24
10	U	209	GLU	C-N-CA	6.06	124.06	120.24
1	A	141	GLN	N-CA-C	-5.74	105.10	111.36
2	B	826	THR	CB-CA-C	5.53	118.12	110.16
11	V	350	ILE	O-C-N	5.42	127.13	121.87
8	P	636	GLU	CB-CA-C	5.41	119.61	109.71
2	O	248	ILE	N-CA-C	-5.40	108.01	113.47
2	O	589	THR	CA-CB-OG1	-5.33	101.60	109.60
2	B	525	ASN	CA-CB-CG	-5.30	107.30	112.60
2	B	593	PHE	CB-CA-C	-5.28	99.92	110.42
2	B	718	ILE	CA-C-O	-5.25	114.99	120.76
3	C	142	PRO	CA-C-N	5.22	127.34	120.60
3	C	142	PRO	C-N-CA	5.22	127.34	120.60
11	V	344	ILE	N-CA-C	-5.20	104.82	110.23
1	S	963	PHE	CA-CB-CG	-5.11	108.69	113.80
8	Q	579	GLU	CB-CG-CD	5.10	121.27	112.60
8	P	637	GLY	N-CA-C	-5.08	104.34	111.09

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	GLY	Peptide
1	A	138	THR	Peptide
1	A	484	GLU	Peptide
1	A	923	GLU	Peptide
2	B	131	LYS	Peptide
2	B	132	ASP	Peptide
2	B	146	HIS	Peptide
2	B	191	LEU	Peptide
2	B	324	LYS	Peptide
2	B	345	PHE	Peptide
2	B	636	PHE	Peptide
2	B	711	THR	Peptide
2	B	738	LEU	Peptide
2	B	81	CYS	Peptide
2	B	825	GLN	Peptide
3	C	5	SER	Peptide
4	E	319	CYS	Peptide
4	E	352	SER	Peptide
6	G	132	LEU	Peptide
6	G	563	ARG	Peptide
6	H	186	PRO	Peptide
7	L	215	GLU	Peptide
7	M	215	GLU	Peptide
7	M	297	ILE	Peptide
2	O	130	MET	Peptide
2	O	131	LYS	Peptide
2	O	139	GLY	Peptide
2	O	147	VAL	Peptide
2	O	154	SER	Peptide
2	O	170	ILE	Peptide
2	O	216	SER	Peptide
2	O	324	LYS	Peptide
2	O	345	PHE	Peptide
2	O	522	LYS	Peptide
2	O	636	PHE	Peptide
2	O	637	PRO	Peptide
8	P	165	ARG	Peptide
8	P	556	LEU	Peptide
8	P	584	LEU	Peptide
8	P	594	LEU	Peptide
8	P	61	PRO	Peptide
8	P	780	GLY	Peptide
8	P	782	ILE	Peptide

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Mol	Chain	Res	Type	Group
8	Q	147	PRO	Peptide
8	Q	499	SER	Peptide
8	Q	50	GLU	Peptide
8	Q	584	LEU	Peptide
8	Q	585	GLY	Peptide
8	Q	594	LEU	Peptide
8	Q	647	VAL	Peptide
8	Q	719	LEU	Peptide
8	Q	721	ASP	Peptide
8	Q	723	HIS	Peptide
8	Q	726	VAL	Peptide
8	Q	781	PRO	Peptide
8	Q	782	ILE	Peptide
8	Q	857	ALA	Peptide
1	S	29	ARG	Peptide
1	S	31	LYS	Peptide
1	S	484	GLU	Peptide
1	S	495	HIS	Peptide
1	S	561	THR	Peptide
1	S	923	GLU	Peptide
1	S	960	HIS	Peptide
1	S	974	ASP	Peptide
10	U	717	GLU	Peptide
9	W	80	VAL	Peptide
9	W	81	GLY	Peptide
12	X	61	TYR	Peptide
12	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	130	0
1	S	9933	10028	9969	165	0
2	B	5605	5790	5768	139	0
2	O	5594	5759	5740	121	0
3	C	4396	4442	4427	79	0
4	E	3224	3390	3384	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	2726	2740	2729	41	0
6	G	4483	4537	4523	67	0
6	H	4216	4288	4273	56	0
7	L	2974	2977	2972	53	0
7	M	2974	2977	2972	77	0
8	P	5598	5681	5652	135	0
8	Q	5631	5724	5694	130	0
9	W	271	242	195	3	0
10	U	9256	9626	9595	138	0
11	V	9258	9475	9422	165	0
12	X	1199	1200	1175	13	0
13	G	1	0	0	0	0
13	L	2	0	0	0	0
13	M	2	0	0	0	0
All	All	86745	88363	87921	1441	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 8.

All (1441) 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)
2:O:856:LEU:HD23	8:Q:867:LEU:HD21	1.23	1.14
11:V:188:ASP:OD2	11:V:191:ASP:HB3	1.53	1.06
6:H:387:SER:OG	6:H:388:PRO:HD3	1.55	1.06
6:H:387:SER:OG	6:H:388:PRO:CD	2.04	1.05
3:C:192:THR:OG1	5:F:138:ARG:NH2	1.97	0.97
4:E:391:CYS:SG	4:E:398:VAL:HG11	2.07	0.94
1:A:722:LEU:HD22	1:A:753:MET:HE1	1.51	0.93
7:L:322:GLN:OE1	7:L:335:GLN:OE1	1.85	0.93
7:L:354:ILE:HG12	7:L:369:LYS:HG2	1.50	0.91
2:O:856:LEU:HD23	8:Q:867:LEU:CD2	2.00	0.91
8:P:710:VAL:HG21	8:P:808:MET:HE3	1.55	0.88
1:A:162:SER:HG	1:A:165:SER:HG	0.93	0.88
1:S:494:LEU:HD11	1:S:518:LEU:HD11	1.56	0.87
2:O:752:GLU:CG	2:O:859:LEU:HD21	2.06	0.86
11:V:143:ASP:HB2	11:V:187:VAL:HG21	1.54	0.86
7:M:361:TYR:CD1	12:X:101:SER:HB3	2.12	0.85
7:M:256:ALA:HB2	7:M:323:VAL:HG21	1.58	0.84
2:O:505:THR:OG1	8:Q:546:GLN:OE1	1.94	0.83
6:H:374:LEU:HD23	6:H:383:SER:OG	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:206:VAL:HG13	6:H:325:VAL:HG22	1.61	0.80
11:V:263:ARG:NH1	11:V:293:ASP:OD2	2.15	0.80
2:O:752:GLU:HG2	2:O:859:LEU:HD21	1.62	0.80
11:V:965:LEU:HD21	11:V:1027:LEU:HD13	1.64	0.80
2:B:638:LYS:NZ	2:O:697:PRO:O	2.13	0.79
7:M:365:PRO:HB3	10:U:266:HIS:NE2	1.98	0.79
10:U:856:THR:OG1	10:U:858:HIS:O	2.00	0.79
11:V:143:ASP:HB2	11:V:187:VAL:CG2	2.11	0.79
7:L:354:ILE:CG1	7:L:369:LYS:HG2	2.12	0.78
7:M:62:ILE:O	7:M:98:ARG:NH2	2.16	0.78
1:A:30:VAL:HG21	6:H:372:ALA:HB3	1.63	0.78
7:M:256:ALA:HA	7:M:323:VAL:CG2	2.13	0.78
2:B:600:GLN:OE1	8:P:601:THR:HG21	1.84	0.77
1:S:558:PHE:O	1:S:561:THR:O	2.02	0.77
8:Q:736:LEU:O	8:Q:807:ARG:NH1	2.18	0.77
1:A:1410:CYS:SG	1:A:1414:SER:OG	2.43	0.77
2:O:584:LEU:O	2:O:584:LEU:HD23	1.86	0.76
6:H:387:SER:OG	6:H:388:PRO:HD2	1.84	0.75
7:M:208:ASP:O	7:M:295:ARG:NH2	2.19	0.75
1:S:1071:ARG:NH2	1:S:1115:GLU:OE2	2.20	0.75
8:Q:169:GLN:NE2	8:Q:172:GLU:OE2	2.20	0.75
10:U:411:SER:O	10:U:415:ASN:ND2	2.21	0.74
8:Q:873:LEU:O	8:Q:877:SER:OG	2.05	0.74
1:A:1071:ARG:NH2	1:A:1115:GLU:OE2	2.19	0.74
8:Q:752:SER:OG	8:Q:768:VAL:O	2.06	0.74
2:B:338:THR:O	2:B:340:GLN:NE2	2.21	0.73
2:B:7:MET:N	2:B:13:GLU:O	2.21	0.73
6:H:100:LEU:HD22	6:H:125:VAL:HG21	1.69	0.73
8:P:548:LEU:HD23	8:P:562:ALA:HB2	1.71	0.73
2:O:777:ILE:HG21	8:Q:830:LEU:HD13	1.70	0.73
10:U:595:LEU:O	10:U:602:ARG:NE	2.21	0.73
8:Q:27:ARG:NH1	8:Q:65:TRP:O	2.22	0.73
11:V:51:LEU:HD22	11:V:83:LEU:HD11	1.70	0.73
2:O:39:LYS:NZ	2:O:67:ILE:O	2.22	0.73
7:L:354:ILE:CD1	7:L:369:LYS:HG2	2.19	0.72
2:O:423:TYR:HH	8:Q:635:GLN:N	1.87	0.72
2:O:755:LEU:HD12	2:O:859:LEU:HD22	1.71	0.72
1:S:452:PHE:O	1:S:455:SER:OG	2.07	0.72
1:S:749:PHE:O	1:S:752:THR:OG1	2.05	0.72
7:L:108:PRO:O	7:L:112:SER:OG	2.08	0.72
11:V:285:ILE:O	11:V:289:VAL:HG13	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:ASP:OD2	1:A:951:ARG:NH2	2.23	0.71
2:B:753:ASN:OD1	8:P:858:SER:OG	2.04	0.71
4:E:64:LEU:HA	4:E:67:LEU:HD12	1.73	0.71
7:L:357:GLY:O	7:L:366:ILE:HG22	1.91	0.71
5:F:253:ARG:NH2	5:F:300:GLN:O	2.23	0.71
7:L:23:THR:HG23	7:L:24:VAL:HG23	1.73	0.71
1:S:1033:ASP:CG	1:S:1093:SER:HG	1.99	0.71
1:A:1227:ALA:HB2	1:A:1256:LEU:HD12	1.73	0.70
6:G:374:LEU:O	6:G:377:SER:OG	2.08	0.70
7:M:342:LEU:HD23	7:M:345:LEU:HD12	1.73	0.70
1:S:1220:PRO:O	1:S:1253:ARG:NH2	2.24	0.70
1:S:1033:ASP:OD2	1:S:1093:SER:OG	2.09	0.70
2:O:411:HIS:O	8:Q:479:ARG:NH2	2.24	0.70
2:B:502:ASN:ND2	2:B:602:MET:O	2.25	0.69
11:V:282:ILE:HA	11:V:285:ILE:HD12	1.73	0.69
8:P:707:SER:OG	8:P:875:HIS:O	2.07	0.69
1:S:460:ARG:NH2	1:S:510:TYR:OH	2.24	0.69
11:V:771:LEU:O	11:V:779:ARG:NH2	2.26	0.69
6:G:214:ARG:NH1	6:G:328:LEU:O	2.25	0.69
2:B:505:THR:HG22	2:B:506:LEU:N	2.08	0.69
1:S:558:PHE:O	1:S:561:THR:C	2.35	0.69
2:B:139:GLY:O	2:B:141:LEU:N	2.26	0.69
1:S:1276:ASN:O	1:S:1279:THR:OG1	2.06	0.69
6:H:184:TRP:O	6:H:204:LYS:NZ	2.23	0.69
2:B:505:THR:HG23	2:B:525:ASN:HD21	1.57	0.69
2:B:854:GLN:NE2	8:P:593:ASP:OD1	2.26	0.69
3:C:489:HIS:O	3:C:493:ASN:ND2	2.25	0.69
1:S:324:LEU:HA	1:S:327:ILE:HD12	1.75	0.68
7:L:71:GLN:O	7:L:75:GLN:NE2	2.26	0.68
1:A:1184:ARG:NH1	1:S:1027:ASP:OD1	2.25	0.68
7:M:365:PRO:CB	10:U:266:HIS:NE2	2.56	0.68
2:O:829:LYS:N	8:Q:824:ASP:O	2.27	0.68
8:P:769:ARG:NH1	8:P:786:GLU:OE2	2.27	0.68
6:G:104:LEU:HD13	6:G:125:VAL:HG22	1.75	0.68
1:S:121:VAL:HA	1:S:124:ILE:HD12	1.74	0.68
2:B:231:PRO:O	2:B:234:SER:OG	2.08	0.68
1:S:1326:GLN:OE1	1:S:1329:ARG:NH2	2.27	0.67
11:V:294:THR:HG23	11:V:295:LEU:HD12	1.75	0.67
2:B:481:ARG:NH1	2:B:647:ASP:OD1	2.28	0.67
2:O:426:LEU:HD12	8:Q:489:ALA:HB1	1.75	0.67
8:P:516:ARG:NH1	8:P:519:THR:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:30:VAL:O	1:S:32:ARG:NH1	2.27	0.67
1:S:481:VAL:O	1:S:485:SER:OG	2.11	0.67
1:A:330:HIS:O	1:A:388:ARG:NH1	2.28	0.67
4:E:391:CYS:SG	4:E:398:VAL:CG1	2.82	0.67
8:P:476:VAL:O	8:P:480:ASN:ND2	2.27	0.67
2:B:602:MET:HE3	8:P:546:GLN:HE21	1.58	0.67
1:S:989:MET:HE1	1:S:1077:MET:HG2	1.74	0.67
1:A:651:GLY:O	1:A:654:THR:OG1	2.13	0.66
8:P:73:ARG:NH2	8:P:158:PRO:O	2.28	0.66
6:G:39:ARG:NH2	6:G:319:PRO:O	2.27	0.66
8:P:511:SER:OG	8:P:526:THR:OG1	2.14	0.66
11:V:177:VAL:HA	11:V:180:LEU:HD12	1.76	0.66
7:M:70:VAL:HG12	7:M:74:MET:HE2	1.78	0.66
7:M:71:GLN:O	7:M:75:GLN:NE2	2.28	0.66
7:M:256:ALA:CB	7:M:323:VAL:HG21	2.25	0.66
7:M:212:TRP:CD1	7:M:298:LEU:HD12	2.30	0.66
1:S:737:ALA:O	1:S:742:GLN:NE2	2.28	0.66
2:O:493:THR:OG1	2:O:576:GLN:O	2.12	0.66
1:S:977:LEU:HB2	1:S:1028:LEU:HD11	1.78	0.66
2:B:846:GLN:OE1	8:P:877:SER:OG	2.14	0.66
7:M:14:LEU:HD11	7:M:30:SER:OG	1.96	0.66
3:C:87:GLN:N	3:C:87:GLN:OE1	2.29	0.65
3:C:508:VAL:HG12	3:C:512:MET:HE2	1.76	0.65
2:O:523:CYS:SG	2:O:580:ALA:HB1	2.36	0.65
8:Q:768:VAL:HG12	8:Q:787:ILE:HG12	1.78	0.65
10:U:745:LEU:O	10:U:749:VAL:HG23	1.96	0.65
2:B:657:LYS:NZ	8:P:557:ASP:O	2.28	0.65
8:Q:341:TYR:OH	8:Q:385:GLU:O	2.15	0.65
2:B:326:SER:OG	2:B:346:LYS:N	2.28	0.65
3:C:115:GLN:NE2	5:F:98:LEU:O	2.28	0.65
5:F:17:VAL:O	5:F:20:THR:OG1	2.15	0.65
2:O:338:THR:O	2:O:340:GLN:NE2	2.29	0.65
2:O:701:TYR:O	2:O:722:ARG:NH1	2.30	0.65
11:V:243:VAL:HG13	11:V:244:PRO:HD3	1.79	0.65
11:V:654:HIS:O	11:V:658:ASN:ND2	2.29	0.65
2:B:494:THR:OG1	2:B:496:SER:OG	2.02	0.65
8:Q:311:CYS:SG	8:Q:312:LEU:N	2.70	0.64
12:X:3:ARG:NH2	12:X:57:ILE:O	2.29	0.64
2:B:738:LEU:HD13	2:B:742:CYS:HB3	1.78	0.64
8:Q:481:LYS:HG2	8:Q:609:VAL:HG12	1.79	0.64
3:C:501:GLY:O	3:C:502:HIS:ND1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:LYS:NZ	2:B:752:GLU:OE2	2.26	0.64
6:G:469:GLN:NE2	6:G:523:GLU:OE1	2.30	0.64
7:L:342:LEU:HD23	7:L:345:LEU:HD12	1.79	0.64
8:Q:525:ALA:HB2	8:Q:584:LEU:HD11	1.79	0.64
8:Q:642:LEU:HD23	8:Q:642:LEU:O	1.98	0.64
1:A:77:VAL:O	1:A:119:SER:OG	2.10	0.64
1:A:1408:PRO:O	1:A:1439:ARG:NH2	2.30	0.64
4:E:420:LEU:HD23	4:E:423:LEU:HD12	1.78	0.64
7:L:47:GLN:OE1	7:L:49:LYS:N	2.31	0.64
2:O:752:GLU:HG2	2:O:859:LEU:CD2	2.27	0.64
11:V:1077:GLY:O	11:V:1083:ASN:ND2	2.30	0.64
4:E:329:ALA:O	4:E:332:GLN:NE2	2.31	0.64
6:G:242:ARG:NH1	6:G:275:GLU:O	2.30	0.64
1:S:418:ALA:O	1:S:423:GLN:N	2.31	0.64
2:B:106:GLU:OE2	2:B:123:SER:OG	2.16	0.64
10:U:22:GLN:OE1	10:U:64:ARG:NH2	2.31	0.64
1:A:194:GLN:NE2	1:A:241:MET:SD	2.69	0.64
5:F:95:LEU:HA	5:F:98:LEU:HD12	1.80	0.64
1:A:724:THR:O	1:A:728:GLN:NE2	2.31	0.63
3:C:167:ASN:O	3:C:174:ARG:NH1	2.31	0.63
1:S:874:ARG:O	1:S:946:LEU:HD11	1.98	0.63
3:C:27:THR:OG1	3:C:30:THR:OG1	2.10	0.63
6:G:418:GLU:OE2	1:S:19:ARG:N	2.31	0.63
6:H:412:ASP:O	6:H:415:THR:OG1	2.14	0.63
7:M:256:ALA:CA	7:M:323:VAL:CG2	2.76	0.63
7:L:207:ILE:O	7:L:211:THR:OG1	2.14	0.63
10:U:18:GLN:O	10:U:22:GLN:NE2	2.32	0.63
2:B:727:MET:O	2:B:727:MET:SD	2.57	0.63
3:C:5:SER:O	3:C:9:SER:N	2.32	0.63
8:P:710:VAL:HG21	8:P:808:MET:CE	2.28	0.63
1:S:117:VAL:O	1:S:121:VAL:HG23	1.99	0.63
6:H:58:GLN:O	2:O:262:LYS:NZ	2.28	0.63
10:U:364:ILE:O	10:U:368:VAL:HG23	1.99	0.63
3:C:192:THR:HG1	5:F:138:ARG:NH2	1.95	0.63
1:S:497:PRO:O	1:S:510:TYR:OH	2.16	0.63
8:Q:662:HIS:O	8:Q:664:ARG:NH2	2.32	0.63
1:S:1336:TYR:OH	1:S:1357:ALA:O	2.16	0.63
10:U:893:GLU:OE2	10:U:903:SER:OG	2.12	0.63
2:B:326:SER:N	2:B:344:LEU:O	2.32	0.62
3:C:383:THR:O	3:C:386:SER:OG	2.16	0.62
1:A:874:ARG:NH2	1:A:944:ASP:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:856:LEU:CD2	8:Q:867:LEU:HD21	2.13	0.62
2:O:483:ILE:HG22	2:O:484:ASP:H	1.64	0.62
8:P:11:LEU:HD12	8:P:429:LEU:HD22	1.80	0.62
2:B:277:CYS:SG	2:B:278:GLN:N	2.73	0.62
1:A:346:TRP:O	1:A:391:SER:OG	2.16	0.62
2:B:711:THR:O	2:B:713:PHE:N	2.33	0.62
11:V:345:LEU:O	11:V:349:VAL:HG23	2.00	0.62
7:L:266:LYS:O	7:L:270:ASN:ND2	2.32	0.62
2:O:759:MET:HE1	2:O:853:ALA:HB2	1.82	0.62
7:L:110:PHE:O	7:L:114:LEU:HD23	2.00	0.62
2:B:190:CYS:HG	2:B:224:SER:N	1.97	0.62
2:O:755:LEU:CD2	2:O:855:LYS:HB3	2.30	0.62
8:P:868:GLN:O	8:P:872:GLN:NE2	2.33	0.62
10:U:1213:ILE:HD11	10:U:1253:LEU:HD22	1.80	0.62
2:B:523:CYS:SG	2:B:582:THR:HB	2.39	0.61
7:L:15:LEU:O	8:P:487:ASN:ND2	2.33	0.61
8:P:516:ARG:O	8:P:517:LEU:HD22	1.99	0.61
10:U:473:VAL:O	10:U:476:SER:OG	2.15	0.61
8:P:782:ILE:HD12	8:P:881:LEU:HD22	1.81	0.61
10:U:366:GLU:O	10:U:370:ASN:ND2	2.33	0.61
11:V:263:ARG:HG2	11:V:267:MET:HE2	1.82	0.61
2:O:752:GLU:HG3	2:O:859:LEU:HD21	1.81	0.61
11:V:1220:SER:N	11:V:1226:LEU:O	2.33	0.61
1:S:1366:GLN:OE1	1:S:1425:ARG:NH1	2.33	0.61
4:E:487:MET:HE3	11:V:202:ILE:HG21	1.81	0.61
10:U:98:HIS:O	10:U:140:LYS:NZ	2.30	0.61
2:B:145:ARG:NH1	2:B:168:SER:O	2.33	0.61
3:C:95:CYS:O	3:C:98:ILE:HG22	2.00	0.61
1:S:1033:ASP:OD1	1:S:1093:SER:OG	2.17	0.61
10:U:170:ASP:OD1	10:U:172:GLN:N	2.33	0.61
6:G:311:ASN:ND2	1:S:33:GLU:O	2.33	0.61
10:U:751:GLU:OE2	10:U:841:TYR:OH	2.18	0.61
11:V:693:ASP:OD1	11:V:694:GLY:N	2.32	0.61
7:M:232:ASN:HD21	7:M:304:THR:HG21	1.66	0.61
10:U:711:ASN:HA	10:U:714:ILE:HD12	1.83	0.61
1:S:424:LEU:O	1:S:428:VAL:HG23	1.99	0.61
11:V:1119:GLN:O	11:V:1122:HIS:ND1	2.34	0.61
7:L:191:LEU:HA	7:L:194:ILE:HD12	1.81	0.61
8:Q:807:ARG:O	8:Q:810:THR:OG1	2.18	0.61
11:V:200:ILE:O	11:V:208:GLN:NE2	2.33	0.60
1:A:1400:ARG:NH1	1:A:1429:ASP:OD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:444:GLU:O	6:G:487:THR:OG1	2.17	0.60
2:O:664:SER:OG	2:O:667:TYR:O	2.16	0.60
2:O:755:LEU:HD22	2:O:855:LYS:HB3	1.83	0.60
2:B:746:ASN:OD1	2:B:747:LEU:N	2.34	0.60
2:B:841:LYS:O	2:B:845:VAL:HG23	2.01	0.60
2:O:408:LEU:HB3	8:Q:472:LEU:HD22	1.83	0.60
8:P:447:THR:HG1	8:P:450:SER:HG	1.46	0.60
1:S:1033:ASP:CG	1:S:1093:SER:OG	2.44	0.60
10:U:51:PHE:O	10:U:65:ARG:NH2	2.34	0.60
3:C:104:ASN:ND2	3:C:107:GLN:OE1	2.34	0.60
4:E:18:PRO:O	4:E:21:GLN:NE2	2.33	0.60
1:A:102:ALA:HB2	1:A:112:LEU:HD11	1.82	0.60
2:B:679:HIS:O	2:B:696:ARG:NH2	2.34	0.60
2:B:734:LEU:O	2:B:737:ILE:N	2.35	0.60
8:Q:733:LEU:HD22	8:Q:746:VAL:HG11	1.82	0.60
1:A:1075:LEU:HD11	1:A:1115:GLU:HB3	1.83	0.60
7:M:295:ARG:HD2	7:M:298:LEU:HD13	1.82	0.60
2:O:72:SER:OG	2:O:73:HIS:N	2.33	0.60
3:C:259:GLU:O	3:C:263:SER:OG	2.12	0.60
2:O:154:SER:OG	2:O:155:SER:O	2.13	0.60
11:V:64:SER:O	11:V:112:ASN:ND2	2.35	0.60
1:A:452:PHE:O	1:A:455:SER:OG	2.15	0.60
1:A:1184:ARG:NH1	1:S:1027:ASP:O	2.35	0.60
7:L:117:GLU:OE1	7:L:158:TYR:OH	2.18	0.60
1:S:955:HIS:NE2	1:S:1016:ASP:OD2	2.35	0.60
11:V:559:ILE:HD11	11:V:581:MET:SD	2.41	0.60
1:A:424:LEU:O	1:A:428:VAL:HG23	2.03	0.59
8:Q:152:MET:HE1	8:Q:253:VAL:HG11	1.83	0.59
1:S:139:VAL:N	1:S:141:GLN:OE1	2.34	0.59
1:A:48:VAL:HG13	6:H:270:VAL:HG13	1.83	0.59
7:L:178:THR:OG1	7:L:181:SER:N	2.35	0.59
8:Q:349:CYS:SG	8:Q:400:ASN:N	2.76	0.59
1:S:974:ASP:O	1:S:976:ASP:N	2.36	0.59
4:E:317:HIS:O	7:M:72:GLN:NE2	2.35	0.59
6:H:387:SER:CB	6:H:388:PRO:CD	2.80	0.59
11:V:346:LEU:HD11	11:V:350:ILE:HD11	1.83	0.59
1:A:1336:TYR:OH	1:A:1357:ALA:O	2.21	0.59
8:P:552:CYS:SG	8:P:553:ALA:N	2.76	0.59
5:F:181:GLU:OE2	5:F:184:ARG:NH1	2.35	0.59
6:G:302:SER:HA	6:G:305:LEU:HD12	1.85	0.59
7:L:356:PHE:CD1	7:L:367:THR:HG23	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:662:ILE:HG12	2:B:744:LEU:HD13	1.84	0.59
6:G:160:ALA:HB2	6:G:177:LEU:HD21	1.85	0.59
8:P:340:GLU:OE1	8:P:340:GLU:N	2.36	0.59
10:U:438:GLN:NE2	10:U:477:CYS:SG	2.76	0.59
11:V:173:PRO:HA	11:V:176:ILE:HD12	1.83	0.59
2:B:732:HIS:O	2:B:736:ARG:NH1	2.36	0.59
1:A:300:GLY:O	1:A:303:SER:OG	2.18	0.59
6:H:326:GLU:N	6:H:326:GLU:OE2	2.36	0.59
7:M:162:SER:HG	7:M:177:TRP:CD1	2.20	0.59
8:P:245:LEU:HD12	8:P:249:GLN:HG2	1.85	0.59
2:B:167:PHE:CD2	2:B:186:LEU:HG	2.37	0.58
2:B:288:GLN:OE1	2:B:330:ILE:HD13	2.03	0.58
2:B:505:THR:HG23	2:B:525:ASN:ND2	2.18	0.58
11:V:86:HIS:ND1	11:V:87:PRO:O	2.36	0.58
7:M:20:ARG:NH1	2:O:429:LEU:O	2.36	0.58
2:O:766:GLU:OE2	8:Q:874:ARG:NH2	2.36	0.58
11:V:425:TYR:O	11:V:428:LEU:N	2.35	0.58
4:E:22:LEU:O	4:E:27:ARG:NH2	2.36	0.58
8:P:288:LEU:HD21	8:P:352:CYS:SG	2.43	0.58
10:U:903:SER:HG	10:U:905:SER:HG	1.51	0.58
7:M:360:PRO:O	12:X:99:ARG:CZ	2.52	0.58
5:F:115:LEU:HD23	5:F:129:LEU:HD13	1.83	0.58
6:G:140:HIS:CE1	6:G:166:LEU:HD11	2.39	0.58
1:S:661:ARG:O	9:W:79:THR:HG22	2.03	0.58
10:U:263:GLU:N	10:U:263:GLU:OE2	2.36	0.58
6:H:69:LEU:O	6:H:73:VAL:HG23	2.03	0.58
8:P:546:GLN:HG3	8:P:599:SER:OG	2.04	0.58
1:S:271:GLN:HA	1:S:274:LEU:HD12	1.85	0.58
6:G:244:VAL:O	6:G:248:VAL:HG23	2.03	0.58
1:A:737:ALA:HB1	1:A:738:PRO:HD2	1.86	0.58
6:G:21:ASP:OD1	6:G:25:ARG:NH1	2.37	0.58
6:G:415:THR:HG21	1:S:21:ALA:HB1	1.86	0.58
7:M:197:LEU:HD22	7:M:242:PRO:HB2	1.86	0.58
2:O:759:MET:CE	2:O:853:ALA:HB2	2.33	0.58
1:S:1312:ASP:O	1:S:1316:GLY:N	2.37	0.58
7:M:234:VAL:HG11	7:M:259:VAL:CG1	2.34	0.58
10:U:876:ASP:OD1	10:U:879:ARG:NH2	2.37	0.58
1:A:1020:ARG:NH1	1:A:1023:GLU:OE2	2.37	0.57
1:S:163:ARG:NE	1:S:190:ILE:O	2.30	0.57
3:C:190:LEU:HD22	5:F:142:ALA:HB2	1.86	0.57
6:H:333:ASP:O	6:H:336:SER:OG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1308:LEU:HD11	1:S:1319:LEU:HD23	1.86	0.57
10:U:757:ASN:HA	10:U:760:ILE:HD12	1.86	0.57
6:G:469:GLN:OE1	6:G:527:SER:OG	2.15	0.57
2:O:759:MET:SD	2:O:853:ALA:N	2.77	0.57
1:S:998:TYR:HB3	1:S:1007:VAL:HG13	1.86	0.57
6:G:414:LEU:HD21	6:G:462:ALA:HB3	1.87	0.57
10:U:1054:HIS:HA	10:U:1151:THR:HG22	1.85	0.57
1:A:331:SER:O	1:A:385:HIS:ND1	2.35	0.57
1:A:1025:VAL:HG21	1:A:1085:LEU:HD13	1.85	0.57
2:B:136:VAL:O	2:B:137:LEU:HD23	2.03	0.57
2:B:747:LEU:HD23	2:B:859:LEU:HD11	1.87	0.57
11:V:197:MET:HE3	11:V:230:GLU:HB3	1.87	0.57
12:X:5:SER:O	12:X:9:ARG:NH1	2.37	0.57
8:Q:552:CYS:SG	8:Q:553:ALA:N	2.78	0.57
1:S:184:HIS:HA	1:S:187:VAL:HG12	1.85	0.57
10:U:184:VAL:O	10:U:223:LYS:NZ	2.35	0.57
10:U:438:GLN:HA	10:U:441:LEU:HD23	1.87	0.57
11:V:60:LYS:N	11:V:66:ASN:OD1	2.37	0.57
2:O:850:ASP:OD1	8:Q:870:TYR:OH	2.22	0.57
10:U:165:CYS:SG	10:U:166:SER:N	2.78	0.57
1:A:180:GLU:OE2	1:A:184:HIS:NE2	2.38	0.56
3:C:140:TYR:CE2	5:F:169:LEU:HD22	2.40	0.56
6:G:496:ALA:O	6:G:498:ASN:ND2	2.37	0.56
8:P:28:VAL:HG22	8:P:37:LEU:HA	1.87	0.56
10:U:488:LEU:HD11	10:U:496:VAL:HG13	1.87	0.56
11:V:273:ILE:HD13	11:V:281:ILE:HD13	1.86	0.56
11:V:689:TYR:OH	11:V:693:ASP:OD2	2.21	0.56
6:H:257:ARG:O	6:H:292:GLN:NE2	2.37	0.56
11:V:813:LEU:HA	11:V:816:LEU:HD12	1.87	0.56
2:B:749:SER:O	2:B:755:LEU:HD21	2.05	0.56
3:C:41:PHE:CE2	3:C:45:LEU:HD11	2.40	0.56
8:P:50:GLU:N	8:P:50:GLU:OE1	2.38	0.56
8:P:429:LEU:HD23	8:P:430:MET:N	2.19	0.56
1:S:652:GLN:O	1:S:683:ARG:NH2	2.38	0.56
1:S:989:MET:HE1	1:S:1077:MET:CG	2.35	0.56
10:U:474:LEU:HD12	10:U:506:LEU:HD21	1.88	0.56
11:V:60:LYS:NZ	11:V:61:THR:OG1	2.38	0.56
11:V:1235:PHE:CD1	11:V:1281:LEU:HD11	2.40	0.56
2:O:57:PHE:HB2	2:O:354:LEU:HD21	1.87	0.56
8:P:860:CYS:SG	8:P:861:ALA:N	2.78	0.56
1:S:1262:PHE:CD2	1:S:1319:LEU:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:888:ILE:CG2	10:U:892:VAL:HG21	2.36	0.56
7:M:16:LEU:HD13	8:Q:486:LEU:HD22	1.86	0.56
8:P:515:SER:OG	8:P:516:ARG:N	2.38	0.56
11:V:247:ASP:O	11:V:250:SER:OG	2.19	0.56
2:B:602:MET:HE3	8:P:546:GLN:NE2	2.20	0.56
4:E:444:LEU:O	4:E:475:LYS:NZ	2.37	0.56
7:M:295:ARG:CD	7:M:298:LEU:HD13	2.35	0.56
2:O:267:SER:OG	2:O:274:LYS:O	2.23	0.56
2:O:661:GLN:HB2	2:O:747:LEU:HD11	1.88	0.56
1:S:1183:CYS:SG	1:S:1184:ARG:N	2.78	0.56
10:U:280:LYS:HG3	10:U:319:ILE:HD11	1.86	0.56
8:P:245:LEU:HD12	8:P:249:GLN:CG	2.36	0.56
8:Q:569:VAL:HA	8:Q:578:ARG:HH12	1.69	0.56
10:U:756:TYR:CE2	10:U:760:ILE:HD11	2.41	0.56
10:U:1218:ASN:OD1	10:U:1219:LYS:N	2.39	0.56
1:A:393:VAL:HA	1:A:396:LEU:HD12	1.88	0.56
2:B:640:LYS:NZ	2:B:695:GLU:OE2	2.25	0.56
1:S:240:GLN:HA	1:S:311:ILE:HD11	1.87	0.56
7:M:121:LEU:HD11	7:M:183:LEU:HB3	1.87	0.55
8:P:37:LEU:HD22	8:P:45:TYR:HD2	1.71	0.55
10:U:219:VAL:O	10:U:222:SER:OG	2.19	0.55
11:V:197:MET:HA	11:V:200:ILE:HG22	1.88	0.55
7:M:360:PRO:O	12:X:99:ARG:NH1	2.38	0.55
8:P:423:LEU:HD12	8:P:428:ARG:O	2.06	0.55
8:Q:329:ASP:O	8:Q:335:VAL:HG21	2.06	0.55
1:A:1022:GLN:NE2	1:S:1022:GLN:OE1	2.37	0.55
8:Q:73:ARG:NH1	8:Q:159:CYS:O	2.40	0.55
10:U:753:LEU:O	10:U:757:ASN:ND2	2.39	0.55
2:O:422:SER:CB	8:Q:486:LEU:HD11	2.35	0.55
2:O:520:LEU:HD11	8:Q:565:TYR:HB3	1.88	0.55
10:U:473:VAL:HG23	10:U:474:LEU:HD23	1.88	0.55
2:B:15:LEU:HD22	2:B:24:VAL:HG22	1.88	0.55
2:B:759:MET:HE3	2:B:763:LEU:HD11	1.89	0.55
3:C:344:THR:HG21	3:C:396:LEU:HD22	1.88	0.55
2:O:584:LEU:HD23	2:O:584:LEU:C	2.30	0.55
3:C:148:GLY:O	3:C:152:ASN:ND2	2.38	0.55
6:G:121:LEU:O	6:G:125:VAL:HG23	2.06	0.55
7:M:13:PRO:O	7:M:16:LEU:HD21	2.07	0.55
2:O:408:LEU:HB2	8:Q:472:LEU:HD13	1.89	0.55
8:Q:515:SER:O	8:Q:522:VAL:N	2.39	0.55
1:S:665:THR:HA	9:W:80:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:990:ASP:OD1	1:S:1055:ARG:NH2	2.39	0.55
11:V:346:LEU:CD1	11:V:350:ILE:HD11	2.36	0.55
1:A:384:VAL:HG13	1:A:389:VAL:HG21	1.89	0.55
7:M:256:ALA:CA	7:M:323:VAL:HG21	2.36	0.55
1:S:938:GLU:O	1:S:1011:ARG:NH1	2.40	0.55
7:L:356:PHE:CE1	7:L:367:THR:HG23	2.42	0.55
2:O:857:SER:HB3	8:Q:795:ALA:HB2	1.88	0.55
10:U:379:THR:HA	10:U:382:LEU:HD12	1.88	0.55
7:L:103:ALA:C	7:L:104:LEU:HD22	2.32	0.55
10:U:144:LEU:O	10:U:151:LEU:N	2.40	0.55
1:A:428:VAL:HG22	1:A:476:PHE:CZ	2.42	0.55
4:E:375:LEU:O	4:E:416:GLN:NE2	2.39	0.55
8:Q:62:ASP:OD2	8:Q:83:ARG:N	2.41	0.55
3:C:382:GLN:NE2	3:C:387:CYS:O	2.37	0.54
6:G:103:VAL:HG11	6:G:125:VAL:HG13	1.89	0.54
8:P:486:LEU:CD2	8:P:490:MET:HE3	2.37	0.54
8:P:655:PHE:CZ	8:P:754:ILE:HD12	2.43	0.54
10:U:492:PRO:O	10:U:496:VAL:HG23	2.07	0.54
11:V:526:PRO:HA	11:V:529:ILE:HD12	1.89	0.54
1:A:1084:ARG:NH2	1:S:952:GLN:HE21	2.05	0.54
2:B:766:GLU:HA	2:B:845:VAL:HG11	1.90	0.54
6:H:411:GLN:O	6:H:411:GLN:NE2	2.40	0.54
2:O:110:LEU:HD23	2:O:120:MET:HA	1.88	0.54
8:P:472:LEU:O	8:P:476:VAL:HG23	2.07	0.54
2:B:350:ASN:ND2	2:B:355:THR:OG1	2.41	0.54
7:M:7:SER:O	7:M:11:GLN:NE2	2.40	0.54
2:O:82:VAL:HG13	2:O:83:SER:H	1.72	0.54
1:S:510:TYR:HA	1:S:513:LEU:HD12	1.90	0.54
11:V:415:GLN:OE1	11:V:415:GLN:N	2.37	0.54
4:E:99:MET:HE2	4:E:133:LEU:HD12	1.90	0.54
8:P:280:GLU:OE2	8:P:318:HIS:N	2.41	0.54
8:Q:366:LEU:HD13	8:Q:398:SER:OG	2.07	0.54
5:F:255:LEU:HD12	5:F:260:LEU:HD21	1.89	0.54
2:O:328:VAL:HG22	2:O:343:LEU:HD23	1.90	0.54
8:Q:143:LEU:HD13	8:Q:197:LEU:HD21	1.89	0.54
8:Q:487:ASN:O	8:Q:491:ASN:ND2	2.41	0.54
2:B:683:GLU:N	2:B:695:GLU:OE1	2.41	0.54
3:C:87:GLN:HA	3:C:90:LEU:HD12	1.89	0.54
1:S:720:ASP:O	1:S:724:THR:HG23	2.07	0.54
11:V:347:PHE:HA	11:V:350:ILE:HD12	1.89	0.54
11:V:1313:LEU:HD11	11:V:1374:MET:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:CD1	1:A:518:LEU:HD11	2.37	0.54
2:B:836:ARG:O	2:B:839:THR:OG1	2.24	0.54
8:P:24:GLY:O	8:P:27:ARG:NH1	2.41	0.54
1:S:155:LEU:HD23	1:S:160:MET:HE3	1.90	0.54
11:V:58:ILE:HD12	11:V:67:GLN:HB2	1.90	0.54
1:A:30:VAL:HG21	6:H:372:ALA:CB	2.33	0.54
1:A:361:ARG:O	1:A:365:MET:HE3	2.08	0.54
8:P:880:LEU:O	8:P:881:LEU:HD23	2.07	0.54
1:S:428:VAL:HG22	1:S:476:PHE:CZ	2.43	0.54
1:A:749:PHE:O	1:A:752:THR:OG1	2.14	0.54
3:C:82:ALA:O	5:F:138:ARG:NH1	2.41	0.54
1:A:268:ASP:OD2	1:A:272:ARG:NH2	2.40	0.53
1:A:1252:GLU:O	1:A:1298:ARG:NH2	2.40	0.53
4:E:501:GLN:HA	4:E:504:ILE:HD12	1.89	0.53
7:L:270:ASN:HB3	7:L:273:LEU:HD12	1.90	0.53
2:O:266:ILE:HA	2:O:276:VAL:HG22	1.89	0.53
8:Q:494:CYS:O	8:Q:498:SER:OG	2.18	0.53
2:B:596:THR:HG22	2:B:597:VAL:H	1.72	0.53
3:C:462:LEU:O	3:C:504:ILE:HD13	2.07	0.53
8:P:782:ILE:CD1	8:P:881:LEU:HD22	2.38	0.53
10:U:1262:LYS:HA	10:U:1265:ILE:HD12	1.90	0.53
11:V:435:ILE:HG23	11:V:457:LEU:HD22	1.89	0.53
11:V:518:LEU:HA	11:V:521:LEU:HD21	1.90	0.53
11:V:945:ILE:HD12	11:V:1034:PHE:CD1	2.42	0.53
11:V:1177:ILE:HG22	11:V:1182:LEU:HD11	1.89	0.53
7:L:58:GLN:O	7:L:61:THR:OG1	2.26	0.53
11:V:515:LYS:HD3	11:V:551:ILE:HG22	1.89	0.53
1:A:108:PRO:HG2	1:A:111:ILE:HD12	1.89	0.53
2:B:520:LEU:HD12	8:P:567:ILE:HB	1.91	0.53
2:O:422:SER:HB2	8:Q:486:LEU:HD11	1.91	0.53
1:S:1410:CYS:O	1:S:1439:ARG:NH2	2.42	0.53
3:C:312:ILE:HG23	3:C:398:ILE:HG23	1.90	0.53
6:H:83:SER:O	6:H:86:GLN:NE2	2.41	0.53
6:H:540:SER:OG	6:H:550:THR:OG1	2.06	0.53
8:P:655:PHE:CE1	8:P:754:ILE:HD12	2.43	0.53
10:U:660:LEU:HD12	10:U:741:ILE:HG23	1.90	0.53
2:B:710:ARG:NH2	2:B:711:THR:OG1	2.42	0.53
5:F:294:TRP:NE1	5:F:349:ASP:OD2	2.42	0.53
8:P:28:VAL:N	8:P:400:ASN:OD1	2.42	0.53
8:P:523:LEU:HD11	8:P:652:CYS:SG	2.48	0.53
10:U:668:LEU:CD1	10:U:749:VAL:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:16:TRP:CZ3	6:G:60:LEU:HD11	2.44	0.53
1:A:663:SER:O	1:A:669:GLN:NE2	2.42	0.53
8:P:708:ILE:HD12	8:P:804:VAL:HG11	1.90	0.53
2:B:505:THR:CG2	2:B:506:LEU:N	2.72	0.53
1:S:1410:CYS:SG	1:S:1414:SER:OG	2.67	0.53
10:U:978:ASN:ND2	10:U:981:GLU:OE1	2.42	0.53
11:V:306:ASP:OD1	11:V:307:LEU:N	2.32	0.53
11:V:371:THR:HG22	11:V:374:VAL:HB	1.91	0.53
2:B:329:LEU:C	2:B:330:ILE:HD12	2.34	0.53
7:M:55:CYS:HB3	7:M:59:LEU:HD23	1.91	0.53
2:O:483:ILE:HB	2:O:486:SER:OG	2.09	0.53
2:O:614:TYR:CG	8:Q:639:CYS:HB3	2.44	0.53
8:Q:227:LEU:HD21	8:Q:336:PRO:HB3	1.89	0.53
11:V:1017:PHE:CE1	11:V:1072:LEU:HD11	2.43	0.53
1:A:684:LEU:HD11	1:A:688:LEU:HD21	1.91	0.52
5:F:9:ASP:OD1	5:F:10:ARG:N	2.41	0.52
2:O:57:PHE:CB	2:O:354:LEU:HD21	2.39	0.52
8:P:68:GLU:HB3	8:P:135:LEU:HD12	1.91	0.52
10:U:651:ILE:HG12	10:U:741:ILE:HG21	1.90	0.52
10:U:1051:GLN:OE1	10:U:1071:HIS:NE2	2.42	0.52
11:V:387:ILE:HA	11:V:431:MET:HE1	1.90	0.52
11:V:1017:PHE:O	11:V:1021:THR:OG1	2.26	0.52
1:A:664:MET:CE	1:A:733:ALA:HB2	2.39	0.52
4:E:293:GLN:O	4:E:297:THR:HG23	2.09	0.52
7:M:29:ILE:HD11	7:M:88:LYS:CG	2.39	0.52
10:U:706:LEU:O	10:U:710:THR:HG23	2.09	0.52
2:B:252:LEU:HD23	2:B:253:ARG:N	2.24	0.52
2:B:505:THR:HG22	2:B:506:LEU:H	1.73	0.52
2:B:596:THR:HG22	2:B:597:VAL:N	2.24	0.52
2:B:728:PHE:O	2:B:731:LEU:N	2.42	0.52
6:H:586:LEU:HA	6:H:589:LEU:HD22	1.91	0.52
7:L:326:ASN:HD22	7:L:364:LYS:HG3	1.74	0.52
8:Q:727:PRO:O	8:Q:728:LEU:HD23	2.09	0.52
10:U:1209:CYS:SG	10:U:1253:LEU:HD21	2.49	0.52
11:V:977:GLU:O	11:V:981:THR:OG1	2.13	0.52
4:E:357:LEU:HD11	4:E:396:TYR:CE2	2.44	0.52
8:P:523:LEU:CD1	8:P:652:CYS:SG	2.98	0.52
8:P:756:GLY:N	8:P:764:VAL:O	2.42	0.52
10:U:592:ARG:NH2	10:U:626:THR:OG1	2.43	0.52
3:C:182:SER:O	3:C:186:VAL:HG23	2.09	0.52
2:O:745:LYS:NZ	2:O:752:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:28:VAL:C	8:P:29:LEU:HD12	2.33	0.52
10:U:668:LEU:HD12	10:U:749:VAL:HG22	1.92	0.52
11:V:343:ILE:O	11:V:346:LEU:HB3	2.10	0.52
11:V:1127:SER:OG	11:V:1130:CYS:SG	2.56	0.52
2:B:614:TYR:O	2:B:615:VAL:HG23	2.10	0.52
2:B:728:PHE:CZ	8:P:676:VAL:HG22	2.45	0.52
3:C:42:GLN:HA	3:C:45:LEU:HD12	1.90	0.52
6:H:515:ALA:HB1	6:H:596:TYR:HE2	1.75	0.52
10:U:488:LEU:HD12	10:U:491:LEU:HD12	1.91	0.52
10:U:898:LYS:NZ	10:U:899:GLU:OE1	2.43	0.52
11:V:742:GLU:OE2	11:V:802:GLN:NE2	2.43	0.52
11:V:1125:ILE:HD11	11:V:1134:LEU:HD13	1.91	0.52
1:A:31:LYS:NZ	6:H:376:ASP:O	2.41	0.52
1:A:510:TYR:HA	1:A:513:LEU:HD12	1.90	0.52
6:G:179:LEU:O	6:G:183:THR:HG23	2.10	0.52
6:G:389:PRO:O	6:G:501:GLN:NE2	2.43	0.52
2:O:484:ASP:OD1	2:O:485:ASP:N	2.41	0.52
10:U:909:LEU:HA	10:U:912:LEU:HD12	1.91	0.52
3:C:178:GLU:N	3:C:178:GLU:OE2	2.43	0.52
4:E:109:LEU:HB2	4:E:114:LEU:HD11	1.92	0.52
8:P:150:TRP:HB2	8:P:175:LEU:HD12	1.92	0.52
8:P:772:ALA:HB2	8:P:783:GLN:HA	1.91	0.52
1:S:770:ARG:NH1	1:S:821:LEU:O	2.42	0.52
11:V:583:GLY:CA	11:V:638:LEU:HD11	2.40	0.52
3:C:434:ASP:OD1	4:E:177:ARG:NH1	2.42	0.52
6:G:151:LEU:O	6:G:214:ARG:NH2	2.43	0.52
7:L:21:SER:O	7:L:23:THR:HG22	2.10	0.52
1:S:837:CYS:SG	1:S:864:LEU:HD22	2.50	0.52
11:V:111:ARG:HA	11:V:114:LEU:HD12	1.92	0.52
11:V:224:HIS:O	11:V:227:VAL:HB	2.09	0.52
2:B:54:THR:OG1	2:B:56:VAL:HG22	2.10	0.52
5:F:67:ARG:NH1	5:F:70:GLY:O	2.41	0.52
2:O:146:HIS:O	2:O:148:LYS:N	2.36	0.52
11:V:417:LEU:HD13	11:V:453:PHE:CZ	2.45	0.52
11:V:1197:LEU:HD13	11:V:1270:MET:HG3	1.92	0.52
1:A:1274:THR:HG22	1:A:1275:SER:H	1.76	0.51
2:B:416:GLU:HA	2:B:419:ILE:HD12	1.92	0.51
3:C:16:MET:HE3	3:C:16:MET:O	2.10	0.51
8:P:643:SER:OG	8:P:644:ARG:N	2.43	0.51
1:S:603:PHE:O	1:S:606:SER:OG	2.22	0.51
1:A:334:LEU:HD13	1:A:346:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:TRP:CZ3	1:A:429:THR:HG23	2.45	0.51
1:A:513:LEU:O	1:A:516:THR:OG1	2.24	0.51
8:P:74:ARG:HA	8:P:90:LEU:HD12	1.93	0.51
8:Q:420:LEU:C	8:Q:421:LEU:HD12	2.35	0.51
11:V:650:GLU:O	11:V:654:HIS:ND1	2.42	0.51
11:V:1226:LEU:HD22	11:V:1234:PHE:HE2	1.76	0.51
1:A:299:PHE:O	1:A:361:ARG:NH1	2.42	0.51
1:A:386:TRP:HZ3	1:A:429:THR:HG23	1.75	0.51
2:B:69:GLU:OE1	2:B:71:ASN:ND2	2.43	0.51
2:B:657:LYS:NZ	8:P:557:ASP:OD1	2.40	0.51
8:Q:433:SER:C	8:Q:434:LEU:HD12	2.35	0.51
1:S:113:SER:O	1:S:117:VAL:HG23	2.10	0.51
5:F:293:ILE:HD12	5:F:295:VAL:CG1	2.40	0.51
2:O:706:THR:O	2:O:717:LEU:HD12	2.11	0.51
1:S:666:ASP:OD2	1:S:668:SER:OG	2.26	0.51
12:X:93:PRO:O	12:X:95:LYS:N	2.44	0.51
6:G:564:ARG:O	6:G:568:THR:OG1	2.12	0.51
2:O:7:MET:O	2:O:76:ILE:HD12	2.11	0.51
12:X:26:GLN:NE2	12:X:33:ASP:O	2.44	0.51
1:A:471:VAL:HG22	1:A:510:TYR:OH	2.10	0.51
6:H:510:GLN:OE1	6:H:513:ARG:NH1	2.44	0.51
7:L:6:ALA:HB1	7:L:10:ARG:NH1	2.26	0.51
7:M:115:ILE:HD13	8:Q:458:LEU:HD13	1.93	0.51
2:O:489:VAL:O	2:O:579:THR:OG1	2.24	0.51
2:O:732:HIS:HA	2:O:735:ILE:HG22	1.93	0.51
10:U:711:ASN:O	10:U:715:LYS:NZ	2.38	0.51
1:A:481:VAL:O	1:A:521:LEU:HD11	2.10	0.51
2:B:87:THR:O	8:P:45:TYR:OH	2.23	0.51
5:F:246:GLU:OE2	5:F:246:GLU:N	2.43	0.51
7:L:204:MET:HA	7:L:207:ILE:HD12	1.92	0.51
2:O:836:ARG:O	2:O:839:THR:OG1	2.26	0.51
11:V:132:SER:OG	11:V:133:LYS:N	2.44	0.51
11:V:382:LEU:HA	11:V:385:LEU:HD12	1.93	0.51
6:G:148:ALA:HB1	6:G:328:LEU:HD21	1.93	0.51
6:H:374:LEU:HD23	6:H:383:SER:HG	1.76	0.51
6:H:524:TRP:O	6:H:529:GLN:N	2.43	0.51
7:M:279:SER:O	7:M:283:ASN:ND2	2.44	0.51
2:O:847:LEU:HD11	8:Q:805:VAL:HB	1.92	0.51
8:Q:200:VAL:HG11	8:Q:220:LEU:HD11	1.93	0.51
8:Q:563:ILE:CG2	8:Q:565:TYR:HE1	2.23	0.51
1:S:375:LEU:HD11	1:S:392:PHE:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:556:HIS:HA	11:V:559:ILE:HD12	1.92	0.51
11:V:801:CYS:SG	11:V:802:GLN:N	2.83	0.51
2:O:769:THR:O	2:O:772:SER:OG	2.14	0.51
1:S:57:LEU:CB	1:S:116:MET:HE1	2.41	0.51
1:S:874:ARG:O	1:S:875:LEU:HD23	2.10	0.51
10:U:587:ILE:O	10:U:590:SER:OG	2.21	0.51
2:B:583:SER:OG	2:B:584:LEU:N	2.44	0.51
7:L:274:TRP:HH2	7:L:280:VAL:HG13	1.75	0.51
7:M:361:TYR:CE1	12:X:101:SER:HA	2.45	0.51
8:Q:494:CYS:SG	8:Q:495:ALA:N	2.84	0.51
10:U:298:GLN:N	10:U:298:GLN:OE1	2.44	0.51
2:B:700:PHE:O	2:B:703:THR:OG1	2.15	0.50
6:G:147:ALA:HB1	6:G:159:LEU:HD11	1.93	0.50
7:L:38:LEU:HD12	7:L:39:ARG:H	1.75	0.50
8:Q:733:LEU:CD2	8:Q:746:VAL:HG11	2.41	0.50
1:S:1050:GLU:OE1	1:S:1053:ARG:NH1	2.44	0.50
10:U:462:LEU:HD11	10:U:466:ILE:HD11	1.93	0.50
10:U:589:ASP:OD1	10:U:592:ARG:NH1	2.44	0.50
11:V:572:LEU:HA	11:V:575:ILE:HD12	1.93	0.50
1:A:1101:ILE:HD13	1:A:1154:PHE:CE2	2.46	0.50
3:C:193:LEU:HD22	5:F:138:ARG:HG2	1.92	0.50
1:S:1393:VAL:HA	1:S:1396:ILE:HD12	1.92	0.50
10:U:747:MET:HG3	10:U:781:LEU:HD13	1.93	0.50
11:V:264:GLN:HA	11:V:267:MET:HE3	1.92	0.50
1:A:1406:LEU:O	1:A:1409:ARG:N	2.43	0.50
2:B:524:GLN:OE1	8:P:560:CYS:SG	2.69	0.50
2:O:759:MET:SD	2:O:852:ALA:HB3	2.51	0.50
8:P:424:SER:O	8:P:427:GLY:N	2.39	0.50
8:P:648:ASP:CG	8:P:803:ALA:HB2	2.35	0.50
1:S:993:GLN:HE22	1:S:1074:GLU:HB2	1.76	0.50
10:U:207:LEU:HD13	10:U:210:ILE:HD12	1.92	0.50
3:C:367:THR:HG21	3:C:403:TRP:CZ3	2.47	0.50
4:E:525:LYS:NZ	11:V:152:THR:O	2.44	0.50
6:H:266:LEU:O	6:H:270:VAL:HG23	2.11	0.50
8:P:423:LEU:HD12	8:P:428:ARG:C	2.37	0.50
1:S:513:LEU:O	1:S:516:THR:OG1	2.20	0.50
11:V:686:LEU:HD21	11:V:815:ARG:HD3	1.94	0.50
3:C:508:VAL:CG1	3:C:512:MET:HE2	2.42	0.50
6:H:365:GLU:HA	6:H:368:LEU:HD12	1.92	0.50
7:L:34:ARG:NH1	7:L:104:LEU:HD23	2.27	0.50
8:P:17:PRO:HD2	8:P:21:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:623:GLN:O	1:S:626:SER:OG	2.25	0.50
10:U:473:VAL:HG23	10:U:474:LEU:CD2	2.41	0.50
10:U:977:PHE:O	10:U:979:SER:N	2.44	0.50
1:A:392:PHE:CE2	1:A:396:LEU:HD11	2.47	0.50
1:A:424:LEU:HD21	1:A:472:PHE:HB3	1.94	0.50
1:A:463:HIS:CD2	1:A:473:LEU:HD11	2.47	0.50
8:P:735:TRP:O	8:P:807:ARG:NH1	2.44	0.50
11:V:236:ILE:HG22	11:V:265:LEU:HD13	1.93	0.50
2:B:423:TYR:CG	8:P:606:LEU:HD13	2.46	0.50
6:G:461:GLN:OE1	6:G:596:TYR:OH	2.24	0.50
6:G:510:GLN:NE2	6:G:543:MET:O	2.44	0.50
2:O:47:ARG:NH1	2:O:116:ASN:OD1	2.44	0.50
11:V:1122:HIS:HA	11:V:1125:ILE:HD12	1.93	0.50
7:L:302:ASP:OD2	7:L:304:THR:OG1	2.14	0.50
1:S:158:HIS:HB2	1:S:160:MET:HE2	1.94	0.50
1:S:291:THR:HA	1:S:294:ILE:HD12	1.92	0.50
7:L:38:LEU:HD12	7:L:39:ARG:N	2.26	0.50
7:L:322:GLN:O	7:L:333:PHE:N	2.45	0.50
7:M:256:ALA:HA	7:M:323:VAL:HG22	1.91	0.50
8:Q:523:LEU:HD22	8:Q:584:LEU:HB2	1.94	0.50
10:U:1082:PRO:HG2	10:U:1083:THR:HG23	1.94	0.50
6:H:61:PRO:O	6:H:102:ARG:NE	2.45	0.49
6:H:100:LEU:CD2	6:H:125:VAL:HG21	2.40	0.49
8:P:424:SER:HB2	8:P:430:MET:HE2	1.94	0.49
8:Q:141:VAL:HG22	8:Q:154:LEU:CD1	2.42	0.49
8:Q:467:GLU:O	8:Q:470:SER:OG	2.26	0.49
8:Q:486:LEU:O	8:Q:486:LEU:HD23	2.12	0.49
8:Q:648:ASP:OD2	8:Q:651:GLN:NE2	2.45	0.49
11:V:792:TRP:NE1	11:V:796:ILE:HD11	2.26	0.49
4:E:20:ALA:N	4:E:21:GLN:OE1	2.45	0.49
6:H:30:ALA:HB2	6:H:42:LEU:HD23	1.94	0.49
7:M:253:PHE:HB2	7:M:260:VAL:HG13	1.94	0.49
1:S:166:PHE:CZ	1:S:170:LEU:HD11	2.47	0.49
1:S:1283:LYS:O	1:S:1287:VAL:HG23	2.12	0.49
10:U:500:LEU:HA	10:U:503:VAL:HG12	1.94	0.49
10:U:1056:HIS:CE1	10:U:1069:THR:HG22	2.48	0.49
1:A:193:LEU:HD23	1:A:241:MET:HE2	1.92	0.49
1:A:235:LEU:HG	1:A:301:VAL:HG11	1.93	0.49
1:A:874:ARG:HG3	1:A:875:LEU:HD23	1.93	0.49
2:B:774:SER:HA	2:B:777:ILE:HD12	1.94	0.49
2:O:745:LYS:HE3	2:O:859:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:362:THR:OG1	8:P:363:PRO:HD2	2.11	0.49
1:S:360:ARG:O	1:S:364:VAL:HG23	2.13	0.49
1:S:737:ALA:HB1	1:S:738:PRO:CD	2.42	0.49
10:U:88:GLU:O	10:U:92:LEU:HD23	2.12	0.49
10:U:591:LEU:HD22	10:U:605:LEU:HD11	1.94	0.49
10:U:662:GLU:OE2	10:U:667:LEU:HD22	2.12	0.49
10:U:1267:LEU:O	10:U:1271:SER:OG	2.22	0.49
8:P:143:LEU:HD11	8:P:175:LEU:HD11	1.95	0.49
10:U:1076:ASN:O	10:U:1080:ALA:N	2.43	0.49
1:A:158:HIS:O	1:A:159:SER:OG	2.24	0.49
2:B:106:GLU:O	2:B:125:LYS:N	2.46	0.49
2:B:170:ILE:HD11	2:B:183:LEU:HB3	1.94	0.49
2:B:622:LEU:HD23	2:B:623:SER:N	2.27	0.49
3:C:344:THR:HG21	3:C:396:LEU:CD2	2.42	0.49
6:G:266:LEU:O	6:G:270:VAL:HG23	2.12	0.49
7:L:305:MET:SD	7:L:305:MET:N	2.85	0.49
7:M:266:LYS:O	7:M:270:ASN:ND2	2.46	0.49
8:Q:563:ILE:HG21	8:Q:565:TYR:HE1	1.78	0.49
1:S:163:ARG:CG	1:S:191:VAL:HG22	2.42	0.49
10:U:66:ARG:HG3	10:U:104:LEU:HD22	1.95	0.49
1:A:153:GLN:NE2	1:A:188:GLN:O	2.46	0.49
3:C:286:CYS:O	3:C:340:TYR:OH	2.23	0.49
3:C:372:SER:HB3	3:C:425:LEU:HD13	1.94	0.49
8:P:125:LEU:O	8:P:127:ASP:N	2.44	0.49
8:Q:801:HIS:O	8:Q:805:VAL:HG23	2.11	0.49
1:S:384:VAL:HG11	1:S:386:TRP:CZ3	2.47	0.49
1:S:732:ALA:O	1:S:735:SER:OG	2.21	0.49
10:U:1213:ILE:HD11	10:U:1253:LEU:CD2	2.43	0.49
2:B:704:LEU:HB2	2:B:720:TYR:HB2	1.94	0.49
4:E:384:THR:O	4:E:388:THR:HG23	2.12	0.49
2:O:506:LEU:HD23	2:O:507:SER:N	2.28	0.49
2:O:591:SER:OG	2:O:624:LEU:HD12	2.12	0.49
8:Q:569:VAL:HA	8:Q:578:ARG:NH1	2.27	0.49
10:U:606:TYR:OH	10:U:662:GLU:OE2	2.30	0.49
11:V:282:ILE:HG22	11:V:286:LEU:CD1	2.43	0.49
12:X:19:PRO:HB2	12:X:22:ILE:HD12	1.94	0.49
1:A:200:HIS:ND1	1:A:202:ASP:O	2.46	0.49
2:B:654:ALA:O	2:B:655:PHE:HD1	1.95	0.49
7:L:203:VAL:HG21	7:L:245:PRO:HB2	1.94	0.49
7:M:338:LEU:HD23	7:M:368:LEU:HD13	1.95	0.49
8:P:28:VAL:O	8:P:29:LEU:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:451:ALA:O	8:P:455:ILE:HD12	2.12	0.49
8:Q:288:LEU:O	8:Q:310:ASP:N	2.42	0.49
1:A:137:LEU:HD13	1:A:141:GLN:HB2	1.93	0.49
1:A:291:THR:HA	1:A:294:ILE:HD12	1.94	0.49
2:B:731:LEU:O	2:B:735:ILE:HG22	2.12	0.49
5:F:82:ASN:H	5:F:85:ALA:HB3	1.77	0.49
6:H:483:LEU:HD11	6:H:509:LEU:HD11	1.95	0.49
2:O:426:LEU:C	2:O:426:LEU:HD23	2.38	0.49
8:P:125:LEU:O	8:P:125:LEU:HD12	2.13	0.49
8:P:220:LEU:HD13	8:P:224:LEU:HD22	1.94	0.49
10:U:544:LEU:HD21	10:U:587:ILE:HD13	1.93	0.49
11:V:61:THR:OG1	11:V:63:GLU:OE1	2.26	0.49
1:S:361:ARG:C	1:S:365:MET:HE3	2.37	0.49
1:S:414:LEU:HD21	1:S:429:THR:HB	1.95	0.49
1:S:504:ARG:HA	1:S:507:LEU:HD12	1.94	0.49
1:S:1025:VAL:HG11	1:S:1085:LEU:HD22	1.94	0.49
11:V:223:GLN:N	11:V:223:GLN:OE1	2.45	0.49
2:B:753:ASN:OD1	8:P:858:SER:CB	2.61	0.48
2:O:94:ILE:O	2:O:109:LEU:HD12	2.13	0.48
2:O:529:LYS:O	2:O:530:LEU:HD23	2.13	0.48
8:P:170:ILE:CG2	8:P:259:VAL:HG13	2.43	0.48
11:V:1206:VAL:HG21	11:V:1223:PHE:HB2	1.95	0.48
8:P:520:GLN:OE1	8:P:520:GLN:N	2.46	0.48
8:Q:324:ILE:HG23	8:Q:338:LEU:CD2	2.44	0.48
1:S:407:LEU:O	1:S:411:VAL:HG23	2.13	0.48
1:A:1323:ALA:HB1	1:A:1324:PRO:HD2	1.94	0.48
1:A:1339:LEU:HD22	1:A:1343:HIS:ND1	2.27	0.48
5:F:245:SER:O	5:F:249:ALA:N	2.46	0.48
7:M:9:LEU:HD21	8:Q:490:MET:SD	2.54	0.48
7:M:233:ASN:ND2	7:M:304:THR:HG22	2.28	0.48
8:Q:849:ASP:O	8:Q:853:THR:HG23	2.13	0.48
10:U:675:LEU:HD12	10:U:702:LEU:HD23	1.95	0.48
10:U:1210:TYR:HA	10:U:1213:ILE:HD12	1.95	0.48
1:A:1369:VAL:O	6:H:531:THR:OG1	2.27	0.48
4:E:382:LEU:HD11	11:V:309:HIS:CE1	2.49	0.48
8:P:706:ALA:HB2	8:P:797:ILE:HG23	1.95	0.48
8:Q:130:LEU:HA	8:Q:144:VAL:HG23	1.96	0.48
8:Q:850:ARG:O	8:Q:853:THR:OG1	2.30	0.48
1:S:928:THR:HG22	1:S:929:TYR:N	2.28	0.48
11:V:112:ASN:HA	11:V:115:LEU:HD12	1.93	0.48
11:V:432:CYS:HG	11:V:465:PHE:HD2	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:LEU:C	2:B:509:LEU:HD12	2.39	0.48
2:O:526:ARG:NE	8:Q:559:ALA:O	2.47	0.48
1:S:1355:HIS:CE1	1:S:1421:LEU:HD21	2.47	0.48
10:U:317:THR:HG22	10:U:326:VAL:HB	1.95	0.48
11:V:1226:LEU:HD22	11:V:1234:PHE:CE2	2.49	0.48
1:A:769:LEU:HD13	1:A:821:LEU:HD11	1.96	0.48
6:G:249:TYR:HB2	6:G:272:ALA:HB2	1.96	0.48
6:H:287:SER:HB2	6:H:303:LEU:HD11	1.95	0.48
1:A:872:MET:HE2	1:A:911:TRP:HB2	1.95	0.48
1:A:1080:ARG:HD3	1:S:952:GLN:OE1	2.13	0.48
7:M:110:PHE:O	7:M:114:LEU:HD23	2.13	0.48
7:M:326:ASN:HD22	7:M:364:LYS:HG3	1.78	0.48
7:M:365:PRO:HB3	10:U:266:HIS:CD2	2.48	0.48
1:S:1160:GLN:NE2	1:S:1196:GLU:OE2	2.43	0.48
1:S:1255:GLU:OE2	1:S:1314:ARG:NH1	2.47	0.48
1:S:1432:VAL:HG12	1:S:1436:LEU:HD12	1.96	0.48
10:U:344:LEU:O	10:U:351:GLN:NE2	2.44	0.48
10:U:754:ILE:HG23	10:U:771:ILE:HG23	1.96	0.48
2:B:22:VAL:C	2:B:23:LEU:HD12	2.39	0.48
3:C:210:GLU:N	3:C:210:GLU:OE1	2.47	0.48
4:E:521:THR:HG22	4:E:522:PHE:O	2.13	0.48
7:M:234:VAL:HG11	7:M:259:VAL:HG11	1.95	0.48
8:P:352:CYS:O	8:P:403:SER:OG	2.30	0.48
11:V:532:LEU:O	11:V:535:VAL:HB	2.13	0.48
7:L:256:ALA:O	7:L:260:VAL:HG23	2.13	0.48
7:M:124:ASP:OD1	2:O:386:ASN:ND2	2.47	0.48
7:M:311:TYR:O	12:X:9:ARG:NE	2.47	0.48
8:Q:227:LEU:HD22	8:Q:334:LEU:CD2	2.44	0.48
8:Q:290:THR:OG1	8:Q:325:LYS:NZ	2.46	0.48
8:Q:782:ILE:HD12	8:Q:881:LEU:HD22	1.95	0.48
1:S:1108:PHE:O	1:S:1112:VAL:HG23	2.14	0.48
4:E:379:ALA:HB2	4:E:419:LEU:HD11	1.96	0.48
10:U:380:GLN:NE2	10:U:380:GLN:O	2.46	0.48
10:U:665:ASP:N	10:U:665:ASP:OD1	2.47	0.48
11:V:447:ASP:HB3	11:V:450:ILE:HD12	1.96	0.48
1:A:361:ARG:C	1:A:365:MET:HE3	2.39	0.47
1:S:944:ASP:OD1	1:S:945:ALA:N	2.47	0.47
10:U:9:ALA:HA	10:U:17:LEU:HD11	1.96	0.47
11:V:243:VAL:HG13	11:V:244:PRO:CD	2.43	0.47
11:V:1115:VAL:HG11	11:V:1142:LEU:HG	1.96	0.47
6:G:104:LEU:HD21	6:G:124:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:121:LEU:O	6:G:124:SER:OG	2.28	0.47
6:G:249:TYR:HA	6:G:252:LEU:HD12	1.95	0.47
2:O:229:ILE:HG22	2:O:268:PHE:CD2	2.49	0.47
1:S:669:GLN:O	1:S:673:ILE:HD12	2.14	0.47
10:U:852:GLN:OE1	10:U:860:SER:N	2.47	0.47
10:U:1028:LEU:HD23	10:U:1074:ILE:CD1	2.43	0.47
11:V:432:CYS:HA	11:V:435:ILE:HD12	1.96	0.47
11:V:1132:LEU:HA	11:V:1135:ILE:HG22	1.95	0.47
1:A:102:ALA:HB2	1:A:112:LEU:CD1	2.43	0.47
1:A:135:VAL:HG12	1:A:179:LEU:HB2	1.95	0.47
1:A:494:LEU:HD11	1:A:518:LEU:HD11	1.95	0.47
1:A:1211:LEU:HD12	1:A:1233:ALA:HB1	1.96	0.47
4:E:109:LEU:CB	4:E:114:LEU:HD11	2.45	0.47
7:L:354:ILE:HD13	7:L:369:LYS:HG2	1.96	0.47
8:P:486:LEU:HD21	8:P:490:MET:HE3	1.95	0.47
8:Q:772:ALA:HB1	8:Q:781:PRO:CG	2.44	0.47
10:U:487:TYR:O	10:U:491:LEU:HG	2.14	0.47
11:V:1099:LYS:NZ	11:V:1113:GLN:OE1	2.46	0.47
1:A:427:MET:HE3	1:A:476:PHE:CD2	2.49	0.47
7:M:143:ALA:HB3	7:M:198:LYS:HE3	1.96	0.47
1:S:715:GLU:O	1:S:719:VAL:HG23	2.15	0.47
10:U:19:GLU:OE2	10:U:19:GLU:N	2.47	0.47
11:V:301:LEU:HD11	11:V:305:LEU:HD11	1.95	0.47
3:C:64:PHE:O	3:C:67:ILE:HG22	2.14	0.47
4:E:113:GLY:O	4:E:117:VAL:HG23	2.14	0.47
8:P:220:LEU:HD13	8:P:224:LEU:CD2	2.45	0.47
2:B:664:SER:OG	2:B:742:CYS:SG	2.64	0.47
6:G:551:TYR:CD2	6:G:574:LEU:HD21	2.50	0.47
7:M:241:ASP:OD2	7:M:244:HIS:ND1	2.39	0.47
2:O:484:ASP:OD1	2:O:484:ASP:N	2.48	0.47
8:P:123:CYS:SG	8:P:124:ILE:N	2.87	0.47
8:P:488:GLU:O	8:P:492:VAL:HG23	2.14	0.47
1:S:759:PRO:O	1:S:763:THR:HG23	2.14	0.47
10:U:823:GLN:O	10:U:823:GLN:NE2	2.47	0.47
11:V:462:PHE:HB2	11:V:473:VAL:HG11	1.96	0.47
11:V:930:ILE:HD11	11:V:1004:LEU:HD13	1.96	0.47
1:A:142:ARG:NH1	1:A:180:GLU:OE2	2.48	0.47
1:A:418:ALA:O	1:A:423:GLN:N	2.47	0.47
2:B:40:THR:HG21	2:B:69:GLU:O	2.15	0.47
3:C:143:ILE:HG21	5:F:92:LEU:CD2	2.45	0.47
2:O:415:LYS:HB2	8:Q:479:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:317:HIS:O	8:Q:347:VAL:N	2.48	0.47
8:Q:542:THR:HA	8:Q:569:VAL:HG23	1.97	0.47
1:S:190:ILE:HG22	1:S:191:VAL:HG23	1.95	0.47
1:S:428:VAL:HG22	1:S:476:PHE:CE1	2.49	0.47
11:V:246:LEU:HD22	11:V:284:PHE:CD2	2.50	0.47
3:C:277:LYS:NZ	3:C:324:GLU:OE2	2.48	0.47
3:C:333:LEU:HD21	4:E:48:ARG:HD2	1.96	0.47
3:C:405:GLU:N	3:C:405:GLU:OE1	2.48	0.47
7:M:104:LEU:HD13	2:O:404:SER:CB	2.45	0.47
11:V:46:SER:OG	11:V:49:VAL:HG12	2.15	0.47
11:V:960:LEU:HD21	11:V:965:LEU:HD13	1.96	0.47
3:C:523:ILE:HG23	3:C:551:LEU:HD11	1.97	0.47
8:Q:136:LEU:HD13	8:Q:139:VAL:HB	1.96	0.47
10:U:828:SER:O	10:U:831:VAL:HG22	2.13	0.47
2:B:673:LYS:O	2:B:677:LEU:HD23	2.15	0.47
2:B:682:CYS:HB3	2:B:692:TYR:HB3	1.97	0.47
5:F:158:GLN:N	5:F:158:GLN:OE1	2.46	0.47
6:G:13:LEU:HD21	6:G:66:VAL:HA	1.95	0.47
6:H:393:MET:HE3	6:H:397:PHE:CE1	2.51	0.47
2:O:7:MET:N	2:O:13:GLU:O	2.48	0.47
8:Q:361:SER:HA	8:Q:366:LEU:HD12	1.95	0.47
10:U:840:ARG:O	10:U:844:ASN:ND2	2.48	0.47
10:U:990:THR:HA	10:U:1031:LEU:HD13	1.96	0.47
1:A:1156:LEU:HD12	1:A:1196:GLU:HB2	1.96	0.46
2:B:83:SER:O	2:B:83:SER:OG	2.32	0.46
7:L:357:GLY:O	7:L:366:ILE:CG2	2.62	0.46
2:O:266:ILE:HG21	2:O:268:PHE:CE1	2.50	0.46
8:P:739:GLU:OE2	8:P:807:ARG:HD3	2.15	0.46
1:S:202:ASP:O	1:S:206:VAL:HG23	2.15	0.46
11:V:210:ASP:O	11:V:213:THR:HG22	2.14	0.46
2:B:287:VAL:HG12	2:B:301:VAL:HG22	1.96	0.46
8:Q:570:ASP:H	8:Q:578:ARG:HH12	1.63	0.46
11:V:540:ALA:HA	11:V:551:ILE:HD11	1.96	0.46
1:A:219:GLU:HG3	1:A:294:ILE:HD11	1.97	0.46
2:B:505:THR:CG2	2:B:506:LEU:H	2.28	0.46
6:G:417:CYS:SG	6:G:455:THR:HG23	2.55	0.46
2:O:426:LEU:HD12	8:Q:489:ALA:CB	2.44	0.46
11:V:306:ASP:OD2	11:V:309:HIS:ND1	2.49	0.46
6:H:64:VAL:HA	6:H:67:LEU:HD13	1.96	0.46
2:O:745:LYS:NZ	2:O:859:LEU:HD11	2.30	0.46
8:P:649:MET:HE1	8:P:759:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:361:ARG:O	1:S:365:MET:HE3	2.16	0.46
11:V:235:LEU:HD11	11:V:242:THR:HG22	1.96	0.46
1:A:348:PHE:CZ	1:A:356:THR:HG23	2.51	0.46
2:B:292:SER:O	2:B:292:SER:OG	2.31	0.46
1:S:587:LEU:O	1:S:589:THR:N	2.48	0.46
1:S:1174:TRP:CD2	1:S:1200:LEU:HD22	2.50	0.46
11:V:367:ALA:O	11:V:371:THR:OG1	2.22	0.46
11:V:392:ASN:N	11:V:392:ASN:OD1	2.48	0.46
11:V:639:ILE:O	11:V:743:ARG:NH2	2.49	0.46
1:A:1283:LYS:O	1:A:1287:VAL:HG23	2.15	0.46
3:C:151:LYS:O	3:C:155:LEU:HD13	2.16	0.46
3:C:515:THR:O	3:C:519:THR:OG1	2.33	0.46
3:C:526:LEU:HB2	3:C:551:LEU:HD13	1.98	0.46
6:H:388:PRO:HD2	6:H:389:PRO:HD3	1.97	0.46
1:S:327:ILE:O	1:S:388:ARG:NH1	2.48	0.46
1:S:1171:LEU:O	1:S:1204:ARG:NH1	2.45	0.46
1:A:34:LYS:NZ	6:H:381:ARG:NH2	2.63	0.46
1:A:476:PHE:CE2	1:A:480:LEU:HD11	2.51	0.46
2:B:187:LYS:O	2:B:228:ILE:HG21	2.15	0.46
3:C:292:ARG:HG3	4:E:103:MET:HE1	1.97	0.46
4:E:73:VAL:O	4:E:81:LEU:HD12	2.16	0.46
7:L:293:PRO:HB2	7:L:296:ALA:HB2	1.98	0.46
7:M:29:ILE:HD11	7:M:88:LYS:HG3	1.98	0.46
2:O:141:LEU:HD12	2:O:153:ILE:O	2.15	0.46
8:P:771:VAL:HG21	8:P:786:GLU:HB3	1.98	0.46
1:S:753:MET:HA	1:S:757:VAL:HG11	1.97	0.46
1:S:1400:ARG:NH2	1:S:1431:GLU:OE1	2.47	0.46
11:V:51:LEU:HD22	11:V:83:LEU:CD1	2.42	0.46
11:V:110:PHE:CZ	11:V:114:LEU:HD11	2.51	0.46
11:V:684:TYR:O	11:V:815:ARG:NH1	2.48	0.46
1:A:102:ALA:HB1	1:A:107:VAL:O	2.16	0.46
1:A:790:HIS:NE2	1:A:843:TYR:OH	2.39	0.46
1:A:1335:PHE:CE1	1:A:1339:LEU:HD12	2.50	0.46
3:C:35:CYS:O	3:C:38:VAL:HG12	2.16	0.46
3:C:418:PRO:HG3	3:C:450:LEU:HD13	1.97	0.46
7:M:233:ASN:H	7:M:305:MET:HE3	1.81	0.46
2:O:412:LEU:O	8:Q:479:ARG:NH2	2.49	0.46
2:O:759:MET:HA	2:O:852:ALA:HB1	1.98	0.46
8:P:841:LEU:O	8:P:845:GLN:HG3	2.16	0.46
8:Q:125:LEU:O	8:Q:127:ASP:N	2.49	0.46
10:U:832:LEU:O	10:U:835:SER:OG	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:920:GLN:O	10:U:924:GLN:NE2	2.45	0.46
11:V:278:LEU:N	11:V:279:PRO:HD2	2.31	0.46
2:B:228:ILE:HG22	2:B:229:ILE:H	1.81	0.46
2:B:614:TYR:OH	8:P:638:VAL:HA	2.16	0.46
3:C:407:VAL:HG11	3:C:426:LEU:HB2	1.97	0.46
7:M:67:HIS:O	7:M:71:GLN:NE2	2.49	0.46
7:M:244:HIS:ND1	10:U:511:MET:HE2	2.31	0.46
7:M:256:ALA:CB	7:M:323:VAL:CG2	2.93	0.46
8:P:843:GLU:OE2	8:P:865:ARG:NE	2.49	0.46
8:Q:703:PRO:O	8:Q:705:VAL:HG23	2.16	0.46
1:S:826:THR:HG22	1:S:828:ASP:H	1.79	0.46
10:U:814:LEU:HD21	10:U:842:ALA:HB1	1.98	0.46
11:V:1186:LEU:HB2	11:V:1237:VAL:HG11	1.98	0.46
2:B:532:THR:HG23	2:B:687:GLU:O	2.15	0.46
2:B:850:ASP:OD1	8:P:870:TYR:HE1	1.99	0.46
5:F:188:PHE:CZ	5:F:192:LEU:HD11	2.51	0.46
7:M:25:TYR:HB2	7:M:40:ILE:HG23	1.97	0.46
2:O:759:MET:HE3	2:O:763:LEU:HG	1.97	0.46
1:S:733:ALA:HB1	1:S:742:GLN:CD	2.41	0.46
1:S:1402:PHE:CE2	1:S:1406:LEU:HD11	2.50	0.46
10:U:1140:THR:O	10:U:1143:THR:OG1	2.29	0.46
11:V:792:TRP:CE2	11:V:796:ILE:HD11	2.51	0.46
11:V:822:LEU:HD23	11:V:825:ILE:HD12	1.98	0.46
1:A:769:LEU:HD13	1:A:821:LEU:CD1	2.46	0.45
2:B:82:VAL:O	2:B:83:SER:OG	2.31	0.45
2:B:764:GLU:O	2:B:768:VAL:HG23	2.15	0.45
6:G:100:LEU:HB2	6:G:121:LEU:HD21	1.98	0.45
6:H:374:LEU:CD2	6:H:383:SER:OG	2.58	0.45
6:H:387:SER:HG	6:H:388:PRO:HD3	1.73	0.45
1:S:1075:LEU:HD11	1:S:1115:GLU:HB3	1.98	0.45
11:V:277:ASP:O	11:V:280:VAL:N	2.43	0.45
1:A:37:PRO:O	1:A:40:ALA:HB3	2.16	0.45
1:A:827:ARG:HB2	1:A:945:ALA:HB2	1.98	0.45
6:H:464:VAL:HG22	6:H:523:GLU:OE2	2.16	0.45
7:M:207:ILE:HA	7:M:281:LEU:HD11	1.99	0.45
8:Q:563:ILE:CG2	8:Q:565:TYR:CE1	2.99	0.45
1:S:124:ILE:HD13	1:S:145:LEU:CD2	2.47	0.45
10:U:216:GLN:HA	10:U:219:VAL:HG22	1.99	0.45
1:A:359:TYR:HA	1:A:362:LEU:HD12	1.99	0.45
1:A:1314:ARG:HH21	1:A:1315:LEU:HD11	1.82	0.45
2:B:315:SER:O	2:B:315:SER:OG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:VAL:HG13	7:L:133:PHE:HE1	1.80	0.45
2:B:835:TYR:O	2:B:839:THR:HG23	2.15	0.45
7:M:315:LEU:O	7:M:318:THR:OG1	2.19	0.45
2:O:176:ILE:HD12	2:O:182:VAL:HG21	1.98	0.45
1:S:752:THR:OG1	1:S:753:MET:N	2.49	0.45
11:V:228:GLY:HA2	11:V:231:LEU:HD12	1.97	0.45
11:V:452:SER:O	11:V:455:SER:OG	2.20	0.45
11:V:793:PHE:HA	11:V:796:ILE:HD12	1.98	0.45
1:A:733:ALA:HB1	1:A:742:GLN:CD	2.41	0.45
3:C:110:LEU:HD11	3:C:114:ILE:HD11	1.98	0.45
4:E:399:CYS:HB3	4:E:437:MET:HE1	1.98	0.45
2:O:184:LEU:HD12	2:O:240:VAL:HG11	1.98	0.45
2:O:481:ARG:NE	2:O:647:ASP:OD1	2.49	0.45
8:Q:651:GLN:O	8:Q:740:ASN:ND2	2.49	0.45
8:Q:675:PRO:O	8:Q:678:THR:OG1	2.33	0.45
1:S:875:LEU:CD2	1:S:946:LEU:HD21	2.46	0.45
1:S:1254:GLU:OE2	1:S:1298:ARG:NH2	2.50	0.45
10:U:234:ILE:O	10:U:238:SER:OG	2.31	0.45
3:C:111:ASN:HA	3:C:114:ILE:HD12	1.99	0.45
6:G:118:LEU:HD23	6:G:121:LEU:HD23	1.97	0.45
7:L:356:PHE:CE1	7:L:367:THR:CG2	2.99	0.45
8:P:792:SER:OG	8:P:793:SER:N	2.48	0.45
11:V:244:PRO:O	11:V:245:ILE:C	2.57	0.45
1:A:25:LEU:HD11	6:H:416:LEU:HA	1.99	0.45
1:A:198:GLU:OE1	1:A:262:MET:N	2.50	0.45
2:B:850:ASP:OD1	8:P:870:TYR:CE1	2.70	0.45
3:C:303:LEU:HD21	3:C:391:PHE:CE1	2.52	0.45
6:G:203:LEU:O	6:G:207:LEU:HD23	2.16	0.45
7:M:354:ILE:HD11	10:U:435:MET:HE3	1.99	0.45
2:O:184:LEU:CD1	2:O:240:VAL:HG11	2.46	0.45
8:P:480:ASN:O	8:P:484:THR:HG23	2.17	0.45
8:P:704:SER:OG	8:P:793:SER:O	2.34	0.45
2:B:590:PHE:CD2	8:Q:682:THR:HG21	2.52	0.45
3:C:465:GLN:O	3:C:469:THR:HG23	2.17	0.45
4:E:50:LEU:HD22	4:E:55:TRP:HE1	1.82	0.45
11:V:606:GLN:O	11:V:610:VAL:HG23	2.17	0.45
3:C:201:GLU:OE1	3:C:202:ALA:N	2.49	0.45
4:E:487:MET:CE	11:V:202:ILE:HG21	2.47	0.45
6:G:295:ASP:OD2	1:S:54:HIS:NE2	2.47	0.45
6:G:555:LEU:HD21	6:G:570:LEU:HB2	1.99	0.45
6:H:118:LEU:HD23	6:H:121:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:143:LEU:HD12	2:O:151:PHE:O	2.16	0.45
1:S:415:MET:HE2	1:S:451:TRP:CZ2	2.52	0.45
11:V:145:LEU:O	11:V:148:ALA:HB3	2.16	0.45
2:B:777:ILE:HD13	8:P:830:LEU:HD13	1.98	0.45
3:C:273:GLU:OE1	3:C:531:TYR:OH	2.30	0.45
5:F:127:GLU:OE1	5:F:132:SER:OG	2.27	0.45
8:Q:193:PHE:O	8:Q:194:LEU:HD23	2.17	0.45
8:Q:229:PHE:CE2	8:Q:240:VAL:HG21	2.52	0.45
1:S:992:HIS:CD2	1:S:1077:MET:HE2	2.52	0.45
10:U:463:LEU:O	10:U:467:VAL:HG23	2.16	0.45
2:B:57:PHE:CB	2:B:354:LEU:HD21	2.46	0.45
2:B:423:TYR:CZ	8:P:606:LEU:HB3	2.52	0.45
3:C:124:ALA:O	5:F:140:ARG:NH1	2.49	0.45
2:O:745:LYS:HZ1	2:O:859:LEU:HD11	1.82	0.45
8:Q:359:TYR:CD1	8:Q:368:VAL:HG23	2.52	0.45
8:Q:609:VAL:O	8:Q:610:VAL:HG23	2.17	0.45
1:S:1239:GLU:HA	1:S:1242:ILE:HD12	1.99	0.45
1:S:1274:THR:HG22	1:S:1275:SER:H	1.82	0.45
11:V:505:SER:OG	11:V:506:ALA:N	2.50	0.45
11:V:689:TYR:CZ	11:V:693:ASP:OD2	2.70	0.45
1:A:1404:LEU:HD21	1:A:1432:VAL:HG12	1.98	0.44
2:B:856:LEU:HD23	8:P:867:LEU:HD21	2.00	0.44
7:M:57:TRP:O	7:M:61:THR:HG23	2.16	0.44
2:O:593:PHE:CD1	2:O:593:PHE:C	2.95	0.44
8:P:36:PHE:HD1	8:P:46:VAL:HG22	1.82	0.44
8:P:317:HIS:O	8:P:347:VAL:N	2.39	0.44
8:Q:125:LEU:O	8:Q:125:LEU:HD12	2.17	0.44
1:A:476:PHE:CZ	1:A:480:LEU:HD11	2.52	0.44
3:C:167:ASN:OD1	7:L:343:ARG:NH1	2.50	0.44
3:C:319:THR:O	3:C:323:VAL:HG23	2.18	0.44
2:O:62:THR:OG1	2:O:63:GLY:N	2.48	0.44
2:O:408:LEU:CB	8:Q:472:LEU:HD13	2.47	0.44
2:O:520:LEU:HD12	8:Q:567:ILE:HG22	1.99	0.44
8:P:649:MET:HE1	8:P:759:PRO:HD2	1.98	0.44
8:Q:143:LEU:CD1	8:Q:197:LEU:HD21	2.47	0.44
1:S:556:MET:HE2	1:S:998:TYR:CD1	2.52	0.44
10:U:174:VAL:HG11	10:U:201:MET:HE2	1.99	0.44
11:V:208:GLN:O	11:V:212:ILE:HG22	2.17	0.44
1:A:170:LEU:HD22	1:A:177:LEU:HD21	2.00	0.44
4:E:176:ARG:HB3	4:E:178:LEU:HD21	2.00	0.44
4:E:403:LEU:CD1	4:E:420:LEU:HD22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:346:ILE:O	5:F:350:LEU:HD23	2.16	0.44
6:G:212:ALA:O	6:G:231:SER:OG	2.33	0.44
7:M:29:ILE:HD11	7:M:88:LYS:HG2	2.00	0.44
2:O:287:VAL:HG12	2:O:301:VAL:HG13	2.00	0.44
8:Q:711:SER:N	8:Q:881:LEU:HD23	2.31	0.44
1:S:57:LEU:HD22	1:S:98:LEU:HD21	1.99	0.44
1:S:575:ARG:O	1:S:579:TYR:N	2.43	0.44
1:S:1043:SER:OG	1:S:1044:GLN:N	2.50	0.44
10:U:315:SER:OG	10:U:377:HIS:ND1	2.50	0.44
11:V:86:HIS:ND1	11:V:92:ILE:HG21	2.32	0.44
11:V:277:ASP:N	11:V:277:ASP:OD1	2.47	0.44
2:B:57:PHE:HB3	2:B:354:LEU:HD21	1.99	0.44
5:F:163:MET:HE2	5:F:166:GLN:OE1	2.17	0.44
8:P:714:LEU:HD23	8:P:815:GLN:CD	2.42	0.44
1:S:37:PRO:O	1:S:40:ALA:HB3	2.17	0.44
1:S:124:ILE:HD13	1:S:145:LEU:HD21	1.99	0.44
10:U:350:LEU:HD11	10:U:1098:GLU:HB3	1.98	0.44
11:V:1066:LEU:HD13	11:V:1134:LEU:HB2	1.98	0.44
2:B:622:LEU:HD23	2:B:622:LEU:C	2.42	0.44
3:C:331:LYS:O	7:L:254:LEU:HD21	2.17	0.44
6:H:229:LEU:HD11	6:H:259:MET:SD	2.58	0.44
2:O:54:THR:OG1	2:O:56:VAL:HG22	2.17	0.44
1:S:683:ARG:O	1:S:686:ALA:HB3	2.17	0.44
10:U:462:LEU:CD1	10:U:466:ILE:HD11	2.47	0.44
10:U:635:TYR:HA	10:U:645:LEU:HD23	2.00	0.44
10:U:768:PHE:CE1	10:U:832:LEU:HD11	2.52	0.44
11:V:933:PHE:CE2	11:V:972:LEU:HD13	2.52	0.44
1:A:94:ILE:HG21	1:A:151:PHE:CE2	2.53	0.44
1:A:675:ALA:O	1:A:679:VAL:HG23	2.18	0.44
2:B:414:LEU:HD21	7:L:37:HIS:ND1	2.32	0.44
2:B:727:MET:SD	2:B:727:MET:C	3.00	0.44
4:E:50:LEU:HD22	4:E:55:TRP:NE1	2.32	0.44
6:G:220:LEU:HD13	6:G:255:CYS:SG	2.58	0.44
6:H:30:ALA:O	6:H:39:ARG:NH1	2.51	0.44
7:L:3:VAL:HG13	7:L:5:GLU:HG2	1.99	0.44
8:P:708:ILE:HG22	8:P:709:LYS:N	2.32	0.44
11:V:348:ASP:O	11:V:351:LYS:HB3	2.18	0.44
4:E:141:ARG:HG2	4:E:146:VAL:HG23	1.98	0.44
6:G:67:LEU:HD23	6:G:103:VAL:HG22	1.98	0.44
7:L:15:LEU:HD21	7:L:25:TYR:HB3	2.00	0.44
8:P:11:LEU:HD12	8:P:429:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:508:CYS:CB	8:Q:642:LEU:HD22	2.48	0.44
1:S:57:LEU:HB2	1:S:116:MET:HE1	1.99	0.44
10:U:463:LEU:HA	10:U:466:ILE:HD12	2.00	0.44
11:V:473:VAL:O	11:V:474:VAL:C	2.60	0.44
11:V:940:LEU:HG	11:V:1027:LEU:HD22	1.98	0.44
2:B:185:GLY:O	2:B:186:LEU:HD23	2.17	0.44
5:F:256:PRO:HD2	5:F:259:LEU:HD23	2.00	0.44
7:M:144:SER:OG	7:M:146:ARG:NH2	2.50	0.44
8:P:37:LEU:HD21	8:P:39:THR:CG2	2.48	0.44
10:U:295:VAL:HG22	10:U:302:ASN:CG	2.43	0.44
10:U:1081:ALA:HB3	10:U:1082:PRO:HD3	1.99	0.44
8:P:523:LEU:HD23	8:P:523:LEU:C	2.43	0.44
8:Q:711:SER:HB3	8:Q:714:LEU:HD12	1.99	0.44
1:S:340:VAL:N	1:S:484:GLU:OE1	2.43	0.44
1:S:1224:TRP:CD2	1:S:1318:LEU:HD13	2.52	0.44
10:U:265:ARG:CZ	10:U:370:ASN:OD1	2.65	0.44
11:V:136:ILE:HG22	11:V:140:LEU:HD12	1.99	0.44
1:A:137:LEU:HD13	1:A:141:GLN:CB	2.48	0.43
2:B:694:CYS:HB2	2:B:705:PHE:HE2	1.83	0.43
3:C:334:ARG:HD3	7:L:252:PHE:CE2	2.52	0.43
5:F:291:LYS:O	5:F:293:ILE:N	2.48	0.43
2:O:235:SER:O	2:O:261:ARG:NH1	2.51	0.43
8:Q:712:ALA:HB1	8:Q:728:LEU:HD11	1.99	0.43
8:Q:874:ARG:NE	8:Q:874:ARG:HA	2.33	0.43
1:S:183:TRP:CE3	1:S:234:MET:HE2	2.53	0.43
11:V:364:TRP:CE2	11:V:384:MET:HG2	2.53	0.43
11:V:469:CYS:O	11:V:470:GLN:C	2.61	0.43
2:B:728:PHE:CE1	8:P:676:VAL:HG22	2.53	0.43
3:C:191:ILE:HD11	3:C:223:VAL:HG22	1.99	0.43
3:C:402:GLY:N	3:C:405:GLU:OE1	2.51	0.43
7:M:203:VAL:HG12	7:M:207:ILE:HD12	1.99	0.43
2:O:745:LYS:CE	2:O:859:LEU:HD11	2.49	0.43
8:P:486:LEU:HD23	8:P:486:LEU:O	2.18	0.43
8:P:502:GLY:O	8:P:504:ARG:N	2.51	0.43
8:Q:74:ARG:HD2	8:Q:90:LEU:HD12	1.99	0.43
1:S:548:LEU:HA	1:S:551:VAL:HG12	2.00	0.43
10:U:1264:LEU:HD23	10:U:1279:MET:HE2	1.99	0.43
1:A:275:ILE:HG23	1:A:330:HIS:CE1	2.52	0.43
3:C:99:ASN:OD1	3:C:107:GLN:NE2	2.51	0.43
4:E:487:MET:O	4:E:490:ALA:HB3	2.18	0.43
6:G:249:TYR:CB	6:G:272:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:78:CYS:SG	2:O:79:CYS:N	2.91	0.43
2:O:651:LEU:HD12	2:O:704:LEU:HD11	2.00	0.43
8:P:315:PHE:CE2	8:P:347:VAL:HG11	2.53	0.43
1:S:384:VAL:HG11	1:S:386:TRP:CE3	2.54	0.43
1:S:651:GLY:O	1:S:654:THR:OG1	2.26	0.43
10:U:521:LEU:HD22	10:U:536:ALA:HA	1.99	0.43
10:U:619:LEU:O	10:U:623:VAL:HG23	2.19	0.43
11:V:186:VAL:HG23	11:V:186:VAL:O	2.18	0.43
11:V:278:LEU:HA	11:V:281:ILE:HD12	2.01	0.43
11:V:1139:MET:HE2	11:V:1188:ILE:HG23	2.00	0.43
2:B:724:GLN:O	2:B:724:GLN:HG2	2.17	0.43
5:F:188:PHE:CE2	5:F:192:LEU:HD11	2.53	0.43
5:F:289:LEU:CD1	6:G:480:LEU:HD13	2.48	0.43
7:M:200:PHE:CE1	7:M:204:MET:HE3	2.53	0.43
8:P:37:LEU:C	8:P:37:LEU:HD23	2.44	0.43
8:Q:77:TYR:HB3	8:Q:85:LEU:HD21	2.00	0.43
10:U:115:ALA:HB1	10:U:121:LEU:HD21	2.00	0.43
11:V:86:HIS:HD1	11:V:92:ILE:HG21	1.84	0.43
2:B:646:GLU:OE1	2:B:646:GLU:N	2.50	0.43
3:C:228:LEU:HD11	3:C:253:ALA:CB	2.48	0.43
4:E:52:SER:OG	7:L:217:GLU:OE2	2.33	0.43
3:C:142:PRO:HA	3:C:145:TYR:CE1	2.53	0.43
5:F:27:ASP:N	5:F:27:ASP:OD1	2.52	0.43
8:P:360:HIS:O	8:P:366:LEU:HD12	2.18	0.43
8:Q:483:LEU:HD23	8:Q:484:THR:N	2.32	0.43
1:S:54:HIS:ND1	1:S:54:HIS:O	2.52	0.43
10:U:33:LEU:O	10:U:36:GLN:NE2	2.52	0.43
10:U:202:PHE:HE1	10:U:210:ILE:HG23	1.83	0.43
10:U:805:LEU:HD12	10:U:845:VAL:HG11	1.99	0.43
10:U:814:LEU:HD23	10:U:817:LEU:HD12	2.00	0.43
11:V:188:ASP:OD2	11:V:191:ASP:CB	2.44	0.43
11:V:242:THR:O	11:V:246:LEU:N	2.44	0.43
2:B:292:SER:OG	2:B:361:ASP:OD2	2.35	0.43
6:G:97:GLN:OE1	6:G:121:LEU:HD22	2.18	0.43
6:G:122:TRP:HZ3	6:G:139:LEU:HD11	1.83	0.43
6:H:55:HIS:O	2:O:264:GLN:NE2	2.52	0.43
2:O:109:LEU:N	2:O:122:LEU:O	2.52	0.43
8:P:366:LEU:HD12	8:P:367:CYS:H	1.84	0.43
1:S:684:LEU:HD21	1:S:757:VAL:HG22	2.01	0.43
6:G:393:MET:HG2	8:P:236:LEU:HD21	2.01	0.43
6:H:301:GLU:O	6:H:305:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:287:VAL:HG12	2:O:301:VAL:HG22	2.00	0.43
8:P:785:VAL:HG12	8:P:786:GLU:N	2.34	0.43
10:U:420:LYS:O	10:U:424:ASN:ND2	2.51	0.43
10:U:651:ILE:HG21	10:U:658:ILE:HD11	2.00	0.43
10:U:1083:THR:OG1	10:U:1084:VAL:N	2.52	0.43
1:A:1060:THR:HG22	1:A:1062:GLY:H	1.83	0.43
2:B:507:SER:O	2:B:508:LEU:HD23	2.19	0.43
7:M:357:GLY:O	7:M:366:ILE:HG22	2.18	0.43
2:O:483:ILE:HG22	2:O:484:ASP:N	2.34	0.43
1:S:271:GLN:OE1	1:S:326:GLN:NE2	2.52	0.43
1:S:281:LEU:HD21	1:S:354:LEU:HD12	2.01	0.43
1:S:1085:LEU:HB3	1:S:1086:PRO:HD2	2.01	0.43
12:X:59:GLU:N	12:X:59:GLU:OE1	2.52	0.43
1:A:239:VAL:HG21	1:A:301:VAL:HG21	2.01	0.43
2:B:475:VAL:HG12	2:B:476:GLU:C	2.43	0.43
2:B:581:VAL:HG12	2:B:582:THR:N	2.33	0.43
2:O:523:CYS:SG	2:O:581:VAL:N	2.92	0.43
8:P:565:TYR:CE2	8:P:582:LEU:HD22	2.54	0.43
8:Q:154:LEU:CD1	8:Q:255:LEU:HD22	2.48	0.43
1:A:22:TRP:HH2	6:H:375:LEU:HD13	1.84	0.42
1:A:344:ARG:O	1:A:350:ARG:NH1	2.52	0.42
2:B:423:TYR:CE2	8:P:606:LEU:HB3	2.54	0.42
2:B:731:LEU:N	2:B:731:LEU:HD23	2.34	0.42
2:B:838:ILE:O	2:B:842:VAL:HG23	2.19	0.42
6:G:29:VAL:O	6:G:33:SER:OG	2.36	0.42
2:O:424:LYS:O	2:O:428:ASN:ND2	2.51	0.42
8:Q:75:LEU:HD22	8:Q:87:CYS:SG	2.58	0.42
8:Q:820:SER:OG	8:Q:821:SER:N	2.52	0.42
1:A:1117:ARG:NH1	1:A:1323:ALA:O	2.51	0.42
4:E:476:LEU:O	4:E:489:TYR:OH	2.22	0.42
2:O:582:THR:HG22	2:O:583:SER:N	2.35	0.42
8:P:60:PHE:CE1	8:P:118:VAL:HG21	2.54	0.42
8:Q:565:TYR:N	8:Q:565:TYR:CD1	2.87	0.42
1:S:837:CYS:O	1:S:841:ILE:HD12	2.19	0.42
1:S:872:MET:HG3	1:S:911:TRP:CE3	2.54	0.42
1:S:1211:LEU:HD12	1:S:1233:ALA:HB1	2.01	0.42
2:B:507:SER:C	2:B:508:LEU:HD23	2.43	0.42
4:E:278:LEU:HD21	4:E:323:GLN:HA	2.00	0.42
4:E:446:TRP:CG	4:E:450:THR:HG21	2.53	0.42
5:F:189:LEU:HD13	5:F:240:TRP:CG	2.53	0.42
2:O:711:THR:OG1	2:O:714:GLU:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:1139:GLY:O	10:U:1143:THR:HG23	2.19	0.42
11:V:88:SER:O	11:V:92:ILE:HG23	2.19	0.42
11:V:637:ASN:O	11:V:641:HIS:ND1	2.52	0.42
11:V:1062:TYR:CE2	11:V:1066:LEU:HD11	2.54	0.42
11:V:1115:VAL:HG11	11:V:1142:LEU:CG	2.49	0.42
1:A:209:TRP:O	1:A:213:ASN:ND2	2.52	0.42
1:A:265:VAL:O	1:A:269:VAL:HG23	2.20	0.42
1:A:925:VAL:HG12	1:A:925:VAL:O	2.18	0.42
2:B:736:ARG:NH1	2:B:736:ARG:HB2	2.34	0.42
8:Q:875:HIS:HB3	8:Q:876:PRO:HD3	2.01	0.42
10:U:115:ALA:O	10:U:119:GLY:N	2.52	0.42
12:X:54:GLU:HB2	12:X:71:LEU:HD21	2.01	0.42
1:A:162:SER:OG	1:A:165:SER:OG	1.99	0.42
2:B:356:SER:O	2:B:356:SER:OG	2.37	0.42
4:E:122:GLN:O	4:E:134:ARG:NH2	2.49	0.42
6:G:245:LEU:HD11	6:G:249:TYR:CZ	2.55	0.42
7:L:62:ILE:HD11	7:L:102:TYR:OH	2.19	0.42
8:P:399:LEU:N	8:P:399:LEU:HD23	2.35	0.42
8:P:595:PRO:HG3	8:P:802:HIS:CE1	2.54	0.42
8:Q:537:LEU:HD12	8:Q:541:TRP:CD1	2.54	0.42
1:S:477:LEU:O	1:S:481:VAL:HG23	2.20	0.42
1:S:1046:HIS:CD2	1:S:1089:VAL:HG13	2.54	0.42
10:U:280:LYS:CG	10:U:319:ILE:HD11	2.50	0.42
1:A:340:VAL:N	1:A:484:GLU:OE1	2.53	0.42
6:G:79:ILE:HG13	6:G:145:LEU:HD21	2.01	0.42
6:G:354:CYS:O	6:G:357:THR:OG1	2.38	0.42
6:H:250:THR:HG21	6:H:282:PRO:HD3	2.00	0.42
6:H:377:SER:O	6:H:382:PHE:HD1	2.03	0.42
7:M:147:GLU:N	7:M:147:GLU:OE1	2.53	0.42
7:M:277:GLU:OE2	7:M:277:GLU:N	2.53	0.42
8:P:170:ILE:HG23	8:P:259:VAL:HG13	2.01	0.42
8:P:284:PHE:CG	8:P:350:ALA:HB3	2.55	0.42
8:P:870:TYR:HA	8:P:873:LEU:HD12	2.01	0.42
8:Q:54:LEU:HD12	8:Q:55:THR:C	2.45	0.42
1:S:57:LEU:HB3	1:S:116:MET:HE1	2.01	0.42
1:S:342:MET:HE2	1:S:342:MET:N	2.34	0.42
1:S:494:LEU:CD1	1:S:518:LEU:HD11	2.39	0.42
10:U:658:ILE:HG23	10:U:737:ILE:HG21	2.00	0.42
11:V:365:ILE:O	11:V:366:LYS:C	2.63	0.42
1:A:218:CYS:HB3	1:A:294:ILE:HA	2.02	0.42
1:A:760:ALA:O	1:A:763:THR:OG1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:488:VAL:HG22	2:B:581:VAL:HG22	2.00	0.42
2:O:144:TRP:HH2	2:O:160:VAL:HG13	1.84	0.42
8:P:258:LEU:HD23	8:P:258:LEU:O	2.20	0.42
8:P:373:ARG:NH1	8:P:385:GLU:OE2	2.53	0.42
8:P:603:PHE:HD1	8:P:639:CYS:SG	2.43	0.42
1:S:947:SER:OG	1:S:948:ASP:N	2.53	0.42
10:U:312:LEU:O	10:U:316:VAL:HG23	2.19	0.42
10:U:437:ARG:HA	10:U:440:ILE:HD12	2.02	0.42
11:V:1234:PHE:O	11:V:1238:MET:HB2	2.19	0.42
1:A:244:LEU:HD23	1:A:245:ARG:N	2.35	0.42
7:M:104:LEU:HD13	2:O:404:SER:HB3	2.00	0.42
8:P:540:GLY:O	8:P:605:SER:OG	2.34	0.42
8:Q:517:LEU:O	8:Q:518:GLN:HG2	2.20	0.42
8:Q:526:THR:HB	8:Q:579:GLU:OE2	2.20	0.42
3:C:84:ASP:O	3:C:87:GLN:NE2	2.52	0.42
3:C:305:THR:O	3:C:307:GLY:N	2.51	0.42
4:E:357:LEU:HD11	4:E:396:TYR:CD2	2.53	0.42
7:L:17:PRO:HB3	7:L:25:TYR:CE1	2.54	0.42
7:M:15:LEU:O	7:M:16:LEU:HD23	2.20	0.42
7:M:300:LYS:NZ	7:M:301:SER:O	2.53	0.42
2:O:69:GLU:O	2:O:71:ASN:N	2.53	0.42
1:S:661:ARG:C	9:W:79:THR:HG22	2.44	0.42
10:U:903:SER:OG	10:U:905:SER:OG	2.28	0.42
11:V:223:GLN:O	11:V:227:VAL:HG23	2.20	0.42
5:F:259:LEU:O	5:F:263:VAL:HG23	2.20	0.42
6:G:558:LEU:O	6:G:562:ASP:C	2.63	0.42
7:M:256:ALA:HB2	7:M:323:VAL:CG2	2.41	0.42
11:V:452:SER:O	11:V:456:LEU:HD23	2.20	0.42
11:V:487:ALA:O	11:V:488:GLU:C	2.63	0.42
2:B:294:GLY:O	2:B:409:ARG:NH1	2.46	0.41
4:E:446:TRP:CD1	4:E:475:LYS:HZ3	2.38	0.41
2:O:289:LEU:HD23	2:O:290:MET:C	2.45	0.41
2:O:668:ALA:O	2:O:670:ASN:ND2	2.53	0.41
2:O:693:PHE:HA	2:O:704:LEU:HD23	2.02	0.41
2:O:699:SER:O	2:O:722:ARG:NH1	2.51	0.41
8:Q:678:THR:O	8:Q:682:THR:OG1	2.23	0.41
1:S:1101:ILE:HG21	1:S:1154:PHE:CZ	2.55	0.41
11:V:434:SER:OG	11:V:435:ILE:N	2.50	0.41
11:V:524:ILE:HG22	11:V:529:ILE:HG13	2.02	0.41
2:B:850:ASP:OD1	8:P:874:ARG:HD2	2.21	0.41
3:C:61:ILE:HD12	3:C:64:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:PHE:N	3:C:65:PRO:HD2	2.35	0.41
6:G:273:LEU:HD23	6:G:279:TRP:HB2	2.01	0.41
6:H:342:THR:HG22	6:H:343:GLN:N	2.35	0.41
7:M:115:ILE:HG21	8:Q:455:ILE:HD11	2.02	0.41
7:M:309:ILE:HD11	7:M:333:PHE:CD1	2.56	0.41
2:O:755:LEU:HD21	2:O:855:LYS:HB3	2.00	0.41
8:P:510:THR:HA	8:P:526:THR:O	2.19	0.41
8:Q:525:ALA:CB	8:Q:584:LEU:HD11	2.48	0.41
1:S:429:THR:O	1:S:433:VAL:HG23	2.20	0.41
10:U:588:MET:HA	10:U:591:LEU:HD12	2.02	0.41
10:U:658:ILE:HD13	10:U:734:SER:O	2.20	0.41
11:V:1085:ASN:OD1	11:V:1086:LEU:N	2.53	0.41
2:B:259:LEU:HD23	2:B:259:LEU:N	2.35	0.41
4:E:409:ALA:O	4:E:412:THR:OG1	2.37	0.41
5:F:176:GLU:OE2	5:F:177:VAL:HG23	2.20	0.41
6:G:184:TRP:O	6:G:204:LYS:NZ	2.51	0.41
7:L:270:ASN:ND2	7:L:289:GLU:OE2	2.47	0.41
7:L:326:ASN:ND2	7:L:364:LYS:HG3	2.34	0.41
8:P:37:LEU:HD21	8:P:39:THR:HG22	2.03	0.41
8:P:531:ASN:ND2	8:P:573:GLY:O	2.52	0.41
8:P:842:ARG:O	8:P:846:THR:HG23	2.20	0.41
8:Q:154:LEU:HD13	8:Q:255:LEU:HD22	2.01	0.41
8:Q:459:LEU:HD23	8:Q:462:ILE:HD12	2.02	0.41
8:Q:752:SER:OG	8:Q:768:VAL:HG23	2.20	0.41
1:S:650:LEU:O	1:S:654:THR:HG23	2.20	0.41
1:S:737:ALA:HB1	1:S:738:PRO:HD2	2.00	0.41
10:U:487:TYR:HB3	10:U:491:LEU:HD21	2.02	0.41
10:U:496:VAL:HG12	10:U:500:LEU:HD12	2.02	0.41
11:V:763:THR:OG1	11:V:764:ASP:N	2.53	0.41
2:B:587:LEU:O	2:B:589:THR:N	2.52	0.41
5:F:68:GLN:O	5:F:74:ARG:NH2	2.54	0.41
8:Q:677:ALA:HA	8:Q:680:LEU:HD12	2.03	0.41
1:S:614:PRO:CG	1:S:617:LEU:HD12	2.50	0.41
1:S:769:LEU:HD22	1:S:832:PHE:HZ	1.84	0.41
11:V:794:ARG:NE	11:V:926:ARG:O	2.41	0.41
1:A:1080:ARG:CG	1:S:952:GLN:OE1	2.69	0.41
2:B:239:TYR:HB3	2:B:259:LEU:HD21	2.02	0.41
4:E:446:TRP:CD1	4:E:450:THR:HG21	2.55	0.41
5:F:274:TYR:CE2	5:F:278:LEU:HD11	2.55	0.41
8:Q:286:GLY:O	8:Q:312:LEU:HD12	2.21	0.41
8:Q:649:MET:HE1	8:Q:759:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:167:CYS:HA	1:S:170:LEU:HD12	2.02	0.41
11:V:1162:PHE:O	11:V:1167:TRP:NE1	2.52	0.41
4:E:407:LEU:O	4:E:447:LYS:NZ	2.35	0.41
6:G:562:ASP:OD1	6:G:562:ASP:N	2.52	0.41
6:H:232:LEU:HB3	6:H:252:LEU:HD21	2.02	0.41
8:P:227:LEU:HB2	8:P:334:LEU:HD21	2.02	0.41
1:S:673:ILE:O	1:S:677:VAL:HG23	2.21	0.41
1:S:1359:ASP:HA	1:S:1362:LEU:HD12	2.03	0.41
10:U:647:LEU:HD13	10:U:721:PHE:CE1	2.55	0.41
11:V:282:ILE:HG22	11:V:286:LEU:HD12	2.03	0.41
11:V:636:ALA:HB1	11:V:739:LEU:CD1	2.51	0.41
1:A:916:PHE:CE2	1:A:920:LEU:HD11	2.56	0.41
2:B:15:LEU:CD2	2:B:24:VAL:HG22	2.51	0.41
3:C:128:ASP:OD1	3:C:129:LYS:N	2.53	0.41
3:C:212:GLN:O	4:E:92:ARG:NH1	2.53	0.41
3:C:228:LEU:HD11	3:C:253:ALA:HB2	2.02	0.41
4:E:467:GLU:O	4:E:470:SER:OG	2.33	0.41
6:G:250:THR:HG23	6:G:282:PRO:HA	2.03	0.41
6:G:548:ARG:HH21	6:G:609:LEU:HD13	1.85	0.41
2:O:277:CYS:HB2	2:O:316:PHE:HB3	2.03	0.41
2:O:769:THR:HG22	2:O:842:VAL:HG22	2.03	0.41
10:U:31:ASN:O	10:U:34:GLN:NE2	2.53	0.41
10:U:668:LEU:HB3	10:U:752:VAL:HG11	2.03	0.41
11:V:51:LEU:HD23	11:V:54:ILE:HD11	2.03	0.41
11:V:311:VAL:O	11:V:338:SER:HB3	2.21	0.41
11:V:492:ALA:O	11:V:495:VAL:HB	2.20	0.41
1:A:1171:LEU:HD13	1:A:1229:ALA:HB2	2.03	0.41
5:F:58:LEU:O	5:F:62:LEU:HD23	2.21	0.41
6:G:140:HIS:NE2	6:G:166:LEU:HD11	2.36	0.41
6:G:150:TRP:O	6:G:155:ARG:N	2.52	0.41
7:L:55:CYS:HB3	7:L:59:LEU:HD23	2.03	0.41
8:P:366:LEU:HD12	8:P:367:CYS:N	2.36	0.41
8:Q:28:VAL:HB	8:Q:402:CYS:SG	2.61	0.41
1:S:455:SER:O	1:S:460:ARG:N	2.48	0.41
10:U:496:VAL:HG12	10:U:500:LEU:CD1	2.51	0.41
11:V:242:THR:O	11:V:245:ILE:HB	2.20	0.41
2:B:593:PHE:CD2	2:B:593:PHE:C	2.93	0.41
2:B:740:ILE:N	2:B:740:ILE:HD12	2.36	0.41
3:C:243:TRP:HZ3	3:C:249:SER:HB3	1.86	0.41
3:C:405:GLU:OE2	3:C:528:GLN:NE2	2.54	0.41
3:C:462:LEU:O	3:C:504:ILE:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:349:LEU:HD23	4:E:393:LYS:HD3	2.03	0.41
5:F:286:HIS:O	5:F:295:VAL:HG22	2.21	0.41
6:G:12:CYS:SG	6:G:13:LEU:N	2.90	0.41
6:G:24:VAL:HG13	6:G:197:LEU:HG	2.02	0.41
6:H:220:LEU:HD23	6:H:220:LEU:C	2.46	0.41
7:M:228:ILE:HG21	7:M:292:PHE:CE2	2.56	0.41
2:O:84:ASP:O	2:O:88:GLY:N	2.50	0.41
2:O:767:LEU:HD13	8:Q:841:LEU:HA	2.01	0.41
1:S:959:ILE:HG22	1:S:960:HIS:CE1	2.56	0.41
10:U:82:GLN:O	10:U:86:VAL:HG23	2.21	0.41
11:V:301:LEU:HD11	11:V:305:LEU:CD1	2.51	0.41
11:V:1190:LEU:O	11:V:1196:ILE:HG23	2.21	0.41
1:A:415:MET:HE3	1:A:419:PHE:CZ	2.56	0.41
2:B:164:SER:OG	2:B:165:GLY:N	2.53	0.41
2:B:520:LEU:CD1	8:P:567:ILE:HB	2.50	0.41
3:C:38:VAL:HG13	3:C:39:ALA:N	2.35	0.41
3:C:372:SER:CB	3:C:425:LEU:HD13	2.51	0.41
6:G:104:LEU:CD1	6:G:125:VAL:HG22	2.47	0.41
6:H:163:LEU:O	6:H:167:ASN:ND2	2.54	0.41
8:P:390:LEU:N	8:P:390:LEU:HD23	2.36	0.41
1:S:521:LEU:O	1:S:524:SER:N	2.53	0.41
1:A:163:ARG:NH2	1:A:190:ILE:O	2.54	0.40
1:A:777:SER:O	1:A:781:VAL:HG23	2.21	0.40
1:A:1084:ARG:NH2	1:S:952:GLN:NE2	2.69	0.40
1:A:1094:SER:O	1:A:1094:SER:OG	2.36	0.40
2:B:330:ILE:HD12	2:B:330:ILE:N	2.37	0.40
2:B:392:PRO:O	2:B:396:THR:OG1	2.34	0.40
3:C:134:PHE:CE2	3:C:138:LEU:HD12	2.56	0.40
5:F:167:ALA:HB1	5:F:208:ALA:HA	2.02	0.40
6:G:551:TYR:CG	6:G:574:LEU:HD21	2.56	0.40
6:H:483:LEU:HD11	6:H:509:LEU:CD1	2.50	0.40
8:Q:508:CYS:HB2	8:Q:642:LEU:HD22	2.03	0.40
11:V:432:CYS:SG	11:V:465:PHE:CD2	3.14	0.40
11:V:432:CYS:SG	11:V:465:PHE:HD2	2.43	0.40
1:A:313:THR:HG22	1:A:313:THR:O	2.21	0.40
2:B:266:ILE:HG21	2:B:268:PHE:CZ	2.57	0.40
2:B:289:LEU:HD23	2:B:290:MET:N	2.36	0.40
3:C:32:GLN:NE2	3:C:216:GLN:OE1	2.54	0.40
6:G:476:PHE:HB3	6:G:520:ARG:HD3	2.03	0.40
6:H:62:ALA:O	6:H:67:LEU:HD11	2.20	0.40
7:L:279:SER:OG	7:L:282:GLN:N	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:15:LEU:HD13	7:M:84:MET:HE2	2.01	0.40
8:Q:485:SER:OG	8:Q:609:VAL:HG11	2.20	0.40
1:S:163:ARG:HG3	1:S:191:VAL:HG22	2.03	0.40
2:B:40:THR:HG21	2:B:70:GLU:HA	2.03	0.40
2:B:240:VAL:HG13	2:B:256:LEU:HD21	2.04	0.40
7:M:326:ASN:ND2	7:M:364:LYS:HG3	2.36	0.40
7:M:354:ILE:HG12	7:M:369:LYS:HG2	2.03	0.40
8:P:545:ILE:HG22	8:P:546:GLN:N	2.35	0.40
8:Q:359:TYR:HD1	8:Q:368:VAL:HG23	1.86	0.40
8:Q:565:TYR:HE2	8:Q:582:LEU:HB2	1.86	0.40
1:S:348:PHE:CZ	1:S:356:THR:HG23	2.57	0.40
10:U:1201:SER:OG	10:U:1260:TYR:OH	2.37	0.40
11:V:199:LEU:O	11:V:202:ILE:HG12	2.20	0.40
1:A:195:GLU:O	1:A:199:SER:OG	2.36	0.40
1:A:1262:PHE:CG	1:A:1319:LEU:HD23	2.57	0.40
2:B:757:ASP:O	2:B:760:ALA:HB3	2.22	0.40
2:B:766:GLU:OE1	2:B:846:GLN:HG2	2.22	0.40
5:F:20:THR:O	5:F:100:ASN:ND2	2.52	0.40
7:M:360:PRO:O	12:X:99:ARG:HD2	2.21	0.40
2:O:29:LYS:NZ	2:O:39:LYS:O	2.53	0.40
2:O:266:ILE:HG22	2:O:267:SER:N	2.36	0.40
8:Q:178:TYR:CD2	8:Q:245:LEU:HD22	2.55	0.40
11:V:273:ILE:HG22	11:V:274:ARG:O	2.22	0.40
4:E:21:GLN:OE1	4:E:21:GLN:N	2.54	0.40
4:E:110:PRO:C	4:E:114:LEU:HD12	2.46	0.40
8:Q:141:VAL:HG22	8:Q:154:LEU:HD12	2.03	0.40
10:U:1007:LEU:HA	10:U:1035:LEU:HD13	2.03	0.40
11:V:157:LEU:HD23	11:V:157:LEU:C	2.47	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%)	1066 (92%)	94 (8%)	0	100	100
1	S	1224/1477 (83%)	1130 (92%)	91 (7%)	3 (0%)	43	77
2	B	685/884 (78%)	581 (85%)	99 (14%)	5 (1%)	18	55
2	O	685/884 (78%)	588 (86%)	89 (13%)	8 (1%)	10	42
3	C	546/583 (94%)	490 (90%)	56 (10%)	0	100	100
4	E	411/555 (74%)	390 (95%)	21 (5%)	0	100	100
5	F	336/399 (84%)	304 (90%)	32 (10%)	0	100	100
6	G	567/641 (88%)	518 (91%)	49 (9%)	0	100	100
6	H	532/641 (83%)	495 (93%)	35 (7%)	2 (0%)	30	66
7	L	368/394 (93%)	332 (90%)	35 (10%)	1 (0%)	36	71
7	M	368/394 (93%)	329 (89%)	38 (10%)	1 (0%)	36	71
8	P	726/906 (80%)	623 (86%)	99 (14%)	4 (1%)	21	58
8	Q	732/906 (81%)	627 (86%)	102 (14%)	3 (0%)	30	66
9	W	21/39 (54%)	15 (71%)	4 (19%)	2 (10%)	0	8
10	U	1150/1328 (87%)	1064 (92%)	85 (7%)	1 (0%)	48	83
11	V	1131/1451 (78%)	1038 (92%)	89 (8%)	4 (0%)	30	66
12	X	151/197 (77%)	138 (91%)	10 (7%)	3 (2%)	6	31
All	All	10793/13156 (82%)	9728 (90%)	1028 (10%)	37 (0%)	37	71

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	132	ASP
2	O	132	ASP
2	O	147	VAL
2	O	218	GLU
8	P	781	PRO
8	Q	781	PRO
6	H	387	SER
7	M	216	PRO
8	P	518	GLN
12	X	94	PRO
2	O	637	PRO
1	S	975	GLY
10	U	978	ASN
12	X	93	PRO
2	B	637	PRO

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Mol	Chain	Res	Type
6	H	61	PRO
2	O	325	LEU
8	P	148	ALA
1	S	29	ARG
11	V	448	GLN
2	B	347	ASP
7	L	216	PRO
2	O	148	LYS
8	Q	63	GLN
11	V	392	ASN
2	O	70	GLU
2	O	217	LEU
9	W	80	VAL
2	B	140	PRO
12	X	62	PRO
2	B	712	PRO
8	P	166	PRO
1	S	30	VAL
9	W	81	GLY
11	V	278	LEU
8	Q	758	ALA
11	V	1288	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1034/1282 (81%)	1032 (100%)	2 (0%)	87	85
1	S	1092/1282 (85%)	1089 (100%)	3 (0%)	86	84
2	B	644/810 (80%)	642 (100%)	2 (0%)	86	84
2	O	641/810 (79%)	639 (100%)	2 (0%)	86	84
3	C	480/507 (95%)	479 (100%)	1 (0%)	87	85
4	E	358/467 (77%)	358 (100%)	0	100	100
5	F	288/336 (86%)	288 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	483/538 (90%)	483 (100%)	0	100	100
6	H	454/538 (84%)	454 (100%)	0	100	100
7	L	334/354 (94%)	334 (100%)	0	100	100
7	M	334/354 (94%)	334 (100%)	0	100	100
8	P	627/749 (84%)	626 (100%)	1 (0%)	87	85
8	Q	630/749 (84%)	626 (99%)	4 (1%)	78	80
9	W	22/22 (100%)	22 (100%)	0	100	100
10	U	1066/1204 (88%)	1066 (100%)	0	100	100
11	V	1065/1324 (80%)	1064 (100%)	1 (0%)	88	88
12	X	125/175 (71%)	125 (100%)	0	100	100
All	All	9677/11501 (84%)	9661 (100%)	16 (0%)	85	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1274	THR
1	A	1308	LEU
2	B	507	SER
2	B	577	ILE
3	C	201	GLU
2	O	401	CYS
2	O	600	GLN
8	P	224	LEU
8	Q	565	TYR
8	Q	566	THR
8	Q	567	ILE
8	Q	610	VAL
1	S	1068	SER
1	S	1183	CYS
1	S	1274	THR
11	V	390	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	101	GLN

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Mol	Chain	Res	Type
1	A	168	GLN
1	A	248	GLN
1	A	780	HIS
1	A	1113	ASN
1	A	1160	GLN
1	A	1231	HIS
1	A	1326	GLN
1	A	1355	HIS
1	A	1440	GLN
2	B	178	ASN
2	B	350	ASN
2	B	366	ASN
2	B	410	GLN
2	B	525	ASN
3	C	32	GLN
3	C	58	ASN
3	C	104	ASN
3	C	107	GLN
3	C	165	HIS
3	C	216	GLN
3	C	366	GLN
3	C	382	GLN
3	C	528	GLN
4	E	34	GLN
4	E	163	GLN
4	E	335	GLN
5	F	64	ASN
6	G	32	ASN
6	G	41	GLN
6	G	291	GLN
6	G	411	GLN
6	G	498	ASN
6	G	577	GLN
6	H	55	HIS
6	H	167	ASN
6	H	224	ASN
6	H	247	GLN
6	H	261	ASN
6	H	311	ASN
6	H	343	GLN
6	H	411	GLN
7	L	244	HIS

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Mol	Chain	Res	Type
7	L	328	GLN
7	L	331	GLN
7	M	232	ASN
7	M	270	ASN
7	M	282	GLN
7	M	331	GLN
7	M	350	GLN
2	O	44	HIS
2	O	251	GLN
2	O	514	HIS
2	O	661	GLN
2	O	670	ASN
8	P	237	GLN
8	P	491	ASN
8	P	546	GLN
8	P	872	GLN
8	Q	49	GLN
8	Q	237	GLN
8	Q	308	HIS
8	Q	464	ASN
8	Q	491	ASN
8	Q	571	GLN
8	Q	783	GLN
8	Q	802	HIS
1	S	99	GLN
1	S	305	HIS
1	S	326	GLN
1	S	652	GLN
1	S	767	GLN
1	S	992	HIS
1	S	993	GLN
1	S	1003	ASN
1	S	1032	GLN
1	S	1046	HIS
1	S	1110	HIS
1	S	1355	HIS
10	U	172	GLN
10	U	438	GLN
10	U	465	ASN
10	U	475	GLN
10	U	618	GLN
10	U	680	ASN

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Mol	Chain	Res	Type
10	U	844	ASN
10	U	1017	ASN
10	U	1127	ASN
10	U	1185	GLN
11	V	72	GLN
11	V	81	GLN
11	V	370	ASN
11	V	609	GLN
11	V	658	ASN
11	V	1269	ASN
12	X	12	HIS
12	X	26	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	2
7	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	9:UNK	C	73:GLU	N	36.32
1	W	95:TRP	C	101:UNK	N	6.15
1	L	330:GLY	C	331:GLN	N	1.19

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23087. These allow visual inspection of the internal detail of the map and identification of artifacts.

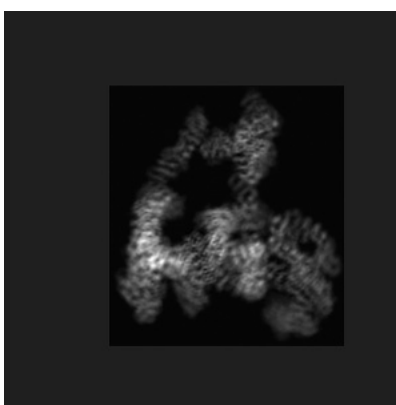
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

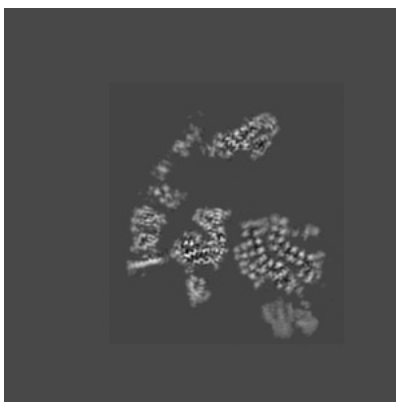
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

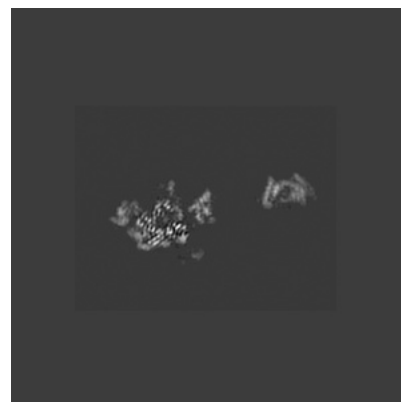
6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

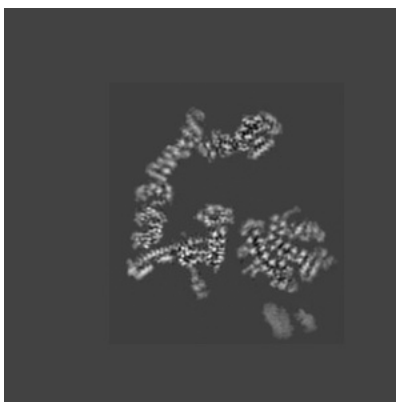
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

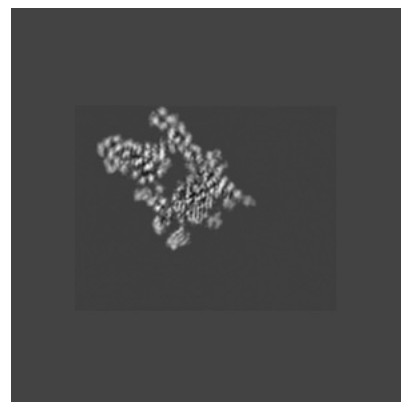
6.3.1 Primary map



X Index: 168



Y Index: 229



Z Index: 163

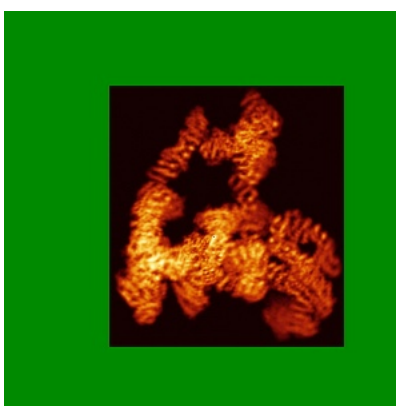
The images above show the largest variance slices of the map in three orthogonal directions.

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

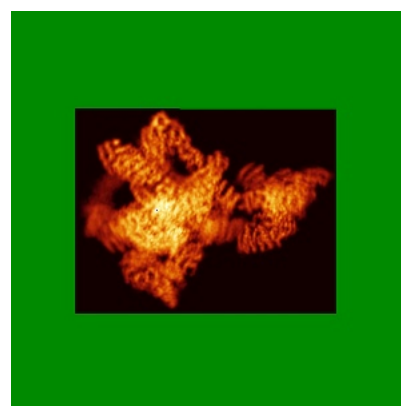
6.4.1 Primary map



X



Y

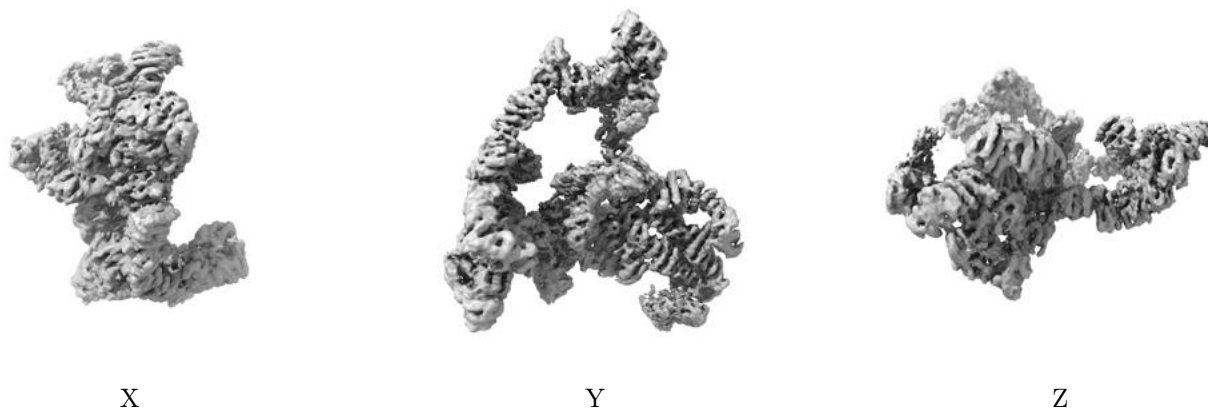


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

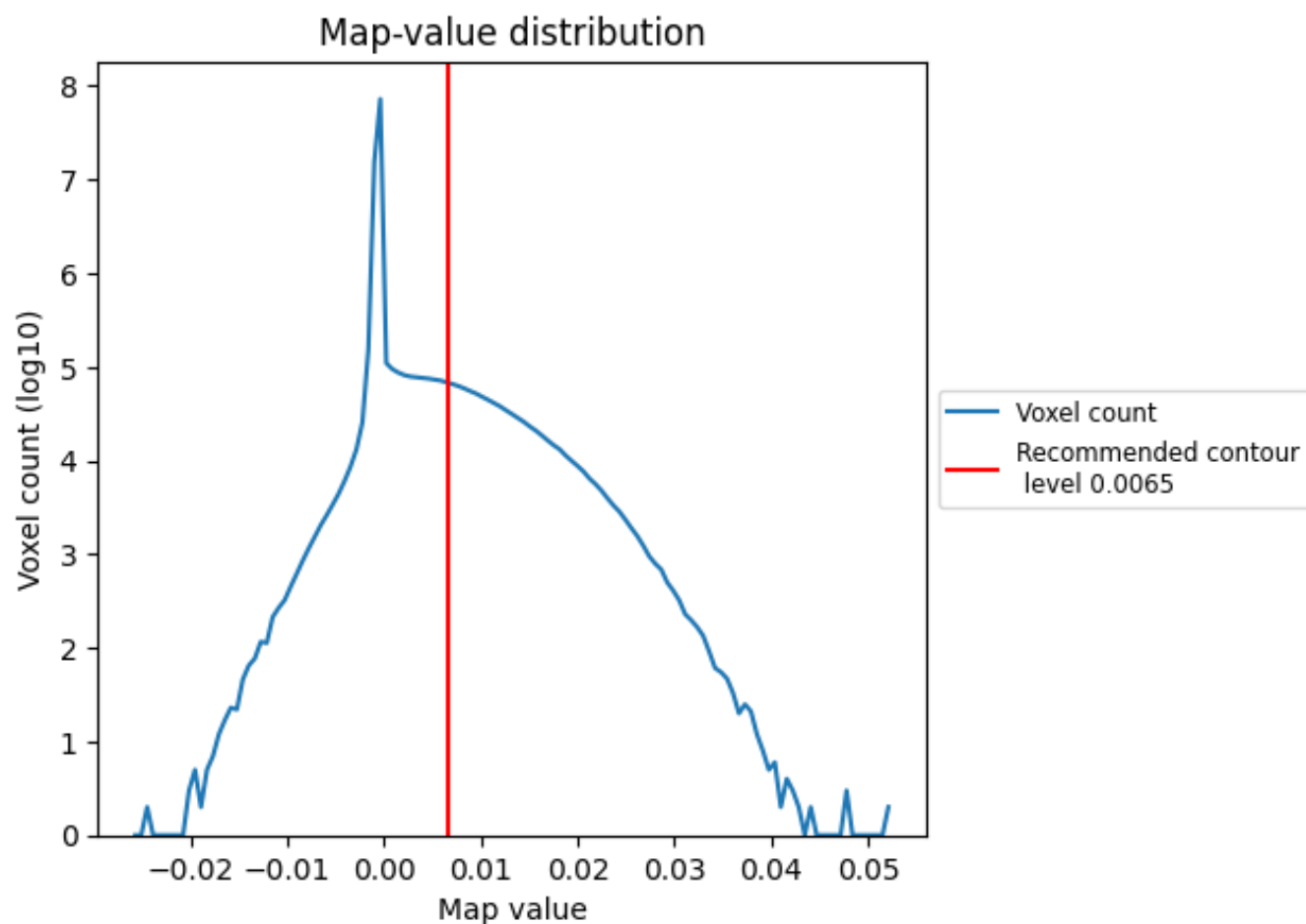
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

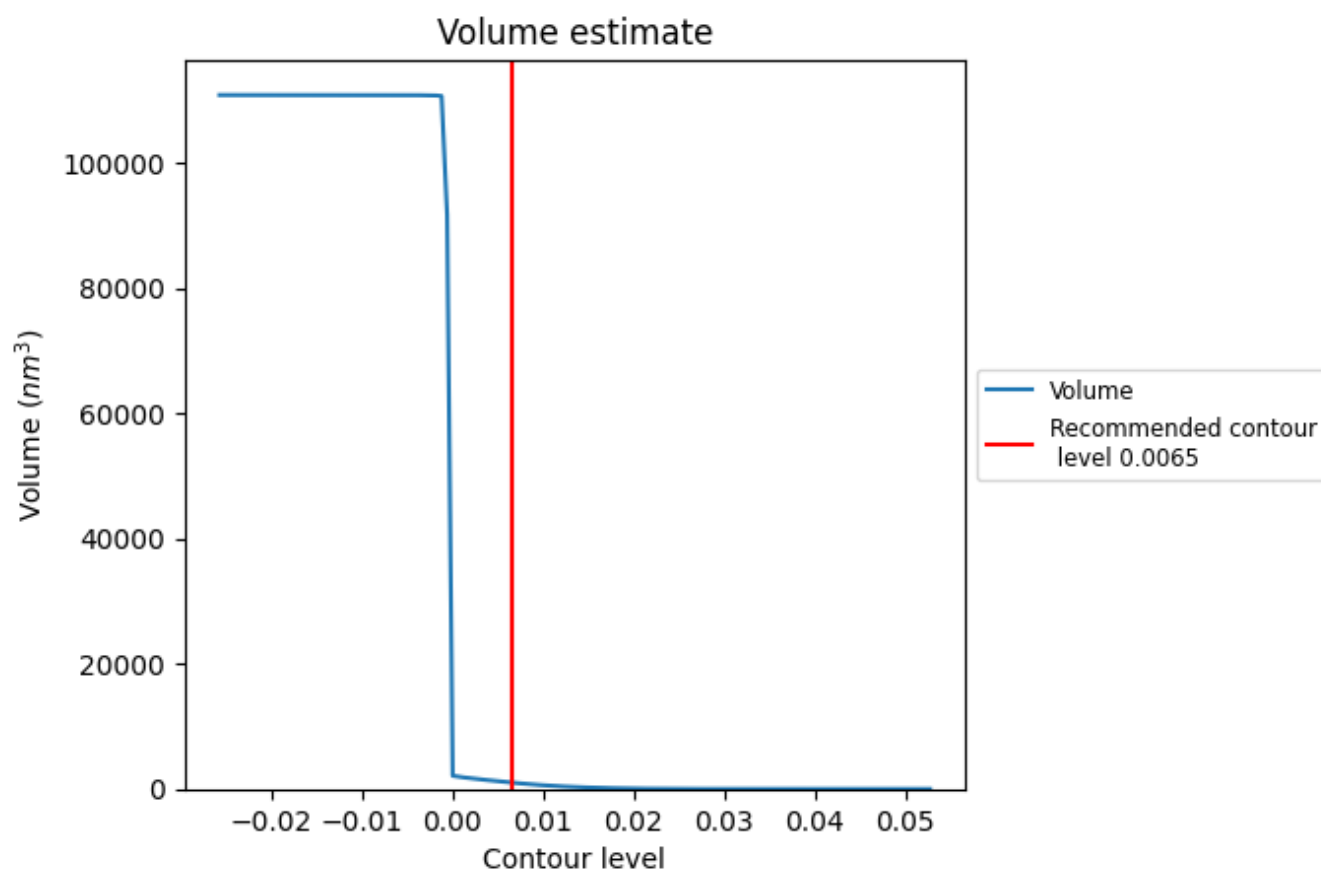
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

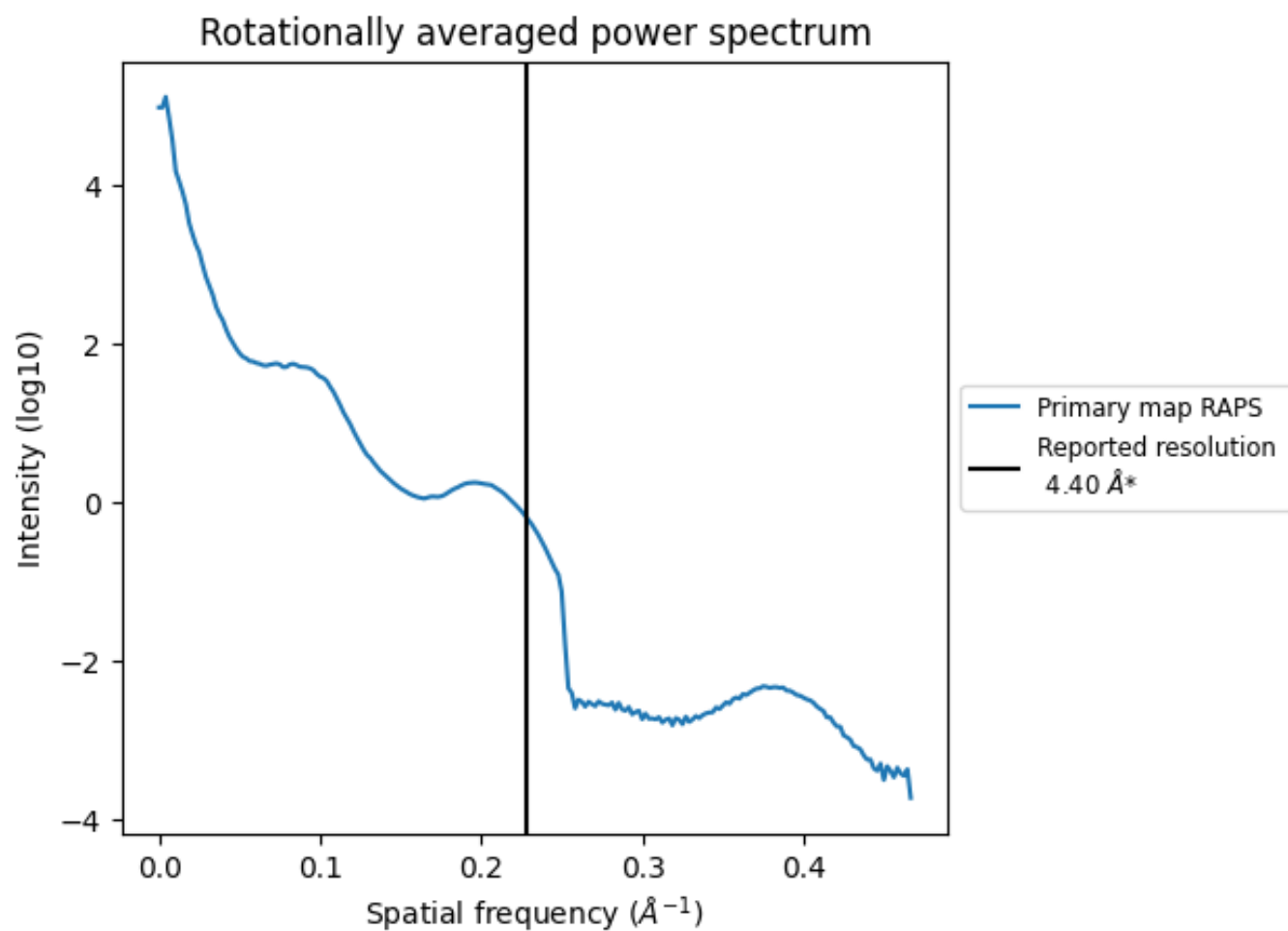
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1020 nm^3 ; this corresponds to an approximate mass of 921 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

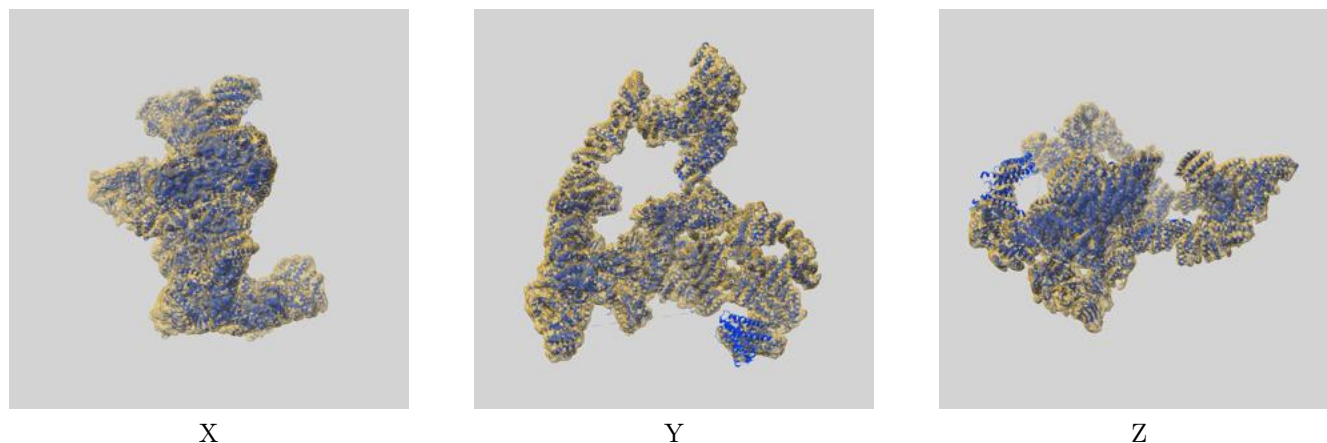
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

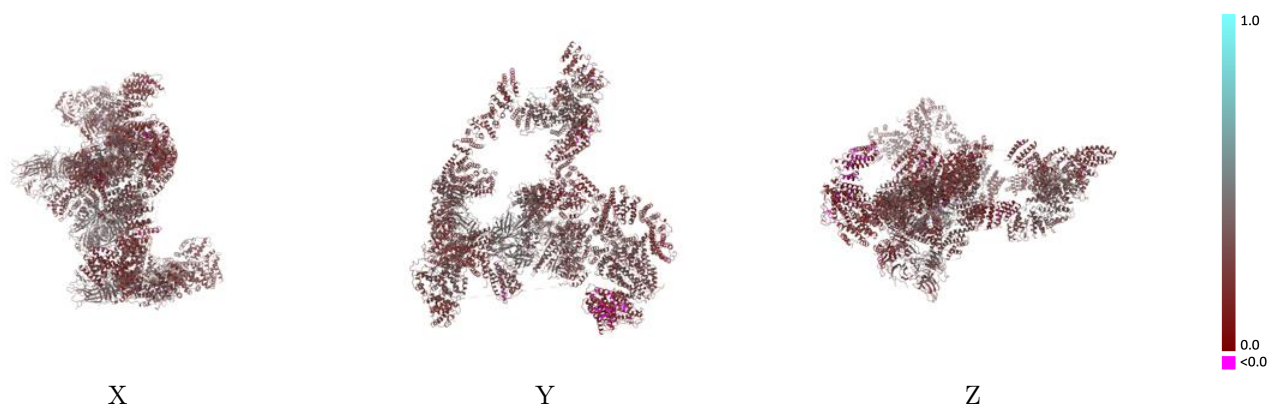
This section contains information regarding the fit between EMDB map EMD-23087 and PDB model 7KZR. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



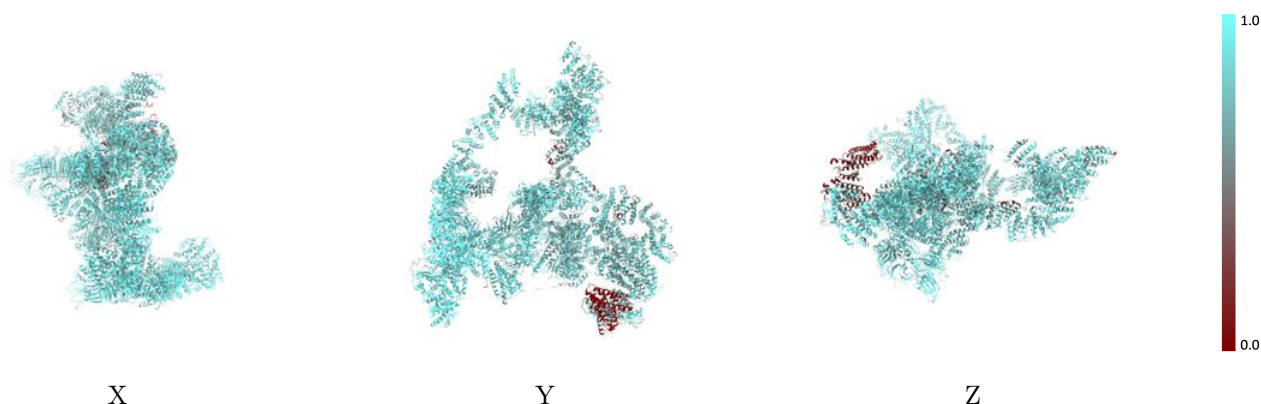
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



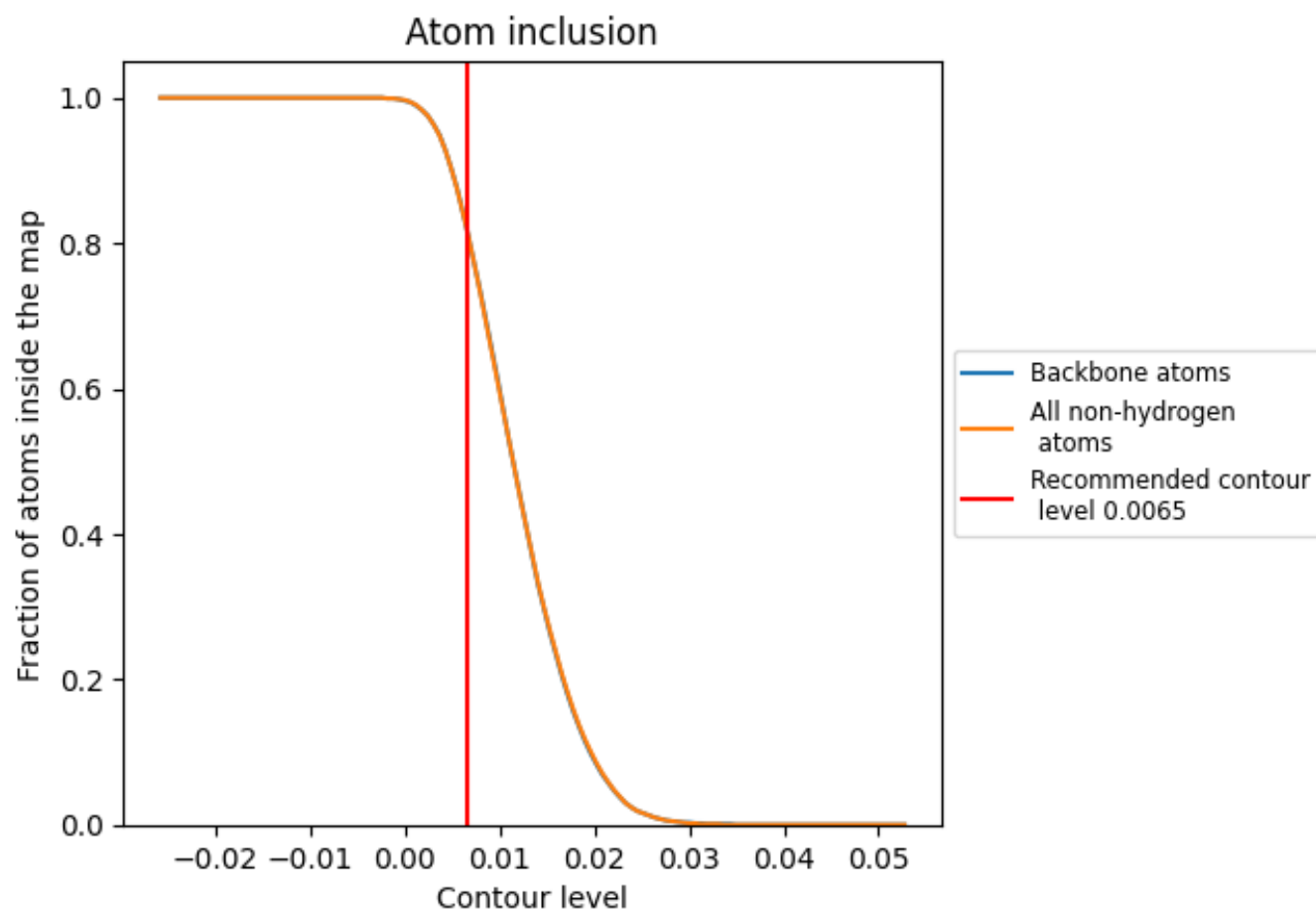
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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	 0.8230	 0.2980
A	 0.8320	 0.2990
B	 0.9060	 0.3700
C	 0.9260	 0.3030
E	 0.8210	 0.2730
F	 0.9180	 0.2900
G	 0.8820	 0.2980
H	 0.7810	 0.2720
L	 0.8990	 0.3020
M	 0.8460	 0.2760
O	 0.9070	 0.3320
P	 0.9220	 0.3930
Q	 0.8960	 0.3260
S	 0.8370	 0.3100
U	 0.7800	 0.2580
V	 0.5930	 0.2210
W	 0.7880	 0.3490
X	 0.7030	 0.2300

