



# Full wwPDB EM Validation Report ⓘ

Aug 27, 2024 – 12:57 AM JST

PDB ID : 8WKQ  
EMDB ID : EMD-37605  
Title : Cryo-EM structure of the MS ring (C1) with export apparatus and proximal rod within the flagellar motor-hook complex in the CW state.  
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2023-09-28  
Resolution : 3.80 Å(reported)  
Based on initial models : ?, .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev112  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

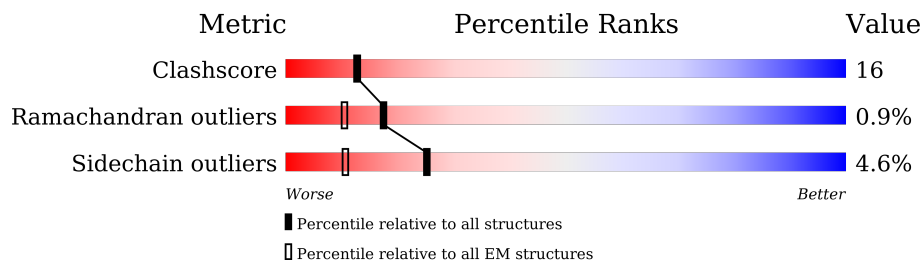
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	0	560	23% 6% 71%
1	1	560	22% 7% 71%
1	2	560	22% 6% 71%
1	3	560	23% 6% 71%
1	4	560	23% 6% 71%
1	5	560	23% 6% 71%
1	6	560	22% 7% 71%
1	7	560	22% 7% 71%

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Mol	Chain	Length	Quality of chain
1	8	560	23% 6% 71%
1	9	560	23% 6% 71%
1	AA	560	23% 6% 71%
1	AB	560	22% 6% 71%
1	AC	560	23% 6% 71%
1	AD	560	22% 7% 71%
1	AE	560	23% 6% 71%
1	AF	560	23% 6% 71%
1	AG	560	23% 6% 71%
1	AH	560	22% 6% 71%
1	AI	560	23% 6% 71%
1	AJ	560	23% 6% 71%
1	AK	560	23% 6% 71%
1	AL	560	23% 6% 71%
1	AM	560	23% 6% 71%
1	AN	560	23% 6% 71%
1	AO	560	22% 7% 71%
1	AP	560	22% 6% 71%
1	AQ	560	23% 6% 71%
1	UI	560	8% 18% 8% 72%
1	UJ	560	10% 17% 9% 72%
1	UK	560	14% 18% 8% 72%
1	UL	560	16% 17% 9% 72%
1	UM	560	20% 17% 9% 72%
1	UN	560	16% 17% 9% 72%

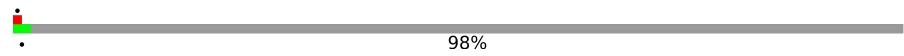
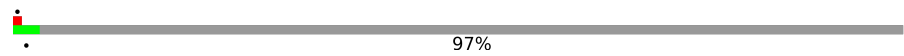
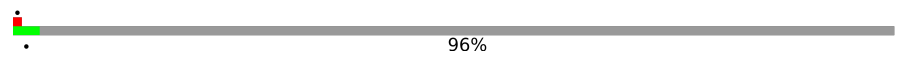
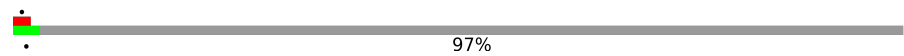
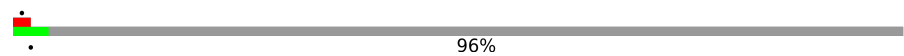
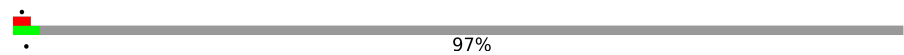
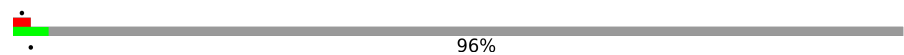
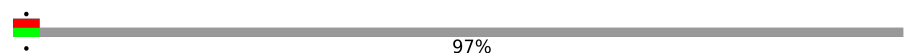
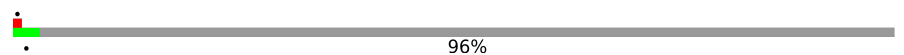
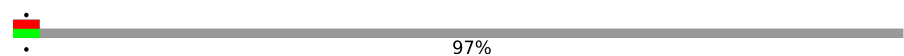
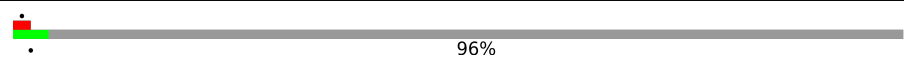


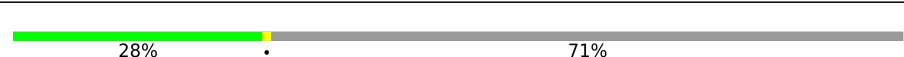
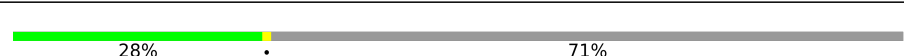
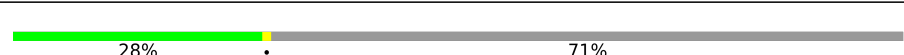
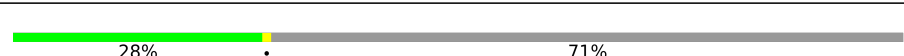

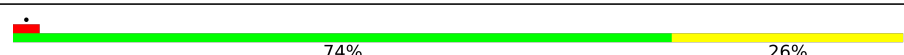
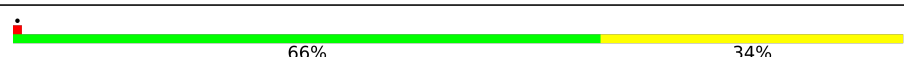
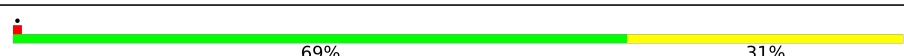



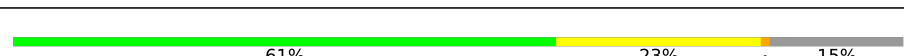
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Mol	Chain	Length	Quality of chain
1	UO	560	12% 18% 8% 72%
1	UP	560	10% 18% 8% 72%
1	WA	560	11% 8% 80%
1	WB	560	11% 7% 80%
1	WC	560	10% 8% 81%
1	WD	560	10% 8% 80%
1	WE	560	12% 7% 80%
1	WF	560	11% 8% 80%
1	WG	560	10% 9% 80%
1	WH	560	10% 6% 83%
1	WI	560	8% 8% 83%
1	WJ	560	10% 7% 82%
1	WK	560	9% 8% 82%
1	WL	560	8% 6% 85%
1	WM	560	9% 6% 85%
1	WN	560	9% 6% 85%
1	WO	560	10% 7% 83%
1	WP	560	9% 7% 82%
1	WQ	560	10% 9% 80%
1	WR	560	10% 8% 80%
1	WS	560	9% 9% 80%
1	WT	560	10% 8% 80%
1	WU	560	11% 8% 80%
1	WV	560	10% 8% 80%
1	WW	560	9% 9% 80%




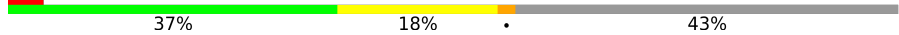















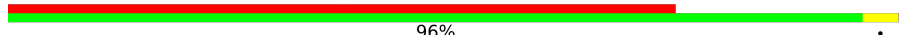
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Mol	Chain	Length	Quality of chain
1	b	560	 98%
1	c	560	 97%
1	d	560	 96%
1	e	560	 97%
1	f	560	 96%
1	g	560	 97%
1	h	560	 96%
1	i	560	 97%
1	j	560	 96%
1	k	560	 97%
1	l	560	 96%
1	t	560	 28% 71%
1	u	560	 28% 71%
1	v	560	 28% 71%
1	w	560	 28% 71%
1	x	560	 28% 71%
1	y	560	 28% 71%
1	z	560	 28% 71%
2	A	89	 74% 26%
2	B	89	 66% 34%
2	C	89	 69% 31%
2	D	89	 67% 33%
3	E	264	 65% 28%
4	F	245	 53% 30% 16%
4	G	245	 61% 23% 15%

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Mol	Chain	Length	Quality of chain
4	H	245	 64% 19% 15%
4	I	245	 62% 20% 15%
4	J	245	 58% 26% 15%
5	K	104	 37% 18% 43%
5	L	104	 71% 14% 12%
5	M	104	 71% 13% 5% 11%
5	N	104	 69% 19% 11%
5	O	104	 68% 20% 11%
5	P	104	 68% 18% 12%
6	Q	138	 70% 26% ..
6	R	138	 67% 20% 12%
6	S	138	 5% 63% 25% 9%
6	T	138	 8% 72% 20% 8%
6	U	138	 15% 67% 20% 11%
7	V	134	 40% 84% 16% .
7	W	134	 49% 81% 16% ..
7	X	134	 55% 84% 16% .
7	Y	134	 63% 83% 16% ..
7	Z	134	 67% 77% 22% .
7	a	134	 75% 96% ..

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 99073 atoms, of which 0 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 Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	UI	155	1172	733	211	226	2	0	0
1	UJ	155	1172	733	211	226	2	0	0
1	UK	155	1172	733	211	226	2	0	0
1	UL	155	1172	733	211	226	2	0	0
1	UM	155	1172	733	211	226	2	0	0
1	UN	155	1172	733	211	226	2	0	0
1	UO	155	1172	733	211	226	2	0	0
1	UP	155	1172	733	211	226	2	0	0
1	WA	113	849	534	148	166	1	0	0
1	WB	111	836	526	146	163	1	0	0
1	WC	108	812	510	142	159	1	0	0
1	WD	110	827	522	144	160	1	0	0
1	WE	112	843	531	147	164	1	0	0
1	WF	111	834	526	145	162	1	0	0
1	WG	112	843	531	147	164	1	0	0
1	WH	95	703	439	126	137	1	0	0
1	WI	95	703	439	126	137	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	WJ	99	737	462	131	143	1	0	0
1	WK	98	729	456	130	142	1	0	0
1	WL	85	622	389	110	122	1	0	0
1	WM	82	596	372	107	116	1	0	0
1	WN	84	611	380	109	121	1	0	0
1	WO	96	714	448	127	138	1	0	0
1	WP	100	741	464	132	144	1	0	0
1	WQ	111	834	526	145	162	1	0	0
1	WR	111	834	526	145	162	1	0	0
1	WS	111	834	526	145	162	1	0	0
1	WT	111	834	526	145	162	1	0	0
1	WU	112	843	531	147	164	1	0	0
1	WV	110	827	521	144	161	1	0	0
1	WW	111	834	526	145	162	1	0	0
1	b	13	81	50	15	16		0	0
1	c	16	103	64	19	20		0	0
1	d	20	133	83	23	27		0	0
1	e	16	103	64	19	20		0	0
1	f	21	140	88	24	28		0	0
1	g	16	103	64	19	20		0	0
1	h	21	140	88	24	28		0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	16	Total	C	N	O	0	0	
			103	64	19	20			
1	j	20	Total	C	N	O	0	0	
			133	83	23	27			
1	k	16	Total	C	N	O	0	0	
			103	64	19	20			
1	l	21	Total	C	N	O	0	0	
			140	88	24	28			
1	t	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	u	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	v	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	w	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	x	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	y	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	z	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	1	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	2	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	3	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	4	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	5	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	6	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	7	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	8	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	9	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	0	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AB	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AC	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AD	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AE	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AF	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AG	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AH	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AI	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AJ	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AK	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AL	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AM	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AN	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AO	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AP	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AQ	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

- Molecule 2 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
2	B	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
2	D	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

- Molecule 3 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	253	Total	C	N	O	S	0	0
			1945	1305	307	318	15		

- Molecule 4 is a protein called Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	207	Total	C	N	O	S	0	0
			1605	1072	249	272	12		
4	G	209	Total	C	N	O	S	0	0
			1626	1086	252	276	12		
4	H	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
4	I	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
4	J	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	59	Total	C	N	O	S	0	0
			429	265	74	83	7		
5	L	91	Total	C	N	O	S	0	0
			672	415	121	129	7		
5	M	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
5	N	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
5	O	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
5	P	92	Total	C	N	O	S	0	0
			679	420	122	130	7		

- Molecule 6 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	134	Total	C	N	O	S	0	0
			1030	633	189	203	5		
6	R	121	Total	C	N	O	S	0	0
			942	583	172	182	5		
6	S	125	Total	C	N	O	S	0	0
			967	598	177	187	5		
6	T	127	Total	C	N	O	S	0	0
			982	606	182	189	5		
6	U	123	Total	C	N	O	S	0	0
			950	588	172	185	5		

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	W	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
7	X	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	Y	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	Z	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	a	133	Total	C	N	O	S	0	0
			969	604	167	193	5		

















MET	GLN	Q129	C204	ASP	PRO	VAL	GLN	ARG	LEU
SER	ASP	V130	L206	PHE	PRO	ASN	GLN	LEU	SER
ALA	GLY	R134	P206	ALA	THR	THR	GLN	SER	ALA
THR	GLY	A135	P207	ASN	LYS	LYS	THR	LYS	THR
ALA	ALA	E139	T211	LYS	GLM	THR	PHE	ASP	ALA
THR	ILE	L140	L212	GLY	GLN	ALA	GLN	GLN	GLN
ALA	VAL	L141	V213	THR	ALA	ASP	LEU	LEU	LEU
ALA	ALA	R142	L220	GLU	GLM	ASP	GLY	GLN	GLN
GLN	GLN	T143	THR	GLU	ASN	LYS	LEU	GLN	GLN
PRO	THR	I144	THR	GLU	THR	THR	ALA	ARG	ARG
LYS	THR	E145	THR	HIS	THR	ALA	ALA	GLY	GLY
GLN	GLN	T146	THR	THR	THR	THR	THR	THR	THR
PRO	GLN	E147	THR	THR	THR	THR	THR	THR	THR
PRO	MET	P148	THR	ASP	THR	THR	THR	THR	THR
LEU	ASN	P149	THR	GLY	THR	THR	THR	THR	THR
LEU	ASN	S152	THR	ALA	THR	THR	THR	THR	THR
LEU	ILE	A153	THR	ARG	ASN	THR	THR	THR	THR
LEU	ARG	R154	THR	LYS	SER	THR	THR	THR	THR
LEU	ALA	V155	THR	ALA	ASN	THR	THR	THR	THR
LEU	GLY	H156	THR	ALA	ASN	THR	THR	THR	THR
LEU	ALA	H157	THR	LEU	ALA	THR	THR	THR	THR
LEU	GLY	L157	THR	GLY	ALA	THR	THR	THR	THR
LEU	ALA	A158	THR	ARG	GLY	THR	THR	THR	THR
LEU	ILE	L164	THR	ARG	PRO	THR	THR	THR	THR
PRO	VAL	F165	THR	THR	ARG	THR	THR	THR	THR
PRO	VAL	V166	THR	LEU	ARG	THR	THR	THR	THR
LEU	VAL	R167	THR	LEU	GLN	THR	THR	THR	THR
LEU	PRO	E168	THR	ILE	ALA	THR	THR	THR	THR
LEU	ASP	Q169	THR	ILE	ALA	THR	THR	THR	THR
LEU	VAL	K170	THR	ARG	VAL	THR	THR	THR	THR
LEU	VAL	P172	THR	THR	THR	THR	THR	THR	THR
LEU	HIS	S175	THR	GLY	THR	THR	THR	THR	THR
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LEU	ALA	R184	THR	VAL	THR	THR	THR	THR	THR
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LEU	THR	Q190	THR	ALA	THR	THR	THR	THR	THR
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LEU	PRO	S192	THR	THR	THR	THR	THR	THR	THR
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LEU	THR	V202	THR	THR	THR	THR	THR	THR	THR
LEU	THR	A203	THR	THR	THR	THR	THR	THR	THR

• Molecule 1: Flagellar M-ring protein



MET	GLN	Y132	Q222	THR	PRO	LEU	ALA	LEU	ALA
SER	ASP	Q133	SER	SER	GLN	PRO	GLY	PRO	GLY
ALA	GLY	R134	THR	THR	THR	THR	THR	THR	THR
THR	GLY	A135	THR	ASN	THR	THR	THR	THR	THR
ALA	ALA	E139	GLY	GLY	ALA	THR	THR	THR	THR
THR	ILE	L140	ARG	ALA	THR	THR	THR	THR	THR
ALA	VAL	A141	ASP	ASP	ASN	THR	THR	THR	THR
ALA	ALA	R142	THR	THR	GLN	THR	THR	THR	THR
GLN	GLN	T143	THR	ASN	ASN	THR	THR	THR	THR
PRO	THR	I144	ASP	ALA	THR	THR	THR	THR	THR
LYS	THR	E145	ALA	ALA	THR	THR	THR	THR	THR
GLN	GLN	T146	GLN	GLY	ALA	THR	THR	THR	THR
LEU	ASN	R154	LEU	SER	PRO	THR	THR	THR	THR
LEU	ILE	V155	LEU	ARG	ARG	THR	THR	THR	THR
LEU	THR	H156	THR	THR	THR	THR	THR	THR	THR
LEU	TYR	L157	ALA	LEU	THR	THR	THR	THR	THR
LEU	THR	A158	THR	ASN	ALA	THR	THR	THR	THR
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LEU	GLY	P162	ARG	THR	THR	THR	THR	THR	THR
LEU	SER	S163	SER	VAL	THR	THR	THR	THR	THR
LEU	GLY	L164	THR	GLY	ASN	THR	THR	THR	THR
LEU	ALA	F165	ARG	GLY	ALA	THR	THR	THR	THR
LEU	ILE	R166	ARG	THR	THR	THR	THR	THR	THR
LEU	GLU	V166	THR	THR	THR	THR	THR	THR	THR
LEU	VAL	R167	ILE	THR	THR	THR	THR	THR	THR
LEU	PRO	K170	ALA	GLY	THR	THR	THR	THR	THR
LEU	ALA	S175	THR	THR	THR	THR	THR	THR	THR
LEU	VAL	E181	LEU	THR	THR	THR	THR	THR	THR
LEU	HIS	P182	SER	ALA	THR	THR	THR	THR	THR
LEU	THR	G183	ILE	THR	THR	THR	THR	THR	THR
LEU	GLY	R184	GLY	THR	THR	THR	THR	THR	THR
LEU	ASN	D187	ASN	THR	THR	THR	THR	THR	THR
LEU	THR	H196	GLY	THR	THR	THR	THR	THR	THR
LEU	VAL	L197	THR	ALA	THR	THR	THR	THR	THR
LEU	ALA	V198	VAL	THR	THR	THR	THR	THR	THR
LEU	GLN	S199	ALA	THR	THR	THR	THR	THR	THR
LEU	GLY	S200	GLN	THR	THR	THR	THR	THR	THR
LEU	THR	A201	VAL	THR	THR	THR	THR	THR	THR
LEU	THR	L205	THR	THR	THR	THR	THR	THR	THR
LEU	ALA	P206	THR	THR	THR	THR	THR	THR	THR
LEU	ALA	P207	PHE	THR	THR	THR	THR	THR	THR
LEU	THR	G112	ALA	THR	THR	THR	THR	THR	THR
LEU	THR	F113	THR	THR	THR	THR	THR	THR	THR
LEU	THR	E114	THR	THR	THR	THR	THR	THR	THR
LEU	THR	L115	THR	THR	THR	THR	THR	THR	THR
LEU	THR	L116	THR	THR	THR	THR	THR	THR	THR
LEU	THR	T1123	THR	THR	THR	THR	THR	THR	THR
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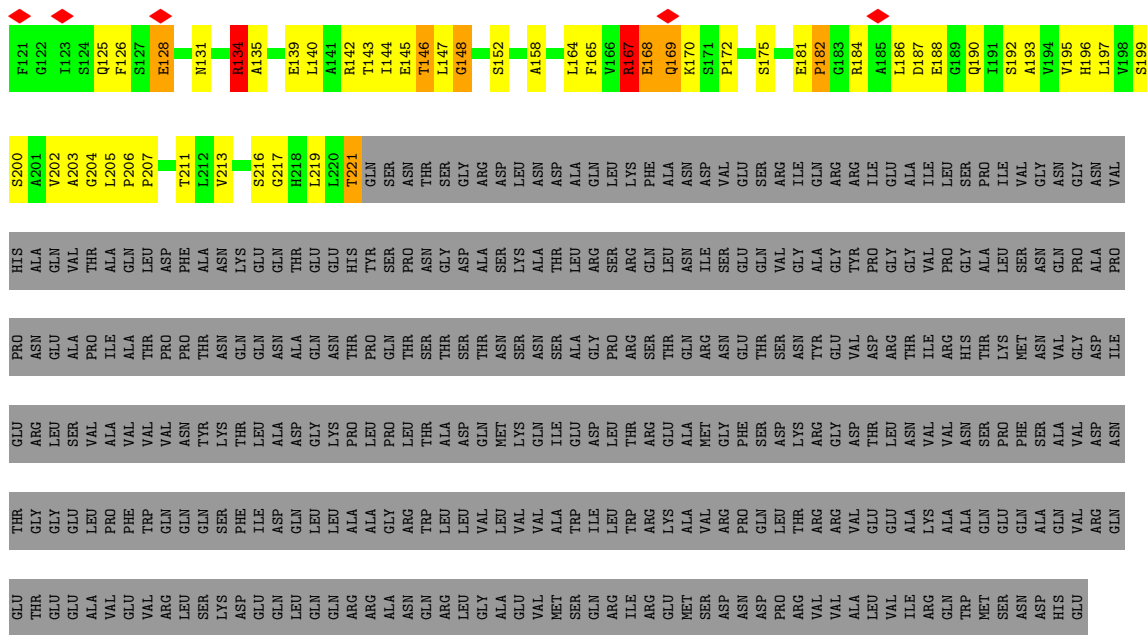




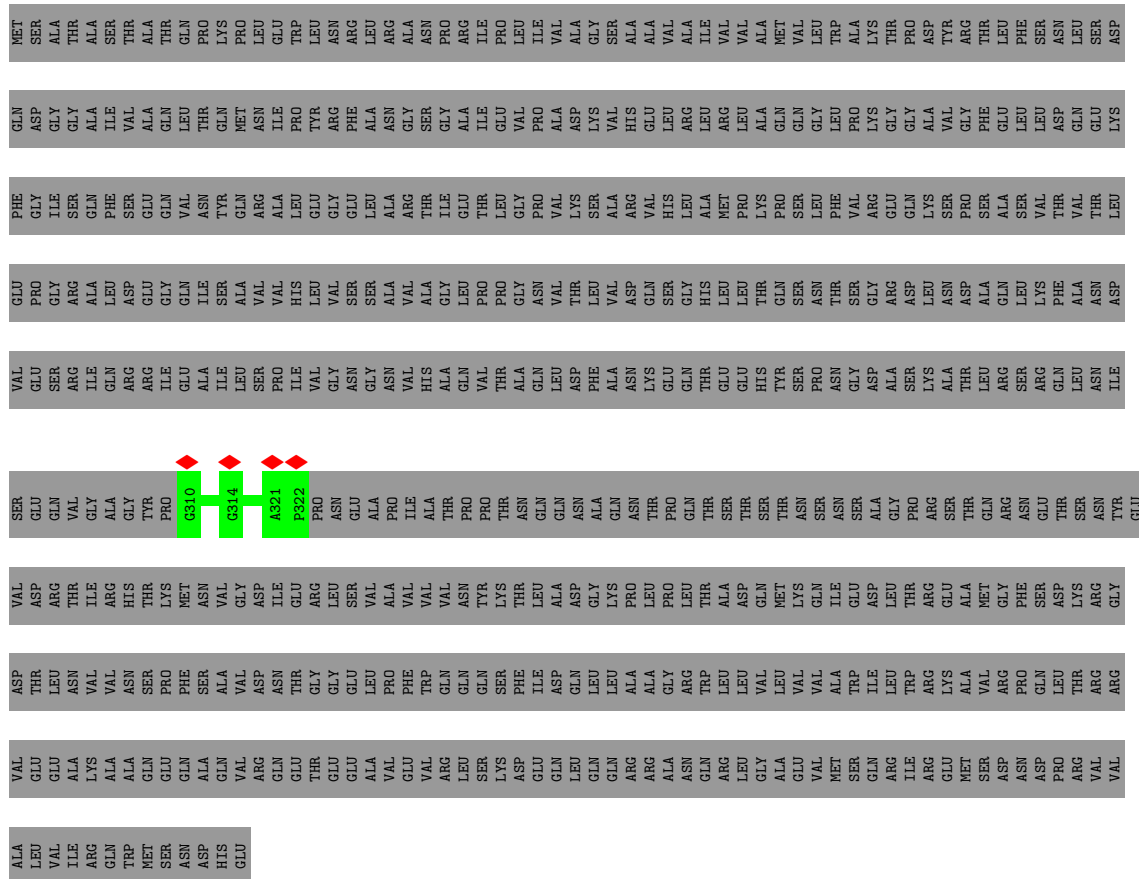








• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein















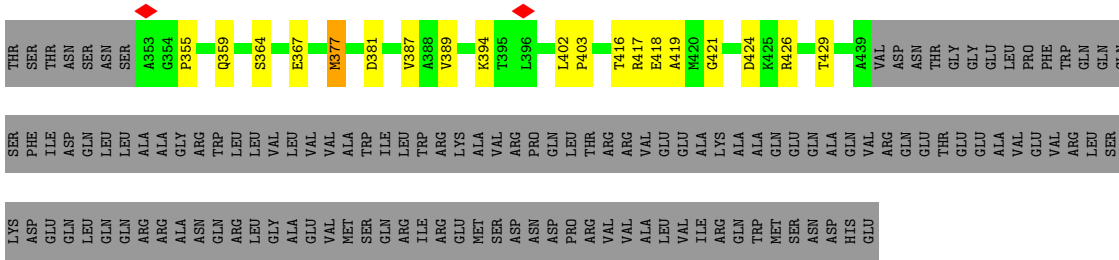




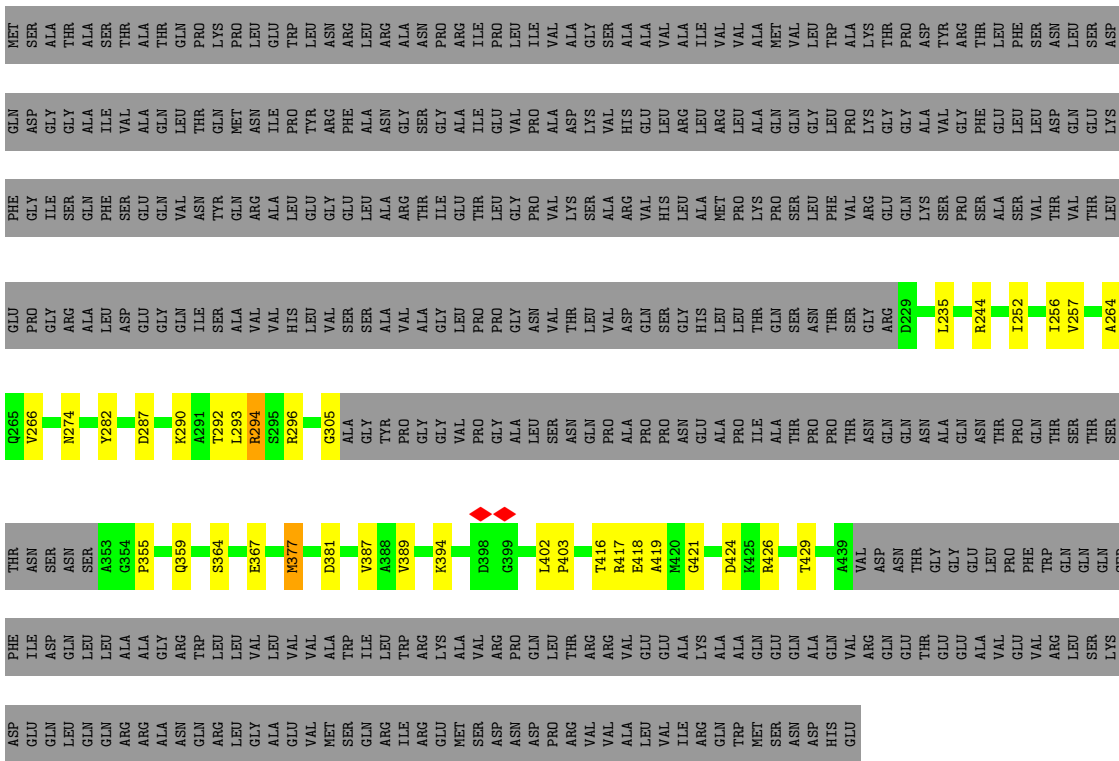




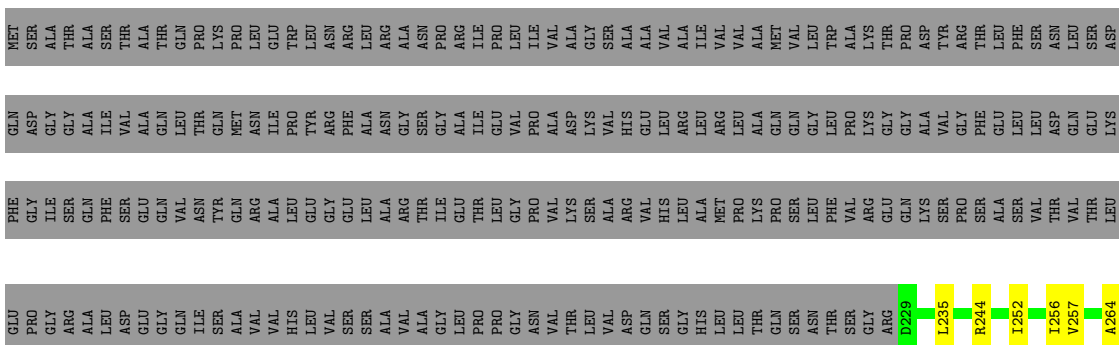


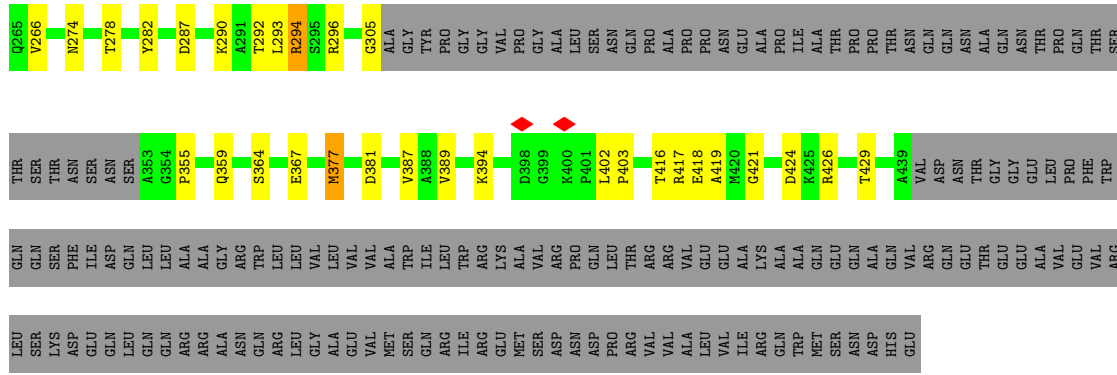


• Molecule 1: Flagellar M-ring protein

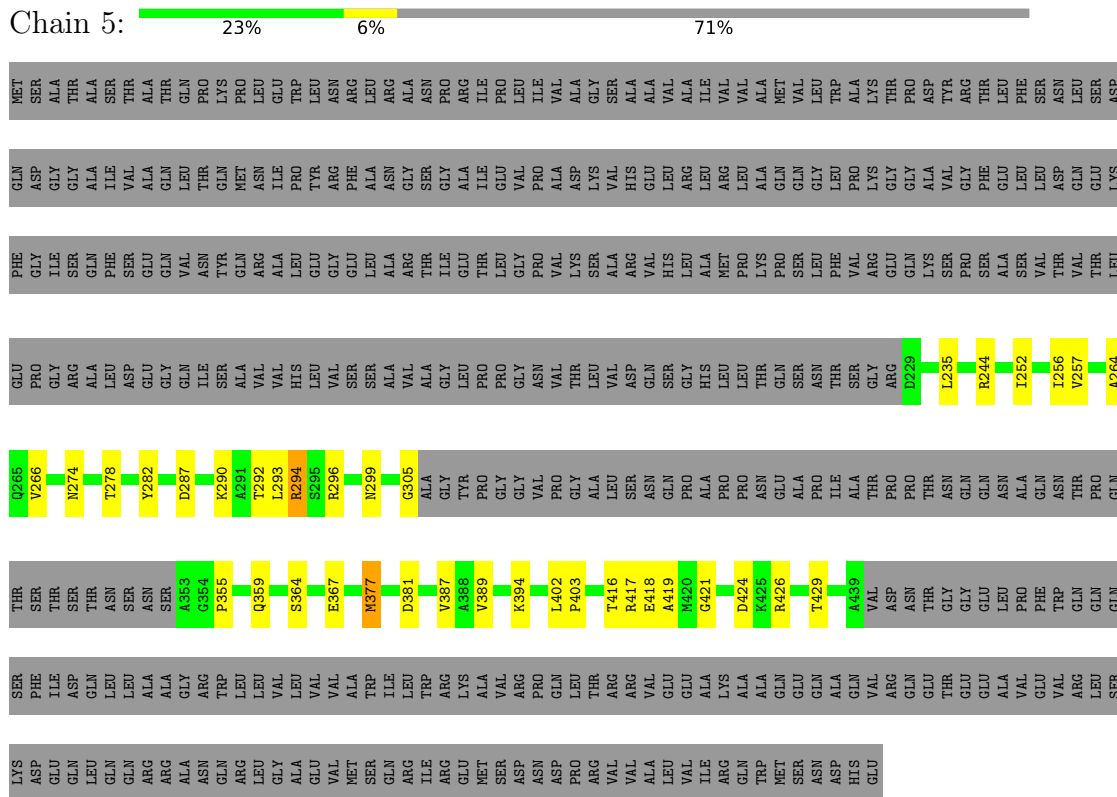


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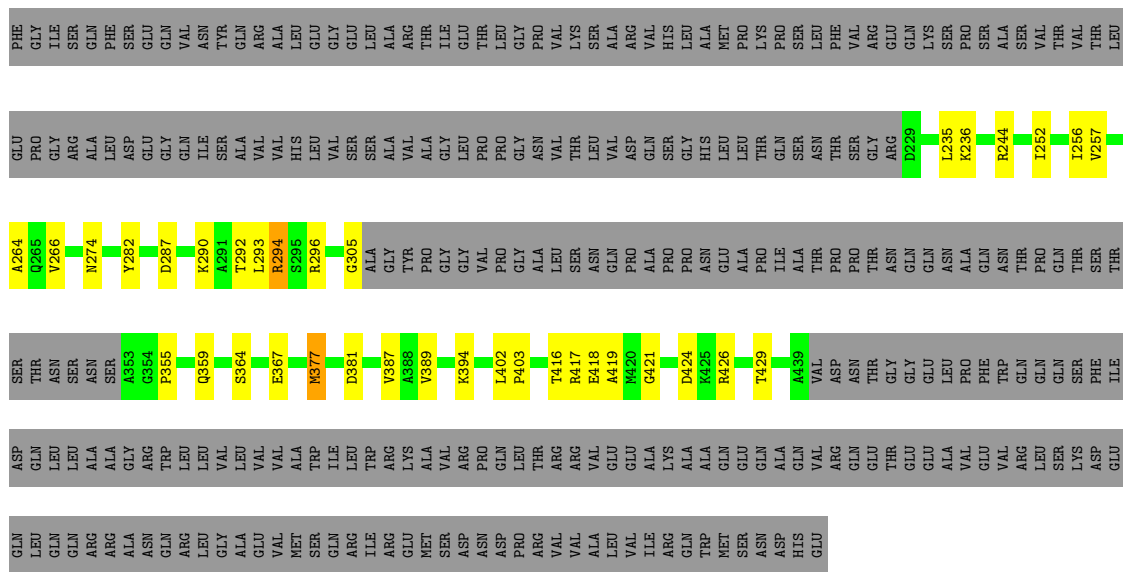


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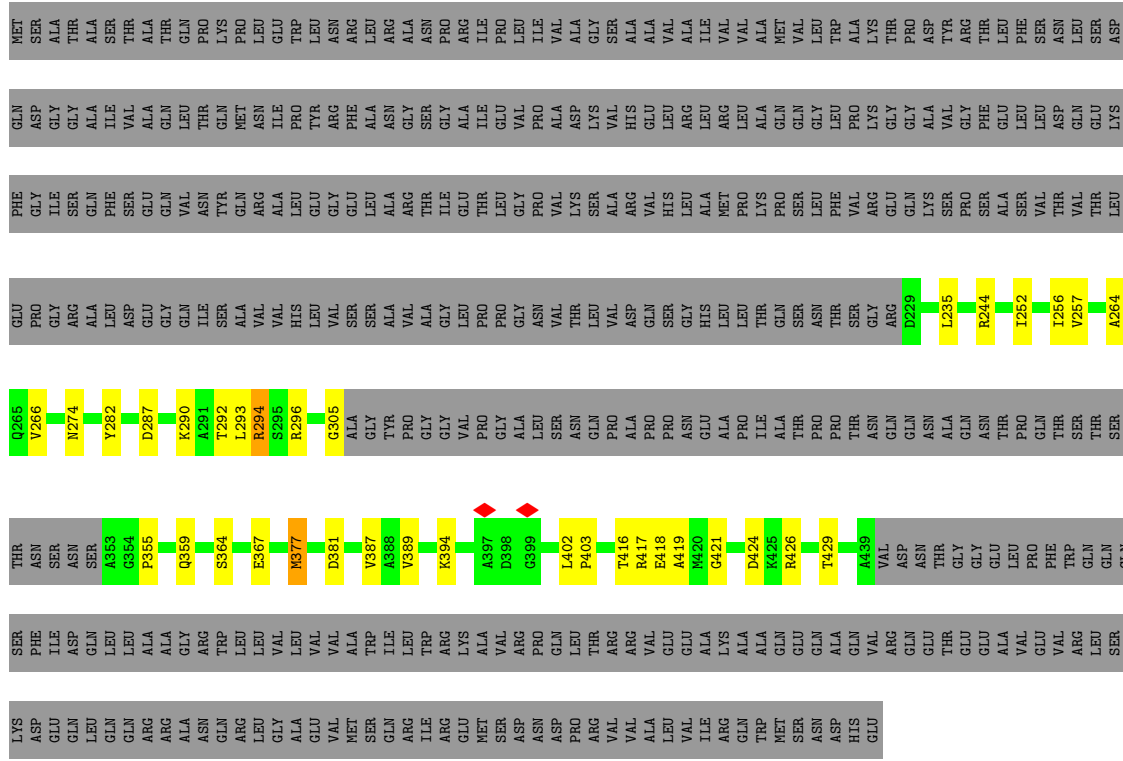


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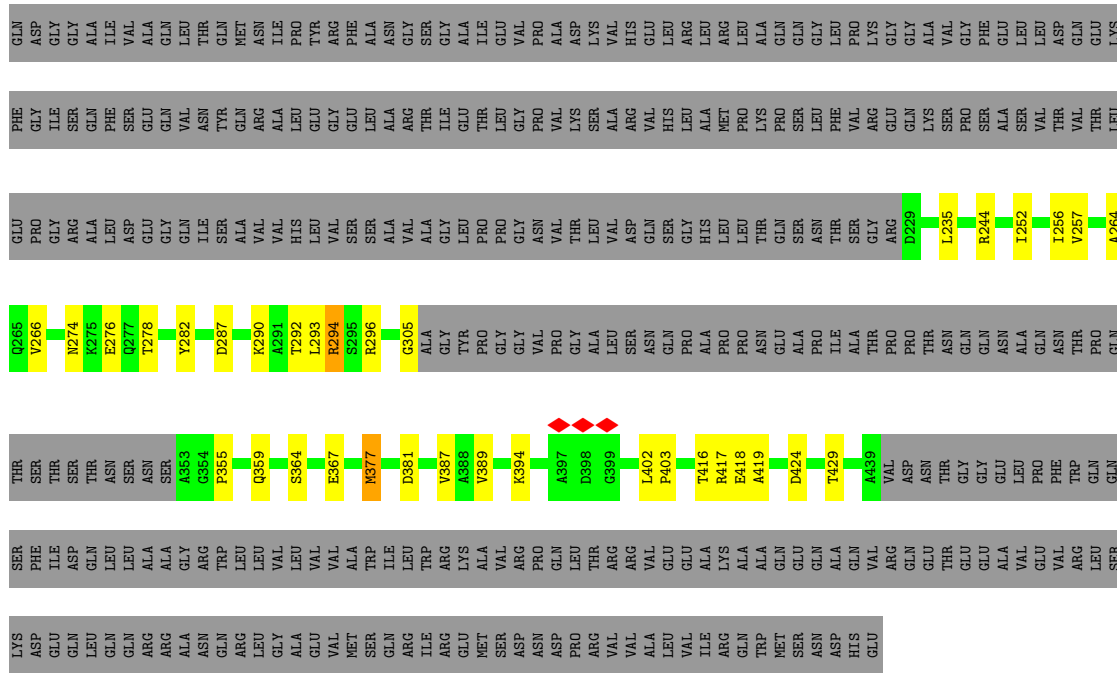


• Molecule 1: Flagellar M-ring protein

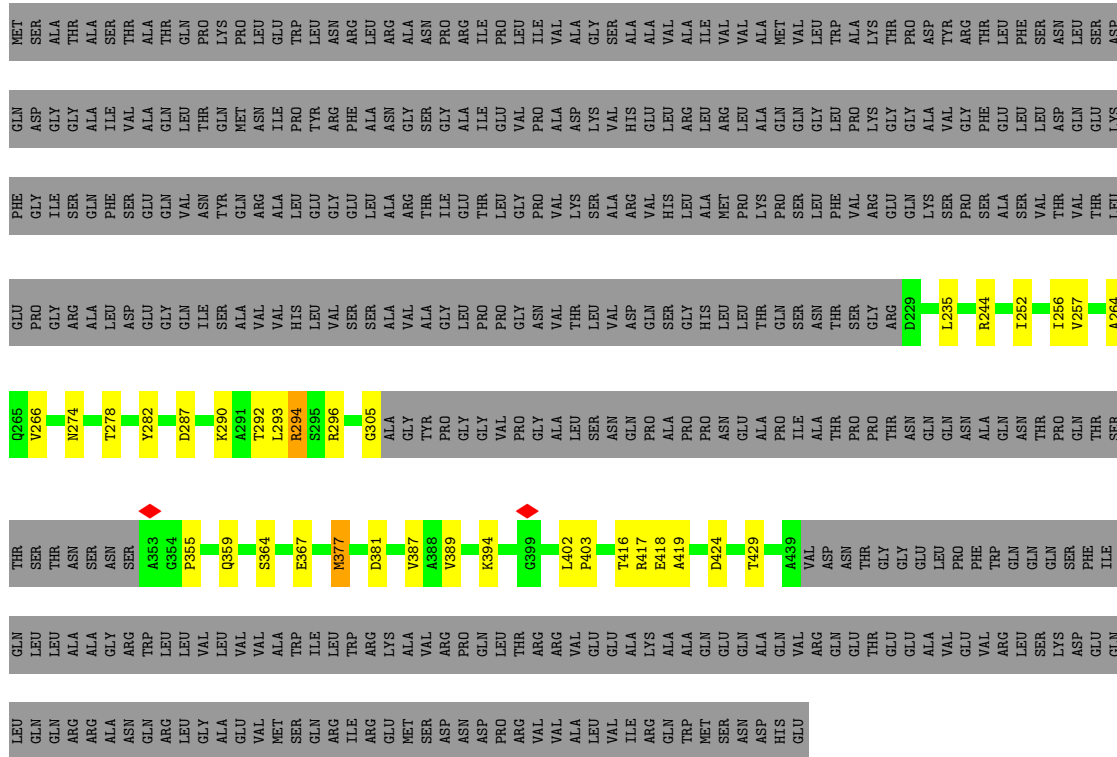


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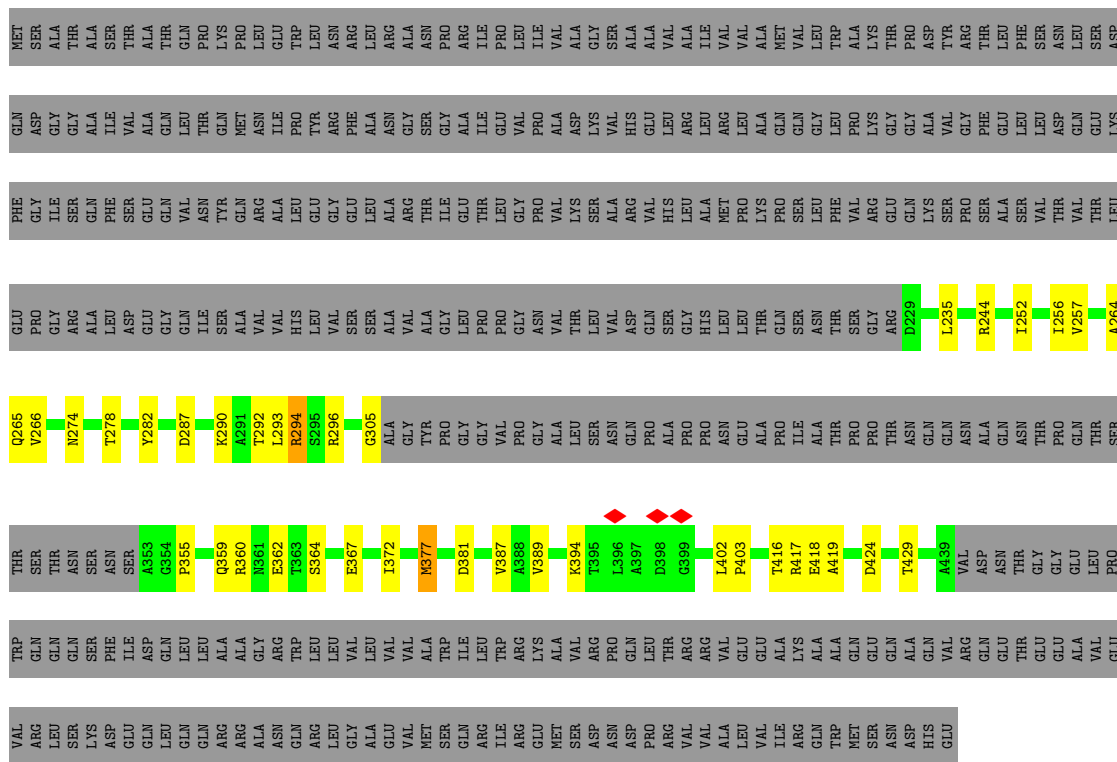


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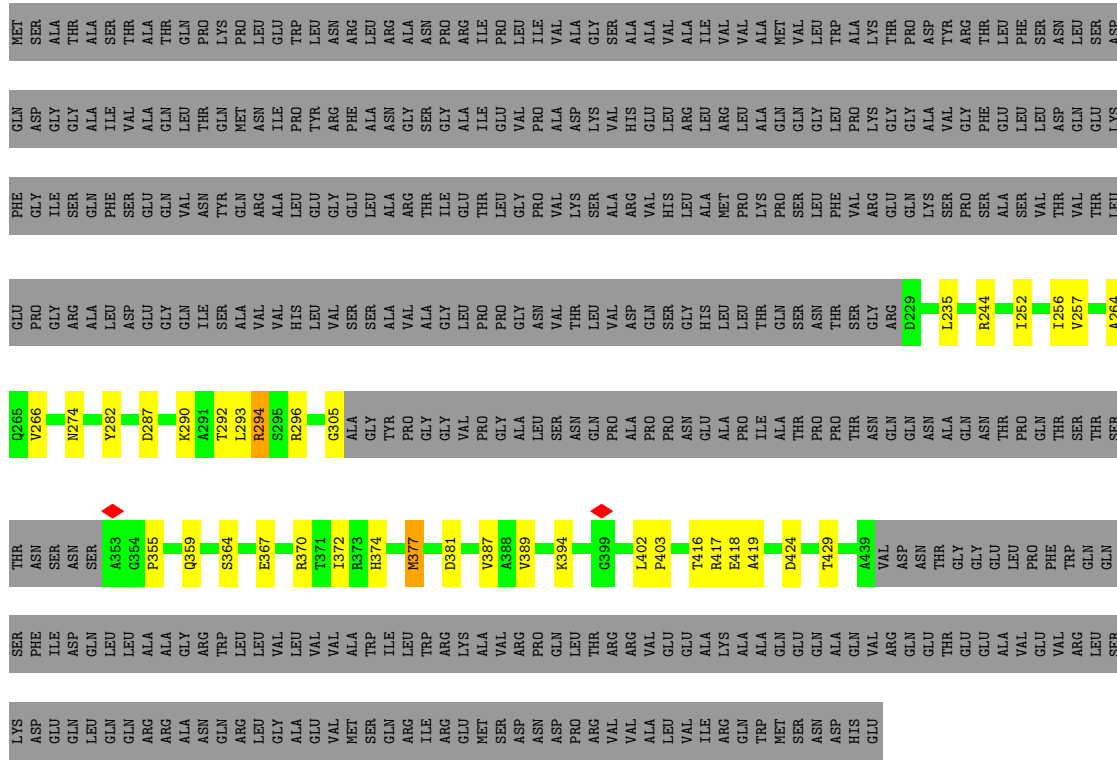


• Molecule 1: Flagellar M-ring protein





• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein





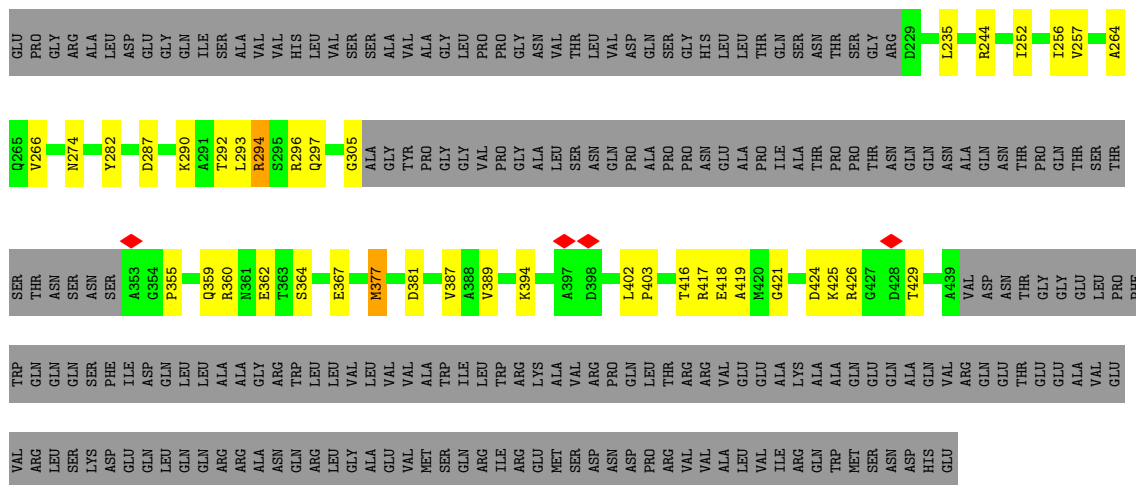




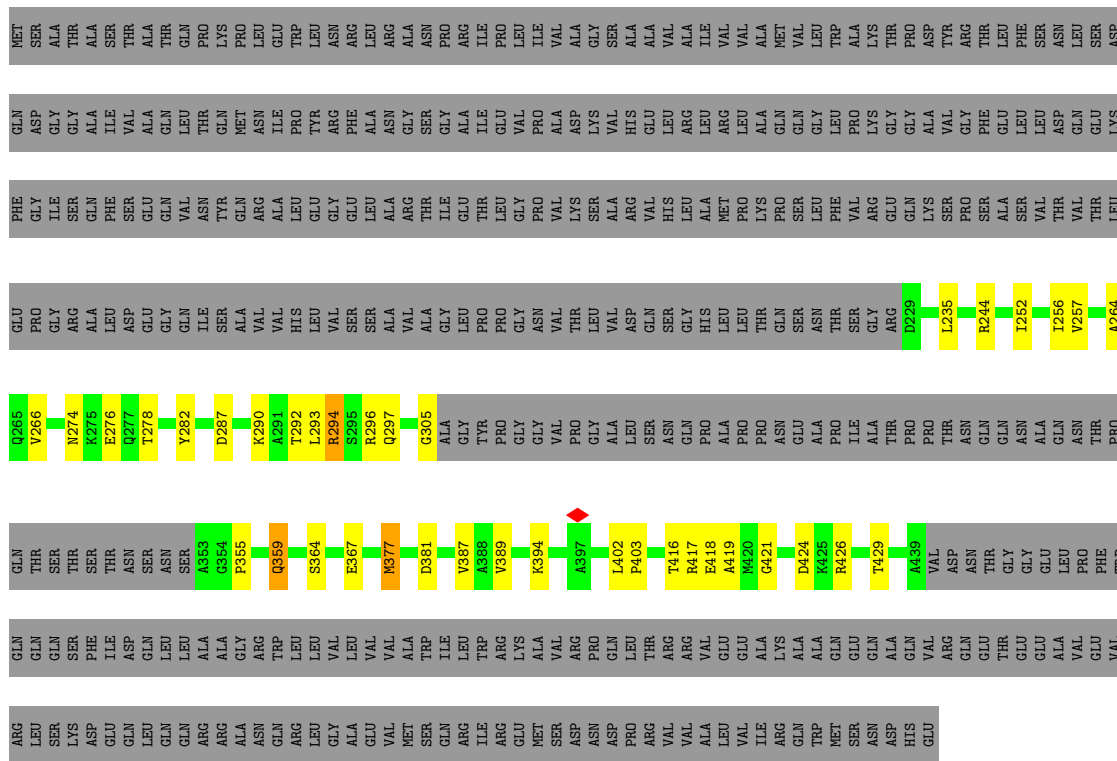




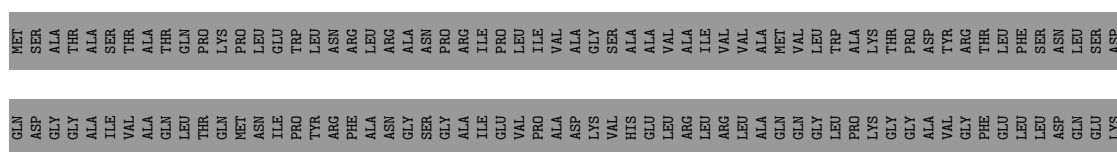




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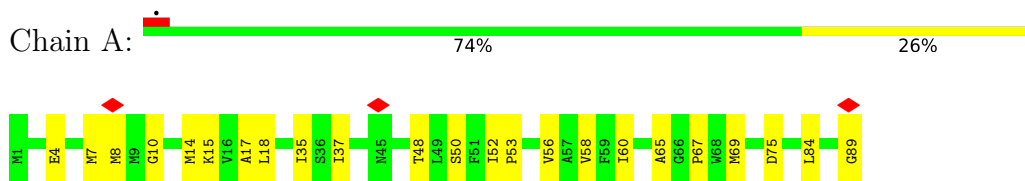


• Molecule 1: Flagellar M-ring protein

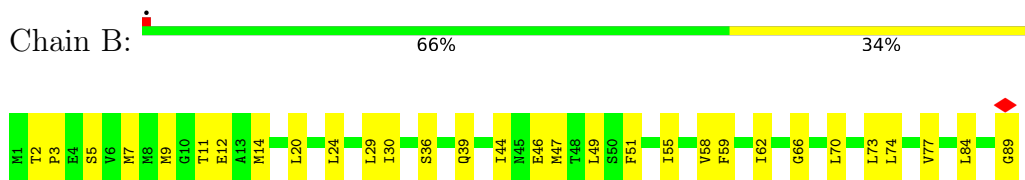




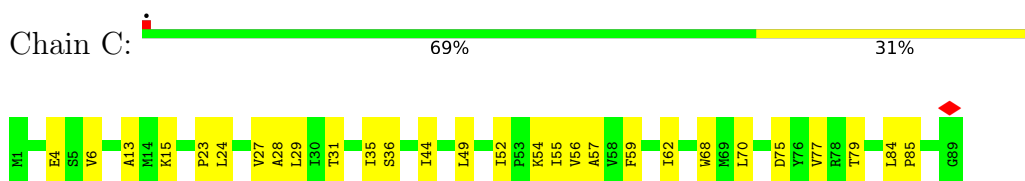
• Molecule 2: Flagellar biosynthetic protein FliQ



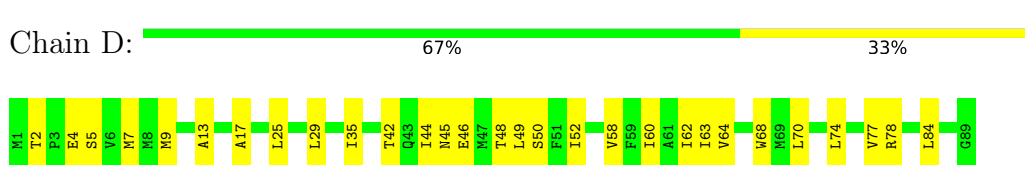
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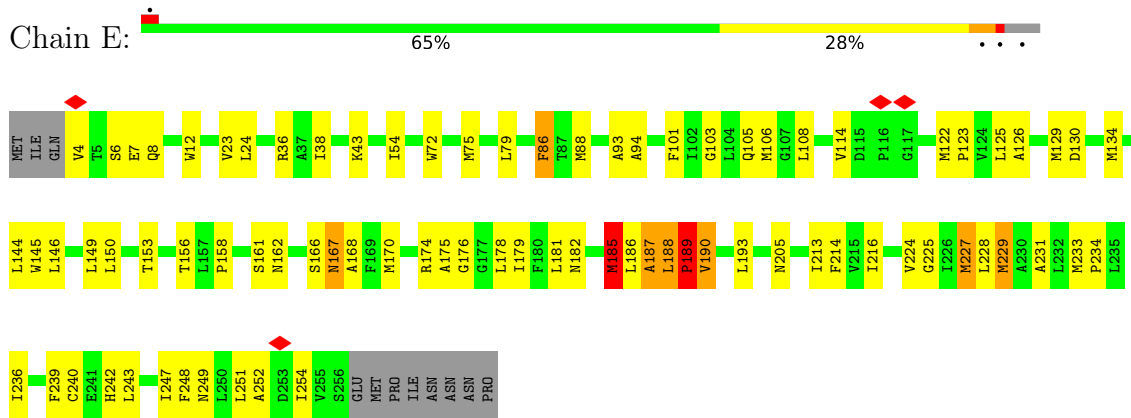
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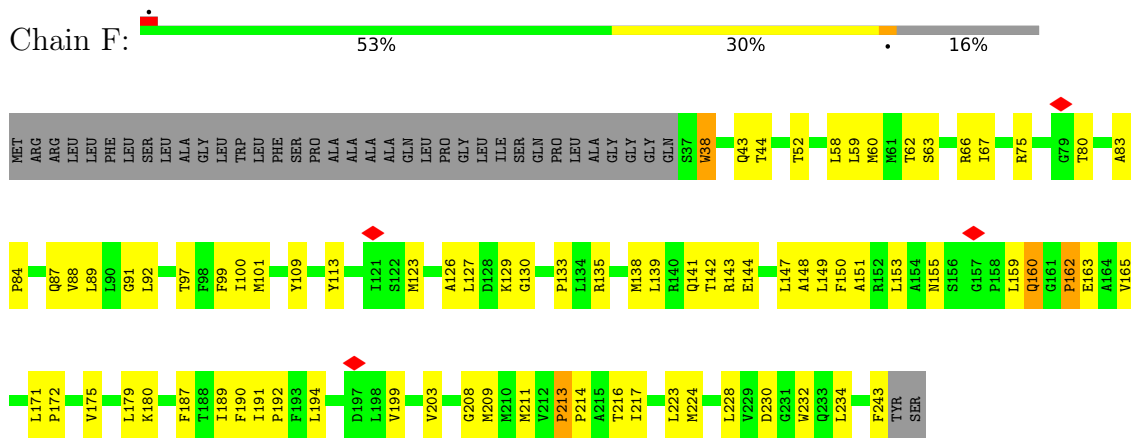
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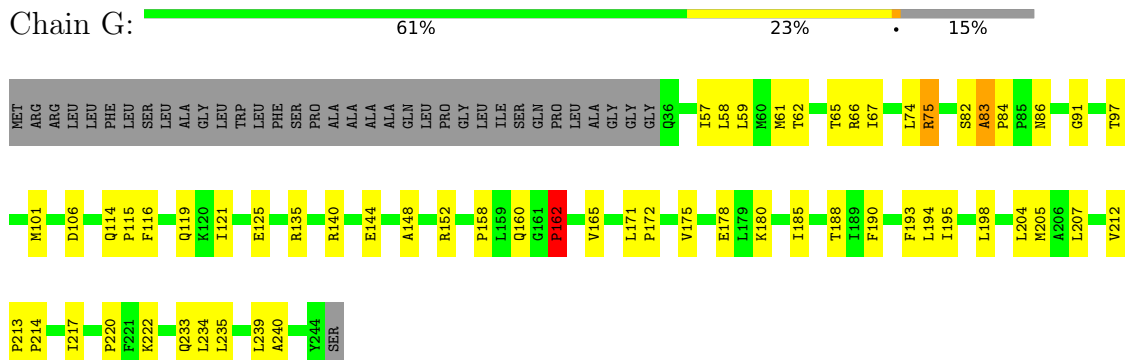
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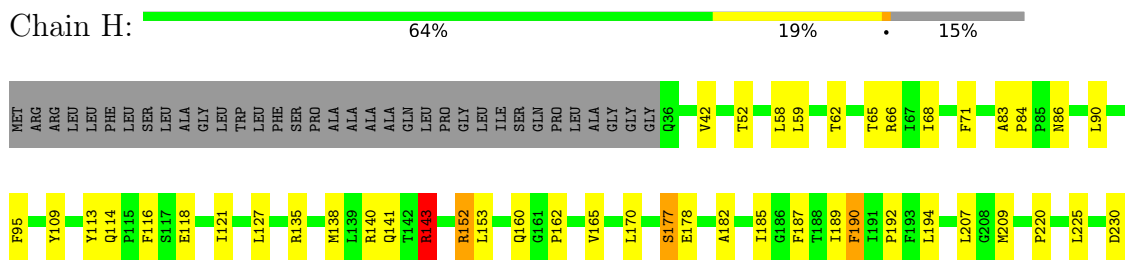
• Molecule 4: Flagellar biosynthetic protein FlIP



• Molecule 4: Flagellar biosynthetic protein FlIP



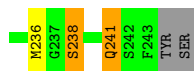
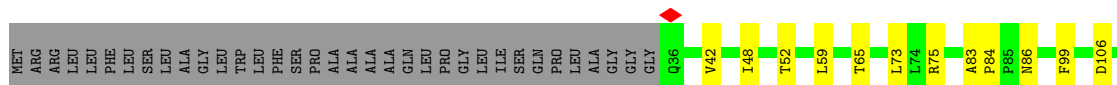
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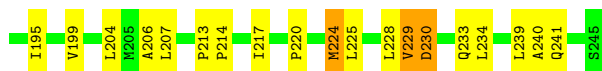
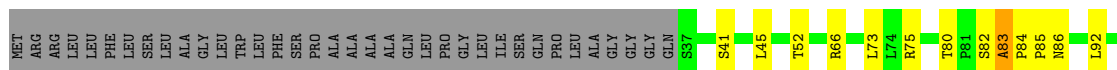




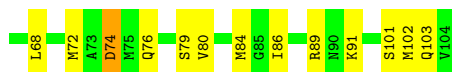
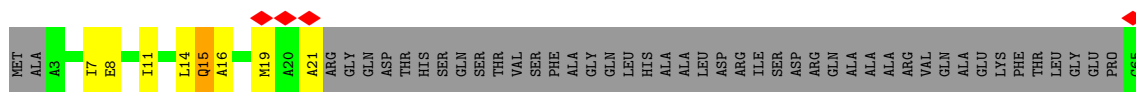
• Molecule 4: Flagellar biosynthetic protein FliP



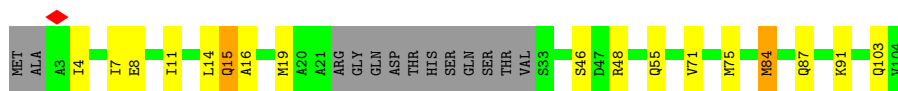
• Molecule 4: Flagellar biosynthetic protein FliP



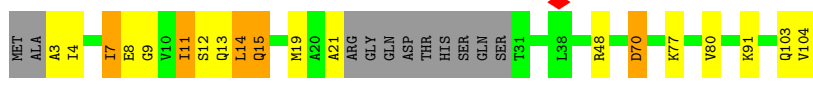
• Molecule 5: Flagellar hook-basal body complex protein FliE



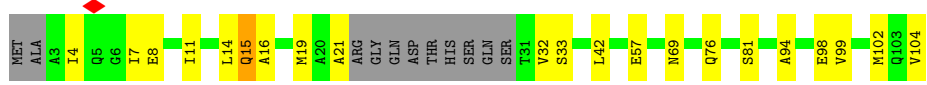
• Molecule 5: Flagellar hook-basal body complex protein FliE



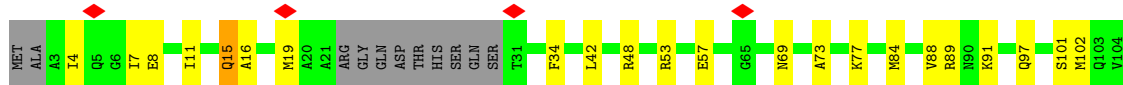
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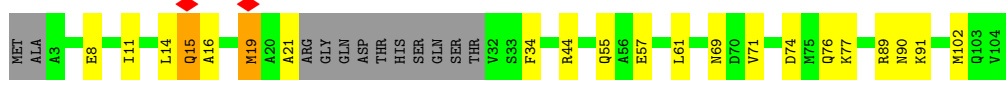
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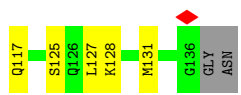
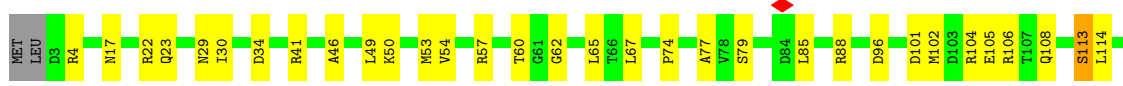
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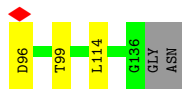
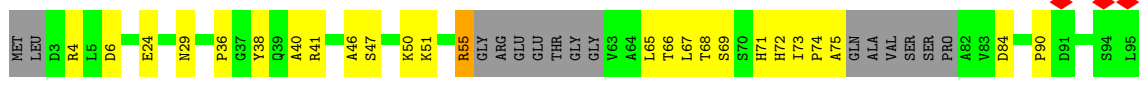
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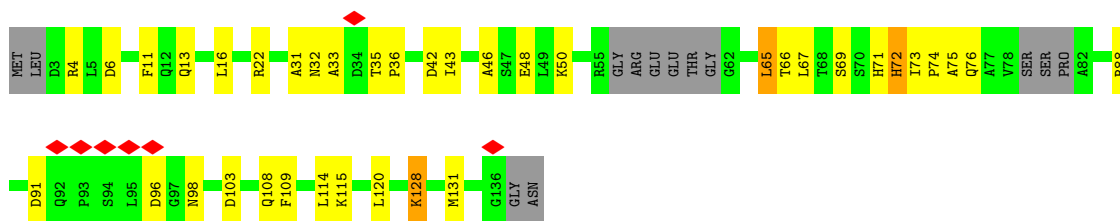
• Molecule 6: Flagellar basal body rod protein FlgB



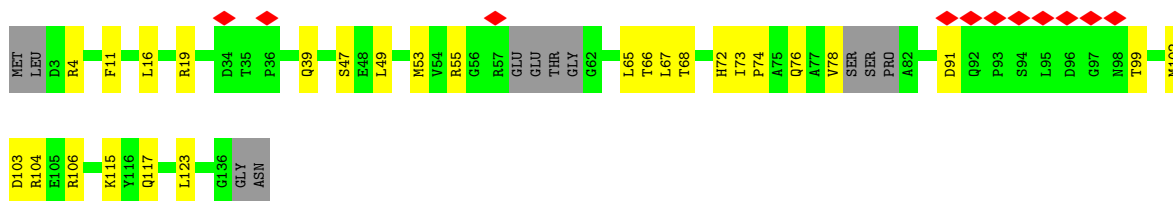
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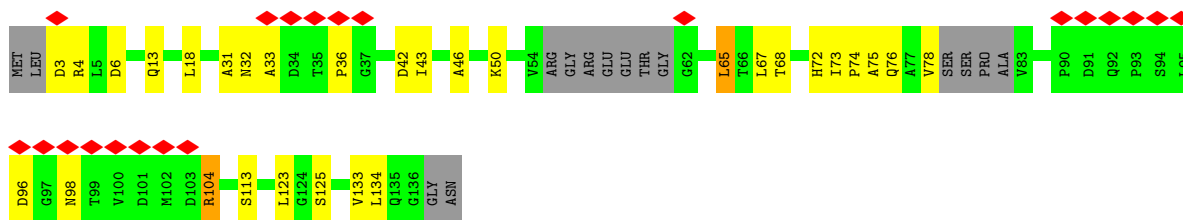
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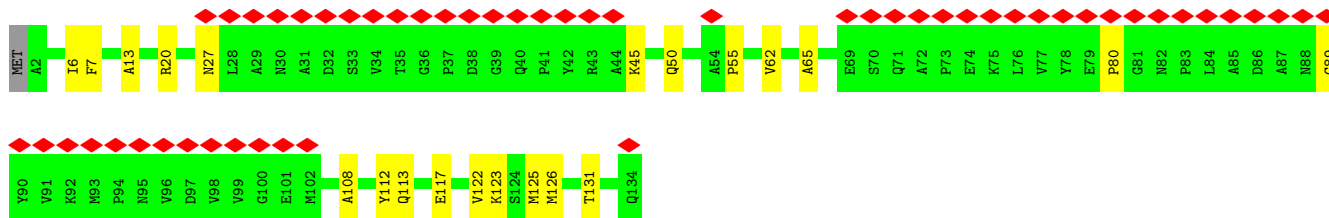
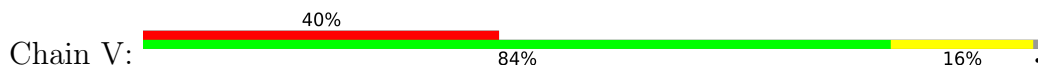
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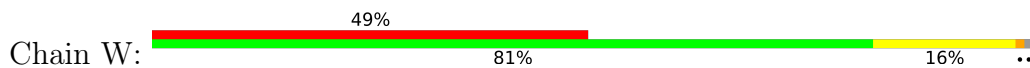
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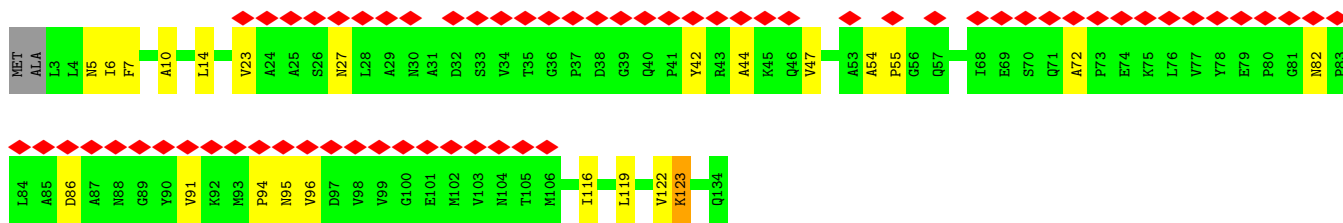


• Molecule 7: Flagellar basal-body rod protein FlgC

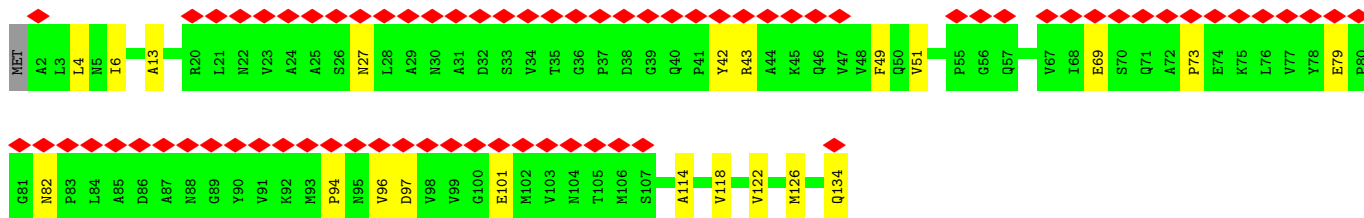
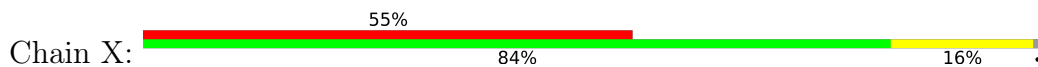


• Molecule 7: Flagellar basal-body rod protein FlgC

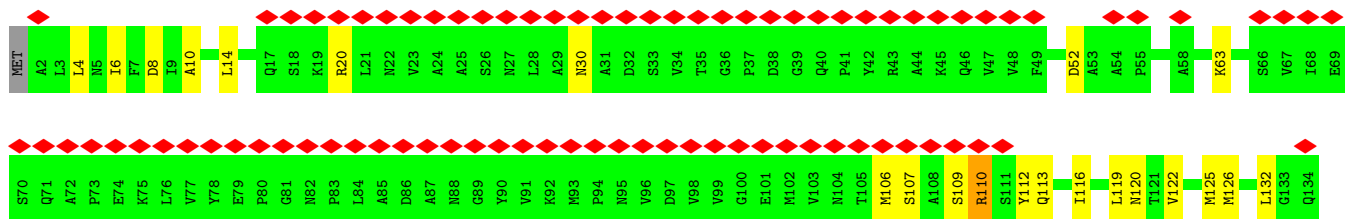
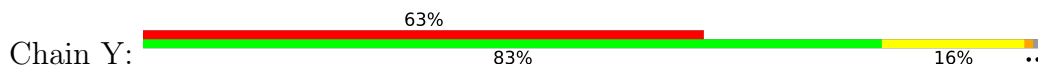




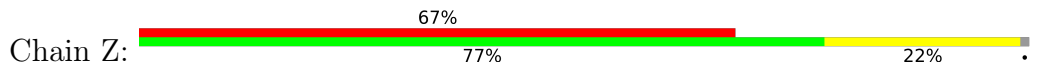
• Molecule 7: Flagellar basal-body rod protein FlgC



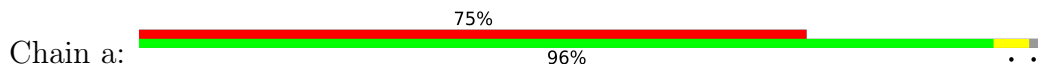
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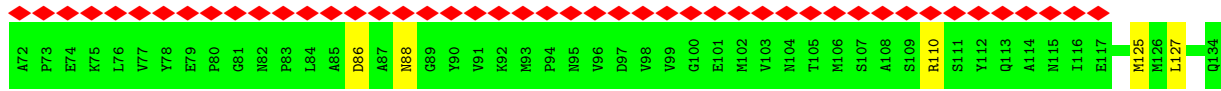


• Molecule 7: Flagellar basal-body rod protein FlgC



• Molecule 7: Flagellar basal-body rod protein FlgC





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0	0.26	0/1289	0.53	0/1741
1	1	0.26	0/1289	0.53	0/1741
1	2	0.27	0/1289	0.53	0/1741
1	3	0.27	0/1289	0.53	0/1741
1	4	0.27	0/1289	0.53	0/1741
1	5	0.27	0/1289	0.53	0/1741
1	6	0.27	0/1289	0.53	0/1741
1	7	0.27	0/1289	0.53	0/1741
1	8	0.27	0/1289	0.53	0/1741
1	9	0.26	0/1289	0.53	0/1741
1	AA	0.27	0/1289	0.53	0/1741
1	AB	0.27	0/1289	0.53	0/1741
1	AC	0.27	0/1289	0.53	0/1741
1	AD	0.27	0/1289	0.53	0/1741
1	AE	0.27	0/1289	0.53	0/1741
1	AF	0.26	0/1289	0.53	0/1741
1	AG	0.27	0/1289	0.53	0/1741
1	AH	0.27	0/1289	0.53	0/1741
1	AI	0.26	0/1289	0.53	0/1741
1	AJ	0.27	0/1289	0.53	0/1741
1	AK	0.26	0/1289	0.53	0/1741
1	AL	0.27	0/1289	0.53	0/1741
1	AM	0.27	0/1289	0.53	0/1741
1	AN	0.26	0/1289	0.53	0/1741
1	AO	0.27	0/1289	0.53	0/1741
1	AP	0.27	0/1289	0.53	0/1741
1	AQ	0.26	0/1289	0.53	0/1741
1	UI	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UJ	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UK	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UL	0.82	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UM	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UN	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UO	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	UP	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	WA	0.60	0/863	0.72	1/1172 (0.1%)
1	WB	0.59	0/850	0.69	0/1154
1	WC	0.59	0/825	0.68	0/1121
1	WD	0.61	0/841	0.68	0/1142
1	WE	0.60	0/857	0.71	0/1164
1	WF	0.60	0/848	0.69	0/1152
1	WG	0.60	0/857	0.68	0/1164
1	WH	0.60	0/714	0.69	0/973
1	WI	0.59	0/714	0.74	0/973
1	WJ	0.61	0/749	0.72	1/1020 (0.1%)
1	WK	0.60	0/741	0.69	0/1009
1	WL	0.60	0/631	0.70	0/860
1	WM	0.59	0/604	0.70	0/824
1	WN	0.60	0/619	0.70	0/844
1	WO	0.60	0/726	0.72	1/989 (0.1%)
1	WP	0.60	0/753	0.69	0/1025
1	WQ	0.60	0/848	0.69	0/1152
1	WR	0.60	0/848	0.69	0/1152
1	WS	0.60	0/848	0.69	0/1152
1	WT	0.60	0/848	0.70	0/1152
1	WU	0.60	0/857	0.67	0/1164
1	WV	0.61	0/841	0.69	0/1142
1	WW	0.60	0/848	0.70	0/1152
1	b	0.52	0/83	0.63	0/114
1	c	0.26	0/107	0.38	0/148
1	d	0.31	0/137	0.49	0/191
1	e	0.28	0/107	0.56	0/148
1	f	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
1	g	0.33	0/107	0.51	0/148
1	h	0.26	0/145	0.44	0/203
1	i	0.30	0/107	0.38	0/148
1	j	0.30	0/137	0.57	0/191
1	k	0.30	0/107	0.37	0/148
1	l	0.29	0/145	0.45	0/203
1	t	0.26	0/1289	0.53	0/1741
1	u	0.26	0/1289	0.53	0/1741
1	v	0.27	0/1289	0.53	0/1741
1	w	0.27	0/1289	0.53	0/1741
1	x	0.27	0/1289	0.53	0/1741
1	y	0.26	0/1289	0.53	0/1741
1	z	0.27	0/1289	0.53	0/1741
2	A	0.29	0/681	0.47	0/930



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	B	0.26	0/681	0.49	0/930
2	C	0.28	0/681	0.48	0/930
2	D	0.29	0/681	0.49	0/930
3	E	0.38	1/1994 (0.1%)	0.56	1/2724 (0.0%)
4	F	0.36	0/1643	0.62	2/2237 (0.1%)
4	G	0.29	0/1665	0.49	1/2267 (0.0%)
4	H	0.29	0/1652	0.48	0/2249
4	I	0.28	0/1652	0.46	0/2249
4	J	0.30	0/1662	0.49	0/2263
5	K	0.42	0/428	0.53	0/572
5	L	0.36	0/675	0.49	0/905
5	M	0.36	0/689	0.52	0/925
5	N	0.36	0/689	0.50	0/925
5	O	0.37	0/689	0.53	0/925
5	P	0.37	0/682	0.51	0/915
6	Q	0.36	0/1042	0.55	0/1408
6	R	0.33	0/951	0.50	0/1282
6	S	0.35	0/976	0.56	0/1316
6	T	0.34	0/991	0.54	0/1335
6	U	0.34	0/959	0.50	0/1293
7	V	0.28	0/981	0.44	0/1334
7	W	0.26	0/976	0.46	0/1327
7	X	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
7	Y	0.28	0/981	0.52	1/1334 (0.1%)
7	Z	0.26	0/981	0.47	0/1334
7	a	0.28	0/981	0.47	0/1334
All	All	0.44	20/100455 (0.0%)	0.60	46/136142 (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	UI	0	2
1	UJ	0	2
1	UK	0	3
1	UL	0	3
1	UM	0	2
1	UN	0	2
1	UO	0	2
1	UP	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	WA	0	3
1	WB	0	4
1	WC	0	3
1	WD	0	1
1	WE	0	2
1	WF	0	3
1	WG	0	3
1	WI	0	1
1	WJ	0	3
1	WK	0	2
1	WL	0	2
1	WM	0	1
1	WN	0	1
1	WO	0	1
1	WP	0	3
1	WQ	0	2
1	WR	0	3
1	WS	0	1
1	WT	0	2
1	WU	0	2
1	WV	0	3
1	WW	0	2
4	H	0	1
6	Q	0	1
6	U	0	1
7	Y	0	1
7	a	0	1
All	All	0	72

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	331	PRO	CG-CD	-14.23	1.03	1.50
7	X	73	PRO	CG-CD	-12.74	1.08	1.50
1	UL	172	PRO	N-CD	-9.53	1.34	1.47
1	UM	172	PRO	N-CD	-9.52	1.34	1.47
1	UP	172	PRO	N-CD	-9.50	1.34	1.47
1	UN	172	PRO	N-CD	-9.47	1.34	1.47
1	UJ	172	PRO	N-CD	-9.47	1.34	1.47
1	UI	172	PRO	N-CD	-9.45	1.34	1.47
1	UO	172	PRO	N-CD	-9.44	1.34	1.47
1	UK	172	PRO	N-CD	-9.42	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UJ	125	GLN	C-N	7.66	1.51	1.34
1	UP	125	GLN	C-N	7.64	1.51	1.34
1	UK	125	GLN	C-N	7.64	1.51	1.34
7	X	73	PRO	CB-CG	-7.64	1.11	1.50
1	UO	125	GLN	C-N	7.62	1.51	1.34
1	UI	125	GLN	C-N	7.60	1.51	1.34
1	UM	125	GLN	C-N	7.60	1.51	1.34
1	UL	125	GLN	C-N	7.59	1.51	1.34
1	UN	125	GLN	C-N	7.56	1.51	1.34
3	E	185	MET	C-O	6.34	1.35	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	73	PRO	CB-CG-CD	18.81	179.86	106.50
7	X	73	PRO	N-CD-CG	-18.80	75.00	103.20
1	f	331	PRO	N-CD-CG	-16.10	79.05	103.20
7	X	73	PRO	CA-CB-CG	-14.00	77.40	104.00
4	F	162	PRO	CA-N-CD	-12.05	94.62	111.50
1	f	331	PRO	CA-CB-CG	-9.00	86.91	104.00
1	UO	126	PHE	O-C-N	8.82	136.82	122.70
1	UL	126	PHE	O-C-N	8.82	136.82	122.70
1	UK	126	PHE	O-C-N	8.81	136.79	122.70
1	UI	126	PHE	O-C-N	8.80	136.78	122.70
1	UN	126	PHE	O-C-N	8.79	136.77	122.70
1	UJ	126	PHE	O-C-N	8.79	136.76	122.70
1	UM	126	PHE	O-C-N	8.78	136.74	122.70
1	UP	126	PHE	O-C-N	8.76	136.72	122.70
1	f	331	PRO	N-CA-CB	-7.03	94.86	103.30
1	UK	126	PHE	CA-C-N	-6.79	102.26	117.20
1	UL	126	PHE	CA-C-N	-6.77	102.31	117.20
1	UJ	126	PHE	CA-C-N	-6.76	102.32	117.20
1	UM	126	PHE	CA-C-N	-6.76	102.33	117.20
1	UO	126	PHE	CA-C-N	-6.76	102.33	117.20
1	UI	126	PHE	CA-C-N	-6.75	102.36	117.20
1	UN	126	PHE	CA-C-N	-6.73	102.39	117.20
1	UP	126	PHE	CA-C-N	-6.73	102.40	117.20
4	F	162	PRO	N-CD-CG	-6.53	93.41	103.20
1	UK	129	GLN	O-C-N	6.38	132.90	122.70
1	UP	129	GLN	O-C-N	6.37	132.89	122.70
1	UO	129	GLN	O-C-N	6.33	132.83	122.70
1	UJ	129	GLN	O-C-N	6.31	132.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	UM	129	GLN	O-C-N	6.30	132.78	122.70
1	WA	162	PRO	N-CA-C	6.29	128.46	112.10
1	UI	129	GLN	O-C-N	6.29	132.76	122.70
1	UN	129	GLN	O-C-N	6.29	132.76	122.70
1	UL	129	GLN	O-C-N	6.28	132.75	122.70
1	UL	126	PHE	C-N-CA	-5.75	107.33	121.70
1	UO	126	PHE	C-N-CA	-5.74	107.36	121.70
1	UK	126	PHE	C-N-CA	-5.73	107.37	121.70
1	UM	126	PHE	C-N-CA	-5.73	107.37	121.70
1	UI	126	PHE	C-N-CA	-5.72	107.39	121.70
1	UN	126	PHE	C-N-CA	-5.72	107.39	121.70
1	UP	126	PHE	C-N-CA	-5.72	107.39	121.70
1	UJ	126	PHE	C-N-CA	-5.72	107.40	121.70
3	E	189	PRO	CA-N-CD	-5.50	103.80	111.50
4	G	162	PRO	N-CA-CB	-5.28	96.80	102.60
1	WJ	214	ASP	CB-CA-C	-5.21	99.99	110.40
7	Y	8	ASP	CB-CG-OD2	5.10	122.89	118.30
1	WO	168	GLU	CB-CA-C	-5.06	100.28	110.40

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	143	ARG	Sidechain
6	Q	106	ARG	Sidechain
6	U	104	ARG	Sidechain
1	UI	221	THR	Mainchain
1	UI	50	ASP	Mainchain
1	UJ	270	THR	Mainchain
1	UJ	50	ASP	Mainchain
1	UK	167	ARG	Sidechain
1	UK	221	THR	Mainchain
1	UK	50	ASP	Mainchain
1	UL	167	ARG	Sidechain
1	UL	221	THR	Mainchain
1	UL	50	ASP	Mainchain
1	UM	221	THR	Mainchain
1	UM	50	ASP	Mainchain
1	UN	221	THR	Mainchain
1	UN	50	ASP	Mainchain
1	UO	221	THR	Mainchain
1	UO	50	ASP	Mainchain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	UP	167	ARG	Sidechain
1	UP	221	THR	Mainchain
1	UP	50	ASP	Mainchain
1	WA	134	ARG	Sidechain
1	WA	142	ARG	Sidechain
1	WA	167	ARG	Sidechain
1	WB	134	ARG	Sidechain
1	WB	142	ARG	Sidechain
1	WB	154	ARG	Sidechain
1	WB	167	ARG	Sidechain
1	WC	134	ARG	Sidechain
1	WC	142	ARG	Sidechain
1	WC	167	ARG	Sidechain
1	WD	134	ARG	Sidechain
1	WE	134	ARG	Sidechain
1	WE	142	ARG	Sidechain
1	WF	134	ARG	Sidechain
1	WF	142	ARG	Sidechain
1	WF	167	ARG	Sidechain
1	WG	134	ARG	Sidechain
1	WG	142	ARG	Sidechain
1	WG	167	ARG	Sidechain
1	WI	142	ARG	Sidechain
1	WJ	134	ARG	Sidechain
1	WJ	142	ARG	Sidechain
1	WJ	167	ARG	Sidechain
1	WK	134	ARG	Sidechain
1	WK	142	ARG	Sidechain
1	WL	134	ARG	Sidechain
1	WL	157	LEU	Mainchain
1	WM	134	ARG	Sidechain
1	WN	134	ARG	Sidechain
1	WO	134	ARG	Sidechain
1	WP	134	ARG	Sidechain
1	WP	142	ARG	Sidechain
1	WP	154	ARG	Sidechain
1	WQ	134	ARG	Sidechain
1	WQ	142	ARG	Sidechain
1	WR	134	ARG	Sidechain
1	WR	142	ARG	Sidechain
1	WR	167	ARG	Sidechain
1	WS	167	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	WT	134	ARG	Sidechain
1	WT	142	ARG	Sidechain
1	WU	134	ARG	Sidechain
1	WU	142	ARG	Sidechain
1	WV	134	ARG	Sidechain
1	WV	142	ARG	Sidechain
1	WV	167	ARG	Sidechain
1	WW	134	ARG	Sidechain
1	WW	167	ARG	Sidechain
7	Y	110	ARG	Sidechain
7	a	110	ARG	Sidechain

## 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	0	1275	0	1254	30	0
1	1	1275	0	1254	50	0
1	2	1275	0	1254	36	0
1	3	1275	0	1254	27	0
1	4	1275	0	1254	33	0
1	5	1275	0	1254	35	0
1	6	1275	0	1254	46	0
1	7	1275	0	1254	50	0
1	8	1275	0	1254	30	0
1	9	1275	0	1254	28	0
1	AA	1275	0	1254	26	0
1	AB	1275	0	1254	40	0
1	AC	1275	0	1254	43	0
1	AD	1275	0	1254	43	0
1	AE	1275	0	1254	42	0
1	AF	1275	0	1254	25	0
1	AG	1275	0	1254	25	0
1	AH	1275	0	1254	48	0
1	AI	1275	0	1254	44	0
1	AJ	1275	0	1254	38	0
1	AK	1275	0	1254	37	0
1	AL	1275	0	1254	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	1275	0	1254	31	0
1	AN	1275	0	1254	27	0
1	AO	1275	0	1254	30	0
1	AP	1275	0	1254	35	0
1	AQ	1275	0	1254	24	0
1	UI	1172	0	1181	62	0
1	UJ	1172	0	1181	78	0
1	UK	1172	0	1181	71	0
1	UL	1172	0	1181	68	0
1	UM	1172	0	1181	67	0
1	UN	1172	0	1181	69	0
1	UO	1172	0	1181	62	0
1	UP	1172	0	1181	65	0
1	WA	849	0	860	79	0
1	WB	836	0	846	79	0
1	WC	812	0	826	68	0
1	WD	827	0	840	93	0
1	WE	843	0	855	88	0
1	WF	834	0	847	62	0
1	WG	843	0	855	71	0
1	WH	703	0	722	67	0
1	WI	703	0	722	74	0
1	WJ	737	0	755	90	0
1	WK	729	0	744	85	0
1	WL	622	0	632	59	0
1	WM	596	0	612	48	0
1	WN	611	0	623	56	0
1	WO	714	0	731	51	0
1	WP	741	0	758	71	0
1	WQ	834	0	847	72	0
1	WR	834	0	847	62	0
1	WS	834	0	847	78	0
1	WT	834	0	847	75	0
1	WU	843	0	855	68	0
1	WV	827	0	838	65	0
1	WW	834	0	847	86	0
1	b	81	0	78	0	0
1	c	103	0	99	0	0
1	d	133	0	129	0	0
1	e	103	0	99	0	0
1	f	140	0	136	0	0
1	g	103	0	99	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	140	0	136	0	0
1	i	103	0	99	0	0
1	j	133	0	129	0	0
1	k	103	0	99	0	0
1	l	140	0	136	0	0
1	t	1275	0	1254	0	0
1	u	1275	0	1254	0	0
1	v	1275	0	1254	0	0
1	w	1275	0	1254	0	0
1	x	1275	0	1254	0	0
1	y	1275	0	1254	0	0
1	z	1275	0	1254	0	0
2	A	670	0	739	34	0
2	B	670	0	739	35	0
2	C	670	0	739	31	0
2	D	670	0	739	32	0
3	E	1945	0	2063	113	0
4	F	1605	0	1701	78	0
4	G	1626	0	1718	58	0
4	H	1614	0	1709	52	0
4	I	1614	0	1709	71	0
4	J	1623	0	1715	83	0
5	K	429	0	445	37	0
5	L	672	0	684	49	0
5	M	686	0	700	52	0
5	N	686	0	700	43	0
5	O	686	0	700	22	0
5	P	679	0	693	28	0
6	Q	1030	0	1025	23	0
6	R	942	0	943	35	0
6	S	967	0	968	59	0
6	T	982	0	984	43	0
6	U	950	0	946	51	0
7	V	969	0	981	17	0
7	W	964	0	976	15	0
7	X	969	0	981	14	0
7	Y	969	0	981	15	0
7	Z	969	0	981	19	0
7	a	969	0	981	0	0
All	All	99073	0	99719	3015	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 16.



All (3015) 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)
1:WD:168:GLU:CD	1:WD:170:LYS:HE3	1.40	1.38
1:WC:121:PHE:HZ	2:C:15:LYS:NZ	1.21	1.35
1:UP:103:GLN:HG2	1:WW:182:PRO:CB	1.58	1.33
1:UP:103:GLN:CG	1:WW:182:PRO:HB3	1.56	1.32
5:L:11:ILE:HG22	1:AH:372:ILE:CD1	1.58	1.32
6:U:72:HIS:CD2	1:1:365:ASN:HB3	1.64	1.32
6:S:73:ILE:CD1	1:AE:297:GLN:HB2	1.61	1.31
1:WJ:164:LEU:HD13	3:E:145:TRP:CD1	1.65	1.29
1:WD:168:GLU:CG	1:WD:170:LYS:HE3	1.64	1.28
1:WP:166:VAL:CG2	4:F:160:GLN:HB3	1.63	1.28
6:R:72:HIS:ND1	1:AJ:365:ASN:HB3	1.47	1.25
5:L:7:ILE:HD11	1:AI:370:ARG:NH2	1.54	1.23
1:WQ:197:LEU:HD12	1:WR:175:SER:OG	1.39	1.23
1:WF:197:LEU:HD12	1:WG:175:SER:OG	1.34	1.23
1:WR:197:LEU:HD12	1:WS:175:SER:OG	1.36	1.22
5:K:7:ILE:HG21	1:AM:278:THR:CG2	1.69	1.22
1:WA:128:GLU:HG2	1:WB:126:PHE:CD2	1.74	1.22
1:WA:128:GLU:CG	1:WB:126:PHE:CD2	2.23	1.21
5:L:11:ILE:CG2	1:AH:372:ILE:HG21	1.68	1.21
1:WD:165:PHE:HB2	4:I:142:THR:O	1.35	1.21
1:WK:167:ARG:HG2	3:E:156:THR:HG22	1.22	1.21
1:WA:128:GLU:CG	1:WB:126:PHE:HD2	1.56	1.19
1:WI:197:LEU:HD12	1:WJ:175:SER:CB	1.74	1.18
6:U:78:VAL:CG1	1:1:299:ASN:HD22	1.58	1.17
6:T:72:HIS:CD2	1:7:365:ASN:HB3	1.79	1.16
1:WJ:197:LEU:HD12	1:WK:175:SER:OG	1.42	1.16
5:L:11:ILE:HG21	1:AH:372:ILE:CG2	1.74	1.15
6:U:78:VAL:HG11	1:1:299:ASN:ND2	1.61	1.15
1:WA:158:ALA:HB2	1:WW:200:SER:O	1.44	1.15
1:WR:197:LEU:HD12	1:WS:175:SER:CB	1.75	1.14
1:WK:197:LEU:HD12	1:WL:175:SER:CB	1.77	1.14
1:UJ:103:GLN:HB3	1:WD:182:PRO:HB3	1.20	1.14
1:WI:197:LEU:HD12	1:WJ:175:SER:OG	1.47	1.13
1:WE:166:VAL:CG2	4:I:160:GLN:HA	1.78	1.13
1:WK:193:ALA:HB1	1:WL:213:VAL:HG21	1.28	1.13
6:T:68:THR:HG21	1:7:367:GLU:OE1	1.49	1.13
6:U:68:THR:HG21	1:1:367:GLU:OE1	1.49	1.13
1:WS:200:SER:O	1:WT:158:ALA:HB2	1.46	1.12
1:WA:128:GLU:HG2	1:WB:126:PHE:HD2	0.96	1.12
1:WO:181:GLU:HB2	1:WO:184:ARG:HG3	1.14	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WR:112:GLY:HA2	1:WR:135:ALA:HA	1.27	1.12
5:M:11:ILE:HD12	5:M:12:SER:N	1.64	1.12
1:WJ:164:LEU:HD22	3:E:145:TRP:CD1	1.83	1.12
1:WP:166:VAL:HG22	4:F:160:GLN:CB	1.79	1.12
5:K:14:LEU:HD23	1:AL:278:THR:CG2	1.78	1.12
1:WL:197:LEU:HD12	1:WM:175:SER:OG	1.49	1.11
1:WG:181:GLU:HB2	1:WG:184:ARG:HG3	1.14	1.11
1:WJ:164:LEU:HB2	3:E:145:TRP:NE1	1.65	1.11
1:WK:181:GLU:HB2	1:WK:184:ARG:HG3	1.14	1.11
1:WP:181:GLU:HB2	1:WP:184:ARG:HG3	1.14	1.11
6:U:78:VAL:CG1	1:1:299:ASN:ND2	2.13	1.11
1:WF:181:GLU:HB2	1:WF:184:ARG:HG3	1.14	1.10
1:WO:200:SER:OG	1:WP:175:SER:HB2	1.50	1.10
5:K:7:ILE:HG21	1:AM:278:THR:HG21	1.20	1.10
5:P:19:MET:HA	1:AP:276:GLU:OE2	1.51	1.10
1:WE:181:GLU:HB2	1:WE:184:ARG:HG3	1.14	1.10
1:WU:197:LEU:HD12	1:WV:175:SER:OG	1.51	1.10
5:P:21:ALA:CB	1:AP:278:THR:HG21	1.80	1.10
1:UN:167:ARG:NH2	1:WQ:188:GLU:HB3	1.68	1.09
5:L:14:LEU:HD21	1:AH:370:ARG:HH21	1.07	1.09
1:WA:197:LEU:HD12	1:WB:175:SER:OG	1.50	1.09
1:WD:168:GLU:CD	1:WD:170:LYS:CE	2.21	1.09
1:WU:181:GLU:HB2	1:WU:184:ARG:HG3	1.14	1.09
5:M:7:ILE:HB	1:AB:278:THR:HG21	1.16	1.09
1:WC:121:PHE:CZ	2:C:15:LYS:NZ	2.02	1.09
1:WA:181:GLU:HB2	1:WA:184:ARG:HG3	1.14	1.09
1:WR:181:GLU:HB2	1:WR:184:ARG:HG3	1.14	1.09
5:L:4:ILE:HG12	1:AI:372:ILE:CG2	1.81	1.09
1:WA:158:ALA:CB	1:WW:200:SER:O	2.00	1.08
1:WW:181:GLU:HB2	1:WW:184:ARG:HG3	1.14	1.08
1:WQ:181:GLU:HB2	1:WQ:184:ARG:HG3	1.13	1.08
1:WV:181:GLU:HB2	1:WV:184:ARG:HG3	1.14	1.08
5:P:21:ALA:HB1	1:AP:278:THR:HG21	1.29	1.08
1:WJ:197:LEU:HD12	1:WK:175:SER:CB	1.82	1.08
1:WN:181:GLU:HB2	1:WN:184:ARG:HG3	1.14	1.08
1:WT:181:GLU:HB2	1:WT:184:ARG:HG3	1.14	1.08
1:WE:112:GLY:HA2	1:WE:135:ALA:HA	1.31	1.08
1:WD:181:GLU:HB2	1:WD:184:ARG:HG3	1.14	1.08
1:WL:181:GLU:HB2	1:WL:184:ARG:HG3	1.14	1.08
1:WS:181:GLU:HB2	1:WS:184:ARG:HG3	1.13	1.07
1:WM:181:GLU:HB2	1:WM:184:ARG:HG3	1.14	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:11:ILE:HG22	1:AH:372:ILE:HD13	1.36	1.07
1:WE:166:VAL:HG22	4:I:160:GLN:HA	1.11	1.07
5:K:7:ILE:CG2	1:AM:278:THR:HG21	1.85	1.07
6:S:72:HIS:ND1	1:AD:365:ASN:HB3	1.67	1.07
1:WB:181:GLU:HB2	1:WB:184:ARG:HG3	1.14	1.07
1:WI:181:GLU:HB2	1:WI:184:ARG:HG3	1.14	1.07
5:K:21:ALA:CB	1:AK:278:THR:HG21	1.83	1.07
5:N:21:ALA:CB	1:4:278:THR:HG21	1.84	1.07
1:WN:196:HIS:HB3	1:WO:211:THR:HG21	1.34	1.07
1:UK:207:PRO:HB2	1:WE:187:ASP:OD1	1.56	1.06
1:WG:200:SER:OG	1:WH:175:SER:HB2	1.54	1.06
1:WH:181:GLU:HB2	1:WH:184:ARG:HG3	1.13	1.06
1:WJ:181:GLU:HB2	1:WJ:184:ARG:HG3	1.14	1.06
5:L:7:ILE:CD1	1:AI:370:ARG:HH21	1.67	1.06
1:WK:196:HIS:HB3	1:WL:211:THR:HG21	1.33	1.06
1:WS:164:LEU:HB2	2:A:89:GLY:O	1.54	1.06
6:S:65:LEU:HB2	1:AD:295:SER:HB2	1.35	1.06
1:WC:186:LEU:HD22	1:WC:190:GLN:HG2	1.38	1.05
6:T:68:THR:OG1	6:T:72:HIS:CE1	2.07	1.05
1:UK:207:PRO:CB	1:WE:187:ASP:OD1	2.04	1.05
5:K:14:LEU:HD23	1:AL:278:THR:HG21	1.37	1.05
1:WG:112:GLY:HA2	1:WG:135:ALA:HA	1.36	1.05
1:WS:112:GLY:HA2	1:WS:135:ALA:HA	1.12	1.05
1:UJ:103:GLN:HB3	1:WD:182:PRO:CB	1.85	1.05
1:WN:201:ALA:HA	1:WO:158:ALA:HB2	1.33	1.05
1:WM:143:THR:OG1	1:WN:154:ARG:HG2	1.57	1.04
6:S:72:HIS:CB	1:AE:295:SER:HB3	1.87	1.04
1:WJ:164:LEU:HB2	3:E:145:TRP:HE1	1.14	1.04
1:WF:122:GLY:HA2	2:D:68:TRP:HE1	1.20	1.04
5:M:11:ILE:HG22	1:AB:372:ILE:CG2	1.87	1.04
1:WD:200:SER:O	1:WE:158:ALA:HB2	1.58	1.04
5:L:11:ILE:HG22	1:AH:372:ILE:HD12	1.38	1.04
1:WJ:164:LEU:CD1	3:E:145:TRP:CD1	2.41	1.03
1:WM:200:SER:OG	1:WN:175:SER:HB2	1.58	1.03
5:L:7:ILE:HD11	1:AI:370:ARG:HH21	1.00	1.03
1:WE:166:VAL:HG22	4:I:160:GLN:CA	1.86	1.03
1:WK:197:LEU:HD12	1:WL:175:SER:HB3	1.07	1.03
6:T:55:ARG:NH2	1:5:299:ASN:ND2	2.06	1.03
1:WJ:128:GLU:HG2	1:WK:126:PHE:HD2	1.22	1.03
1:WL:197:LEU:HD12	1:WM:175:SER:CB	1.88	1.03
1:WV:112:GLY:HA2	1:WV:135:ALA:HA	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:73:ILE:HG13	1:AK:295:SER:HB2	1.38	1.02
1:WL:197:LEU:CD1	1:WM:175:SER:OG	2.06	1.02
1:WO:197:LEU:HD12	1:WP:175:SER:OG	1.58	1.02
1:WD:168:GLU:CG	1:WD:170:LYS:CE	2.37	1.02
1:WR:197:LEU:CD1	1:WS:175:SER:OG	2.07	1.02
1:WT:197:LEU:HD12	1:WU:175:SER:OG	1.57	1.02
1:WN:200:SER:O	1:WO:158:ALA:CB	2.07	1.02
1:UK:207:PRO:HD2	1:WE:187:ASP:CG	1.80	1.02
1:WF:197:LEU:HD12	1:WG:175:SER:CB	1.89	1.02
1:WH:203:ALA:HB1	1:WI:160:PRO:HB3	1.39	1.02
1:WA:128:GLU:HG3	1:WB:126:PHE:CE2	1.95	1.01
1:WW:165:PHE:HE1	2:B:89:GLY:HA2	1.20	1.01
6:U:65:LEU:CD2	1:1:297:GLN:HB2	1.90	1.01
1:UJ:103:GLN:OE1	1:WD:182:PRO:HB3	1.58	1.01
1:WW:164:LEU:HD12	2:B:89:GLY:O	1.60	1.01
1:WE:167:ARG:HD3	4:I:161:GLY:HA2	1.40	1.01
1:WG:164:LEU:O	4:J:241:GLN:HG2	1.58	1.01
1:WJ:164:LEU:HD22	3:E:145:TRP:HD1	1.26	1.01
1:WN:200:SER:O	1:WO:158:ALA:HB3	1.59	1.01
1:WT:196:HIS:HB3	1:WU:211:THR:HG21	1.41	1.01
1:WA:112:GLY:HA2	1:WA:135:ALA:HA	1.41	1.00
5:N:21:ALA:HB3	1:4:278:THR:HG21	1.43	1.00
1:WA:160:PRO:HB3	1:WW:203:ALA:HB1	1.38	1.00
1:WJ:164:LEU:CD2	3:E:145:TRP:HD1	1.74	1.00
6:U:78:VAL:HG11	1:1:299:ASN:HD22	0.86	1.00
1:UP:62:ASP:OD2	1:WV:184:ARG:NH2	1.95	1.00
1:WS:200:SER:O	1:WT:158:ALA:CB	2.09	1.00
1:WD:168:GLU:HG2	1:WD:170:LYS:HE3	1.42	0.99
5:M:11:ILE:CG2	1:AB:372:ILE:HG21	1.92	0.99
1:WC:164:LEU:O	4:I:241:GLN:HG2	1.61	0.99
1:WH:200:SER:O	1:WI:158:ALA:HB2	1.62	0.99
1:WJ:197:LEU:CD1	1:WK:175:SER:OG	2.11	0.99
1:WD:200:SER:OG	1:WE:175:SER:HB2	1.59	0.99
1:WM:193:ALA:HB1	1:WN:213:VAL:HG11	1.44	0.99
1:UK:207:PRO:HD2	1:WE:187:ASP:OD2	1.61	0.99
1:WA:128:GLU:HG3	1:WB:126:PHE:CD2	1.96	0.98
1:UM:125:GLN:O	1:UM:129:GLN:N	1.97	0.98
1:UK:73:MET:CE	1:UK:99:ARG:HD3	1.93	0.98
1:UN:125:GLN:O	1:UN:129:GLN:N	1.97	0.98
1:UO:125:GLN:O	1:UO:129:GLN:N	1.97	0.98
5:M:11:ILE:CG2	1:AB:372:ILE:CG2	2.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UN:73:MET:CE	1:UN:99:ARG:HD3	1.93	0.98
1:UP:125:GLN:O	1:UP:129:GLN:N	1.97	0.98
1:WF:197:LEU:CD1	1:WG:175:SER:OG	2.11	0.98
1:UJ:73:MET:CE	1:UJ:99:ARG:HD3	1.93	0.98
1:UP:73:MET:CE	1:UP:99:ARG:HD3	1.93	0.98
1:WK:164:LEU:HD12	3:E:248:PHE:HB3	1.46	0.98
3:E:185:MET:O	3:E:189:PRO:HD2	1.64	0.97
1:WC:164:LEU:O	4:I:241:GLN:CG	2.12	0.97
1:UL:73:MET:CE	1:UL:99:ARG:HD3	1.93	0.97
1:UO:73:MET:CE	1:UO:99:ARG:HD3	1.93	0.97
5:M:14:LEU:HB3	1:AA:278:THR:HG21	1.45	0.97
1:UI:73:MET:CE	1:UI:99:ARG:HD3	1.93	0.97
5:M:11:ILE:HD12	5:M:11:ILE:C	1.84	0.97
1:WI:197:LEU:CD1	1:WJ:175:SER:OG	2.12	0.97
5:L:11:ILE:HG21	1:AH:372:ILE:HG21	1.34	0.97
1:WT:197:LEU:HD12	1:WU:175:SER:CB	1.94	0.96
1:UI:125:GLN:O	1:UI:129:GLN:N	1.97	0.96
1:UM:73:MET:CE	1:UM:99:ARG:HD3	1.93	0.96
1:WC:121:PHE:HZ	2:C:15:LYS:CE	1.76	0.96
1:UK:125:GLN:O	1:UK:129:GLN:N	1.97	0.96
1:WI:196:HIS:HB3	1:WJ:211:THR:HG21	1.45	0.96
1:WP:166:VAL:HG22	4:F:160:GLN:HB3	0.99	0.96
6:T:78:VAL:O	1:7:299:ASN:ND2	1.99	0.96
1:UL:125:GLN:O	1:UL:129:GLN:N	1.97	0.96
1:WK:164:LEU:HD12	3:E:248:PHE:CB	1.96	0.96
1:WE:197:LEU:HD12	1:WF:175:SER:OG	1.63	0.96
5:M:11:ILE:HG22	1:AB:372:ILE:HG21	1.44	0.96
6:U:72:HIS:HD2	1:1:365:ASN:HB3	0.98	0.96
1:UJ:125:GLN:O	1:UJ:129:GLN:N	1.97	0.96
1:WT:112:GLY:HA2	1:WT:135:ALA:HA	1.48	0.95
1:WA:200:SER:OG	1:WB:175:SER:HB2	1.64	0.95
5:L:4:ILE:CG1	1:AI:372:ILE:CG2	2.44	0.95
1:WH:200:SER:OG	1:WI:175:SER:HB2	1.67	0.95
5:L:11:ILE:CG2	1:AH:372:ILE:CG2	2.38	0.95
6:R:72:HIS:CE1	1:AJ:365:ASN:HB3	2.02	0.95
1:UP:133:GLN:NE2	1:UP:157:LEU:O	2.00	0.95
1:WC:200:SER:O	1:WD:158:ALA:HB2	1.64	0.95
1:WD:165:PHE:HB3	4:I:143:ARG:HA	1.48	0.95
1:WK:197:LEU:CD1	1:WL:175:SER:HB3	1.96	0.95
1:UI:133:GLN:NE2	1:UI:157:LEU:O	2.00	0.94
1:UJ:133:GLN:NE2	1:UJ:157:LEU:O	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WE:200:SER:OG	1:WF:175:SER:HB2	1.67	0.94
1:WH:193:ALA:HB1	1:WI:213:VAL:HG11	1.46	0.94
1:UK:133:GLN:NE2	1:UK:157:LEU:O	2.00	0.94
1:UM:133:GLN:NE2	1:UM:157:LEU:O	2.00	0.94
1:UN:133:GLN:NE2	1:UN:157:LEU:O	2.00	0.94
1:UL:133:GLN:NE2	1:UL:157:LEU:O	2.00	0.94
1:UO:103:GLN:CD	1:WU:182:PRO:HB3	1.87	0.94
1:WI:197:LEU:HD12	1:WJ:175:SER:HB3	1.47	0.94
1:UM:62:ASP:OD2	1:WP:184:ARG:NH2	1.99	0.94
1:WS:112:GLY:CA	1:WS:135:ALA:HA	1.97	0.94
6:T:78:VAL:C	1:7:299:ASN:HD21	1.70	0.94
1:WT:200:SER:O	1:WU:158:ALA:CB	2.15	0.93
6:Q:65:LEU:HD22	1:AQ:295:SER:HB2	1.49	0.93
1:UO:133:GLN:NE2	1:UO:157:LEU:O	2.00	0.93
6:S:72:HIS:HB2	1:AE:295:SER:HB3	1.48	0.93
1:UK:207:PRO:CG	1:WE:187:ASP:OD1	2.16	0.93
5:L:4:ILE:HD11	1:AI:372:ILE:HG22	1.49	0.93
5:L:4:ILE:HG12	1:AI:372:ILE:CB	1.98	0.92
1:WP:200:SER:OG	1:WQ:175:SER:HB2	1.69	0.92
1:WS:112:GLY:HA2	1:WS:135:ALA:CA	1.99	0.92
6:T:72:HIS:HD2	1:7:365:ASN:HB3	1.15	0.92
1:WA:197:LEU:HD12	1:WB:175:SER:CB	1.99	0.92
1:WR:112:GLY:CA	1:WR:135:ALA:HA	2.00	0.92
1:WS:124:SER:HB2	2:A:8:MET:CE	2.00	0.92
1:UN:62:ASP:OD2	1:WR:184:ARG:NH2	2.02	0.92
1:WF:181:GLU:CB	1:WF:184:ARG:HG3	2.00	0.91
1:WP:181:GLU:CB	1:WP:184:ARG:HG3	2.01	0.91
1:WT:181:GLU:CB	1:WT:184:ARG:HG3	2.00	0.91
1:WA:181:GLU:CB	1:WA:184:ARG:HG3	2.01	0.91
1:WM:181:GLU:CB	1:WM:184:ARG:HG3	2.01	0.91
1:WE:181:GLU:CB	1:WE:184:ARG:HG3	2.01	0.91
1:WB:181:GLU:CB	1:WB:184:ARG:HG3	2.01	0.91
1:WI:164:LEU:HD22	4:J:148:ALA:HB2	1.50	0.91
1:WS:121:PHE:HE1	1:WT:120:LYS:HZ3	0.94	0.91
5:L:14:LEU:CD2	1:AH:370:ARG:HH21	1.83	0.90
1:WQ:181:GLU:CB	1:WQ:184:ARG:HG3	2.00	0.90
5:K:14:LEU:CD2	1:AL:278:THR:HG21	2.01	0.90
1:WU:181:GLU:CB	1:WU:184:ARG:HG3	2.00	0.90
1:WI:181:GLU:CB	1:WI:184:ARG:HG3	2.01	0.90
1:WG:181:GLU:CB	1:WG:184:ARG:HG3	2.01	0.90
1:WD:181:GLU:CB	1:WD:184:ARG:HG3	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:73:ILE:HD13	1:AE:297:GLN:HB2	1.54	0.90
1:WJ:164:LEU:CD2	3:E:145:TRP:CD1	2.53	0.90
1:UM:103:GLN:CD	1:WQ:182:PRO:HB3	1.93	0.90
1:WG:165:PHE:CZ	4:I:153:LEU:HD21	2.07	0.90
1:WG:165:PHE:HE1	4:J:240:ALA:HB3	1.36	0.90
1:WH:181:GLU:CB	1:WH:184:ARG:HG3	2.00	0.89
1:WM:197:LEU:HD12	1:WN:175:SER:OG	1.72	0.89
1:WJ:128:GLU:CG	1:WK:126:PHE:HD2	1.84	0.89
1:WK:181:GLU:CB	1:WK:184:ARG:HG3	2.01	0.89
1:WD:168:GLU:HG2	1:WD:170:LYS:CE	2.00	0.89
1:WV:181:GLU:CB	1:WV:184:ARG:HG3	2.01	0.89
3:E:158:PRO:HG2	3:E:162:ASN:HD21	1.35	0.89
5:K:14:LEU:HD23	1:AL:278:THR:HG22	1.55	0.89
1:WB:197:LEU:HD12	1:WC:175:SER:OG	1.72	0.89
1:WD:115:LEU:HD22	1:WD:134:ARG:HD2	1.54	0.89
1:WR:197:LEU:HD12	1:WS:175:SER:HB3	1.54	0.89
1:WW:165:PHE:CE1	2:B:89:GLY:HA2	2.07	0.89
6:T:55:ARG:CZ	1:5:299:ASN:ND2	2.35	0.89
1:WD:200:SER:O	1:WE:158:ALA:CB	2.20	0.89
1:WI:164:LEU:HD22	4:J:148:ALA:CB	2.02	0.89
1:WO:181:GLU:CB	1:WO:184:ARG:HG3	2.00	0.89
1:WJ:181:GLU:CB	1:WJ:184:ARG:HG3	2.00	0.88
1:WR:181:GLU:CB	1:WR:184:ARG:HG3	2.01	0.88
1:WW:181:GLU:CB	1:WW:184:ARG:HG3	2.01	0.88
6:S:65:LEU:HB2	1:AD:295:SER:CB	2.03	0.88
1:UM:126:PHE:CE1	1:UM:130:VAL:HG21	2.09	0.88
1:WN:181:GLU:CB	1:WN:184:ARG:HG3	2.01	0.88
1:UN:126:PHE:O	1:UN:130:VAL:N	2.07	0.88
1:UP:126:PHE:CE1	1:UP:130:VAL:HG21	2.09	0.88
1:UK:126:PHE:CE1	1:UK:130:VAL:HG21	2.09	0.88
1:UM:126:PHE:O	1:UM:130:VAL:N	2.07	0.87
1:UO:126:PHE:CE1	1:UO:130:VAL:HG21	2.09	0.87
1:WS:181:GLU:CB	1:WS:184:ARG:HG3	2.00	0.87
6:T:72:HIS:HD2	1:7:365:ASN:CB	1.87	0.87
1:UO:126:PHE:O	1:UO:130:VAL:N	2.07	0.87
1:WT:121:PHE:CZ	1:WU:122:GLY:O	2.27	0.87
1:UI:126:PHE:CE1	1:UI:130:VAL:HG21	2.09	0.87
1:WL:181:GLU:CB	1:WL:184:ARG:HG3	2.01	0.87
5:L:4:ILE:HG12	1:AI:372:ILE:HB	1.54	0.87
1:UK:126:PHE:O	1:UK:130:VAL:N	2.07	0.87
1:WV:200:SER:O	1:WW:158:ALA:HB2	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UJ:126:PHE:CE1	1:UJ:130:VAL:HG21	2.09	0.87
1:UL:126:PHE:CE1	1:UL:130:VAL:HG21	2.09	0.87
1:WD:165:PHE:HE2	4:I:141:GLN:HA	1.39	0.87
1:UN:126:PHE:CE1	1:UN:130:VAL:HG21	2.09	0.87
1:UP:126:PHE:O	1:UP:130:VAL:N	2.07	0.87
1:UJ:126:PHE:O	1:UJ:130:VAL:N	2.07	0.86
1:WK:200:SER:O	1:WL:158:ALA:HB3	1.75	0.86
1:WC:121:PHE:CZ	2:C:15:LYS:CE	2.56	0.86
1:WD:203:ALA:HB1	1:WE:160:PRO:HB3	1.57	0.86
6:S:73:ILE:HD12	1:AE:297:GLN:HB2	1.57	0.86
1:WC:200:SER:O	1:WD:158:ALA:CB	2.23	0.86
1:WM:139:GLU:HB3	1:WN:154:ARG:HH21	1.39	0.86
5:L:4:ILE:HG12	1:AI:372:ILE:HG21	1.57	0.86
1:WK:132:TYR:HB2	1:WL:126:PHE:HZ	1.40	0.86
1:WA:196:HIS:HB3	1:WB:211:THR:HG21	1.57	0.86
1:WB:200:SER:OG	1:WC:175:SER:HB2	1.76	0.86
1:WK:193:ALA:HB1	1:WL:213:VAL:CG2	2.06	0.86
1:WS:124:SER:HB2	2:A:8:MET:HE2	1.57	0.86
1:WO:166:VAL:HG23	4:F:139:LEU:O	1.75	0.86
1:WS:121:PHE:HE1	1:WT:120:LYS:NZ	1.74	0.86
5:L:4:ILE:CG1	1:AI:372:ILE:HG21	2.04	0.86
1:UL:126:PHE:O	1:UL:130:VAL:N	2.07	0.85
1:UJ:103:GLN:CB	1:WD:182:PRO:HB3	2.04	0.85
1:WR:196:HIS:HB3	1:WS:211:THR:HG21	1.56	0.85
1:WR:200:SER:O	1:WS:158:ALA:CB	2.24	0.85
5:K:21:ALA:HB1	1:AK:278:THR:HG21	1.56	0.85
1:UI:126:PHE:O	1:UI:130:VAL:N	2.07	0.85
1:UJ:126:PHE:O	1:UJ:130:VAL:HG23	1.77	0.85
1:UM:103:GLN:CG	1:WQ:182:PRO:HB3	2.06	0.85
1:WH:200:SER:O	1:WI:158:ALA:CB	2.23	0.85
1:WK:167:ARG:CG	3:E:156:THR:HG22	2.04	0.85
6:U:65:LEU:HD22	1:I:297:GLN:HB2	1.57	0.85
1:UI:126:PHE:O	1:UI:130:VAL:HG23	1.77	0.85
1:WV:200:SER:O	1:WW:158:ALA:CB	2.25	0.85
1:WM:197:LEU:HD12	1:WN:175:SER:CB	2.05	0.84
1:WS:125:GLN:HB2	2:A:4:GLU:HB2	1.57	0.84
1:WJ:164:LEU:CD1	3:E:145:TRP:HD1	1.82	0.84
6:T:68:THR:HG1	6:T:72:HIS:CE1	1.94	0.84
1:UN:126:PHE:O	1:UN:130:VAL:HG23	1.77	0.84
1:WU:197:LEU:HD12	1:WV:175:SER:CB	2.07	0.84
6:T:78:VAL:HG12	1:6:361:ASN:HD22	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WC:165:PHE:HD2	4:H:152:ARG:HH21	1.21	0.84
1:WA:175:SER:HB2	1:WW:200:SER:OG	1.76	0.84
1:WA:175:SER:CB	1:WW:197:LEU:HD12	2.08	0.84
1:WF:122:GLY:HA2	2:D:68:TRP:NE1	1.93	0.84
1:UK:126:PHE:O	1:UK:130:VAL:HG23	1.77	0.84
1:UO:103:GLN:NE2	1:WU:182:PRO:HB3	1.92	0.84
1:UP:126:PHE:O	1:UP:130:VAL:HG23	1.77	0.84
1:UL:126:PHE:O	1:UL:130:VAL:HG23	1.77	0.84
5:L:4:ILE:CD1	1:AI:372:ILE:HG22	2.08	0.84
6:Q:88:ARG:NH1	6:Q:105:GLU:OE1	2.10	0.84
1:WT:200:SER:O	1:WU:158:ALA:HB2	1.77	0.84
6:S:76:GLN:O	1:AD:297:GLN:OE1	1.96	0.84
1:UJ:167:ARG:NH2	1:WB:188:GLU:HB3	1.92	0.83
3:E:182:ASN:HB3	3:E:239:PHE:HZ	1.43	0.83
5:M:7:ILE:HB	1:AB:278:THR:CG2	2.07	0.83
1:UO:126:PHE:O	1:UO:130:VAL:HG23	1.77	0.83
1:UJ:103:GLN:OE1	1:WD:182:PRO:CB	2.26	0.83
1:UM:126:PHE:O	1:UM:130:VAL:HG23	1.77	0.83
1:UN:94:HIS:HB3	1:UN:146:THR:HG21	1.60	0.83
1:WJ:164:LEU:CG	3:E:145:TRP:HD1	1.91	0.83
1:WQ:200:SER:OG	1:WR:175:SER:HB2	1.78	0.83
1:UP:94:HIS:HB3	1:UP:146:THR:HG21	1.61	0.83
1:UL:94:HIS:HB3	1:UL:146:THR:HG21	1.60	0.83
5:L:14:LEU:HD21	1:AH:370:ARG:NH2	1.91	0.83
1:UO:94:HIS:HB3	1:UO:146:THR:HG21	1.60	0.83
1:WP:166:VAL:CG2	4:F:160:GLN:CB	2.46	0.83
6:T:55:ARG:NH2	1:5:299:ASN:HD22	1.75	0.83
1:WG:200:SER:O	1:WH:158:ALA:HB2	1.79	0.83
1:WT:197:LEU:CD1	1:WU:175:SER:OG	2.27	0.82
1:WJ:164:LEU:CG	3:E:145:TRP:CD1	2.62	0.82
5:L:7:ILE:HD11	1:AI:370:ARG:CZ	2.08	0.82
1:UI:94:HIS:HB3	1:UI:146:THR:HG21	1.60	0.82
1:UJ:167:ARG:HH22	1:WB:188:GLU:HB3	1.44	0.82
1:UK:207:PRO:CD	1:WE:187:ASP:OD1	2.27	0.82
1:WW:125:GLN:OE1	2:B:2:THR:CG2	2.28	0.82
5:M:21:ALA:HB1	1:0:278:THR:HG21	1.62	0.82
5:N:11:ILE:HG22	1:6:372:ILE:HD12	1.62	0.82
7:Z:6:ILE:HG21	7:Z:122:VAL:HG11	1.59	0.82
6:U:78:VAL:HG12	1:1:299:ASN:ND2	1.93	0.82
1:UL:128:GLU:O	1:UL:132:TYR:N	2.13	0.81
1:UP:127:SER:O	1:UP:131:ASN:N	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UK:128:GLU:O	1:UK:132:TYR:N	2.13	0.81
1:UL:73:MET:HE1	1:UL:99:ARG:HD3	1.59	0.81
1:UO:127:SER:O	1:UO:131:ASN:N	2.13	0.81
1:WK:196:HIS:CB	1:WL:211:THR:HG21	2.10	0.81
1:UM:103:GLN:HG2	1:WQ:182:PRO:HB3	1.61	0.81
1:WJ:164:LEU:CD2	3:E:144:LEU:HB2	2.10	0.81
2:C:28:ALA:HB1	2:C:54:LYS:HE3	1.60	0.81
5:P:21:ALA:HB1	1:AP:278:THR:CG2	2.10	0.81
1:UI:127:SER:O	1:UI:131:ASN:N	2.13	0.81
1:UJ:94:HIS:HB3	1:UJ:146:THR:HG21	1.60	0.81
1:UL:127:SER:O	1:UL:131:ASN:N	2.13	0.81
1:UM:94:HIS:HB3	1:UM:146:THR:HG21	1.60	0.81
1:WI:200:SER:O	1:WJ:158:ALA:CB	2.29	0.81
6:U:33:ALA:O	6:U:98:ASN:ND2	2.13	0.81
1:UJ:128:GLU:O	1:UJ:132:TYR:N	2.13	0.81
1:UK:94:HIS:HB3	1:UK:146:THR:HG21	1.60	0.81
1:UN:127:SER:O	1:UN:131:ASN:N	2.13	0.81
1:UJ:127:SER:O	1:UJ:131:ASN:N	2.13	0.80
1:UK:127:SER:O	1:UK:131:ASN:N	2.13	0.80
1:UM:127:SER:O	1:UM:131:ASN:N	2.13	0.80
1:WA:197:LEU:CD1	1:WB:175:SER:OG	2.28	0.80
1:WK:143:THR:CB	1:WL:156:HIS:HE2	1.94	0.80
6:U:72:HIS:HD2	1:1:365:ASN:CB	1.88	0.80
1:WK:165:PHE:HA	3:E:149:LEU:HD13	1.62	0.80
1:WP:200:SER:O	1:WQ:158:ALA:HB2	1.80	0.80
1:UI:128:GLU:O	1:UI:132:TYR:N	2.13	0.80
1:WT:121:PHE:CE1	1:WU:122:GLY:O	2.34	0.80
4:F:100:ILE:HG23	4:F:101:MET:HE2	1.63	0.80
1:WG:165:PHE:CE1	4:J:240:ALA:HB3	2.17	0.80
1:WH:143:THR:OG1	1:WI:154:ARG:HG2	1.82	0.80
5:M:11:ILE:HG22	1:AB:372:ILE:CB	2.11	0.80
5:P:14:LEU:HB3	1:AQ:278:THR:HG21	1.64	0.80
1:UK:73:MET:HE3	1:UK:99:ARG:HD3	1.62	0.80
1:WJ:164:LEU:CD2	3:E:144:LEU:CB	2.60	0.80
5:M:7:ILE:HD11	1:AC:370:ARG:HE	1.46	0.80
1:WU:200:SER:OG	1:WV:175:SER:HB2	1.82	0.79
1:WV:197:LEU:HD12	1:WW:175:SER:CB	2.12	0.79
7:Y:6:ILE:HG21	7:Y:122:VAL:HG21	1.62	0.79
1:WG:197:LEU:HD12	1:WH:175:SER:OG	1.82	0.79
1:WH:181:GLU:HB2	1:WH:184:ARG:CG	2.07	0.79
1:UN:73:MET:HE1	1:UN:99:ARG:HD3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WM:181:GLU:HB2	1:WM:184:ARG:CG	2.07	0.79
4:J:83:ALA:HB3	4:J:84:PRO:HD3	1.62	0.79
1:WB:164:LEU:O	4:H:152:ARG:HD3	1.81	0.79
1:WJ:181:GLU:HB2	1:WJ:184:ARG:CG	2.07	0.79
1:UK:207:PRO:CD	1:WE:187:ASP:CG	2.51	0.79
1:WF:200:SER:OG	1:WG:175:SER:HB2	1.81	0.79
1:WG:143:THR:OG1	1:WH:154:ARG:HG2	1.83	0.79
1:WO:181:GLU:HB2	1:WO:184:ARG:CG	2.07	0.79
1:UM:128:GLU:O	1:UM:132:TYR:N	2.13	0.79
1:WA:175:SER:OG	1:WW:197:LEU:HD12	1.83	0.79
1:WJ:197:LEU:HD12	1:WK:175:SER:HB3	1.63	0.79
1:WP:165:PHE:HB3	4:F:160:GLN:O	1.83	0.79
1:WN:201:ALA:CA	1:WO:158:ALA:HB2	2.13	0.79
1:WA:175:SER:HB3	1:WW:197:LEU:HD12	1.64	0.79
1:UO:128:GLU:O	1:UO:132:TYR:N	2.14	0.78
1:WI:181:GLU:HB2	1:WI:184:ARG:CG	2.07	0.78
1:UI:98:LEU:HD22	1:UI:147:LEU:HD21	1.66	0.78
1:UJ:98:LEU:HD22	1:UJ:147:LEU:HD21	1.66	0.78
1:WE:167:ARG:CD	4:I:161:GLY:HA2	2.12	0.78
1:WQ:113:PHE:HB3	1:WR:134:ARG:HE	1.48	0.78
2:B:39:GLN:NE2	2:B:46:GLU:O	2.13	0.78
6:S:35:THR:HG22	7:X:49:PHE:HB3	1.65	0.78
1:WL:181:GLU:HB2	1:WL:184:ARG:CG	2.07	0.78
1:UJ:103:GLN:HB3	1:WD:182:PRO:CA	2.13	0.78
1:WK:162:PRO:HB2	3:E:249:ASN:HB2	1.64	0.78
1:WP:197:LEU:HD12	1:WQ:175:SER:OG	1.84	0.78
1:WV:120:LYS:NZ	1:WV:123:ILE:HD11	1.99	0.78
5:N:11:ILE:HG22	1:6:372:ILE:CD1	2.14	0.78
1:UP:128:GLU:O	1:UP:132:TYR:N	2.13	0.78
4:F:141:GLN:HE22	4:F:243:PHE:HB3	1.48	0.78
6:R:67:LEU:HD11	6:R:74:PRO:HA	1.64	0.78
1:UK:207:PRO:CD	1:WE:187:ASP:OD2	2.31	0.78
1:WP:200:SER:O	1:WQ:158:ALA:CB	2.31	0.78
1:UL:73:MET:HE1	1:UL:99:ARG:CD	2.14	0.78
1:WS:200:SER:OG	1:WT:175:SER:HB2	1.83	0.78
1:WU:197:LEU:CD1	1:WV:175:SER:OG	2.29	0.78
1:WA:167:ARG:NH2	1:WA:168:GLU:OE2	2.17	0.78
1:UO:98:LEU:HD22	1:UO:147:LEU:HD21	1.66	0.77
6:S:72:HIS:HA	1:AE:295:SER:OG	1.83	0.77
1:WJ:143:THR:OG1	1:WK:154:ARG:HG2	1.83	0.77
1:UM:98:LEU:HD22	1:UM:147:LEU:HD21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UP:73:MET:HE1	1:UP:99:ARG:HD3	1.65	0.77
1:WF:187:ASP:HB3	1:WF:190:GLN:HG3	1.66	0.77
1:WJ:128:GLU:CG	1:WK:126:PHE:CD2	2.67	0.77
1:UK:98:LEU:HD22	1:UK:147:LEU:HD21	1.66	0.77
1:UP:98:LEU:HD22	1:UP:147:LEU:HD21	1.66	0.77
1:WF:128:GLU:HG2	1:WG:126:PHE:HD2	1.48	0.77
1:WT:197:LEU:HD12	1:WU:175:SER:HB3	1.65	0.77
1:WD:197:LEU:HD12	1:WE:175:SER:OG	1.85	0.77
6:S:72:HIS:ND1	1:AD:365:ASN:CB	2.47	0.77
1:UJ:167:ARG:HH11	1:2:236:LYS:NZ	1.83	0.77
5:P:19:MET:CA	1:AP:276:GLU:OE2	2.32	0.77
1:UJ:261:LEU:HB3	1:UJ:270:THR:HG23	1.67	0.77
1:UL:98:LEU:HD22	1:UL:147:LEU:HD21	1.66	0.77
1:UN:128:GLU:O	1:UN:132:TYR:N	2.13	0.77
1:UN:167:ARG:HH22	1:WQ:188:GLU:HB3	1.47	0.77
1:WK:165:PHE:HA	3:E:149:LEU:CD1	2.15	0.77
1:WK:197:LEU:CD1	1:WL:175:SER:CB	2.59	0.77
1:WO:203:ALA:HB1	1:WP:160:PRO:HB3	1.66	0.77
6:S:73:ILE:HD11	1:AE:297:GLN:HB2	1.63	0.77
1:WJ:125:GLN:HG3	3:E:242:HIS:ND1	1.99	0.76
1:WM:197:LEU:HD12	1:WN:175:SER:HB3	1.67	0.76
5:N:21:ALA:HB1	1:4:278:THR:HG21	1.65	0.76
1:UP:212:LEU:HB3	1:UP:221:THR:HG23	1.67	0.76
1:WK:181:GLU:HB2	1:WK:184:ARG:CG	2.07	0.76
1:WQ:181:GLU:HB2	1:WQ:184:ARG:CG	2.07	0.76
1:WD:193:ALA:HB1	1:WE:213:VAL:HG11	1.67	0.76
1:WN:200:SER:HA	1:WO:173:SER:OG	1.85	0.76
1:WT:200:SER:O	1:WU:158:ALA:HB3	1.84	0.76
1:UL:167:ARG:NH1	1:WF:188:GLU:OE2	2.19	0.76
1:WQ:197:LEU:CD1	1:WR:175:SER:OG	2.26	0.76
1:WW:125:GLN:HB2	2:B:2:THR:HG21	1.66	0.76
5:M:21:ALA:CB	1:0:278:THR:HG21	2.15	0.76
1:WP:196:HIS:HB3	1:WQ:211:THR:HG21	1.66	0.76
6:U:73:ILE:HG13	1:2:295:SER:HB2	1.67	0.76
1:UM:73:MET:HE1	1:UM:99:ARG:HD3	1.66	0.76
6:R:73:ILE:HG13	1:AK:295:SER:CB	2.14	0.76
1:UM:212:LEU:HB3	1:UM:221:THR:HG23	1.67	0.76
1:UN:98:LEU:HD22	1:UN:147:LEU:HD21	1.66	0.76
1:WA:211:THR:HG21	1:WW:196:HIS:HB3	1.67	0.76
1:WN:197:LEU:HD12	1:WO:175:SER:HB3	1.68	0.76
1:WW:181:GLU:HB2	1:WW:184:ARG:CG	2.07	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UI:212:LEU:HB3	1:UI:221:THR:HG23	1.67	0.76
1:WA:181:GLU:HB2	1:WA:184:ARG:CG	2.07	0.76
1:WP:181:GLU:HB2	1:WP:184:ARG:CG	2.07	0.76
1:UN:212:LEU:HB3	1:UN:221:THR:HG23	1.67	0.76
1:WB:163:SER:HB2	1:WB:166:VAL:HG22	1.67	0.76
1:WT:160:PRO:HD3	1:WT:172:PRO:HA	1.66	0.76
1:UL:212:LEU:HB3	1:UL:221:THR:HG23	1.67	0.75
1:UO:212:LEU:HB3	1:UO:221:THR:HG23	1.67	0.75
1:WA:199:SER:HA	1:WA:205:LEU:HD23	1.69	0.75
1:WC:199:SER:HA	1:WC:205:LEU:HD23	1.69	0.75
1:WD:112:GLY:HA2	1:WD:135:ALA:HA	1.67	0.75
1:WD:199:SER:HA	1:WD:205:LEU:HD23	1.69	0.75
5:N:7:ILE:CG2	1:6:278:THR:HG21	2.17	0.75
1:WF:196:HIS:HB3	1:WG:211:THR:HG21	1.67	0.75
1:WN:199:SER:HA	1:WN:205:LEU:HD23	1.69	0.75
1:WE:199:SER:HA	1:WE:205:LEU:HD23	1.68	0.75
1:WP:199:SER:HA	1:WP:205:LEU:HD23	1.69	0.75
6:U:68:THR:CG2	1:1:294:ARG:CD	2.65	0.75
1:WF:199:SER:HA	1:WF:205:LEU:HD23	1.69	0.75
1:WC:200:SER:OG	1:WD:175:SER:HB2	1.86	0.75
1:WI:199:SER:HA	1:WI:205:LEU:HD23	1.69	0.75
1:WO:166:VAL:HG11	4:F:147:LEU:HD12	1.66	0.75
1:WW:199:SER:HA	1:WW:205:LEU:HD23	1.69	0.75
1:WO:199:SER:HA	1:WO:205:LEU:HD23	1.69	0.75
1:WR:181:GLU:HB2	1:WR:184:ARG:CG	2.07	0.75
1:UM:139:GLU:OE1	1:UM:142:ARG:NH2	2.20	0.75
1:WB:199:SER:HA	1:WB:205:LEU:HD23	1.68	0.75
1:WJ:128:GLU:HG2	1:WK:126:PHE:CD2	2.15	0.75
1:WW:125:GLN:OE1	2:B:2:THR:HG22	1.86	0.75
5:M:4:ILE:HD12	1:AC:374:HIS:HB2	1.68	0.75
5:N:7:ILE:HG21	1:6:278:THR:CG2	2.15	0.75
1:UK:212:LEU:HB3	1:UK:221:THR:HG23	1.67	0.74
1:WG:199:SER:HA	1:WG:205:LEU:HD23	1.69	0.74
6:T:55:ARG:CZ	1:5:299:ASN:HD21	1.97	0.74
1:WI:200:SER:O	1:WJ:158:ALA:HB3	1.87	0.74
1:WR:200:SER:O	1:WS:158:ALA:HB2	1.87	0.74
1:UK:94:HIS:CB	1:UK:146:THR:HG21	2.17	0.74
1:WC:193:ALA:HB1	1:WD:213:VAL:HG11	1.68	0.74
1:WD:149:PRO:HG2	1:WD:190:GLN:HE22	1.52	0.74
1:WJ:164:LEU:HB2	3:E:145:TRP:CD1	2.22	0.74
4:G:135:ARG:NH2	4:G:165:VAL:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:6:ILE:HG21	7:X:122:VAL:HG21	1.69	0.74
1:UO:94:HIS:CB	1:UO:146:THR:HG21	2.17	0.74
1:WT:199:SER:HA	1:WT:205:LEU:HD23	1.69	0.74
1:WV:197:LEU:HD12	1:WW:175:SER:OG	1.88	0.74
1:WN:197:LEU:HD12	1:WO:175:SER:CB	2.17	0.74
1:WO:164:LEU:O	4:F:144:GLU:N	2.21	0.74
5:K:21:ALA:HB1	1:AK:278:THR:CG2	2.17	0.74
1:UL:94:HIS:CB	1:UL:146:THR:HG21	2.17	0.74
1:WQ:199:SER:HA	1:WQ:205:LEU:HD23	1.69	0.74
1:WR:199:SER:HA	1:WR:205:LEU:HD23	1.69	0.74
1:WS:199:SER:HA	1:WS:205:LEU:HD23	1.69	0.74
1:WV:199:SER:HA	1:WV:205:LEU:HD23	1.69	0.74
3:E:23:VAL:HA	3:E:150:LEU:HD21	1.69	0.74
5:M:4:ILE:HG12	1:AC:372:ILE:HB	1.68	0.74
1:WJ:199:SER:HA	1:WJ:205:LEU:HD23	1.69	0.74
1:WN:181:GLU:HB2	1:WN:184:ARG:CG	2.07	0.74
1:UI:73:MET:HE3	1:UI:99:ARG:HD3	1.67	0.74
1:WB:163:SER:HB3	1:WB:169:GLN:HG2	1.70	0.74
1:WK:199:SER:HA	1:WK:205:LEU:HD23	1.69	0.74
1:UN:94:HIS:CB	1:UN:146:THR:HG21	2.17	0.74
1:UO:139:GLU:OE1	1:UO:142:ARG:NH2	2.20	0.74
1:WH:199:SER:HA	1:WH:205:LEU:HD23	1.69	0.74
1:WP:164:LEU:HD13	4:F:148:ALA:HA	1.69	0.74
1:UJ:94:HIS:CB	1:UJ:146:THR:HG21	2.17	0.73
1:UL:139:GLU:OE1	1:UL:142:ARG:NH2	2.20	0.73
1:WC:197:LEU:HD12	1:WD:175:SER:OG	1.88	0.73
1:WK:143:THR:HG1	1:WL:156:HIS:CE1	2.04	0.73
6:U:65:LEU:HB2	1:1:295:SER:HB2	1.69	0.73
1:UJ:73:MET:HE1	1:UJ:99:ARG:HD3	1.69	0.73
1:UK:103:GLN:NE2	1:WF:182:PRO:HB3	2.01	0.73
1:UM:94:HIS:CB	1:UM:146:THR:HG21	2.17	0.73
1:WE:166:VAL:HG21	4:I:160:GLN:HG2	1.69	0.73
5:K:89:ARG:NH1	5:P:102:MET:SD	2.61	0.73
5:N:94:ALA:O	5:N:98:GLU:HG3	1.88	0.73
1:UL:73:MET:CE	1:UL:99:ARG:CD	2.66	0.73
1:UN:73:MET:CE	1:UN:99:ARG:CD	2.66	0.73
1:WB:197:LEU:HD12	1:WC:175:SER:CB	2.18	0.73
1:UI:94:HIS:CB	1:UI:146:THR:HG21	2.17	0.73
1:WB:181:GLU:HB2	1:WB:184:ARG:CG	2.07	0.73
1:WW:167:ARG:HD2	4:H:140:ARG:O	1.87	0.73
7:X:79:GLU:HG2	7:X:82:ASN:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:6:ILE:HD13	7:Z:122:VAL:HG21	1.71	0.73
1:UK:73:MET:CE	1:UK:99:ARG:CD	2.66	0.73
1:WA:158:ALA:HB3	1:WW:200:SER:O	1.87	0.73
1:WJ:164:LEU:HD21	3:E:144:LEU:CB	2.17	0.73
1:WR:200:SER:OG	1:WS:175:SER:HB2	1.88	0.73
1:WU:199:SER:HA	1:WU:205:LEU:HD23	1.69	0.73
7:V:55:PRO:HG3	1:AP:359:GLN:NE2	2.04	0.73
1:UN:139:GLU:OE1	1:UN:142:ARG:NH2	2.20	0.73
1:WD:164:LEU:O	4:I:144:GLU:HG2	1.88	0.73
1:WP:123:ILE:HG23	2:A:67:PRO:HB3	1.70	0.73
2:C:29:LEU:HB2	2:D:52:ILE:HG13	1.71	0.73
6:S:73:ILE:CD1	1:AE:297:GLN:CB	2.56	0.73
1:UN:73:MET:HE1	1:UN:99:ARG:CD	2.17	0.73
1:UP:94:HIS:CB	1:UP:146:THR:HG21	2.17	0.73
1:WT:200:SER:OG	1:WU:175:SER:HB2	1.88	0.73
1:UK:139:GLU:OE1	1:UK:142:ARG:NH2	2.20	0.73
1:UP:73:MET:CE	1:UP:99:ARG:CD	2.66	0.73
1:WK:193:ALA:CB	1:WL:213:VAL:HG21	2.13	0.73
5:K:21:ALA:CB	1:AK:278:THR:CG2	2.64	0.73
6:S:42:ASP:OD2	6:S:43:ILE:N	2.22	0.73
2:B:11:THR:HA	2:B:14:MET:HE3	1.69	0.73
1:UP:139:GLU:OE1	1:UP:142:ARG:NH2	2.20	0.73
1:WM:200:SER:O	1:WN:158:ALA:CB	2.37	0.73
1:UI:139:GLU:OE1	1:UI:142:ARG:NH2	2.20	0.72
1:WK:132:TYR:HB2	1:WL:126:PHE:CZ	2.23	0.72
1:UM:73:MET:CE	1:UM:99:ARG:CD	2.66	0.72
1:UI:73:MET:CE	1:UI:99:ARG:CD	2.66	0.72
1:WL:199:SER:HA	1:WL:205:LEU:HD23	1.69	0.72
1:WM:199:SER:HA	1:WM:205:LEU:HD23	1.69	0.72
1:WS:181:GLU:HB2	1:WS:184:ARG:CG	2.07	0.72
1:WC:197:LEU:HD12	1:WD:175:SER:CB	2.18	0.72
1:WU:181:GLU:HB2	1:WU:184:ARG:CG	2.07	0.72
5:L:11:ILE:CG2	1:AH:372:ILE:HD13	2.16	0.72
1:WM:197:LEU:HA	1:WN:175:SER:OG	1.89	0.72
5:M:4:ILE:HG13	1:AC:372:ILE:CG2	2.20	0.72
1:WG:181:GLU:HB2	1:WG:184:ARG:CG	2.07	0.72
5:L:11:ILE:CG2	1:AH:372:ILE:CB	2.67	0.72
1:UO:73:MET:CE	1:UO:99:ARG:CD	2.66	0.72
5:L:11:ILE:HG21	1:AH:372:ILE:CB	2.18	0.72
5:M:11:ILE:C	5:M:11:ILE:CD1	2.57	0.72
6:R:46:ALA:O	6:R:50:LYS:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UJ:73:MET:CE	1:UJ:99:ARG:CD	2.66	0.72
1:WD:197:LEU:HA	1:WE:175:SER:OG	1.89	0.72
1:WV:181:GLU:HB2	1:WV:184:ARG:CG	2.07	0.72
5:K:7:ILE:CG2	1:AM:278:THR:CG2	2.53	0.72
7:W:6:ILE:HG21	7:W:122:VAL:HG21	1.72	0.72
1:UJ:98:LEU:CD1	1:UJ:146:THR:OG1	2.38	0.71
1:WE:181:GLU:HB2	1:WE:184:ARG:CG	2.07	0.71
1:UL:98:LEU:CD1	1:UL:146:THR:OG1	2.39	0.71
1:UJ:139:GLU:OE1	1:UJ:142:ARG:NH2	2.20	0.71
1:WJ:164:LEU:HD21	3:E:144:LEU:HB3	1.72	0.71
5:P:76:GLN:HE21	7:V:123:LYS:HB2	1.54	0.71
1:UM:98:LEU:CD1	1:UM:146:THR:OG1	2.39	0.71
1:WC:165:PHE:CD2	4:H:152:ARG:NH2	2.52	0.71
6:U:72:HIS:CE1	1:2:294:ARG:HG3	2.25	0.71
1:UI:62:ASP:OD2	1:WA:184:ARG:NH2	2.24	0.71
1:UI:98:LEU:CD1	1:UI:146:THR:OG1	2.38	0.71
1:UN:126:PHE:CD1	1:UN:130:VAL:HG21	2.26	0.71
1:WC:165:PHE:HD2	4:H:152:ARG:NH2	1.88	0.71
1:UP:126:PHE:CD1	1:UP:130:VAL:HG21	2.26	0.71
1:WT:181:GLU:HB2	1:WT:184:ARG:CG	2.07	0.71
1:WV:197:LEU:HD12	1:WW:175:SER:HB3	1.71	0.71
4:J:139:LEU:O	4:J:142:THR:HG22	1.89	0.71
5:K:21:ALA:HB3	1:AK:278:THR:HG21	1.71	0.71
5:M:4:ILE:CD1	1:AC:374:HIS:HB2	2.20	0.71
1:WH:193:ALA:HB1	1:WI:213:VAL:CG1	2.18	0.71
2:D:48:THR:OG1	4:I:206:ALA:O	2.08	0.71
1:UK:126:PHE:CD1	1:UK:130:VAL:HG21	2.26	0.71
1:UP:73:MET:HE1	1:UP:99:ARG:CD	2.20	0.71
1:WD:181:GLU:HB2	1:WD:184:ARG:CG	2.07	0.71
6:R:72:HIS:ND1	1:AJ:365:ASN:CB	2.40	0.71
1:UN:98:LEU:CD1	1:UN:146:THR:OG1	2.39	0.71
1:WF:181:GLU:HB2	1:WF:184:ARG:CG	2.07	0.71
1:WK:200:SER:HA	1:WL:173:SER:OG	1.91	0.71
2:B:39:GLN:HE21	2:B:49:LEU:HD12	1.56	0.71
6:T:78:VAL:HG12	1:6:361:ASN:ND2	2.06	0.71
1:WR:200:SER:O	1:WS:158:ALA:HB3	1.90	0.71
6:U:68:THR:HG22	1:1:294:ARG:HD3	1.73	0.71
1:UK:98:LEU:CD1	1:UK:146:THR:OG1	2.38	0.70
1:UL:103:GLN:HG2	1:WH:182:PRO:HB3	1.72	0.70
1:UM:126:PHE:CD1	1:UM:130:VAL:HG21	2.26	0.70
1:UP:98:LEU:CD1	1:UP:146:THR:OG1	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WJ:164:LEU:C	4:J:152:ARG:HH22	1.95	0.70
1:UK:126:PHE:O	1:UK:130:VAL:CG2	2.40	0.70
1:WD:190:GLN:HG3	1:WE:217:GLY:HA3	1.72	0.70
1:WE:128:GLU:HB3	1:WF:126:PHE:CE2	2.25	0.70
2:D:84:LEU:HD21	4:J:185:ILE:HG23	1.72	0.70
6:U:68:THR:HG21	1:1:294:ARG:HD2	1.71	0.70
1:UJ:73:MET:HE3	1:UJ:99:ARG:HD3	1.73	0.70
1:UO:126:PHE:CD1	1:UO:130:VAL:HG21	2.26	0.70
1:WE:197:LEU:HD12	1:WF:175:SER:CB	2.21	0.70
1:WM:139:GLU:HB3	1:WN:154:ARG:NH2	2.06	0.70
1:UI:126:PHE:O	1:UI:130:VAL:CG2	2.40	0.70
1:UJ:126:PHE:O	1:UJ:130:VAL:CG2	2.40	0.70
1:WA:200:SER:O	1:WB:158:ALA:CB	2.40	0.70
1:UO:73:MET:HE1	1:UO:99:ARG:HD3	1.71	0.70
1:WB:200:SER:O	1:WC:158:ALA:HB2	1.91	0.70
1:WD:165:PHE:CE2	4:I:141:GLN:HA	2.26	0.70
1:WP:193:ALA:HB1	1:WQ:213:VAL:HG11	1.74	0.70
6:R:71:HIS:HB2	1:AK:294:ARG:HG2	1.74	0.70
1:UN:126:PHE:O	1:UN:130:VAL:CG2	2.40	0.70
1:UO:98:LEU:CD1	1:UO:146:THR:OG1	2.38	0.70
2:D:13:ALA:HB1	4:J:195:ILE:HD11	1.73	0.70
1:UI:167:ARG:HH22	1:WW:188:GLU:HB3	1.57	0.70
1:WD:165:PHE:CB	4:I:143:ARG:HA	2.22	0.70
1:WW:167:ARG:CD	4:H:140:ARG:O	2.40	0.70
1:WR:112:GLY:HA2	1:WR:135:ALA:CA	2.16	0.70
3:E:182:ASN:HB3	3:E:239:PHE:CZ	2.26	0.70
5:K:14:LEU:HB3	1:AL:278:THR:HG21	1.72	0.70
1:WS:121:PHE:CE1	1:WT:120:LYS:NZ	2.55	0.69
1:UL:62:ASP:OD2	1:WG:184:ARG:NH2	2.25	0.69
1:UL:126:PHE:CD1	1:UL:130:VAL:HG21	2.26	0.69
1:WM:193:ALA:HB1	1:WN:213:VAL:CG1	2.22	0.69
6:T:91:ASP:OD2	6:T:104:ARG:NH1	2.25	0.69
1:UJ:126:PHE:CD1	1:UJ:130:VAL:HG21	2.26	0.69
1:WJ:164:LEU:CB	3:E:145:TRP:HE1	1.99	0.69
1:UI:126:PHE:CD1	1:UI:130:VAL:HG21	2.26	0.69
1:UL:126:PHE:O	1:UL:130:VAL:CG2	2.40	0.69
6:S:72:HIS:HB3	1:AE:295:SER:HB3	1.72	0.69
1:UL:126:PHE:O	1:UL:130:VAL:CB	2.41	0.69
1:WA:175:SER:OG	1:WW:197:LEU:HA	1.93	0.69
1:WE:166:VAL:HG21	4:I:160:GLN:CG	2.23	0.69
1:UI:126:PHE:O	1:UI:130:VAL:CB	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UN:126:PHE:O	1:UN:130:VAL:CB	2.41	0.69
1:UO:73:MET:HE3	1:UO:99:ARG:HD3	1.71	0.69
1:UO:126:PHE:O	1:UO:130:VAL:CG2	2.40	0.69
3:E:188:LEU:HB3	3:E:189:PRO:CD	2.22	0.69
4:J:143:ARG:HB3	4:J:146:ASP:OD2	1.92	0.69
1:UJ:126:PHE:O	1:UJ:130:VAL:CB	2.41	0.69
1:WL:197:LEU:HD13	1:WM:175:SER:OG	1.91	0.69
5:M:77:LYS:NZ	6:S:13:GLN:OE1	2.26	0.69
1:UM:126:PHE:O	1:UM:130:VAL:CB	2.41	0.69
1:WK:164:LEU:HD12	3:E:248:PHE:HB2	1.74	0.69
1:WN:200:SER:CA	1:WO:173:SER:OG	2.41	0.69
2:C:13:ALA:HB1	4:I:195:ILE:HD11	1.75	0.69
5:M:11:ILE:HG22	1:AB:372:ILE:HB	1.74	0.69
1:WA:167:ARG:HH21	4:H:162:PRO:CD	2.06	0.69
4:H:153:LEU:HD22	4:I:99:PHE:HB3	1.75	0.69
6:U:76:GLN:N	1:1:297:GLN:HE22	1.91	0.69
1:WA:128:GLU:HG3	1:WB:126:PHE:HE2	1.54	0.69
1:WA:213:VAL:HG11	1:WW:193:ALA:HB1	1.73	0.69
1:WG:165:PHE:CZ	4:I:153:LEU:CD2	2.75	0.69
1:WK:197:LEU:HA	1:WL:175:SER:HB2	1.74	0.69
1:WP:190:GLN:HG2	1:WQ:217:GLY:HA3	1.75	0.69
5:M:4:ILE:CG1	1:AC:372:ILE:CG2	2.70	0.69
1:UM:126:PHE:O	1:UM:130:VAL:CG2	2.40	0.68
1:UO:126:PHE:O	1:UO:130:VAL:CB	2.41	0.68
1:UP:126:PHE:O	1:UP:130:VAL:CG2	2.40	0.68
1:WD:196:HIS:HB3	1:WE:211:THR:HG21	1.75	0.68
1:UM:73:MET:HE1	1:UM:99:ARG:CD	2.21	0.68
6:R:68:THR:CG2	1:AJ:294:ARG:HD3	2.23	0.68
1:UJ:167:ARG:HH11	1:2:236:LYS:HZ3	1.40	0.68
1:UP:126:PHE:O	1:UP:130:VAL:CB	2.41	0.68
1:WC:197:LEU:HD12	1:WD:175:SER:HB3	1.76	0.68
1:UK:73:MET:HE3	1:UK:99:ARG:CD	2.22	0.68
1:WA:167:ARG:HH21	4:H:162:PRO:HD3	1.58	0.68
4:F:109:TYR:HA	4:F:113:TYR:HB2	1.74	0.68
1:WB:193:ALA:HB1	1:WC:213:VAL:HG11	1.76	0.68
1:WD:197:LEU:HD12	1:WE:175:SER:CB	2.23	0.68
1:UK:126:PHE:O	1:UK:130:VAL:CB	2.41	0.68
1:WS:197:LEU:HD12	1:WT:175:SER:OG	1.94	0.68
1:WS:197:LEU:HD12	1:WT:175:SER:CB	2.24	0.68
1:UJ:125:GLN:HA	1:UJ:128:GLU:HB2	1.76	0.68
1:UL:98:LEU:HD12	1:UL:146:THR:OG1	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WD:193:ALA:HB1	1:WE:213:VAL:CG1	2.23	0.68
1:WJ:125:GLN:CB	3:E:242:HIS:HB2	2.23	0.68
1:WA:128:GLU:CG	1:WB:126:PHE:CE2	2.64	0.67
1:WD:165:PHE:CB	4:I:142:THR:O	2.29	0.67
1:WN:200:SER:O	1:WO:173:SER:OG	2.12	0.67
1:WW:164:LEU:CD1	2:B:89:GLY:O	2.40	0.67
2:B:58:VAL:HG21	4:H:207:LEU:HD11	1.75	0.67
1:UM:125:GLN:HA	1:UM:128:GLU:HB2	1.76	0.67
1:WE:134:ARG:HB3	1:WE:134:ARG:HH21	1.57	0.67
1:UM:98:LEU:HD12	1:UM:146:THR:OG1	1.94	0.67
1:UP:98:LEU:HD12	1:UP:146:THR:OG1	1.94	0.67
5:L:4:ILE:CG1	1:AI:372:ILE:HG22	2.25	0.67
1:WP:197:LEU:HD12	1:WQ:175:SER:CB	2.25	0.67
1:WV:120:LYS:HZ2	1:WV:123:ILE:HD11	1.58	0.67
1:UL:125:GLN:HA	1:UL:128:GLU:HB2	1.76	0.67
1:UO:125:GLN:HA	1:UO:128:GLU:HB2	1.76	0.67
1:WE:166:VAL:CG2	4:I:160:GLN:HG2	2.25	0.67
1:WQ:197:LEU:HD12	1:WR:175:SER:CB	2.23	0.67
1:UN:98:LEU:HD12	1:UN:146:THR:OG1	1.94	0.67
1:UN:103:GLN:HG2	1:WS:182:PRO:HB3	1.75	0.67
1:WG:200:SER:O	1:WH:158:ALA:CB	2.42	0.67
2:B:14:MET:HG3	2:C:59:PHE:HE1	1.58	0.67
1:UJ:98:LEU:HD12	1:UJ:146:THR:OG1	1.94	0.67
1:WE:112:GLY:HA3	1:WE:139:GLU:OE1	1.95	0.67
1:WF:197:LEU:HD12	1:WG:175:SER:HB3	1.74	0.67
5:O:7:ILE:HD11	1:1:370:ARG:HE	1.58	0.67
1:UJ:73:MET:HE1	1:UJ:99:ARG:CD	2.24	0.67
1:WA:197:LEU:HD12	1:WB:175:SER:HB3	1.75	0.67
1:WD:115:LEU:CD2	1:WD:134:ARG:HD2	2.24	0.67
1:WH:164:LEU:O	4:J:143:ARG:HG3	1.95	0.67
1:UI:125:GLN:HA	1:UI:128:GLU:HB2	1.76	0.67
1:UK:98:LEU:HD12	1:UK:146:THR:OG1	1.94	0.67
1:WA:200:SER:O	1:WB:158:ALA:HB3	1.95	0.67
1:WO:167:ARG:O	1:WO:168:GLU:HB2	1.93	0.67
1:WR:113:PHE:HA	1:WS:134:ARG:HH12	1.58	0.67
3:E:166:SER:O	3:E:168:ALA:N	2.26	0.67
5:P:21:ALA:HB3	1:AP:278:THR:HG21	1.73	0.67
6:U:36:PRO:HB3	6:U:96:ASP:HB2	1.77	0.67
1:WW:186:LEU:HA	1:WW:190:GLN:OE1	1.96	0.66
4:H:68:ILE:HD11	5:M:104:VAL:HG22	1.76	0.66
6:U:65:LEU:HD21	1:1:297:GLN:HB2	1.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UI:73:MET:HE1	1:UI:99:ARG:HD3	1.76	0.66
1:UO:98:LEU:HD12	1:UO:146:THR:OG1	1.94	0.66
1:WB:190:GLN:HG2	1:WC:216:SER:O	1.94	0.66
1:WD:168:GLU:OE2	1:WD:170:LYS:HE3	1.94	0.66
1:WE:112:GLY:HA2	1:WE:135:ALA:CA	2.18	0.66
4:F:43:GLN:OE1	6:Q:4:ARG:NH1	2.28	0.66
1:UO:62:ASP:OD2	1:WT:184:ARG:NH2	2.28	0.66
1:UP:125:GLN:HA	1:UP:128:GLU:HB2	1.76	0.66
1:WS:124:SER:HB2	2:A:8:MET:HE3	1.75	0.66
3:E:193:LEU:HD22	3:E:228:LEU:HD11	1.77	0.66
5:N:14:LEU:HB3	1:5:278:THR:HG21	1.77	0.66
5:P:15:GLN:HB2	1:AQ:374:HIS:CD2	2.30	0.66
3:E:187:ALA:O	3:E:188:LEU:C	2.34	0.66
5:K:7:ILE:CB	1:AM:278:THR:HG21	2.24	0.66
4:I:194:LEU:HD11	4:J:220:PRO:HG2	1.77	0.66
7:V:6:ILE:HG21	7:V:122:VAL:HG21	1.76	0.66
1:WF:167:ARG:C	4:I:152:ARG:NH1	2.49	0.66
1:WA:112:GLY:HA3	1:WA:139:GLU:OE1	1.95	0.66
6:U:123:LEU:HD23	7:Z:132:LEU:HD11	1.77	0.66
1:UM:73:MET:HE3	1:UM:99:ARG:HD3	1.76	0.65
5:N:7:ILE:HG21	1:6:278:THR:HG21	1.76	0.65
1:WF:128:GLU:HG2	1:WG:126:PHE:CD2	2.29	0.65
1:WU:167:ARG:HH12	4:G:158:PRO:HD3	1.61	0.65
1:UI:98:LEU:HD12	1:UI:146:THR:OG1	1.94	0.65
1:WH:203:ALA:CB	1:WI:160:PRO:HB3	2.19	0.65
1:WO:197:LEU:HD12	1:WP:175:SER:CB	2.26	0.65
1:UK:125:GLN:HA	1:UK:128:GLU:HB2	1.76	0.65
1:UM:139:GLU:CD	1:UM:142:ARG:HH21	2.00	0.65
1:WS:124:SER:CB	2:A:8:MET:HE2	2.26	0.65
4:H:66:ARG:NH2	4:H:242:SER:OG	2.30	0.65
5:N:7:ILE:HD11	1:7:370:ARG:HH21	1.61	0.65
1:1:389:VAL:HG21	1:1:416:THR:HG21	1.79	0.65
1:3:389:VAL:HG21	1:3:416:THR:HG21	1.79	0.65
1:4:389:VAL:HG21	1:4:416:THR:HG21	1.79	0.65
1:AM:389:VAL:HG21	1:AM:416:THR:HG21	1.79	0.65
1:AI:389:VAL:HG21	1:AI:416:THR:HG21	1.79	0.65
1:AK:389:VAL:HG21	1:AK:416:THR:HG21	1.79	0.65
6:S:72:HIS:HA	1:AE:295:SER:CB	2.27	0.65
6:U:72:HIS:CD2	1:1:365:ASN:CB	2.60	0.65
1:2:389:VAL:HG21	1:2:416:THR:HG21	1.79	0.65
1:AN:389:VAL:HG21	1:AN:416:THR:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UN:125:GLN:HA	1:UN:128:GLU:HB2	1.76	0.65
1:WP:128:GLU:HG3	1:WQ:126:PHE:HE2	1.62	0.65
1:WW:134:ARG:HB3	1:WW:134:ARG:HH21	1.61	0.65
6:U:76:GLN:H	1:1:297:GLN:NE2	1.95	0.65
1:AJ:389:VAL:HG21	1:AJ:416:THR:HG21	1.79	0.65
1:AL:389:VAL:HG21	1:AL:416:THR:HG21	1.79	0.65
1:WM:200:SER:O	1:WN:158:ALA:HB2	1.97	0.65
1:WT:128:GLU:HG2	1:WU:126:PHE:HD2	1.60	0.65
1:6:389:VAL:HG21	1:6:416:THR:HG21	1.79	0.65
1:AG:389:VAL:HG21	1:AG:416:THR:HG21	1.79	0.65
4:F:58:LEU:O	4:F:62:THR:OG1	2.14	0.64
4:H:135:ARG:NH1	4:H:165:VAL:O	2.30	0.64
1:5:389:VAL:HG21	1:5:416:THR:HG21	1.79	0.64
1:7:389:VAL:HG21	1:7:416:THR:HG21	1.79	0.64
1:WA:154:ARG:HG2	1:WW:143:THR:OG1	1.97	0.64
1:WF:167:ARG:C	4:I:152:ARG:HH12	2.00	0.64
1:AP:389:VAL:HG21	1:AP:416:THR:HG21	1.79	0.64
1:UO:139:GLU:CD	1:UO:142:ARG:HH21	2.00	0.64
1:UP:139:GLU:CD	1:UP:142:ARG:HH21	2.00	0.64
1:WE:123:ILE:HB	1:WE:128:GLU:OE1	1.95	0.64
1:WE:166:VAL:CG2	4:I:160:GLN:CA	2.60	0.64
1:WI:167:ARG:HG3	4:J:160:GLN:O	1.98	0.64
1:WP:164:LEU:HD21	4:F:151:ALA:HB2	1.79	0.64
5:M:4:ILE:HG13	1:AC:372:ILE:HG21	1.79	0.64
6:R:36:PRO:HB3	6:R:96:ASP:HB2	1.79	0.64
6:U:68:THR:CG2	1:1:294:ARG:HD2	2.25	0.64
1:AO:389:VAL:HG21	1:AO:416:THR:HG21	1.79	0.64
1:UJ:139:GLU:CD	1:UJ:142:ARG:HH21	2.00	0.64
1:UN:139:GLU:CD	1:UN:142:ARG:HH21	2.00	0.64
1:WR:143:THR:OG1	1:WS:154:ARG:HG2	1.97	0.64
1:8:389:VAL:HG21	1:8:416:THR:HG21	1.79	0.64
1:AE:389:VAL:HG21	1:AE:416:THR:HG21	1.79	0.64
1:AH:389:VAL:HG21	1:AH:416:THR:HG21	1.79	0.64
1:UI:139:GLU:CD	1:UI:142:ARG:HH21	2.00	0.64
1:UP:73:MET:HE3	1:UP:99:ARG:HD3	1.78	0.64
1:AJ:235:LEU:HD22	1:AK:244:ARG:HH12	1.63	0.64
1:AL:235:LEU:HD22	1:AM:244:ARG:HH12	1.63	0.64
1:AM:287:ASP:HB3	1:AM:290:LYS:HE2	1.80	0.64
1:UO:73:MET:HE1	1:UO:99:ARG:CD	2.26	0.64
1:WH:197:LEU:HD11	1:WI:156:HIS:HD2	1.63	0.64
1:WH:197:LEU:HD12	1:WI:175:SER:OG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:55:GLN:NE2	5:P:74:ASP:OD2	2.31	0.64
1:5:394:LYS:HA	1:5:394:LYS:HE3	1.80	0.64
1:8:394:LYS:HA	1:8:394:LYS:HE3	1.80	0.64
1:9:389:VAL:HG21	1:9:416:THR:HG21	1.79	0.64
1:0:394:LYS:HA	1:0:394:LYS:HE3	1.80	0.64
1:AE:394:LYS:HA	1:AE:394:LYS:HE3	1.80	0.64
1:AN:235:LEU:HD22	1:AO:244:ARG:HH12	1.63	0.64
1:AQ:389:VAL:HG21	1:AQ:416:THR:HG21	1.79	0.64
1:WN:196:HIS:CB	1:WO:211:THR:HG21	2.19	0.64
5:N:7:ILE:HD11	1:7:370:ARG:HE	1.62	0.64
1:6:394:LYS:HA	1:6:394:LYS:HE3	1.80	0.64
1:0:235:LEU:HD22	1:AA:244:ARG:HH12	1.63	0.64
1:AB:235:LEU:HD22	1:AC:244:ARG:HH12	1.63	0.64
1:AC:394:LYS:HA	1:AC:394:LYS:HE3	1.80	0.64
1:WH:166:VAL:HG11	4:J:147:LEU:HD12	1.80	0.64
3:E:24:LEU:HB3	5:K:89:ARG:NH2	2.12	0.64
5:P:21:ALA:CB	1:AP:278:THR:CG2	2.67	0.64
6:T:72:HIS:CD2	1:7:365:ASN:CB	2.66	0.64
1:1:235:LEU:HD22	1:2:244:ARG:HH12	1.63	0.64
1:3:394:LYS:HE3	1:3:394:LYS:HA	1.80	0.64
1:7:394:LYS:HA	1:7:394:LYS:HE3	1.80	0.64
1:8:235:LEU:HD22	1:9:244:ARG:HH12	1.63	0.64
1:AA:394:LYS:HE3	1:AA:394:LYS:HA	1.80	0.64
1:AF:389:VAL:HG21	1:AF:416:THR:HG21	1.79	0.64
1:AG:394:LYS:HA	1:AG:394:LYS:HE3	1.80	0.64
1:WF:167:ARG:O	4:I:152:ARG:NH1	2.31	0.64
1:4:287:ASP:HB3	1:4:290:LYS:HE2	1.80	0.64
1:5:287:ASP:HB3	1:5:290:LYS:HE2	1.80	0.64
1:AA:389:VAL:HG21	1:AA:416:THR:HG21	1.79	0.64
1:AB:394:LYS:HA	1:AB:394:LYS:HE3	1.80	0.64
1:AC:389:VAL:HG21	1:AC:416:THR:HG21	1.79	0.64
1:AL:287:ASP:HB3	1:AL:290:LYS:HE2	1.80	0.64
1:WG:139:GLU:HB3	1:WH:154:ARG:HH21	1.63	0.63
4:I:204:LEU:HD22	4:I:212:VAL:HG11	1.78	0.63
5:N:11:ILE:CG2	1:6:372:ILE:HG21	2.28	0.63
1:3:235:LEU:HD22	1:4:244:ARG:HH12	1.63	0.63
1:0:389:VAL:HG21	1:0:416:THR:HG21	1.79	0.63
1:AB:389:VAL:HG21	1:AB:416:THR:HG21	1.79	0.63
1:AD:389:VAL:HG21	1:AD:416:THR:HG21	1.79	0.63
1:AN:287:ASP:HB3	1:AN:290:LYS:HE2	1.80	0.63
1:AP:235:LEU:HD22	1:AQ:244:ARG:HH12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WL:197:LEU:HD12	1:WM:175:SER:HB3	1.80	0.63
2:C:75:ASP:O	2:C:79:THR:HG23	1.98	0.63
3:E:158:PRO:CG	3:E:162:ASN:HD21	2.09	0.63
1:3:287:ASP:HB3	1:3:290:LYS:HE2	1.80	0.63
1:9:394:LYS:HA	1:9:394:LYS:HE3	1.80	0.63
1:AD:394:LYS:HE3	1:AD:394:LYS:HA	1.80	0.63
1:AE:235:LEU:HD22	1:AF:244:ARG:HH12	1.63	0.63
1:UL:139:GLU:CD	1:UL:142:ARG:HH21	2.00	0.63
1:WB:200:SER:O	1:WC:158:ALA:CB	2.45	0.63
1:WH:197:LEU:HD12	1:WI:175:SER:CB	2.28	0.63
1:WH:197:LEU:HA	1:WI:175:SER:OG	1.97	0.63
2:D:58:VAL:HG11	4:J:207:LEU:HD11	1.79	0.63
6:T:66:THR:OG1	1:7:294:ARG:HG2	1.98	0.63
1:1:394:LYS:HA	1:1:394:LYS:HE3	1.80	0.63
1:5:235:LEU:HD22	1:6:244:ARG:HH12	1.63	0.63
1:AD:235:LEU:HD22	1:AE:244:ARG:HH12	1.63	0.63
1:AF:394:LYS:HA	1:AF:394:LYS:HE3	1.80	0.63
1:AH:235:LEU:HD22	1:AI:244:ARG:HH12	1.63	0.63
1:AH:394:LYS:HA	1:AH:394:LYS:HE3	1.80	0.63
1:WB:166:VAL:O	4:H:152:ARG:HD2	1.97	0.63
1:WJ:164:LEU:CD2	3:E:144:LEU:HB3	2.27	0.63
5:K:14:LEU:CD2	1:AL:278:THR:CG2	2.62	0.63
6:S:22:ARG:NH2	6:S:108:GLN:OE1	2.31	0.63
1:2:394:LYS:HA	1:2:394:LYS:HE3	1.80	0.63
1:4:394:LYS:HA	1:4:394:LYS:HE3	1.80	0.63
1:6:235:LEU:HD22	1:7:244:ARG:HH12	1.63	0.63
1:9:287:ASP:HB3	1:9:290:LYS:HE2	1.80	0.63
1:AC:235:LEU:HD22	1:AD:244:ARG:HH12	1.63	0.63
1:AG:235:LEU:HD22	1:AH:244:ARG:HH12	1.63	0.63
1:WO:196:HIS:HB3	1:WP:211:THR:HG21	1.80	0.63
6:U:72:HIS:HE1	1:2:294:ARG:HE	1.43	0.63
1:0:287:ASP:HB3	1:0:290:LYS:HE2	1.80	0.63
1:AO:235:LEU:HD22	1:AP:244:ARG:HH12	1.63	0.63
1:WH:166:VAL:CG1	4:J:147:LEU:HD12	2.28	0.63
1:WP:214:ASP:OD1	1:WP:218:HIS:HB2	1.99	0.63
1:WU:128:GLU:HG2	1:WV:126:PHE:HD2	1.64	0.63
1:6:287:ASP:HB3	1:6:290:LYS:HE2	1.80	0.63
1:7:235:LEU:HD22	1:8:244:ARG:HH12	1.63	0.63
1:9:235:LEU:HD22	1:0:244:ARG:HH12	1.63	0.63
1:AF:235:LEU:HD22	1:AG:244:ARG:HH12	1.63	0.63
1:AH:287:ASP:HB3	1:AH:290:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:394:LYS:HA	1:AI:394:LYS:HE3	1.80	0.63
1:WG:139:GLU:HB3	1:WH:154:ARG:NH2	2.14	0.63
1:WH:166:VAL:HG11	4:J:147:LEU:CD1	2.28	0.63
1:AA:287:ASP:HB3	1:AA:290:LYS:HE2	1.80	0.63
1:AK:287:ASP:HB3	1:AK:290:LYS:HE2	1.80	0.63
1:AO:287:ASP:HB3	1:AO:290:LYS:HE2	1.80	0.63
1:WG:193:ALA:HB1	1:WH:213:VAL:HG11	1.81	0.63
1:4:235:LEU:HD22	1:5:244:ARG:HH12	1.63	0.63
1:8:287:ASP:HB3	1:8:290:LYS:HE2	1.80	0.63
1:AJ:394:LYS:HA	1:AJ:394:LYS:HE3	1.80	0.63
1:UK:139:GLU:CD	1:UK:142:ARG:HH21	2.00	0.63
1:WS:168:GLU:HB3	1:WS:170:LYS:HE3	1.81	0.63
4:H:116:PHE:O	6:S:4:ARG:NH2	2.30	0.63
6:R:65:LEU:HD21	1:AI:363:THR:HG23	1.80	0.63
1:2:287:ASP:HB3	1:2:290:LYS:HE2	1.80	0.63
1:AA:235:LEU:HD22	1:AB:244:ARG:HH12	1.63	0.63
1:AI:235:LEU:HD22	1:AJ:244:ARG:HH12	1.63	0.63
1:AI:287:ASP:HB3	1:AI:290:LYS:HE2	1.80	0.63
1:AM:235:LEU:HD22	1:AN:244:ARG:HH12	1.63	0.63
1:WL:186:LEU:HA	1:WL:190:GLN:OE1	1.99	0.62
6:R:73:ILE:CG1	1:AK:295:SER:HB2	2.22	0.62
6:S:76:GLN:H	1:AD:297:GLN:HE22	1.46	0.62
1:WI:200:SER:OG	1:WJ:175:SER:HB2	1.99	0.62
1:WU:165:PHE:HA	4:G:148:ALA:HB1	1.80	0.62
1:AG:287:ASP:HB3	1:AG:290:LYS:HE2	1.80	0.62
1:AO:394:LYS:HE3	1:AO:394:LYS:HA	1.80	0.62
2:C:23:PRO:O	2:C:27:VAL:HG12	1.99	0.62
5:L:11:ILE:HG23	1:AH:372:ILE:HG21	1.76	0.62
5:M:4:ILE:CG1	1:AC:372:ILE:HG22	2.29	0.62
1:AD:287:ASP:HB3	1:AD:290:LYS:HE2	1.80	0.62
1:AK:235:LEU:HD22	1:AL:244:ARG:HH12	1.63	0.62
1:AK:394:LYS:HA	1:AK:394:LYS:HE3	1.80	0.62
1:UI:167:ARG:NH2	1:WW:188:GLU:HB3	2.13	0.62
1:WQ:128:GLU:HG2	1:WR:126:PHE:CD2	2.34	0.62
6:S:72:HIS:CB	1:AE:295:SER:CB	2.73	0.62
4:F:162:PRO:HD2	4:F:163:GLU:N	2.14	0.62
1:2:235:LEU:HD22	1:3:244:ARG:HH12	1.63	0.62
1:WS:197:LEU:HD12	1:WT:175:SER:HB3	1.81	0.62
3:E:105:GLN:NE2	4:F:216:THR:O	2.33	0.62
4:G:67:ILE:HD12	4:G:239:LEU:HD13	1.81	0.62
4:J:45:LEU:HG	5:P:89:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:287:ASP:HB3	1:AE:290:LYS:HE2	1.80	0.62
1:AP:394:LYS:HA	1:AP:394:LYS:HE3	1.80	0.62
1:WQ:128:GLU:HG2	1:WR:126:PHE:HD2	1.65	0.62
2:B:24:LEU:HD22	2:B:58:VAL:HG13	1.81	0.62
6:U:78:VAL:HG12	1:1:299:ASN:HD21	1.62	0.62
1:7:287:ASP:HB3	1:7:290:LYS:HE2	1.80	0.62
1:AC:287:ASP:HB3	1:AC:290:LYS:HE2	1.80	0.62
1:WE:166:VAL:CG2	4:I:160:GLN:CG	2.78	0.62
1:AJ:287:ASP:HB3	1:AJ:290:LYS:HE2	1.80	0.62
1:WK:197:LEU:HD11	1:WL:156:HIS:HD2	1.63	0.62
4:H:52:THR:OG1	5:M:91:LYS:NZ	2.28	0.62
5:L:4:ILE:HG13	1:AI:372:ILE:HG21	1.82	0.62
6:S:72:HIS:CE1	1:AD:365:ASN:HB3	2.33	0.62
1:AL:394:LYS:HA	1:AL:394:LYS:HE3	1.80	0.62
1:UO:103:GLN:NE2	1:WU:182:PRO:CB	2.63	0.62
1:UP:167:ARG:HH11	1:8:236:LYS:HE2	1.63	0.62
1:AP:287:ASP:HB3	1:AP:290:LYS:HE2	1.80	0.62
1:AQ:394:LYS:HA	1:AQ:394:LYS:HE3	1.80	0.62
1:1:287:ASP:HB3	1:1:290:LYS:HE2	1.80	0.61
1:AB:287:ASP:HB3	1:AB:290:LYS:HE2	1.80	0.61
1:AN:394:LYS:HA	1:AN:394:LYS:HE3	1.80	0.61
1:UI:73:MET:HE3	1:UI:99:ARG:CD	2.27	0.61
1:WT:128:GLU:HG2	1:WU:126:PHE:CD2	2.35	0.61
2:D:46:GLU:HB2	2:D:49:LEU:HD23	1.82	0.61
2:D:70:LEU:O	2:D:74:LEU:HG	2.01	0.61
1:UK:73:MET:HE1	1:UK:99:ARG:HD3	1.80	0.61
1:UN:73:MET:HE3	1:UN:99:ARG:HD3	1.81	0.61
1:WO:197:LEU:CD1	1:WP:175:SER:OG	2.42	0.61
1:AF:287:ASP:HB3	1:AF:290:LYS:HE2	1.80	0.61
1:AM:394:LYS:HA	1:AM:394:LYS:HE3	1.80	0.61
1:AQ:287:ASP:HB3	1:AQ:290:LYS:HE2	1.80	0.61
1:UK:207:PRO:CG	1:WE:187:ASP:CG	2.68	0.61
1:WI:190:GLN:HG2	1:WJ:217:GLY:HA3	1.82	0.61
3:E:114:VAL:HG12	4:G:213:PRO:HB3	1.81	0.61
1:UL:208:GLY:N	1:WG:187:ASP:OD2	2.33	0.61
1:WB:212:LEU:HB3	1:WB:221:THR:HG23	1.81	0.61
1:WI:190:GLN:NE2	1:WJ:216:SER:O	2.33	0.61
1:WO:128:GLU:HG2	1:WP:126:PHE:HD2	1.64	0.61
4:G:82:SER:HA	5:K:103:GLN:NE2	2.15	0.61
5:M:11:ILE:CD1	5:M:12:SER:N	2.55	0.61
1:WW:125:GLN:OE1	2:B:2:THR:HG21	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:11:ILE:HD12	5:M:12:SER:CA	2.31	0.61
1:WP:128:GLU:HG3	1:WQ:126:PHE:CE2	2.35	0.61
1:WP:190:GLN:NE2	1:WQ:216:SER:O	2.33	0.61
4:F:52:THR:OG1	5:K:91:LYS:NZ	2.34	0.61
6:R:51:LYS:NZ	6:R:84:ASP:OD1	2.34	0.61
7:W:27:ASN:OD1	7:W:42:TYR:OH	2.19	0.61
1:WJ:164:LEU:CB	3:E:145:TRP:CD1	2.83	0.61
1:WJ:186:LEU:HA	1:WJ:190:GLN:OE1	2.00	0.61
1:WR:212:LEU:HB3	1:WR:221:THR:HG23	1.82	0.61
2:A:56:VAL:O	2:A:60:ILE:HG12	2.01	0.61
4:G:66:ARG:NE	4:G:178:GLU:OE1	2.33	0.61
1:WC:193:ALA:HB1	1:WD:213:VAL:CG1	2.30	0.60
1:WH:197:LEU:HD12	1:WI:175:SER:HB3	1.83	0.60
1:WM:200:SER:O	1:WN:158:ALA:HB3	2.01	0.60
1:UK:103:GLN:CD	1:WF:182:PRO:HB3	2.21	0.60
1:WI:164:LEU:HD23	1:WI:165:PHE:HB3	1.83	0.60
3:E:106:MET:SD	3:E:225:GLY:HA3	2.40	0.60
7:Z:12:SER:OG	7:Z:62:VAL:O	2.19	0.60
1:UI:73:MET:HE1	1:UI:99:ARG:CD	2.31	0.60
1:UM:126:PHE:CE1	1:UM:130:VAL:CG2	2.84	0.60
1:WA:197:LEU:HA	1:WB:175:SER:OG	2.00	0.60
4:I:83:ALA:HB3	4:I:84:PRO:HD3	1.83	0.60
1:WA:175:SER:CB	1:WW:197:LEU:HA	2.31	0.60
1:UK:127:SER:O	1:UK:131:ASN:CB	2.50	0.60
1:UP:103:GLN:HG2	1:WW:182:PRO:HB3	0.71	0.60
1:WE:197:LEU:CD1	1:WF:175:SER:OG	2.44	0.60
1:WV:164:LEU:HB3	4:G:152:ARG:NH1	2.17	0.60
1:UM:103:GLN:NE2	1:WQ:182:PRO:HB3	2.17	0.60
1:WF:190:GLN:HA	1:WG:217:GLY:O	2.01	0.60
1:WK:197:LEU:HA	1:WL:175:SER:CB	2.32	0.60
1:WR:186:LEU:HA	1:WR:190:GLN:OE1	2.00	0.60
1:4:402:LEU:HD12	1:4:403:PRO:HD2	1.84	0.60
1:AM:402:LEU:HD12	1:AM:403:PRO:HD2	1.84	0.60
1:UP:167:ARG:NH1	1:8:236:LYS:HE2	2.15	0.60
1:WH:193:ALA:CB	1:WI:213:VAL:HG11	2.26	0.60
2:B:14:MET:HG3	2:C:59:PHE:CE1	2.36	0.60
2:D:74:LEU:HD11	4:J:228:LEU:HD13	1.83	0.60
1:5:402:LEU:HD12	1:5:403:PRO:HD2	1.84	0.60
1:WK:197:LEU:HD11	1:WL:156:HIS:CD2	2.35	0.60
1:1:402:LEU:HD12	1:1:403:PRO:HD2	1.84	0.60
1:UI:127:SER:O	1:UI:131:ASN:CB	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WH:167:ARG:HH22	4:J:162:PRO:CG	2.14	0.60
1:WJ:212:LEU:HB3	1:WJ:221:THR:HG23	1.84	0.60
4:J:83:ALA:CB	4:J:84:PRO:HD3	2.30	0.60
6:T:55:ARG:NH2	1:5:299:ASN:HD21	1.91	0.60
1:7:402:LEU:HD12	1:7:403:PRO:HD2	1.84	0.60
1:UK:126:PHE:CE1	1:UK:130:VAL:CG2	2.84	0.60
1:WI:200:SER:O	1:WJ:158:ALA:HB2	2.02	0.60
1:WM:143:THR:OG1	1:WN:154:ARG:CG	2.41	0.60
4:J:184:GLN:O	4:J:188:THR:HG23	2.02	0.60
1:2:402:LEU:HD12	1:2:403:PRO:HD2	1.84	0.60
1:8:402:LEU:HD12	1:8:403:PRO:HD2	1.84	0.60
1:AL:402:LEU:HD12	1:AL:403:PRO:HD2	1.84	0.60
1:UI:126:PHE:CE1	1:UI:130:VAL:CG2	2.84	0.59
1:UN:127:SER:O	1:UN:131:ASN:CB	2.50	0.59
1:UN:208:GLY:N	1:WR:187:ASP:OD1	2.35	0.59
1:UO:126:PHE:CE1	1:UO:130:VAL:CG2	2.84	0.59
1:UP:127:SER:O	1:UP:131:ASN:CB	2.50	0.59
1:WD:168:GLU:CG	1:WD:170:LYS:HE2	2.31	0.59
6:U:32:ASN:ND2	7:Z:60:GLY:O	2.35	0.59
7:Y:109:SER:O	7:Y:113:GLN:HG3	2.02	0.59
1:3:402:LEU:HD12	1:3:403:PRO:HD2	1.84	0.59
1:AG:402:LEU:HD12	1:AG:403:PRO:HD2	1.84	0.59
1:AN:402:LEU:HD12	1:AN:403:PRO:HD2	1.84	0.59
1:UL:127:SER:O	1:UL:131:ASN:CB	2.50	0.59
1:UM:127:SER:O	1:UM:131:ASN:CB	2.50	0.59
1:WG:212:LEU:HB3	1:WG:221:THR:HG23	1.83	0.59
2:C:52:ILE:O	2:C:56:VAL:HG22	2.02	0.59
5:M:11:ILE:CG2	1:AB:372:ILE:HG22	2.31	0.59
6:U:68:THR:CG2	1:1:294:ARG:HD3	2.30	0.59
7:V:20:ARG:HD3	7:V:108:ALA:HB2	1.84	0.59
1:6:402:LEU:HD12	1:6:403:PRO:HD2	1.84	0.59
1:AH:402:LEU:HD12	1:AH:403:PRO:HD2	1.84	0.59
1:WB:197:LEU:CD1	1:WC:175:SER:OG	2.48	0.59
1:WS:193:ALA:HB1	1:WT:213:VAL:HG11	1.84	0.59
1:WV:190:GLN:NE2	1:WW:216:SER:O	2.34	0.59
4:I:232:TRP:O	4:I:236:MET:HG2	2.02	0.59
6:T:65:LEU:HB2	1:7:295:SER:CB	2.32	0.59
1:UJ:127:SER:O	1:UJ:131:ASN:CB	2.50	0.59
1:UO:127:SER:O	1:UO:131:ASN:CB	2.50	0.59
1:WI:186:LEU:HA	1:WI:190:GLN:OE1	2.02	0.59
1:WJ:128:GLU:OE2	1:WK:127:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WJ:164:LEU:HD13	3:E:145:TRP:CG	2.33	0.59
1:WP:128:GLU:HG2	1:WQ:126:PHE:CD2	2.37	0.59
1:WP:212:LEU:HB3	1:WP:221:THR:HG23	1.85	0.59
1:WR:122:GLY:O	1:WR:123:ILE:C	2.39	0.59
6:R:74:PRO:O	6:R:75:ALA:C	2.40	0.59
6:S:115:LYS:HE3	7:Y:4:LEU:HD11	1.84	0.59
1:9:402:LEU:HD12	1:9:403:PRO:HD2	1.84	0.59
1:AF:402:LEU:HD12	1:AF:403:PRO:HD2	1.84	0.59
1:WC:212:LEU:HB3	1:WC:221:THR:HG23	1.84	0.59
1:WD:197:LEU:HD12	1:WE:175:SER:HB3	1.85	0.59
1:WP:193:ALA:HB1	1:WQ:213:VAL:CG1	2.32	0.59
6:Q:46:ALA:O	6:Q:50:LYS:HG3	2.02	0.59
6:R:68:THR:CG2	1:AJ:294:ARG:CD	2.80	0.59
1:0:402:LEU:HD12	1:0:403:PRO:HD2	1.84	0.59
2:B:51:PHE:CZ	2:B:55:ILE:HD11	2.38	0.59
4:F:66:ARG:NH2	4:F:243:PHE:O	2.36	0.59
5:M:3:ALA:C	1:AC:372:ILE:CD1	2.70	0.59
1:AI:402:LEU:HD12	1:AI:403:PRO:HD2	1.84	0.59
1:AO:402:LEU:HD12	1:AO:403:PRO:HD2	1.84	0.59
1:UL:126:PHE:CE1	1:UL:130:VAL:CG2	2.84	0.59
1:WA:212:LEU:HB3	1:WA:221:THR:HG23	1.84	0.59
1:WI:212:LEU:HB3	1:WI:221:THR:HG23	1.84	0.59
1:WS:190:GLN:NE2	1:WT:216:SER:O	2.36	0.59
2:A:84:LEU:HD13	4:G:188:THR:HG21	1.84	0.59
1:AA:402:LEU:HD12	1:AA:403:PRO:HD2	1.84	0.59
1:AK:402:LEU:HD12	1:AK:403:PRO:HD2	1.84	0.59
1:WK:196:HIS:HB3	1:WL:211:THR:CG2	2.22	0.59
5:L:7:ILE:CG2	1:AH:278:THR:HG21	2.33	0.59
1:7:377:MET:SD	1:7:377:MET:N	2.76	0.59
1:WK:197:LEU:CD1	1:WL:175:SER:OG	2.51	0.59
1:9:377:MET:N	1:9:377:MET:SD	2.76	0.59
1:AJ:252:ILE:HD11	1:AJ:419:ALA:HB2	1.85	0.59
1:WK:203:ALA:HB1	1:WL:160:PRO:HA	1.84	0.58
1:AC:252:ILE:HD11	1:AC:419:ALA:HB2	1.85	0.58
1:AD:377:MET:N	1:AD:377:MET:SD	2.76	0.58
1:AF:377:MET:N	1:AF:377:MET:SD	2.76	0.58
1:AH:252:ILE:HD11	1:AH:419:ALA:HB2	1.85	0.58
1:AI:252:ILE:HD11	1:AI:419:ALA:HB2	1.85	0.58
1:WJ:164:LEU:CB	3:E:145:TRP:NE1	2.54	0.58
1:WS:196:HIS:HB3	1:WT:211:THR:HG21	1.84	0.58
1:WT:116:LEU:HD13	1:WT:135:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:377:MET:N	1:5:377:MET:SD	2.76	0.58
1:AH:377:MET:SD	1:AH:377:MET:N	2.76	0.58
1:AQ:377:MET:N	1:AQ:377:MET:SD	2.76	0.58
1:WE:128:GLU:HB3	1:WF:126:PHE:CD2	2.38	0.58
1:WT:212:LEU:HB3	1:WT:221:THR:HG23	1.84	0.58
5:L:7:ILE:HD11	1:AI:370:ARG:NE	2.17	0.58
5:L:11:ILE:CG2	1:AH:372:ILE:HB	2.33	0.58
6:T:65:LEU:HB2	1:7:295:SER:HB2	1.84	0.58
7:V:55:PRO:HG3	1:AP:359:GLN:CD	2.23	0.58
1:1:252:ILE:HD11	1:1:419:ALA:HB2	1.85	0.58
1:9:305:GLY:HA3	1:9:355:PRO:HG2	1.86	0.58
1:AA:377:MET:N	1:AA:377:MET:SD	2.76	0.58
1:AB:402:LEU:HD12	1:AB:403:PRO:HD2	1.84	0.58
1:AC:377:MET:N	1:AC:377:MET:SD	2.76	0.58
1:AD:252:ILE:HD11	1:AD:419:ALA:HB2	1.85	0.58
1:AE:305:GLY:HA3	1:AE:355:PRO:HG2	1.86	0.58
1:AE:402:LEU:HD12	1:AE:403:PRO:HD2	1.84	0.58
1:AN:377:MET:N	1:AN:377:MET:SD	2.76	0.58
1:AO:252:ILE:HD11	1:AO:419:ALA:HB2	1.85	0.58
1:AP:377:MET:SD	1:AP:377:MET:N	2.76	0.58
1:AQ:402:LEU:HD12	1:AQ:403:PRO:HD2	1.84	0.58
1:WK:212:LEU:HB3	1:WK:221:THR:HG23	1.84	0.58
4:F:44:THR:HG23	5:K:84:MET:HE1	1.86	0.58
6:S:67:LEU:HA	6:S:72:HIS:NE2	2.18	0.58
1:3:252:ILE:HD11	1:3:419:ALA:HB2	1.85	0.58
1:4:305:GLY:HA3	1:4:355:PRO:HG2	1.86	0.58
1:AB:377:MET:SD	1:AB:377:MET:N	2.76	0.58
1:AD:305:GLY:HA3	1:AD:355:PRO:HG2	1.86	0.58
1:AK:252:ILE:HD11	1:AK:419:ALA:HB2	1.85	0.58
1:WA:175:SER:OG	1:WW:197:LEU:CD1	2.51	0.58
1:WO:166:VAL:HG22	4:F:142:THR:O	2.03	0.58
6:R:66:THR:OG1	1:AJ:294:ARG:HG2	2.02	0.58
1:3:377:MET:N	1:3:377:MET:SD	2.76	0.58
1:4:252:ILE:HD11	1:4:419:ALA:HB2	1.85	0.58
1:5:305:GLY:HA3	1:5:355:PRO:HG2	1.86	0.58
1:0:305:GLY:HA3	1:0:355:PRO:HG2	1.86	0.58
1:AJ:402:LEU:HD12	1:AJ:403:PRO:HD2	1.84	0.58
1:AP:402:LEU:HD12	1:AP:403:PRO:HD2	1.84	0.58
6:Q:127:LEU:O	6:Q:131:MET:HG2	2.03	0.58
6:S:42:ASP:OD1	6:S:88:ARG:NH2	2.36	0.58
1:AB:252:ILE:HD11	1:AB:419:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:252:ILE:HD11	1:AE:419:ALA:HB2	1.85	0.58
1:AN:252:ILE:HD11	1:AN:419:ALA:HB2	1.85	0.58
1:AO:377:MET:N	1:AO:377:MET:SD	2.76	0.58
1:WE:212:LEU:HB3	1:WE:221:THR:HG23	1.85	0.58
1:WW:125:GLN:CB	2:B:2:THR:HG21	2.34	0.58
2:A:35:ILE:HD11	2:A:53:PRO:HB2	1.85	0.58
1:4:377:MET:SD	1:4:377:MET:N	2.76	0.58
1:6:252:ILE:HD11	1:6:419:ALA:HB2	1.85	0.58
1:AE:377:MET:SD	1:AE:377:MET:N	2.76	0.58
1:AL:377:MET:N	1:AL:377:MET:SD	2.76	0.58
1:AP:252:ILE:HD11	1:AP:419:ALA:HB2	1.85	0.58
1:WU:164:LEU:HA	4:G:152:ARG:HG3	1.84	0.58
1:WU:212:LEU:HB3	1:WU:221:THR:HG23	1.84	0.58
1:WV:134:ARG:HB3	1:WV:134:ARG:HH21	1.69	0.58
2:C:29:LEU:HD22	2:D:52:ILE:HG21	1.84	0.58
4:J:82:SER:OG	5:N:104:VAL:O	2.20	0.58
5:K:11:ILE:CD1	1:AL:276:GLU:OE2	2.52	0.58
5:L:11:ILE:HG22	1:AH:372:ILE:CB	2.32	0.58
5:M:7:ILE:CB	1:AB:278:THR:HG21	2.11	0.58
1:UJ:167:ARG:CZ	1:WB:188:GLU:OE2	2.52	0.58
1:WA:187:ASP:CG	1:WA:190:GLN:HG3	2.24	0.58
1:WE:200:SER:O	1:WF:158:ALA:CB	2.52	0.58
1:WH:167:ARG:NH2	4:J:162:PRO:HG2	2.18	0.58
3:E:187:ALA:O	3:E:190:VAL:HG12	2.04	0.58
4:H:83:ALA:HB3	4:H:84:PRO:HD3	1.85	0.58
7:V:50:GLN:HG3	7:V:65:ALA:HB2	1.85	0.58
1:2:252:ILE:HD11	1:2:419:ALA:HB2	1.85	0.58
1:5:252:ILE:HD11	1:5:419:ALA:HB2	1.85	0.58
1:6:377:MET:N	1:6:377:MET:SD	2.76	0.58
1:0:377:MET:N	1:0:377:MET:SD	2.76	0.58
1:AA:305:GLY:HA3	1:AA:355:PRO:HG2	1.86	0.58
1:AG:252:ILE:HD11	1:AG:419:ALA:HB2	1.85	0.58
1:AI:305:GLY:HA3	1:AI:355:PRO:HG2	1.86	0.58
1:UP:126:PHE:CE1	1:UP:130:VAL:CG2	2.84	0.58
1:WA:213:VAL:CG1	1:WW:193:ALA:HB1	2.32	0.58
1:WB:186:LEU:HA	1:WB:190:GLN:OE1	2.04	0.58
4:I:146:ASP:OD1	4:J:233:GLN:NE2	2.37	0.58
4:J:229:VAL:O	4:J:230:ASP:C	2.41	0.58
1:7:252:ILE:HD11	1:7:419:ALA:HB2	1.85	0.58
1:8:305:GLY:HA3	1:8:355:PRO:HG2	1.86	0.58
1:AC:402:LEU:HD12	1:AC:403:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:305:GLY:HA3	1:AJ:355:PRO:HG2	1.86	0.58
1:AJ:377:MET:N	1:AJ:377:MET:SD	2.76	0.58
1:AM:252:ILE:HD11	1:AM:419:ALA:HB2	1.85	0.58
1:WG:166:VAL:HG12	1:WG:168:GLU:HB3	1.86	0.57
3:E:167:ASN:HD21	3:E:174:ARG:HH12	1.52	0.57
1:3:305:GLY:HA3	1:3:355:PRO:HG2	1.86	0.57
1:6:305:GLY:HA3	1:6:355:PRO:HG2	1.86	0.57
1:AF:305:GLY:HA3	1:AF:355:PRO:HG2	1.86	0.57
1:WD:168:GLU:OE1	1:WD:170:LYS:CE	2.51	0.57
3:E:176:GLY:HA2	3:E:179:ILE:HD12	1.86	0.57
5:M:19:MET:HA	1:0:276:GLU:OE2	2.04	0.57
1:2:377:MET:N	1:2:377:MET:SD	2.76	0.57
1:AD:402:LEU:HD12	1:AD:403:PRO:HD2	1.84	0.57
1:AG:377:MET:N	1:AG:377:MET:SD	2.76	0.57
1:AK:305:GLY:HA3	1:AK:355:PRO:HG2	1.85	0.57
1:WV:212:LEU:HB3	1:WV:221:THR:HG23	1.84	0.57
6:Q:67:LEU:HD11	6:Q:74:PRO:HA	1.85	0.57
1:1:377:MET:N	1:1:377:MET:SD	2.76	0.57
1:AC:305:GLY:HA3	1:AC:355:PRO:HG2	1.86	0.57
1:UN:208:GLY:HA3	1:WR:187:ASP:OD1	2.05	0.57
1:8:377:MET:N	1:8:377:MET:SD	2.76	0.57
1:AH:305:GLY:HA3	1:AH:355:PRO:HG2	1.86	0.57
1:AL:252:ILE:HD11	1:AL:419:ALA:HB2	1.85	0.57
1:AQ:305:GLY:HA3	1:AQ:355:PRO:HG2	1.85	0.57
1:UJ:126:PHE:CE1	1:UJ:130:VAL:CG2	2.84	0.57
1:UL:69:GLN:HE22	1:WH:182:PRO:HG2	1.69	0.57
1:WE:166:VAL:HG22	4:I:160:GLN:N	2.18	0.57
1:WE:167:ARG:CD	4:I:161:GLY:CA	2.81	0.57
1:WG:149:PRO:HG2	1:WG:190:GLN:NE2	2.19	0.57
1:WG:197:LEU:HD12	1:WH:175:SER:CB	2.35	0.57
1:WK:193:ALA:CB	1:WL:213:VAL:CG2	2.76	0.57
1:WV:197:LEU:CD1	1:WW:175:SER:OG	2.53	0.57
3:E:170:MET:O	3:E:174:ARG:N	2.26	0.57
5:M:4:ILE:HG12	1:AC:372:ILE:CB	2.34	0.57
5:P:76:GLN:HG3	7:V:123:LYS:HD2	1.86	0.57
6:T:103:ASP:OD1	7:Z:112:TYR:OH	2.14	0.57
6:U:42:ASP:OD1	6:U:43:ILE:N	2.38	0.57
6:U:72:HIS:HE1	1:2:294:ARG:NE	2.01	0.57
1:AK:377:MET:N	1:AK:377:MET:SD	2.76	0.57
1:UO:73:MET:HE3	1:UO:99:ARG:CD	2.32	0.57
6:S:65:LEU:C	6:S:65:LEU:HD12	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:252:ILE:HD11	1:AF:419:ALA:HB2	1.85	0.57
1:AP:305:GLY:HA3	1:AP:355:PRO:HG2	1.86	0.57
1:WM:197:LEU:CD1	1:WN:175:SER:OG	2.48	0.57
3:E:185:MET:O	3:E:186:LEU:C	2.42	0.57
1:8:252:ILE:HD11	1:8:419:ALA:HB2	1.85	0.57
1:AA:252:ILE:HD11	1:AA:419:ALA:HB2	1.85	0.57
1:AI:377:MET:N	1:AI:377:MET:SD	2.76	0.57
1:UK:161:LYS:O	1:UK:162:PRO:C	2.43	0.57
1:UP:126:PHE:O	1:UP:130:VAL:HB	2.05	0.57
6:S:65:LEU:CD1	1:AD:365:ASN:ND2	2.67	0.57
1:AG:305:GLY:HA3	1:AG:355:PRO:HG2	1.86	0.57
1:WC:196:HIS:HB3	1:WD:211:THR:HG21	1.87	0.57
1:WQ:196:HIS:CD2	1:WR:219:LEU:HD22	2.40	0.57
5:L:11:ILE:HG21	1:AH:372:ILE:HB	1.87	0.57
1:UK:207:PRO:HG2	1:WE:187:ASP:OD2	2.05	0.57
1:UM:161:LYS:O	1:UM:162:PRO:C	2.43	0.57
1:WG:197:LEU:HA	1:WH:175:SER:OG	2.05	0.57
1:WO:200:SER:O	1:WP:158:ALA:HB2	2.04	0.57
1:WU:200:SER:O	1:WV:158:ALA:CB	2.52	0.57
6:R:65:LEU:HD22	1:AJ:295:SER:HB2	1.86	0.57
1:AB:305:GLY:HA3	1:AB:355:PRO:HG2	1.86	0.57
1:AM:377:MET:N	1:AM:377:MET:SD	2.76	0.57
1:AO:305:GLY:HA3	1:AO:355:PRO:HG2	1.86	0.57
1:AQ:252:ILE:HD11	1:AQ:419:ALA:HB2	1.85	0.57
1:UJ:126:PHE:O	1:UJ:130:VAL:HB	2.05	0.56
1:UO:126:PHE:O	1:UO:130:VAL:HB	2.05	0.56
1:WE:167:ARG:HD3	4:I:161:GLY:CA	2.27	0.56
1:WK:187:ASP:OD1	1:WK:187:ASP:N	2.38	0.56
1:WQ:124:SER:O	1:WQ:127:SER:N	2.37	0.56
1:WV:160:PRO:HB2	1:WV:170:LYS:HB2	1.87	0.56
3:E:149:LEU:O	3:E:153:THR:HG23	2.05	0.56
4:J:83:ALA:O	4:J:84:PRO:C	2.39	0.56
7:W:94:PRO:HB2	7:W:96:VAL:HG23	1.86	0.56
1:7:305:GLY:HA3	1:7:355:PRO:HG2	1.86	0.56
1:UI:126:PHE:O	1:UI:130:VAL:HB	2.05	0.56
2:B:9:MET:HA	2:B:12:GLU:OE1	2.05	0.56
5:L:8:GLU:O	5:L:11:ILE:HG13	2.05	0.56
5:O:8:GLU:O	5:O:11:ILE:HG13	2.06	0.56
1:9:252:ILE:HD11	1:9:419:ALA:HB2	1.85	0.56
1:AN:305:GLY:HA3	1:AN:355:PRO:HG2	1.86	0.56
1:UJ:73:MET:HE3	1:UJ:99:ARG:CD	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UN:51:TYR:OH	1:UN:76:PRO:HB2	2.05	0.56
1:UN:126:PHE:O	1:UN:130:VAL:HB	2.05	0.56
1:UO:161:LYS:O	1:UO:162:PRO:C	2.43	0.56
1:WA:121:PHE:HB3	2:C:68:TRP:CD1	2.40	0.56
1:WI:164:LEU:HD13	4:J:148:ALA:HB1	1.88	0.56
5:P:8:GLU:O	5:P:11:ILE:HG13	2.06	0.56
6:R:114:LEU:HD21	7:X:126:MET:SD	2.45	0.56
1:1:305:GLY:HA3	1:1:355:PRO:HG2	1.86	0.56
1:UL:161:LYS:O	1:UL:162:PRO:C	2.43	0.56
1:WA:213:VAL:HG21	1:WW:193:ALA:HB1	1.86	0.56
1:WC:170:LYS:H	1:WC:170:LYS:HD2	1.69	0.56
1:WN:203:ALA:HB2	1:WO:160:PRO:HA	1.86	0.56
1:WU:197:LEU:HD12	1:WV:175:SER:HB3	1.87	0.56
5:K:8:GLU:O	5:K:11:ILE:HG13	2.05	0.56
1:2:305:GLY:HA3	1:2:355:PRO:HG2	1.86	0.56
1:0:252:ILE:HD11	1:0:419:ALA:HB2	1.85	0.56
1:AL:305:GLY:HA3	1:AL:355:PRO:HG2	1.86	0.56
1:UM:51:TYR:OH	1:UM:76:PRO:HB2	2.06	0.56
1:WI:170:LYS:O	1:WI:171:SER:OG	2.21	0.56
2:D:25:LEU:HD23	4:J:206:ALA:HB2	1.86	0.56
5:L:11:ILE:HG22	1:AH:372:ILE:CG1	2.32	0.56
1:UK:73:MET:HE1	1:UK:99:ARG:CD	2.35	0.56
5:M:3:ALA:C	1:AC:372:ILE:HD13	2.26	0.56
1:UI:51:TYR:OH	1:UI:76:PRO:HB2	2.05	0.56
1:UJ:55:PHE:HB2	1:UJ:58:LEU:HD11	1.88	0.56
1:UP:161:LYS:O	1:UP:162:PRO:C	2.43	0.56
1:WR:123:ILE:HB	1:WR:127:SER:OG	2.06	0.56
3:E:205:ASN:HD21	4:F:211:MET:HB2	1.71	0.56
1:UP:51:TYR:OH	1:UP:76:PRO:HB2	2.06	0.56
1:UP:55:PHE:HB2	1:UP:58:LEU:HD11	1.88	0.56
1:WA:216:SER:O	1:WW:190:GLN:NE2	2.39	0.56
1:WB:143:THR:OG1	1:WC:154:ARG:HG2	2.06	0.56
1:WU:200:SER:O	1:WV:158:ALA:HB2	2.06	0.56
4:H:66:ARG:HG3	4:H:182:ALA:HB2	1.87	0.56
7:W:72:ALA:O	7:W:95:ASN:ND2	2.38	0.56
1:AM:305:GLY:HA3	1:AM:355:PRO:HG2	1.86	0.56
1:UI:161:LYS:O	1:UI:162:PRO:C	2.43	0.56
1:UJ:161:LYS:O	1:UJ:162:PRO:C	2.43	0.56
1:UO:51:TYR:OH	1:UO:76:PRO:HB2	2.05	0.56
1:WD:117:ASP:O	1:WD:118:GLN:C	2.44	0.56
1:WJ:200:SER:O	1:WK:158:ALA:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WL:190:GLN:NE2	1:WM:216:SER:O	2.39	0.56
1:WM:190:GLN:HG3	1:WN:217:GLY:HA3	1.88	0.56
1:WT:187:ASP:OD1	1:WT:190:GLN:N	2.39	0.56
3:E:93:ALA:HB2	4:F:88:VAL:HG21	1.87	0.56
1:UI:55:PHE:HB2	1:UI:58:LEU:HD11	1.88	0.56
1:UM:126:PHE:O	1:UM:130:VAL:HB	2.05	0.56
1:UO:55:PHE:HB2	1:UO:58:LEU:HD11	1.88	0.56
1:WS:117:ASP:O	1:WS:118:GLN:C	2.44	0.56
1:WS:165:PHE:CE1	2:A:89:GLY:C	2.79	0.56
5:K:14:LEU:CB	1:AL:278:THR:HG21	2.35	0.56
5:N:14:LEU:HD11	1:6:370:ARG:HH21	1.71	0.56
1:UL:126:PHE:O	1:UL:130:VAL:HB	2.05	0.55
1:UO:102:GLN:HG2	1:UO:193:ALA:HB2	1.88	0.55
1:UP:102:GLN:HG2	1:UP:193:ALA:HB2	1.89	0.55
1:WB:197:LEU:HD12	1:WC:175:SER:HB3	1.87	0.55
1:WJ:139:GLU:HB3	1:WK:154:ARG:HH21	1.70	0.55
1:WV:120:LYS:HZ3	1:WV:123:ILE:HD11	1.71	0.55
1:UJ:126:PHE:CD1	1:UJ:130:VAL:CG2	2.90	0.55
1:UL:126:PHE:CD1	1:UL:130:VAL:CG2	2.90	0.55
1:WA:156:HIS:HD2	1:WW:197:LEU:HD11	1.71	0.55
1:WD:143:THR:OG1	1:WE:154:ARG:HG2	2.06	0.55
1:WG:190:GLN:NE2	1:WH:216:SER:O	2.39	0.55
1:WJ:190:GLN:HG2	1:WK:216:SER:O	2.07	0.55
4:H:58:LEU:O	4:H:62:THR:OG1	2.23	0.55
4:I:59:LEU:HD11	5:N:102:MET:HE1	1.88	0.55
4:J:75:ARG:NH1	4:J:86:ASN:OD1	2.36	0.55
5:L:87:GLN:O	5:L:91:LYS:HG2	2.06	0.55
1:8:264:ALA:HB2	1:8:389:VAL:HG13	1.89	0.55
1:UN:55:PHE:HB2	1:UN:58:LEU:HD11	1.88	0.55
1:WL:197:LEU:CD1	1:WM:175:SER:CB	2.72	0.55
1:WO:128:GLU:HG2	1:WP:126:PHE:CD2	2.40	0.55
1:WO:166:VAL:CG2	4:F:139:LEU:O	2.50	0.55
5:M:12:SER:O	5:M:15:GLN:HG3	2.06	0.55
1:UI:102:GLN:HG2	1:UI:193:ALA:HB2	1.89	0.55
1:UN:126:PHE:CE1	1:UN:130:VAL:CG2	2.84	0.55
1:UN:161:LYS:O	1:UN:162:PRO:C	2.43	0.55
1:WR:197:LEU:HA	1:WS:175:SER:OG	2.07	0.55
1:WS:172:PRO:HD2	1:WS:204:GLY:O	2.07	0.55
4:F:38:TRP:HB2	5:L:46:SER:OG	2.06	0.55
5:P:89:ARG:NH2	5:P:90:ASN:OD1	2.39	0.55
1:AQ:264:ALA:HB2	1:AQ:389:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WO:165:PHE:HE1	4:F:143:ARG:HH11	1.54	0.55
1:WV:128:GLU:HG3	1:WW:126:PHE:CE2	2.42	0.55
5:N:21:ALA:HB1	1:4:278:THR:CG2	2.35	0.55
1:UI:211:THR:HG23	1:UI:219:LEU:HD11	1.89	0.55
1:UK:51:TYR:OH	1:UK:76:PRO:HB2	2.05	0.55
1:UM:102:GLN:HG2	1:UM:193:ALA:HB2	1.89	0.55
1:WM:197:LEU:HD11	1:WN:156:HIS:HD2	1.71	0.55
1:WP:123:ILE:CG2	2:A:67:PRO:HB3	2.35	0.55
3:E:233:MET:O	3:E:236:ILE:HG12	2.06	0.55
4:J:230:ASP:OD2	4:J:230:ASP:N	2.40	0.55
5:L:11:ILE:HG21	1:AH:372:ILE:HG22	1.82	0.55
1:5:264:ALA:HB2	1:5:389:VAL:HG13	1.89	0.55
1:AA:264:ALA:HB2	1:AA:389:VAL:HG13	1.89	0.55
1:UJ:51:TYR:OH	1:UJ:76:PRO:HB2	2.06	0.55
1:UK:126:PHE:O	1:UK:130:VAL:HB	2.05	0.55
1:UM:211:THR:HG23	1:UM:219:LEU:HD11	1.89	0.55
1:UN:102:GLN:HG2	1:UN:193:ALA:HB2	1.88	0.55
1:UO:211:THR:HG23	1:UO:219:LEU:HD11	1.89	0.55
5:N:8:GLU:O	5:N:11:ILE:HG13	2.05	0.55
1:6:264:ALA:HB2	1:6:389:VAL:HG13	1.89	0.55
1:UI:126:PHE:CD1	1:UI:130:VAL:CG2	2.90	0.55
1:UJ:102:GLN:HG2	1:UJ:193:ALA:HB2	1.88	0.55
1:UN:126:PHE:CD1	1:UN:130:VAL:CG2	2.90	0.55
1:WP:197:LEU:HD12	1:WQ:175:SER:HB3	1.89	0.55
1:WP:197:LEU:HA	1:WQ:175:SER:OG	2.07	0.55
7:Z:17:GLN:NE2	7:Z:111:SER:OG	2.39	0.55
1:2:264:ALA:HB2	1:2:389:VAL:HG13	1.89	0.55
1:UK:126:PHE:CD1	1:UK:130:VAL:CG2	2.90	0.55
1:WW:117:ASP:O	1:WW:118:GLN:C	2.44	0.55
4:J:80:THR:HB	4:J:83:ALA:HB2	1.88	0.55
1:AN:264:ALA:HB2	1:AN:389:VAL:HG13	1.89	0.55
1:AP:264:ALA:HB2	1:AP:389:VAL:HG13	1.89	0.55
1:UP:211:THR:HG23	1:UP:219:LEU:HD11	1.89	0.55
1:WB:193:ALA:HB1	1:WC:213:VAL:CG1	2.36	0.55
1:WC:121:PHE:CZ	2:C:15:LYS:HE3	2.40	0.55
1:WF:200:SER:O	1:WG:158:ALA:CB	2.55	0.55
1:WP:165:PHE:CB	4:F:160:GLN:O	2.54	0.55
1:WQ:172:PRO:HD2	1:WQ:204:GLY:O	2.07	0.55
1:9:264:ALA:HB2	1:9:389:VAL:HG13	1.89	0.55
1:UP:103:GLN:CB	1:WW:182:PRO:HB3	2.33	0.54
1:WA:193:ALA:HB1	1:WB:213:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WT:190:GLN:NE2	1:WU:216:SER:O	2.39	0.54
5:K:72:MET:O	5:K:76:GLN:HG2	2.06	0.54
1:UL:51:TYR:OH	1:UL:76:PRO:HB2	2.05	0.54
1:UL:102:GLN:HG2	1:UL:193:ALA:HB2	1.88	0.54
1:UN:211:THR:HG23	1:UN:219:LEU:HD11	1.89	0.54
1:WA:200:SER:O	1:WB:158:ALA:HB2	2.08	0.54
1:WO:197:LEU:HA	1:WP:175:SER:OG	2.07	0.54
1:UP:126:PHE:CD1	1:UP:130:VAL:CG2	2.90	0.54
1:WS:124:SER:CA	2:A:8:MET:HE2	2.37	0.54
1:WS:145:GLU:O	1:WS:147:LEU:N	2.39	0.54
1:WU:130:VAL:O	1:WU:134:ARG:HG3	2.07	0.54
5:N:21:ALA:CB	1:4:278:THR:CG2	2.74	0.54
6:R:90:PRO:HB3	6:R:99:THR:HB	1.88	0.54
7:V:113:GLN:O	7:V:117:GLU:HG2	2.07	0.54
1:1:264:ALA:HB2	1:1:389:VAL:HG13	1.89	0.54
1:3:264:ALA:HB2	1:3:389:VAL:HG13	1.89	0.54
1:0:264:ALA:HB2	1:0:389:VAL:HG13	1.89	0.54
1:UK:102:GLN:HG2	1:UK:193:ALA:HB2	1.88	0.54
1:UL:55:PHE:HB2	1:UL:58:LEU:HD11	1.88	0.54
1:UL:211:THR:HG23	1:UL:219:LEU:HD11	1.89	0.54
1:WH:167:ARG:HH22	4:J:162:PRO:HG3	1.72	0.54
1:WK:171:SER:HB3	1:WK:206:PRO:HG3	1.89	0.54
1:WV:128:GLU:HG3	1:WW:126:PHE:CD2	2.43	0.54
4:F:83:ALA:HB3	4:F:84:PRO:HD3	1.89	0.54
5:O:77:LYS:HE3	6:U:13:GLN:HE22	1.73	0.54
1:UK:55:PHE:HB2	1:UK:58:LEU:HD11	1.88	0.54
1:UM:55:PHE:HB2	1:UM:58:LEU:HD11	1.88	0.54
1:WK:186:LEU:HD22	1:WK:190:GLN:CD	2.28	0.54
6:S:36:PRO:HB3	6:S:96:ASP:HB2	1.89	0.54
1:4:264:ALA:HB2	1:4:389:VAL:HG13	1.89	0.54
1:7:264:ALA:HB2	1:7:389:VAL:HG13	1.89	0.54
1:WM:193:ALA:CB	1:WN:213:VAL:HG11	2.27	0.54
1:WV:113:PHE:O	1:WV:116:LEU:HB3	2.07	0.54
2:B:36:SER:HB3	2:C:44:ILE:HG23	1.89	0.54
1:UJ:260:THR:HG23	1:UJ:268:LEU:HD11	1.89	0.54
1:UK:211:THR:HG23	1:UK:219:LEU:HD11	1.89	0.54
1:UM:103:GLN:NE2	1:WQ:182:PRO:CB	2.71	0.54
1:UM:126:PHE:CD1	1:UM:130:VAL:CG2	2.90	0.54
1:WS:186:LEU:HA	1:WS:190:GLN:OE1	2.08	0.54
3:E:38:ILE:HB	3:E:43:LYS:HE2	1.90	0.54
3:E:236:ILE:O	3:E:240:CYS:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:11:ILE:HG22	1:6:372:ILE:HB	1.88	0.54
5:O:77:LYS:HE3	6:U:13:GLN:NE2	2.23	0.54
1:AC:264:ALA:HB2	1:AC:389:VAL:HG13	1.89	0.54
1:AD:264:ALA:HB2	1:AD:389:VAL:HG13	1.89	0.54
1:UL:73:MET:HE3	1:UL:99:ARG:HD3	1.84	0.54
1:UL:88:VAL:HB	1:UL:89:PRO:HD2	1.90	0.54
1:WI:145:GLU:O	1:WI:147:LEU:N	2.41	0.54
1:WT:166:VAL:HG21	4:G:158:PRO:CB	2.38	0.54
1:WU:114:GLU:O	1:WU:117:ASP:N	2.41	0.54
1:AF:282:TYR:HB3	1:AG:292:THR:HG21	1.90	0.54
1:AK:264:ALA:HB2	1:AK:389:VAL:HG13	1.89	0.54
1:UK:88:VAL:HB	1:UK:89:PRO:HD2	1.90	0.54
1:WE:196:HIS:HB3	1:WF:211:THR:HG21	1.90	0.54
1:WT:145:GLU:O	1:WT:147:LEU:N	2.40	0.54
1:AD:282:TYR:HB3	1:AE:292:THR:HG21	1.90	0.54
1:AE:282:TYR:HB3	1:AF:292:THR:HG21	1.90	0.54
1:AO:264:ALA:HB2	1:AO:389:VAL:HG13	1.89	0.54
1:WF:193:ALA:HB1	1:WG:213:VAL:CG1	2.38	0.54
1:WF:212:LEU:HB3	1:WF:221:THR:HG23	1.90	0.54
1:WK:196:HIS:CG	1:WL:211:THR:HG21	2.42	0.54
5:N:76:GLN:NE2	7:Y:132:LEU:O	2.41	0.54
1:AF:264:ALA:HB2	1:AF:389:VAL:HG13	1.89	0.54
5:N:7:ILE:CG2	1:6:278:THR:CG2	2.80	0.53
6:S:65:LEU:HD13	1:AD:365:ASN:ND2	2.23	0.53
1:AB:282:TYR:HB3	1:AC:292:THR:HG21	1.90	0.53
1:AC:282:TYR:HB3	1:AD:292:THR:HG21	1.90	0.53
1:AG:282:TYR:HB3	1:AH:292:THR:HG21	1.90	0.53
1:AI:264:ALA:HB2	1:AI:389:VAL:HG13	1.89	0.53
1:UN:80:ALA:HB3	1:UN:83:SER:HB3	1.91	0.53
1:WP:145:GLU:HG2	1:WP:152:SER:HA	1.91	0.53
1:WU:196:HIS:HB3	1:WV:211:THR:HG21	1.89	0.53
3:E:186:LEU:HD21	3:E:236:ILE:HG22	1.90	0.53
3:E:188:LEU:O	3:E:190:VAL:N	2.39	0.53
4:I:139:LEU:HG	4:I:170:LEU:HD21	1.90	0.53
1:AB:264:ALA:HB2	1:AB:389:VAL:HG13	1.89	0.53
1:AH:264:ALA:HB2	1:AH:389:VAL:HG13	1.89	0.53
1:AM:264:ALA:HB2	1:AM:389:VAL:HG13	1.89	0.53
1:WE:200:SER:O	1:WF:158:ALA:HB2	2.09	0.53
1:WS:145:GLU:HG2	1:WS:152:SER:HA	1.91	0.53
1:WT:145:GLU:HG2	1:WT:152:SER:HA	1.91	0.53
1:AL:264:ALA:HB2	1:AL:389:VAL:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UP:80:ALA:HB3	1:UP:83:SER:HB3	1.91	0.53
1:WA:166:VAL:HG11	4:H:160:GLN:HE22	1.74	0.53
1:WA:201:ALA:C	1:WB:158:ALA:HB2	2.28	0.53
1:WD:200:SER:OG	1:WE:175:SER:CB	2.47	0.53
1:WI:164:LEU:HD22	4:J:148:ALA:CA	2.39	0.53
1:WJ:190:GLN:NE2	1:WK:216:SER:O	2.41	0.53
1:WU:145:GLU:HG2	1:WU:152:SER:HA	1.91	0.53
2:D:42:THR:HG22	2:D:44:ILE:HG12	1.91	0.53
4:I:163:GLU:N	4:I:163:GLU:OE2	2.39	0.53
6:R:65:LEU:HB3	1:AJ:295:SER:HB2	1.90	0.53
1:1:282:TYR:HB3	1:2:292:THR:HG21	1.90	0.53
1:AA:282:TYR:HB3	1:AB:292:THR:HG21	1.90	0.53
1:AG:264:ALA:HB2	1:AG:389:VAL:HG13	1.89	0.53
1:AH:282:TYR:HB3	1:AI:292:THR:HG21	1.90	0.53
1:UO:126:PHE:CD1	1:UO:130:VAL:CG2	2.90	0.53
1:UP:88:VAL:HB	1:UP:89:PRO:HD2	1.90	0.53
1:WO:145:GLU:HG2	1:WO:152:SER:HA	1.91	0.53
1:WQ:145:GLU:HG2	1:WQ:152:SER:HA	1.91	0.53
4:F:75:ARG:HD2	4:F:84:PRO:HD2	1.89	0.53
5:M:4:ILE:HG12	1:AC:372:ILE:CG2	2.37	0.53
1:3:282:TYR:HB3	1:4:292:THR:HG21	1.90	0.53
1:UN:88:VAL:HB	1:UN:89:PRO:HD2	1.90	0.53
1:UO:80:ALA:HB3	1:UO:83:SER:HB3	1.91	0.53
1:WO:149:PRO:HB3	1:WO:184:ARG:HB3	1.90	0.53
1:WV:145:GLU:HG2	1:WV:152:SER:HA	1.91	0.53
1:0:282:TYR:HB3	1:AA:292:THR:HG21	1.90	0.53
1:AI:282:TYR:HB3	1:AJ:292:THR:HG21	1.90	0.53
1:AJ:264:ALA:HB2	1:AJ:389:VAL:HG13	1.89	0.53
1:UI:159:MET:N	1:UI:159:MET:SD	2.82	0.53
1:UL:80:ALA:HB3	1:UL:83:SER:HB3	1.91	0.53
1:WQ:212:LEU:HB3	1:WQ:221:THR:HG23	1.90	0.53
1:WR:145:GLU:HG2	1:WR:152:SER:HA	1.91	0.53
1:WW:145:GLU:HG2	1:WW:152:SER:HA	1.90	0.53
2:B:77:VAL:HG21	4:H:225:LEU:HD11	1.91	0.53
5:M:11:ILE:HG21	1:AB:372:ILE:HG22	1.91	0.53
1:AJ:282:TYR:HB3	1:AK:292:THR:HG21	1.90	0.53
1:UK:80:ALA:HB3	1:UK:83:SER:HB3	1.91	0.53
1:UM:80:ALA:HB3	1:UM:83:SER:HB3	1.91	0.53
1:WK:163:SER:O	3:E:252:ALA:CB	2.57	0.53
1:WU:160:PRO:HG2	1:WU:170:LYS:O	2.08	0.53
1:WV:193:ALA:HB1	1:WW:213:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ILE:O	2:B:66:GLY:N	2.39	0.53
3:E:54:ILE:HD11	4:J:153:LEU:HB3	1.91	0.53
3:E:101:PHE:CE2	4:F:223:LEU:HD11	2.43	0.53
5:N:11:ILE:CG2	1:6:372:ILE:CG2	2.87	0.53
6:Q:50:LYS:O	6:Q:54:VAL:HG22	2.09	0.53
1:1:293:LEU:HD21	1:1:364:SER:HB3	1.91	0.53
1:3:293:LEU:HD21	1:3:364:SER:HB3	1.91	0.53
1:9:282:TYR:HB3	1:0:292:THR:HG21	1.90	0.53
1:0:293:LEU:HD21	1:0:364:SER:HB3	1.91	0.53
1:AE:264:ALA:HB2	1:AE:389:VAL:HG13	1.89	0.53
1:AK:282:TYR:HB3	1:AL:292:THR:HG21	1.90	0.53
1:UK:207:PRO:HG2	1:WE:187:ASP:CG	2.29	0.53
7:W:23:VAL:HG21	7:W:47:VAL:HG13	1.91	0.53
7:Z:57:GLN:O	7:Z:59:THR:N	2.40	0.53
1:UO:159:MET:N	1:UO:159:MET:SD	2.82	0.53
1:WO:200:SER:O	1:WP:158:ALA:CB	2.56	0.53
1:8:293:LEU:HD21	1:8:364:SER:HB3	1.91	0.53
1:AA:293:LEU:HD21	1:AA:364:SER:HB3	1.91	0.53
1:AC:293:LEU:HD21	1:AC:364:SER:HB3	1.91	0.53
1:UJ:88:VAL:HB	1:UJ:89:PRO:HD2	1.90	0.52
1:WB:145:GLU:HG2	1:WB:152:SER:HA	1.91	0.52
1:WN:145:GLU:HG2	1:WN:152:SER:HA	1.90	0.52
1:WT:145:GLU:C	1:WT:147:LEU:H	2.12	0.52
4:H:194:LEU:HD11	4:I:217:ILE:HA	1.91	0.52
4:I:180:LYS:O	4:I:184:GLN:HG3	2.09	0.52
7:Y:10:ALA:HB3	7:Y:119:LEU:HD13	1.89	0.52
1:5:293:LEU:HD21	1:5:364:SER:HB3	1.91	0.52
1:AE:293:LEU:HD21	1:AE:364:SER:HB3	1.91	0.52
1:UM:88:VAL:HB	1:UM:89:PRO:HD2	1.90	0.52
1:WA:145:GLU:HG2	1:WA:152:SER:HA	1.90	0.52
1:WD:145:GLU:HG2	1:WD:152:SER:HA	1.91	0.52
1:WG:165:PHE:CE1	4:J:240:ALA:CB	2.89	0.52
1:WR:111:VAL:HB	1:WR:114:GLU:HB3	1.92	0.52
3:E:188:LEU:HB3	3:E:189:PRO:HD2	1.91	0.52
4:H:232:TRP:O	4:H:236:MET:HG3	2.10	0.52
4:J:41:SER:HB3	6:U:133:VAL:HG21	1.91	0.52
5:P:76:GLN:NE2	7:V:123:LYS:HB2	2.24	0.52
1:4:293:LEU:HD21	1:4:364:SER:HB3	1.91	0.52
1:6:282:TYR:HB3	1:7:292:THR:HG21	1.90	0.52
1:6:293:LEU:HD21	1:6:364:SER:HB3	1.91	0.52
1:AB:293:LEU:HD21	1:AB:364:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:282:TYR:HB3	1:AM:292:THR:HG21	1.90	0.52
1:WB:164:LEU:O	4:H:152:ARG:CD	2.54	0.52
1:WJ:125:GLN:HB2	3:E:242:HIS:HB2	1.92	0.52
1:WT:124:SER:CB	2:A:4:GLU:OE2	2.57	0.52
4:I:116:PHE:O	6:T:4:ARG:NH2	2.42	0.52
7:V:80:PRO:HB3	7:V:89:GLY:HA3	1.90	0.52
1:2:282:TYR:HB3	1:3:292:THR:HG21	1.90	0.52
1:2:293:LEU:HD21	1:2:364:SER:HB3	1.91	0.52
1:5:282:TYR:HB3	1:6:292:THR:HG21	1.90	0.52
1:AD:293:LEU:HD21	1:AD:364:SER:HB3	1.91	0.52
1:AM:282:TYR:HB3	1:AN:292:THR:HG21	1.90	0.52
1:UM:159:MET:N	1:UM:159:MET:SD	2.82	0.52
1:WJ:141:ALA:O	1:WJ:145:GLU:HG3	2.09	0.52
1:WP:145:GLU:O	1:WP:147:LEU:N	2.42	0.52
1:WV:142:ARG:O	1:WV:146:THR:HG23	2.10	0.52
1:WV:164:LEU:HD23	4:G:152:ARG:HH12	1.75	0.52
4:F:149:LEU:HD22	4:G:233:GLN:HG3	1.92	0.52
4:G:58:LEU:O	4:G:62:THR:OG1	2.22	0.52
4:J:52:THR:OG1	5:O:91:LYS:NZ	2.32	0.52
5:O:73:ALA:HB1	6:U:13:GLN:HE21	1.74	0.52
1:4:282:TYR:HB3	1:5:292:THR:HG21	1.90	0.52
1:8:282:TYR:HB3	1:9:292:THR:HG21	1.90	0.52
1:AG:293:LEU:HD21	1:AG:364:SER:HB3	1.91	0.52
1:UO:88:VAL:HB	1:UO:89:PRO:HD2	1.90	0.52
1:WF:116:LEU:HD21	1:WF:134:ARG:CZ	2.38	0.52
1:WI:145:GLU:HG2	1:WI:152:SER:HA	1.91	0.52
1:WK:145:GLU:HG2	1:WK:152:SER:HA	1.90	0.52
5:N:7:ILE:HG21	1:6:278:THR:HG22	1.91	0.52
1:7:293:LEU:HD21	1:7:364:SER:HB3	1.92	0.52
1:9:293:LEU:HD21	1:9:364:SER:HB3	1.91	0.52
1:UJ:159:MET:N	1:UJ:159:MET:SD	2.82	0.52
1:UK:207:PRO:CG	1:WE:187:ASP:OD2	2.57	0.52
1:WJ:162:PRO:HA	1:WJ:169:GLN:CD	2.30	0.52
1:WP:200:SER:O	1:WQ:158:ALA:HB3	2.09	0.52
7:V:131:THR:O	7:V:131:THR:HG22	2.09	0.52
1:1:235:LEU:HB3	1:2:244:ARG:HH22	1.75	0.52
1:AF:293:LEU:HD21	1:AF:364:SER:HB3	1.91	0.52
1:AO:282:TYR:HB3	1:AP:292:THR:HG21	1.90	0.52
1:UI:80:ALA:HB3	1:UI:83:SER:HB3	1.91	0.52
1:WD:142:ARG:O	1:WD:146:THR:HG23	2.10	0.52
1:WK:170:LYS:O	1:WK:171:SER:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WS:145:GLU:C	1:WS:147:LEU:H	2.12	0.52
1:WU:186:LEU:HA	1:WU:190:GLN:OE1	2.10	0.52
2:B:3:PRO:O	2:B:7:MET:HG2	2.09	0.52
7:Y:20:ARG:NH2	7:Y:107:SER:HB2	2.24	0.52
1:AM:235:LEU:HB3	1:AN:244:ARG:HH22	1.75	0.52
1:UJ:80:ALA:HB3	1:UJ:83:SER:HB3	1.91	0.52
1:UK:159:MET:N	1:UK:159:MET:SD	2.82	0.52
1:WK:162:PRO:CB	3:E:249:ASN:HB2	2.35	0.52
1:WL:145:GLU:HG2	1:WL:152:SER:HA	1.91	0.52
1:WQ:145:GLU:O	1:WQ:147:LEU:N	2.43	0.52
1:WU:113:PHE:HB3	1:WV:134:ARG:CZ	2.39	0.52
2:D:35:ILE:HG21	2:D:50:SER:HA	1.92	0.52
2:D:77:VAL:HG11	4:J:229:VAL:HG21	1.90	0.52
4:F:199:VAL:O	4:F:203:VAL:HG23	2.10	0.52
5:O:48:ARG:NH1	6:U:3:ASP:OD2	2.43	0.52
1:4:235:LEU:HB3	1:5:244:ARG:HH22	1.75	0.52
1:AH:235:LEU:HB3	1:AI:244:ARG:HH22	1.75	0.52
1:UI:88:VAL:HB	1:UI:89:PRO:HD2	1.90	0.52
1:WB:187:ASP:CG	1:WB:190:GLN:HG3	2.30	0.52
1:WF:125:GLN:O	1:WF:128:GLU:N	2.43	0.52
1:WV:186:LEU:HA	1:WV:190:GLN:OE1	2.10	0.52
6:S:46:ALA:O	6:S:50:LYS:HG3	2.09	0.52
1:AN:282:TYR:HB3	1:AO:292:THR:HG21	1.90	0.52
1:AP:282:TYR:HB3	1:AQ:292:THR:HG21	1.90	0.52
1:WD:149:PRO:CG	1:WD:190:GLN:HE22	2.23	0.52
1:WD:168:GLU:OE1	1:WD:170:LYS:NZ	2.42	0.52
1:WD:197:LEU:HA	1:WE:175:SER:CB	2.40	0.52
1:WM:132:TYR:CD1	1:WN:130:VAL:HG22	2.45	0.52
1:WN:200:SER:HB2	1:WO:173:SER:HB2	1.92	0.52
1:WS:190:GLN:HG2	1:WT:217:GLY:HA3	1.91	0.52
4:G:74:LEU:HD22	4:G:235:LEU:HD22	1.91	0.52
4:I:73:LEU:HD13	4:I:186:GLY:HA3	1.92	0.52
1:AE:235:LEU:HB3	1:AF:244:ARG:HH22	1.75	0.52
1:AJ:235:LEU:HB3	1:AK:244:ARG:HH22	1.75	0.52
1:AL:235:LEU:HB3	1:AM:244:ARG:HH22	1.75	0.52
1:AO:235:LEU:HB3	1:AP:244:ARG:HH22	1.75	0.52
1:AP:235:LEU:HB3	1:AQ:244:ARG:HH22	1.75	0.52
1:UJ:103:GLN:CD	1:WD:182:PRO:HB3	2.28	0.51
1:WG:145:GLU:HG2	1:WG:152:SER:HA	1.91	0.51
1:WM:201:ALA:C	1:WN:158:ALA:HB2	2.30	0.51
1:WQ:145:GLU:C	1:WQ:147:LEU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WT:160:PRO:HD3	1:WT:172:PRO:CA	2.38	0.51
1:WT:161:LYS:HB3	1:WT:162:PRO:HD2	1.91	0.51
2:A:65:ALA:O	2:A:69:MET:HG3	2.09	0.51
2:C:4:GLU:C	2:C:6:VAL:H	2.13	0.51
4:G:83:ALA:HB1	4:G:84:PRO:HD2	1.92	0.51
6:R:67:LEU:HG	6:R:72:HIS:HB3	1.92	0.51
1:7:282:TYR:HB3	1:8:292:THR:HG21	1.90	0.51
1:AH:293:LEU:HD21	1:AH:364:SER:HB3	1.91	0.51
1:AI:293:LEU:HD21	1:AI:364:SER:HB3	1.91	0.51
1:WD:118:GLN:O	1:WD:119:GLU:C	2.49	0.51
1:WF:197:LEU:HA	1:WG:175:SER:OG	2.10	0.51
1:WH:145:GLU:HG2	1:WH:152:SER:HA	1.91	0.51
1:WP:145:GLU:C	1:WP:147:LEU:H	2.14	0.51
1:WP:166:VAL:HA	1:WP:169:GLN:HB2	1.91	0.51
1:WQ:125:GLN:O	1:WQ:128:GLU:N	2.43	0.51
3:E:227:MET:SD	3:E:228:LEU:N	2.82	0.51
7:Z:23:VAL:HG21	7:Z:47:VAL:HG13	1.91	0.51
1:2:235:LEU:HB3	1:3:244:ARG:HH22	1.75	0.51
1:AC:235:LEU:HB3	1:AD:244:ARG:HH22	1.75	0.51
1:AK:235:LEU:HB3	1:AL:244:ARG:HH22	1.75	0.51
1:WC:145:GLU:HG2	1:WC:152:SER:HA	1.91	0.51
1:WC:197:LEU:HA	1:WD:175:SER:OG	2.11	0.51
1:WM:145:GLU:HG2	1:WM:152:SER:HA	1.91	0.51
1:WR:190:GLN:NE2	1:WS:216:SER:O	2.43	0.51
6:Q:29:ASN:ND2	6:Q:41:ARG:O	2.36	0.51
1:5:256:ILE:HG13	1:5:257:VAL:N	2.26	0.51
1:0:235:LEU:HB3	1:AA:244:ARG:HH22	1.75	0.51
1:AO:293:LEU:HD21	1:AO:364:SER:HB3	1.91	0.51
1:UP:204:GLY:O	1:UP:206:PRO:HD3	2.11	0.51
1:WC:197:LEU:CD1	1:WD:175:SER:OG	2.58	0.51
1:WJ:128:GLU:HG3	1:WK:126:PHE:CD2	2.43	0.51
2:D:78:ARG:HG3	4:J:234:LEU:HD11	1.91	0.51
4:F:67:ILE:H	4:F:67:ILE:HD12	1.75	0.51
6:Q:62:GLY:HA2	6:Q:79:SER:HB3	1.91	0.51
6:R:68:THR:HG21	1:AJ:294:ARG:HD2	1.92	0.51
7:W:7:PHE:HZ	7:W:123:LYS:HB2	1.76	0.51
7:Z:28:LEU:HD21	7:Z:101:GLU:HB2	1.91	0.51
1:3:235:LEU:HB3	1:4:244:ARG:HH22	1.75	0.51
1:6:235:LEU:HB3	1:7:244:ARG:HH22	1.75	0.51
1:7:235:LEU:HB3	1:8:244:ARG:HH22	1.75	0.51
1:UO:204:GLY:O	1:UO:206:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WA:132:TYR:HB2	1:WB:126:PHE:HZ	1.76	0.51
2:B:59:PHE:HZ	4:G:198:LEU:HD21	1.75	0.51
3:E:130:ASP:O	3:E:134:MET:HG2	2.10	0.51
4:H:42:VAL:HG13	5:N:42:LEU:HD22	1.93	0.51
5:M:8:GLU:O	5:M:11:ILE:HG13	2.09	0.51
5:O:53:ARG:O	5:O:57:GLU:HG2	2.11	0.51
6:U:65:LEU:CB	1:1:295:SER:HB2	2.39	0.51
1:7:256:ILE:HG13	1:7:257:VAL:N	2.26	0.51
1:AA:256:ILE:HG13	1:AA:257:VAL:N	2.26	0.51
1:AG:235:LEU:HB3	1:AH:244:ARG:HH22	1.75	0.51
1:AJ:256:ILE:HG13	1:AJ:257:VAL:N	2.26	0.51
1:AL:256:ILE:HG13	1:AL:257:VAL:N	2.26	0.51
1:UJ:253:GLY:O	1:UJ:255:PRO:HD3	2.11	0.51
1:UL:159:MET:SD	1:UL:159:MET:N	2.82	0.51
1:UL:216:SER:C	1:UL:218:HIS:H	2.14	0.51
1:UM:103:GLN:CD	1:WQ:182:PRO:CB	2.71	0.51
1:WK:200:SER:CA	1:WL:173:SER:OG	2.59	0.51
1:WN:203:ALA:HB1	1:WO:160:PRO:HB3	1.93	0.51
2:D:17:ALA:HB2	4:J:195:ILE:HG23	1.92	0.51
6:S:67:LEU:HA	6:S:72:HIS:HE2	1.74	0.51
1:9:235:LEU:HB3	1:0:244:ARG:HH22	1.75	0.51
1:9:256:ILE:HG13	1:9:257:VAL:N	2.26	0.51
1:AB:235:LEU:HB3	1:AC:244:ARG:HH22	1.75	0.51
1:AL:293:LEU:HD21	1:AL:364:SER:HB3	1.91	0.51
1:UM:73:MET:HE3	1:UM:99:ARG:CD	2.36	0.51
1:WI:145:GLU:C	1:WI:147:LEU:H	2.13	0.51
5:L:7:ILE:CD1	1:AI:370:ARG:HE	2.24	0.51
1:AH:256:ILE:HG13	1:AH:257:VAL:N	2.26	0.51
1:AM:256:ILE:HG13	1:AM:257:VAL:N	2.26	0.51
1:UI:98:LEU:HD22	1:UI:147:LEU:CD2	2.39	0.51
1:UN:204:GLY:O	1:UN:206:PRO:HD3	2.11	0.51
1:WF:116:LEU:CD2	1:WF:134:ARG:HD3	2.41	0.51
1:WR:115:LEU:HD22	1:WR:134:ARG:HH11	1.75	0.51
3:E:88:MET:HG2	3:E:146:LEU:HD11	1.93	0.51
4:F:135:ARG:NH2	4:F:165:VAL:O	2.44	0.51
4:I:75:ARG:NH1	4:I:86:ASN:OD1	2.36	0.51
1:8:256:ILE:HG13	1:8:257:VAL:N	2.26	0.51
1:AF:235:LEU:HB3	1:AG:244:ARG:HH22	1.75	0.51
1:AJ:293:LEU:HD21	1:AJ:364:SER:HB3	1.91	0.51
1:AK:293:LEU:HD21	1:AK:364:SER:HB3	1.91	0.51
1:AN:256:ILE:HG13	1:AN:257:VAL:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:293:LEU:HD21	1:AN:364:SER:HB3	1.92	0.51
1:AQ:293:LEU:HD21	1:AQ:364:SER:HB3	1.91	0.51
1:UI:204:GLY:O	1:UI:206:PRO:HD3	2.11	0.51
1:WP:128:GLU:CG	1:WQ:126:PHE:CE2	2.93	0.51
2:D:2:THR:HG23	2:D:5:SER:H	1.76	0.51
3:E:86:PHE:CZ	4:F:91:GLY:HA3	2.45	0.51
4:G:193:PHE:HB3	4:G:222:LYS:HD3	1.92	0.51
1:2:256:ILE:HG13	1:2:257:VAL:N	2.26	0.51
1:3:256:ILE:HG13	1:3:257:VAL:N	2.26	0.51
1:AF:256:ILE:HG13	1:AF:257:VAL:N	2.26	0.51
1:AO:256:ILE:HG13	1:AO:257:VAL:N	2.26	0.51
1:UM:204:GLY:O	1:UM:206:PRO:HD3	2.11	0.51
1:UO:98:LEU:HD22	1:UO:147:LEU:CD2	2.39	0.51
1:WB:190:GLN:NE2	1:WC:216:SER:O	2.44	0.51
1:WI:193:ALA:HB1	1:WJ:213:VAL:HG21	1.93	0.51
1:WS:118:GLN:O	1:WS:119:GLU:C	2.49	0.51
3:E:166:SER:C	3:E:168:ALA:N	2.64	0.51
1:4:256:ILE:HG13	1:4:257:VAL:N	2.26	0.51
1:AC:256:ILE:HG13	1:AC:257:VAL:N	2.26	0.51
1:WQ:190:GLN:HG2	1:WR:216:SER:O	2.11	0.50
2:D:58:VAL:O	2:D:62:ILE:HD12	2.11	0.50
1:AM:293:LEU:HD21	1:AM:364:SER:HB3	1.91	0.50
1:AP:256:ILE:HG13	1:AP:257:VAL:N	2.26	0.50
1:UL:204:GLY:O	1:UL:206:PRO:HD3	2.11	0.50
1:WG:200:SER:OG	1:WH:175:SER:CB	2.45	0.50
1:WJ:139:GLU:HB3	1:WK:156:HIS:HE1	1.76	0.50
1:WK:160:PRO:HB3	1:WK:170:LYS:HB2	1.94	0.50
3:E:205:ASN:ND2	4:F:211:MET:HB2	2.25	0.50
4:H:65:THR:O	4:H:68:ILE:HG22	2.12	0.50
5:O:84:MET:O	5:O:88:VAL:HG23	2.11	0.50
7:Z:56:GLY:HA3	1:1:303:GLN:HE22	1.76	0.50
1:5:235:LEU:HB3	1:6:244:ARG:HH22	1.75	0.50
1:AD:256:ILE:HG13	1:AD:257:VAL:N	2.26	0.50
1:AI:256:ILE:HG13	1:AI:257:VAL:N	2.26	0.50
1:WE:167:ARG:HH21	4:I:162:PRO:HD2	1.75	0.50
1:WF:116:LEU:HD21	1:WF:134:ARG:HD3	1.93	0.50
4:I:119:GLN:HG3	6:T:4:ARG:HE	1.76	0.50
5:N:11:ILE:HG22	1:6:372:ILE:CB	2.40	0.50
1:AA:235:LEU:HB3	1:AB:244:ARG:HH22	1.75	0.50
1:AE:256:ILE:HG13	1:AE:257:VAL:N	2.26	0.50
1:AN:235:LEU:HB3	1:AO:244:ARG:HH22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:293:LEU:HD21	1:AP:364:SER:HB3	1.92	0.50
1:UK:204:GLY:O	1:UK:206:PRO:HD3	2.11	0.50
1:WD:145:GLU:C	1:WD:147:LEU:H	2.15	0.50
1:WT:162:PRO:O	1:WT:163:SER:HB3	2.11	0.50
2:D:2:THR:O	2:D:5:SER:OG	2.24	0.50
4:I:204:LEU:HD11	4:I:217:ILE:HD12	1.93	0.50
1:6:256:ILE:HG13	1:6:257:VAL:N	2.26	0.50
1:AI:235:LEU:HB3	1:AJ:244:ARG:HH22	1.75	0.50
1:UK:98:LEU:HD22	1:UK:147:LEU:CD2	2.39	0.50
1:WG:115:LEU:HG	1:WG:116:LEU:N	2.25	0.50
1:WV:196:HIS:HB3	1:WW:211:THR:HG21	1.93	0.50
7:W:54:ALA:HB3	7:W:55:PRO:HD3	1.93	0.50
1:AB:256:ILE:HG13	1:AB:257:VAL:N	2.26	0.50
1:AD:235:LEU:HB3	1:AE:244:ARG:HH22	1.75	0.50
1:WD:197:LEU:CD1	1:WE:175:SER:OG	2.59	0.50
1:WH:186:LEU:HD22	1:WH:190:GLN:CD	2.32	0.50
1:WT:166:VAL:HG21	4:G:158:PRO:HB2	1.93	0.50
4:G:180:LYS:NZ	4:H:230:ASP:OD1	2.27	0.50
5:N:57:GLU:HG2	6:S:11:PHE:CE2	2.47	0.50
7:Y:10:ALA:O	7:Y:14:LEU:HG	2.12	0.50
1:1:256:ILE:HG13	1:1:257:VAL:N	2.26	0.50
1:WA:112:GLY:O	1:WA:115:LEU:HB3	2.12	0.50
1:WP:165:PHE:HA	4:F:160:GLN:O	2.12	0.50
3:E:229:MET:O	3:E:233:MET:HG2	2.12	0.50
4:F:143:ARG:HH21	4:F:180:LYS:HB3	1.77	0.50
4:F:224:MET:O	4:F:228:LEU:HB2	2.11	0.50
6:T:123:LEU:HD23	7:Y:132:LEU:HD11	1.92	0.50
1:WC:143:THR:OG1	1:WD:154:ARG:HG2	2.12	0.50
3:E:166:SER:O	3:E:167:ASN:C	2.49	0.50
4:G:75:ARG:NH2	4:G:84:PRO:O	2.44	0.50
4:G:86:ASN:HD21	5:L:103:GLN:HA	1.77	0.50
1:UP:159:MET:SD	1:UP:159:MET:N	2.82	0.50
1:WQ:163:SER:HB3	1:WQ:166:VAL:HG23	1.94	0.50
1:WS:166:VAL:HG22	4:G:144:GLU:HG2	1.94	0.50
1:WU:202:VAL:HB	1:WU:205:LEU:HB2	1.94	0.50
1:WV:200:SER:OG	1:WW:175:SER:HB2	2.11	0.50
4:J:167:MET:HG3	4:J:171:LEU:HG	1.93	0.50
7:Y:106:MET:O	7:Y:110:ARG:HG2	2.12	0.50
1:2:294:ARG:HD2	1:2:367:GLU:OE1	2.12	0.50
1:8:235:LEU:HB3	1:9:244:ARG:HH22	1.75	0.50
1:0:256:ILE:HG13	1:0:257:VAL:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UN:159:MET:N	1:UN:159:MET:SD	2.82	0.49
1:WQ:142:ARG:O	1:WQ:146:THR:HG23	2.13	0.49
1:WQ:202:VAL:HB	1:WQ:205:LEU:HB2	1.94	0.49
1:WS:197:LEU:HA	1:WT:175:SER:OG	2.11	0.49
1:1:294:ARG:HD2	1:1:367:GLU:OE1	2.12	0.49
1:AO:294:ARG:HD2	1:AO:367:GLU:OE1	2.12	0.49
1:AP:294:ARG:HD2	1:AP:367:GLU:OE1	2.12	0.49
1:UP:98:LEU:HD22	1:UP:147:LEU:CD2	2.39	0.49
1:WB:187:ASP:OD1	1:WB:190:GLN:HG3	2.12	0.49
1:WD:149:PRO:HG2	1:WD:190:GLN:NE2	2.23	0.49
5:P:55:GLN:HG2	5:P:71:VAL:HG22	1.94	0.49
6:U:46:ALA:O	6:U:50:LYS:HG2	2.11	0.49
1:AK:256:ILE:HG13	1:AK:257:VAL:N	2.26	0.49
1:AM:294:ARG:HD2	1:AM:367:GLU:OE1	2.13	0.49
1:AN:294:ARG:HD2	1:AN:367:GLU:OE1	2.12	0.49
1:AQ:256:ILE:HG13	1:AQ:257:VAL:N	2.26	0.49
1:AQ:294:ARG:HD2	1:AQ:367:GLU:OE1	2.13	0.49
1:UM:98:LEU:HD22	1:UM:147:LEU:CD2	2.39	0.49
1:UN:69:GLN:HE22	1:WS:182:PRO:HG2	1.77	0.49
1:WH:202:VAL:HB	1:WH:205:LEU:HB2	1.95	0.49
1:WN:202:VAL:HB	1:WN:205:LEU:HB2	1.94	0.49
6:S:66:THR:OG1	1:AD:294:ARG:HG2	2.11	0.49
1:3:294:ARG:HD2	1:3:367:GLU:OE1	2.12	0.49
1:UN:73:MET:HE1	1:UN:99:ARG:HD2	1.95	0.49
1:UN:208:GLY:CA	1:WR:187:ASP:OD1	2.60	0.49
1:UO:103:GLN:CG	1:WU:182:PRO:HB3	2.42	0.49
1:WN:145:GLU:O	1:WN:147:LEU:N	2.46	0.49
1:WA:112:GLY:HA2	1:WA:135:ALA:CA	2.27	0.49
1:WD:200:SER:O	1:WE:158:ALA:HB3	2.10	0.49
1:WE:202:VAL:HB	1:WE:205:LEU:HB2	1.95	0.49
1:WG:219:LEU:HD21	1:WG:222:GLN:O	2.13	0.49
1:WO:142:ARG:O	1:WO:146:THR:HG23	2.11	0.49
1:WP:164:LEU:HD11	4:F:151:ALA:HB3	1.93	0.49
4:I:59:LEU:O	4:I:65:THR:OG1	2.28	0.49
6:S:76:GLN:N	1:AD:297:GLN:HE22	2.08	0.49
1:AL:294:ARG:HD2	1:AL:367:GLU:OE1	2.13	0.49
1:WC:128:GLU:HG2	1:WC:129:GLN:N	2.28	0.49
1:WD:145:GLU:O	1:WD:147:LEU:N	2.46	0.49
1:WF:202:VAL:HB	1:WF:205:LEU:HB2	1.94	0.49
1:WK:202:VAL:HB	1:WK:205:LEU:HB2	1.95	0.49
1:WM:197:LEU:HA	1:WN:175:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WS:202:VAL:HB	1:WS:205:LEU:HB2	1.94	0.49
2:D:77:VAL:CG1	4:J:229:VAL:HG21	2.42	0.49
4:G:66:ARG:NH2	4:G:178:GLU:OE1	2.45	0.49
1:UI:129:GLN:O	1:UI:133:GLN:N	2.29	0.49
1:UL:167:ARG:O	1:UL:168:GLU:C	2.49	0.49
1:UN:80:ALA:CB	1:UN:83:SER:HB3	2.43	0.49
1:WA:213:VAL:CG2	1:WW:193:ALA:HB1	2.42	0.49
1:WF:193:ALA:HB1	1:WG:213:VAL:HG11	1.94	0.49
1:WN:145:GLU:C	1:WN:147:LEU:H	2.15	0.49
3:E:12:TRP:CZ3	5:P:34:PHE:HB2	2.48	0.49
6:T:68:THR:CG2	1:7:294:ARG:CD	2.91	0.49
1:4:294:ARG:HD2	1:4:367:GLU:OE1	2.12	0.49
1:UJ:98:LEU:HD22	1:UJ:147:LEU:CD2	2.39	0.49
1:UK:80:ALA:CB	1:UK:83:SER:HB3	2.43	0.49
1:WA:167:ARG:HH21	4:H:162:PRO:HD2	1.78	0.49
1:WE:112:GLY:O	1:WE:115:LEU:HB3	2.12	0.49
1:WF:116:LEU:HD22	1:WF:131:ASN:HA	1.94	0.49
1:WG:164:LEU:O	4:J:241:GLN:CG	2.47	0.49
1:WL:202:VAL:HB	1:WL:205:LEU:HB2	1.95	0.49
1:WP:144:ILE:O	1:WP:147:LEU:HB2	2.13	0.49
1:WQ:124:SER:O	1:WQ:125:GLN:C	2.50	0.49
2:C:36:SER:OG	2:D:44:ILE:HG23	2.12	0.49
4:F:126:ALA:O	4:F:127:LEU:C	2.48	0.49
6:Q:17:ASN:HD22	6:Q:57:ARG:NH1	2.10	0.49
6:T:102:MET:HB3	6:T:106:ARG:HH21	1.77	0.49
1:AG:256:ILE:HG13	1:AG:257:VAL:N	2.26	0.49
1:AK:294:ARG:HD2	1:AK:367:GLU:OE1	2.12	0.49
1:UJ:80:ALA:CB	1:UJ:83:SER:HB3	2.43	0.49
1:UL:80:ALA:CB	1:UL:83:SER:HB3	2.43	0.49
1:UP:80:ALA:CB	1:UP:83:SER:HB3	2.43	0.49
1:WC:197:LEU:HD11	1:WD:156:HIS:HD2	1.78	0.49
1:WD:186:LEU:HD22	1:WD:190:GLN:CD	2.32	0.49
1:WF:145:GLU:HG2	1:WF:152:SER:HA	1.95	0.49
1:WH:193:ALA:CB	1:WI:213:VAL:CG1	2.88	0.49
6:R:68:THR:HG21	1:AJ:294:ARG:CD	2.42	0.49
1:AB:266:VAL:HG22	1:AB:387:VAL:HG22	1.95	0.49
1:UN:98:LEU:HD22	1:UN:147:LEU:CD2	2.39	0.49
1:WK:143:THR:OG1	1:WL:156:HIS:NE2	1.94	0.49
1:WS:197:LEU:HD11	1:WT:156:HIS:HD2	1.78	0.49
1:WW:115:LEU:HA	1:WW:118:GLN:OE1	2.13	0.49
5:K:7:ILE:HG21	1:AM:278:THR:HG22	1.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:86:ILE:HG12	5:P:102:MET:HE2	1.95	0.49
5:L:11:ILE:CG2	1:AH:372:ILE:HD12	2.28	0.49
1:AA:266:VAL:HG22	1:AA:387:VAL:HG22	1.95	0.49
1:AC:266:VAL:HG22	1:AC:387:VAL:HG22	1.95	0.49
1:UL:73:MET:HE1	1:UL:99:ARG:HD2	1.92	0.48
1:UM:80:ALA:CB	1:UM:83:SER:HB3	2.43	0.48
1:WB:202:VAL:HB	1:WB:205:LEU:HB2	1.94	0.48
1:WV:120:LYS:NZ	1:WV:123:ILE:CD1	2.74	0.48
4:F:179:LEU:HD22	4:G:84:PRO:HG3	1.95	0.48
1:4:266:VAL:HG22	1:4:387:VAL:HG22	1.95	0.48
1:5:294:ARG:HD2	1:5:367:GLU:OE1	2.13	0.48
1:AJ:294:ARG:HD2	1:AJ:367:GLU:OE1	2.12	0.48
1:WJ:200:SER:OG	1:WK:175:SER:HB2	2.13	0.48
2:A:48:THR:HG21	4:F:208:GLY:HA2	1.95	0.48
4:F:92:LEU:HD13	4:F:232:TRP:HZ2	1.77	0.48
4:F:130:GLY:O	4:F:133:PRO:HD2	2.13	0.48
4:J:73:LEU:HD13	4:J:186:GLY:HA3	1.94	0.48
5:N:4:ILE:HG12	1:7:372:ILE:CG2	2.43	0.48
6:R:68:THR:HG21	1:AJ:294:ARG:HH11	1.78	0.48
6:T:49:LEU:O	6:T:53:MET:HG2	2.13	0.48
6:T:67:LEU:HD21	6:T:74:PRO:HB3	1.94	0.48
7:X:94:PRO:HB2	7:X:96:VAL:HG23	1.94	0.48
1:AA:294:ARG:HD2	1:AA:367:GLU:OE1	2.12	0.48
1:AB:294:ARG:HD2	1:AB:367:GLU:OE1	2.12	0.48
1:AC:294:ARG:HD2	1:AC:367:GLU:OE1	2.12	0.48
1:UI:127:SER:O	1:UI:131:ASN:HB2	2.14	0.48
1:UL:98:LEU:HD22	1:UL:147:LEU:CD2	2.39	0.48
1:WD:168:GLU:CD	1:WD:170:LYS:NZ	2.67	0.48
1:WR:165:PHE:HZ	4:G:240:ALA:HB1	1.78	0.48
1:WS:200:SER:O	1:WT:158:ALA:HB3	2.05	0.48
4:I:42:VAL:HG13	5:O:42:LEU:HD22	1.95	0.48
7:X:97:ASP:O	7:X:101:GLU:HG2	2.13	0.48
1:9:294:ARG:HD2	1:9:367:GLU:OE1	2.12	0.48
1:0:294:ARG:HD2	1:0:367:GLU:OE1	2.12	0.48
1:AD:294:ARG:HD2	1:AD:367:GLU:OE1	2.12	0.48
1:AE:294:ARG:HD2	1:AE:367:GLU:OE1	2.12	0.48
1:AG:266:VAL:HG22	1:AG:387:VAL:HG22	1.95	0.48
1:AH:266:VAL:HG22	1:AH:387:VAL:HG22	1.95	0.48
1:UI:80:ALA:CB	1:UI:83:SER:HB3	2.43	0.48
1:WJ:202:VAL:HB	1:WJ:205:LEU:HB2	1.95	0.48
1:WK:132:TYR:CB	1:WL:126:PHE:HZ	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WM:202:VAL:HB	1:WM:205:LEU:HB2	1.94	0.48
1:WP:202:VAL:HB	1:WP:205:LEU:HB2	1.95	0.48
5:N:99:VAL:O	5:N:102:MET:HG2	2.13	0.48
6:S:32:ASN:ND2	7:X:51:VAL:HG12	2.28	0.48
6:S:65:LEU:HD11	1:AD:365:ASN:HD21	1.78	0.48
1:3:266:VAL:HG22	1:3:387:VAL:HG22	1.95	0.48
1:5:266:VAL:HG22	1:5:387:VAL:HG22	1.95	0.48
1:8:294:ARG:HD2	1:8:367:GLU:OE1	2.13	0.48
1:AD:266:VAL:HG22	1:AD:387:VAL:HG22	1.95	0.48
1:AG:294:ARG:HD2	1:AG:367:GLU:OE1	2.12	0.48
1:UJ:256:PRO:HD2	1:WC:187:ASP:HB3	1.94	0.48
1:UK:127:SER:O	1:UK:131:ASN:HB2	2.14	0.48
1:WC:164:LEU:O	4:I:241:GLN:HG3	2.08	0.48
1:WK:193:ALA:CB	1:WL:213:VAL:HG11	2.44	0.48
1:WW:202:VAL:HB	1:WW:205:LEU:HB2	1.95	0.48
1:6:266:VAL:HG22	1:6:387:VAL:HG22	1.95	0.48
1:7:294:ARG:HD2	1:7:367:GLU:OE1	2.13	0.48
1:0:266:VAL:HG22	1:0:387:VAL:HG22	1.95	0.48
1:UJ:127:SER:O	1:UJ:131:ASN:HB2	2.14	0.48
1:WA:142:ARG:O	1:WA:146:THR:HG23	2.13	0.48
1:WA:196:HIS:CD2	1:WB:219:LEU:HD22	2.49	0.48
1:WI:202:VAL:HB	1:WI:205:LEU:HB2	1.94	0.48
1:WV:164:LEU:CB	4:G:152:ARG:HH12	2.27	0.48
3:E:178:LEU:HD13	3:E:181:LEU:HD23	1.95	0.48
4:J:150:PHE:CE1	4:J:172:PRO:HB2	2.48	0.48
5:O:4:ILE:HG12	1:1:372:ILE:CG2	2.42	0.48
1:6:294:ARG:HD2	1:6:367:GLU:OE1	2.13	0.48
1:AI:294:ARG:HD2	1:AI:367:GLU:OE1	2.12	0.48
1:AP:266:VAL:HG22	1:AP:387:VAL:HG22	1.95	0.48
1:UO:80:ALA:CB	1:UO:83:SER:HB3	2.43	0.48
1:WA:193:ALA:HB1	1:WB:213:VAL:CG1	2.43	0.48
1:WC:202:VAL:HB	1:WC:205:LEU:HB2	1.95	0.48
1:WD:167:ARG:HH21	1:WD:168:GLU:HA	1.77	0.48
1:WF:124:SER:O	1:WF:127:SER:N	2.46	0.48
1:WG:142:ARG:O	1:WG:146:THR:HG23	2.14	0.48
1:WR:202:VAL:HB	1:WR:205:LEU:HB2	1.95	0.48
1:WV:192:SER:O	1:WV:195:VAL:N	2.47	0.48
2:C:54:LYS:NZ	2:D:48:THR:HG21	2.29	0.48
3:E:101:PHE:CE2	4:F:80:THR:HG21	2.48	0.48
4:I:159:LEU:O	4:I:160:GLN:HB2	2.14	0.48
6:T:55:ARG:CZ	1:5:299:ASN:HD22	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:27:ASN:OD1	7:X:42:TYR:OH	2.27	0.48
1:2:266:VAL:HG22	1:2:387:VAL:HG22	1.95	0.48
1:AF:266:VAL:HG22	1:AF:387:VAL:HG22	1.95	0.48
1:UK:127:SER:O	1:UK:131:ASN:CG	2.52	0.48
1:UL:127:SER:O	1:UL:131:ASN:CG	2.52	0.48
1:UN:98:LEU:HD12	1:UN:146:THR:HG1	1.78	0.48
1:UN:127:SER:O	1:UN:131:ASN:CG	2.52	0.48
1:UP:167:ARG:NH1	1:8:236:LYS:CE	2.76	0.48
1:WB:128:GLU:HG2	1:WC:126:PHE:HD2	1.79	0.48
1:WB:197:LEU:HA	1:WC:175:SER:OG	2.13	0.48
1:WC:187:ASP:O	1:WC:190:GLN:HB3	2.14	0.48
1:WQ:164:LEU:HD23	4:F:149:LEU:HB2	1.95	0.48
5:L:55:GLN:HG2	5:L:71:VAL:HG22	1.95	0.48
1:AF:294:ARG:HD2	1:AF:367:GLU:OE1	2.13	0.48
1:AH:294:ARG:HD2	1:AH:367:GLU:OE1	2.13	0.48
1:AI:266:VAL:HG22	1:AI:387:VAL:HG22	1.95	0.48
1:AQ:266:VAL:HG22	1:AQ:387:VAL:HG22	1.95	0.48
1:WA:202:VAL:HB	1:WA:205:LEU:HB2	1.94	0.48
1:WJ:171:SER:HB3	1:WJ:206:PRO:HG3	1.96	0.48
1:WV:202:VAL:HB	1:WV:205:LEU:HB2	1.95	0.48
3:E:86:PHE:CZ	4:F:88:VAL:HA	2.48	0.48
5:M:11:ILE:HG23	1:AB:372:ILE:HG21	1.89	0.48
1:AO:266:VAL:HG22	1:AO:387:VAL:HG22	1.95	0.48
1:UJ:103:GLN:HB3	1:WD:182:PRO:HA	1.91	0.48
1:UJ:127:SER:O	1:UJ:131:ASN:CG	2.52	0.48
1:WN:200:SER:CB	1:WO:173:SER:HB2	2.44	0.48
2:D:60:ILE:HA	2:D:63:ILE:HG12	1.96	0.48
3:E:158:PRO:HG2	3:E:162:ASN:ND2	2.16	0.48
7:V:27:ASN:ND2	7:V:45:LYS:O	2.33	0.48
1:AK:296:ARG:HH11	1:AK:296:ARG:HG2	1.79	0.48
1:UJ:129:GLN:O	1:UJ:133:GLN:N	2.29	0.47
1:UO:127:SER:O	1:UO:131:ASN:CG	2.52	0.47
1:WA:216:SER:O	1:WW:190:GLN:HG2	2.14	0.47
1:WH:187:ASP:OD2	1:WH:190:GLN:HB2	2.14	0.47
1:WI:193:ALA:HB1	1:WJ:213:VAL:HG11	1.94	0.47
1:WN:142:ARG:O	1:WN:146:THR:HG23	2.14	0.47
1:WO:202:VAL:HB	1:WO:205:LEU:HB2	1.95	0.47
1:WP:163:SER:C	1:WP:165:PHE:H	2.17	0.47
1:WS:165:PHE:HE1	2:A:89:GLY:C	2.17	0.47
1:WU:113:PHE:CE2	1:WU:139:GLU:HG3	2.48	0.47
2:B:44:ILE:HD13	2:B:44:ILE:HA	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:94:ALA:HB2	3:E:179:ILE:HA	1.96	0.47
5:K:7:ILE:CD1	1:AM:278:THR:HG21	2.44	0.47
6:R:29:ASN:HD21	6:R:41:ARG:H	1.61	0.47
7:W:44:ALA:HB2	7:W:96:VAL:HG22	1.96	0.47
7:Z:42:TYR:O	7:Z:94:PRO:HB3	2.14	0.47
1:9:296:ARG:HG2	1:9:296:ARG:HH11	1.79	0.47
1:AE:266:VAL:HG22	1:AE:387:VAL:HG22	1.95	0.47
1:WB:187:ASP:OD1	1:WB:190:GLN:N	2.41	0.47
1:WG:202:VAL:HB	1:WG:205:LEU:HB2	1.95	0.47
1:WQ:168:GLU:O	1:WQ:169:GLN:C	2.52	0.47
6:T:72:HIS:HD2	1:7:365:ASN:CG	2.16	0.47
1:AD:296:ARG:HG2	1:AD:296:ARG:HH11	1.80	0.47
1:AG:296:ARG:HG2	1:AG:296:ARG:HH11	1.79	0.47
1:AL:266:VAL:HG22	1:AL:387:VAL:HG22	1.95	0.47
1:AN:296:ARG:HG2	1:AN:296:ARG:HH11	1.79	0.47
1:AQ:296:ARG:HG2	1:AQ:296:ARG:HH11	1.79	0.47
1:UL:180:LEU:HB2	1:UL:215:GLN:HE22	1.79	0.47
1:WA:167:ARG:NH2	4:H:162:PRO:HD3	2.26	0.47
1:WH:165:PHE:O	4:J:144:GLU:HG2	2.14	0.47
1:WT:202:VAL:HB	1:WT:205:LEU:HB2	1.95	0.47
1:WU:115:LEU:HD21	1:WU:134:ARG:HD3	1.95	0.47
1:WW:142:ARG:O	1:WW:146:THR:HG23	2.14	0.47
4:G:82:SER:HA	5:K:103:GLN:HE21	1.79	0.47
1:7:266:VAL:HG22	1:7:387:VAL:HG22	1.95	0.47
1:UM:127:SER:O	1:UM:131:ASN:HB2	2.14	0.47
1:UP:127:SER:O	1:UP:131:ASN:CG	2.52	0.47
1:WA:196:HIS:HB3	1:WB:211:THR:CG2	2.36	0.47
1:WD:202:VAL:HB	1:WD:205:LEU:HB2	1.95	0.47
1:WI:193:ALA:HB1	1:WJ:213:VAL:CG2	2.45	0.47
1:WV:112:GLY:HA2	1:WV:135:ALA:CA	2.28	0.47
2:B:70:LEU:O	2:B:74:LEU:HG	2.14	0.47
4:H:190:PHE:CD1	4:I:220:PRO:HG3	2.49	0.47
6:R:24:GLU:OE1	7:W:5:ASN:HB2	2.15	0.47
1:4:296:ARG:HG2	1:4:296:ARG:HH11	1.79	0.47
1:7:296:ARG:HG2	1:7:296:ARG:HH11	1.80	0.47
1:AB:296:ARG:HG2	1:AB:296:ARG:HH11	1.79	0.47
1:AP:296:ARG:HG2	1:AP:296:ARG:HH11	1.79	0.47
1:UL:103:GLN:CG	1:WH:182:PRO:HB3	2.43	0.47
1:WU:142:ARG:O	1:WU:146:THR:HG23	2.14	0.47
2:D:2:THR:OG1	2:D:4:GLU:OE1	2.29	0.47
7:Y:52:ASP:OD1	7:Y:63:LYS:HD3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:266:VAL:HG22	1:1:387:VAL:HG22	1.95	0.47
1:6:296:ARG:HG2	1:6:296:ARG:HH11	1.79	0.47
1:AH:296:ARG:HG2	1:AH:296:ARG:HH11	1.80	0.47
1:AK:266:VAL:HG22	1:AK:387:VAL:HG22	1.95	0.47
1:AM:266:VAL:HG22	1:AM:387:VAL:HG22	1.95	0.47
1:UN:127:SER:O	1:UN:131:ASN:HB2	2.14	0.47
2:B:7:MET:SD	2:C:70:LEU:HD22	2.54	0.47
5:M:4:ILE:HG13	1:AC:372:ILE:HG22	1.92	0.47
1:9:266:VAL:HG22	1:9:387:VAL:HG22	1.95	0.47
1:0:296:ARG:HG2	1:0:296:ARG:HH11	1.79	0.47
1:AA:296:ARG:HG2	1:AA:296:ARG:HH11	1.79	0.47
1:AJ:266:VAL:HG22	1:AJ:387:VAL:HG22	1.95	0.47
1:AJ:296:ARG:HG2	1:AJ:296:ARG:HH11	1.80	0.47
1:UL:98:LEU:HD12	1:UL:146:THR:HG1	1.78	0.47
1:UM:127:SER:O	1:UM:131:ASN:CG	2.52	0.47
1:WF:147:LEU:HA	1:WG:215:GLN:O	2.14	0.47
1:WI:196:HIS:HB3	1:WJ:211:THR:CG2	2.32	0.47
1:WI:197:LEU:HA	1:WJ:175:SER:OG	2.15	0.47
1:WT:186:LEU:HA	1:WT:190:GLN:OE1	2.15	0.47
1:WW:118:GLN:O	1:WW:119:GLU:C	2.49	0.47
1:WW:145:GLU:O	1:WW:147:LEU:N	2.48	0.47
4:F:138:MET:O	4:F:142:THR:OG1	2.16	0.47
4:F:189:ILE:O	4:F:192:PRO:HD2	2.15	0.47
4:G:205:MET:CE	4:H:209:MET:HA	2.45	0.47
5:K:80:VAL:HG22	6:Q:131:MET:SD	2.54	0.47
6:R:96:ASP:OD1	6:R:96:ASP:N	2.39	0.47
6:T:55:ARG:HH22	1:5:299:ASN:HD22	1.59	0.47
6:T:73:ILE:HD12	6:T:74:PRO:HD2	1.95	0.47
1:1:296:ARG:HG2	1:1:296:ARG:HH11	1.80	0.47
1:AC:296:ARG:HG2	1:AC:296:ARG:HH11	1.79	0.47
1:UL:127:SER:O	1:UL:131:ASN:HB2	2.14	0.47
3:E:72:TRP:HE1	3:E:161:SER:HB2	1.80	0.47
5:N:4:ILE:HG12	1:7:372:ILE:HB	1.96	0.47
6:S:72:HIS:CA	1:AE:295:SER:CB	2.93	0.47
6:U:72:HIS:CE1	1:2:294:ARG:CG	2.96	0.47
1:AN:266:VAL:HG22	1:AN:387:VAL:HG22	1.95	0.47
1:UI:127:SER:O	1:UI:131:ASN:CG	2.52	0.47
1:UL:167:ARG:HA	1:UL:167:ARG:HD3	1.74	0.47
1:UO:127:SER:O	1:UO:131:ASN:HB2	2.14	0.47
1:WJ:164:LEU:HD23	3:E:144:LEU:CB	2.43	0.47
6:S:73:ILE:HG22	6:S:75:ALA:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:266:VAL:HG22	1:8:387:VAL:HG22	1.95	0.47
1:AE:296:ARG:HG2	1:AE:296:ARG:HH11	1.80	0.47
1:AL:296:ARG:HG2	1:AL:296:ARG:HH11	1.80	0.47
1:UM:136:LEU:HD23	1:UM:157:LEU:CD1	2.45	0.47
1:UO:129:GLN:O	1:UO:133:GLN:N	2.29	0.47
1:WB:145:GLU:O	1:WB:147:LEU:N	2.48	0.47
1:WF:125:GLN:O	1:WF:126:PHE:C	2.53	0.47
1:WJ:125:GLN:HB2	3:E:242:HIS:CG	2.50	0.47
2:C:31:THR:O	2:C:35:ILE:HG12	2.14	0.47
4:J:138:MET:HB3	4:J:138:MET:HE2	1.61	0.47
5:M:48:ARG:NH2	6:S:6:ASP:OD2	2.48	0.47
6:Q:22:ARG:NH2	6:Q:108:GLN:OE1	2.47	0.47
1:AI:296:ARG:HG2	1:AI:296:ARG:HH11	1.80	0.47
1:AM:296:ARG:HG2	1:AM:296:ARG:HH11	1.79	0.47
1:AO:296:ARG:HG2	1:AO:296:ARG:HH11	1.80	0.47
1:WI:193:ALA:HB1	1:WJ:213:VAL:CG1	2.45	0.46
2:C:4:GLU:C	2:C:6:VAL:N	2.67	0.46
3:E:103:GLY:O	3:E:106:MET:HB2	2.16	0.46
4:F:59:LEU:HD21	5:K:102:MET:HE3	1.97	0.46
5:M:7:ILE:O	5:M:11:ILE:HG23	2.16	0.46
5:N:4:ILE:CG1	1:7:372:ILE:HG21	2.45	0.46
6:U:67:LEU:HD11	6:U:74:PRO:HA	1.97	0.46
7:W:14:LEU:HD21	7:W:116:ILE:HG13	1.97	0.46
1:UJ:98:LEU:HD12	1:UJ:146:THR:HG1	1.80	0.46
1:UO:136:LEU:HD23	1:UO:157:LEU:CD1	2.45	0.46
1:UP:73:MET:HE3	1:UP:99:ARG:CD	2.38	0.46
1:WE:134:ARG:HB3	1:WE:134:ARG:NH2	2.27	0.46
1:WG:112:GLY:HA3	1:WG:139:GLU:OE1	2.15	0.46
1:WG:149:PRO:HG2	1:WG:190:GLN:HE22	1.79	0.46
1:WP:164:LEU:HD21	4:F:151:ALA:CB	2.43	0.46
1:WQ:125:GLN:O	1:WQ:126:PHE:C	2.53	0.46
1:WU:190:GLN:NE2	1:WV:216:SER:O	2.47	0.46
2:A:17:ALA:HB2	4:G:195:ILE:HD12	1.96	0.46
2:B:29:LEU:HD23	2:B:30:ILE:HD13	1.96	0.46
4:I:161:GLY:C	4:I:163:GLU:N	2.69	0.46
5:K:21:ALA:HB3	1:AK:278:THR:CG2	2.39	0.46
6:S:65:LEU:HD13	1:AD:295:SER:OG	2.14	0.46
6:S:114:LEU:HD21	7:Y:126:MET:CE	2.45	0.46
1:3:296:ARG:HG2	1:3:296:ARG:HH11	1.80	0.46
1:WA:170:LYS:H	1:WA:170:LYS:HD2	1.80	0.46
1:WD:187:ASP:OD1	1:WD:190:GLN:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WJ:164:LEU:HD11	3:E:145:TRP:HA	1.97	0.46
1:WK:201:ALA:HA	1:WL:158:ALA:HB2	1.98	0.46
1:WN:197:LEU:CD1	1:WO:175:SER:HB3	2.42	0.46
1:WU:190:GLN:HG2	1:WV:216:SER:O	2.15	0.46
4:F:230:ASP:O	4:F:234:LEU:HG	2.15	0.46
4:J:105:ILE:HD13	5:O:34:PHE:HZ	1.80	0.46
1:2:296:ARG:HH11	1:2:296:ARG:HG2	1.79	0.46
1:UJ:136:LEU:HD23	1:UJ:157:LEU:CD1	2.46	0.46
1:UN:73:MET:HE3	1:UN:99:ARG:CD	2.41	0.46
1:UP:73:MET:HE1	1:UP:99:ARG:HD2	1.97	0.46
1:UP:127:SER:O	1:UP:131:ASN:HB2	2.14	0.46
1:WF:143:THR:OG1	1:WG:154:ARG:HG2	2.14	0.46
1:WJ:200:SER:O	1:WK:158:ALA:HB2	2.15	0.46
1:WN:135:ALA:O	1:WN:139:GLU:HG2	2.16	0.46
4:J:83:ALA:HB3	4:J:84:PRO:CD	2.38	0.46
5:L:15:GLN:HG3	5:L:16:ALA:N	2.30	0.46
1:5:296:ARG:HG2	1:5:296:ARG:HH11	1.79	0.46
1:WD:190:GLN:NE2	1:WE:216:SER:O	2.49	0.46
1:WE:143:THR:HA	1:WE:146:THR:HG23	1.97	0.46
4:F:75:ARG:HD3	4:F:89:LEU:HD11	1.97	0.46
5:O:48:ARG:NH2	6:U:6:ASP:OD1	2.48	0.46
6:S:76:GLN:H	1:AD:297:GLN:NE2	2.12	0.46
7:X:114:ALA:O	7:X:118:VAL:HG23	2.16	0.46
7:Z:47:VAL:HG12	7:Z:67:VAL:HG22	1.96	0.46
1:AF:296:ARG:HG2	1:AF:296:ARG:HH11	1.80	0.46
1:UN:136:LEU:HD23	1:UN:157:LEU:CD1	2.45	0.46
1:WK:135:ALA:O	1:WK:139:GLU:HG2	2.16	0.46
1:WO:135:ALA:O	1:WO:139:GLU:HG2	2.16	0.46
1:WQ:147:LEU:O	1:WQ:148:GLY:C	2.54	0.46
4:J:159:LEU:HD13	4:J:165:VAL:HG22	1.98	0.46
6:R:51:LYS:O	6:R:55:ARG:HG2	2.16	0.46
1:8:235:LEU:HD13	1:9:244:ARG:HH22	1.81	0.46
1:UP:136:LEU:HD23	1:UP:157:LEU:CD1	2.45	0.46
1:WC:135:ALA:O	1:WC:139:GLU:HG2	2.16	0.46
1:WD:135:ALA:O	1:WD:139:GLU:HG2	2.16	0.46
1:WR:165:PHE:C	1:WR:167:ARG:H	2.18	0.46
4:G:59:LEU:O	4:G:65:THR:OG1	2.21	0.46
1:8:296:ARG:HG2	1:8:296:ARG:HH11	1.80	0.46
1:0:235:LEU:HD13	1:AA:244:ARG:HH22	1.81	0.46
1:AH:235:LEU:HD13	1:AI:244:ARG:HH22	1.81	0.46
1:AK:235:LEU:HD13	1:AL:244:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UJ:98:LEU:HD11	1:UJ:143:THR:O	2.16	0.46
1:UM:98:LEU:HD12	1:UM:146:THR:HG1	1.80	0.46
1:WT:197:LEU:HA	1:WU:175:SER:OG	2.16	0.46
4:I:138:MET:O	4:I:142:THR:OG1	2.28	0.46
5:N:11:ILE:CG2	1:6:372:ILE:HB	2.45	0.46
6:Q:113:SER:O	6:Q:117:GLN:HG3	2.15	0.46
6:T:78:VAL:C	1:7:299:ASN:ND2	2.48	0.46
6:U:76:GLN:OE1	1:2:297:GLN:OE1	2.33	0.46
7:X:43:ARG:HD2	7:X:69:GLU:OE2	2.14	0.46
1:3:235:LEU:HD13	1:4:244:ARG:HH22	1.81	0.46
1:AN:235:LEU:HD13	1:AO:244:ARG:HH22	1.81	0.46
1:WH:197:LEU:HA	1:WI:175:SER:CB	2.46	0.46
1:WK:197:LEU:HD13	1:WL:175:SER:OG	2.16	0.46
1:WU:167:ARG:NH1	4:G:158:PRO:HD3	2.30	0.46
1:WW:187:ASP:N	1:WW:190:GLN:HB2	2.31	0.46
2:C:85:PRO:HG3	4:I:238:SER:HA	1.97	0.46
3:E:86:PHE:HZ	4:F:87:GLN:O	1.97	0.46
4:F:150:PHE:CZ	4:F:172:PRO:HB2	2.51	0.46
4:G:97:THR:O	4:G:101:MET:HG2	2.16	0.46
4:G:171:LEU:HB3	4:G:172:PRO:HD3	1.97	0.46
6:U:65:LEU:HG	6:U:75:ALA:CA	2.46	0.46
1:1:235:LEU:HD13	1:2:244:ARG:HH22	1.81	0.46
1:5:235:LEU:HD13	1:6:244:ARG:HH22	1.81	0.46
1:AO:235:LEU:HD13	1:AP:244:ARG:HH22	1.81	0.46
1:UK:136:LEU:HD23	1:UK:157:LEU:CD1	2.45	0.46
1:UL:98:LEU:HD11	1:UL:143:THR:O	2.16	0.46
1:UL:136:LEU:HD23	1:UL:157:LEU:CD1	2.45	0.46
1:UN:103:GLN:CG	1:WS:182:PRO:HB3	2.43	0.46
1:WF:196:HIS:CD2	1:WG:219:LEU:HD22	2.51	0.46
1:WF:200:SER:O	1:WG:158:ALA:HB2	2.16	0.46
1:WI:165:PHE:HB2	4:J:159:LEU:O	2.16	0.46
1:WM:145:GLU:O	1:WM:146:THR:C	2.54	0.46
1:WW:135:ALA:O	1:WW:139:GLU:HG2	2.16	0.46
2:C:15:LYS:HB2	2:C:15:LYS:HE2	1.70	0.46
2:C:24:LEU:HD11	2:C:62:ILE:HD11	1.96	0.46
6:R:66:THR:OG1	1:AJ:294:ARG:CG	2.64	0.46
1:AC:235:LEU:HD13	1:AD:244:ARG:HH22	1.81	0.46
1:WP:142:ARG:O	1:WP:146:THR:HG23	2.16	0.45
1:WP:197:LEU:CD1	1:WQ:175:SER:OG	2.58	0.45
1:WS:124:SER:CB	2:A:8:MET:CE	2.82	0.45
2:A:84:LEU:HD21	4:G:185:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:235:LEU:HD13	1:AC:244:ARG:HH22	1.81	0.45
1:AE:235:LEU:HD13	1:AF:244:ARG:HH22	1.81	0.45
1:UO:162:PRO:O	1:UO:163:SER:C	2.55	0.45
1:UP:162:PRO:O	1:UP:163:SER:C	2.55	0.45
1:WE:135:ALA:O	1:WE:139:GLU:HG2	2.16	0.45
1:WG:135:ALA:O	1:WG:139:GLU:HG2	2.16	0.45
1:WK:145:GLU:O	1:WK:147:LEU:N	2.49	0.45
1:WN:200:SER:HB2	1:WO:173:SER:CB	2.45	0.45
1:WP:135:ALA:O	1:WP:139:GLU:HG2	2.16	0.45
3:E:108:LEU:HA	3:E:108:LEU:HD23	1.76	0.45
4:H:109:TYR:HA	4:H:113:TYR:HB3	1.98	0.45
4:I:48:ILE:HD11	5:O:89:ARG:HH12	1.81	0.45
6:T:115:LYS:HE2	7:Z:4:LEU:HD21	1.97	0.45
1:6:235:LEU:HD13	1:7:244:ARG:HH22	1.81	0.45
1:UI:94:HIS:HB2	1:UI:146:THR:HG21	1.97	0.45
1:UO:94:HIS:HB2	1:UO:146:THR:HG21	1.97	0.45
1:UP:98:LEU:HD11	1:UP:143:THR:O	2.16	0.45
1:WU:112:GLY:HA2	1:WU:139:GLU:OE1	2.17	0.45
1:WU:114:GLU:O	1:WU:115:LEU:C	2.54	0.45
1:WW:145:GLU:C	1:WW:147:LEU:H	2.19	0.45
4:I:190:PHE:CD1	4:J:220:PRO:HG3	2.52	0.45
5:N:7:ILE:HD11	1:7:370:ARG:NH2	2.30	0.45
5:N:69:ASN:HB2	6:T:16:LEU:HD23	1.98	0.45
1:AA:235:LEU:HD13	1:AB:244:ARG:HH22	1.81	0.45
1:AI:235:LEU:HD13	1:AJ:244:ARG:HH22	1.81	0.45
1:UI:162:PRO:O	1:UI:163:SER:C	2.55	0.45
1:UK:98:LEU:HD11	1:UK:143:THR:O	2.16	0.45
1:WA:217:GLY:HA3	1:WW:190:GLN:HG2	1.98	0.45
1:WC:181:GLU:O	1:WC:182:PRO:C	2.54	0.45
1:WH:139:GLU:HB3	1:WI:154:ARG:HH21	1.80	0.45
1:WM:135:ALA:O	1:WM:139:GLU:HG2	2.16	0.45
1:WQ:160:PRO:HG2	1:WQ:170:LYS:O	2.16	0.45
1:WV:190:GLN:HG2	1:WW:217:GLY:HA3	1.97	0.45
3:E:158:PRO:HD2	3:E:162:ASN:ND2	2.32	0.45
4:H:66:ARG:HB2	4:H:178:GLU:OE1	2.17	0.45
5:K:86:ILE:HG12	5:P:102:MET:CE	2.46	0.45
6:Q:104:ARG:O	6:Q:108:GLN:HG2	2.17	0.45
6:S:33:ALA:O	6:S:98:ASN:ND2	2.50	0.45
1:AL:235:LEU:HD13	1:AM:244:ARG:HH22	1.81	0.45
1:UI:136:LEU:HD23	1:UI:157:LEU:CD1	2.45	0.45
1:UK:162:PRO:O	1:UK:163:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UK:207:PRO:HG2	1:WE:187:ASP:OD1	2.10	0.45
1:UL:162:PRO:O	1:UL:163:SER:C	2.55	0.45
1:UL:164:LEU:HD22	1:UL:164:LEU:H	1.81	0.45
1:UM:164:LEU:HD22	1:UM:164:LEU:H	1.82	0.45
1:WC:164:LEU:HB3	4:H:152:ARG:NH2	2.30	0.45
1:WC:193:ALA:HB1	1:WD:213:VAL:HG21	1.98	0.45
1:WQ:135:ALA:O	1:WQ:139:GLU:HG2	2.16	0.45
1:WT:135:ALA:O	1:WT:139:GLU:HG2	2.16	0.45
1:WT:190:GLN:HG2	1:WU:217:GLY:HA3	1.99	0.45
2:A:58:VAL:HG21	4:G:207:LEU:HD21	1.97	0.45
4:F:60:MET:CE	4:G:91:GLY:HA3	2.47	0.45
6:S:128:LYS:HE2	7:X:134:GLN:HG2	1.98	0.45
1:2:235:LEU:HD13	1:3:244:ARG:HH22	1.81	0.45
1:7:235:LEU:HD13	1:8:244:ARG:HH22	1.81	0.45
1:AG:235:LEU:HD13	1:AH:244:ARG:HH22	1.81	0.45
1:AJ:235:LEU:HD13	1:AK:244:ARG:HH22	1.81	0.45
1:UK:80:ALA:N	1:UK:85:ALA:O	2.49	0.45
1:WB:164:LEU:HD23	1:WB:164:LEU:HA	1.75	0.45
1:WF:114:GLU:HA	1:WF:117:ASP:HB2	1.99	0.45
1:WG:190:GLN:HG3	1:WH:217:GLY:HA3	1.99	0.45
1:WI:197:LEU:HD13	1:WJ:175:SER:OG	2.09	0.45
1:WV:135:ALA:O	1:WV:139:GLU:HG2	2.16	0.45
5:N:15:GLN:HG3	5:N:16:ALA:N	2.30	0.45
5:O:15:GLN:HG3	5:O:16:ALA:N	2.30	0.45
5:P:15:GLN:HG3	5:P:16:ALA:N	2.30	0.45
5:P:61:LEU:HD21	6:U:50:LYS:NZ	2.31	0.45
6:T:78:VAL:CG1	1:6:361:ASN:ND2	2.78	0.45
1:UM:94:HIS:HB2	1:UM:146:THR:HG21	1.97	0.45
1:UN:52:ARG:O	1:UN:88:VAL:N	2.38	0.45
1:WA:187:ASP:OD2	1:WA:190:GLN:HG3	2.16	0.45
1:WF:128:GLU:CG	1:WG:126:PHE:CD2	2.98	0.45
1:WJ:135:ALA:O	1:WJ:139:GLU:HG2	2.16	0.45
1:WS:137:GLU:HG3	1:WS:155:VAL:O	2.16	0.45
1:WT:167:ARG:HG2	1:WT:168:GLU:N	2.31	0.45
1:WW:219:LEU:HG	1:WW:221:THR:H	1.82	0.45
4:G:204:LEU:HD12	4:G:214:PRO:HB3	1.99	0.45
4:G:205:MET:HE3	4:H:209:MET:HA	1.99	0.45
7:X:4:LEU:N	7:X:126:MET:HE3	2.31	0.45
1:UJ:162:PRO:O	1:UJ:163:SER:C	2.55	0.45
1:UM:162:PRO:O	1:UM:163:SER:C	2.55	0.45
1:UN:162:PRO:O	1:UN:163:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WB:112:GLY:HA2	1:WB:139:GLU:OE1	2.17	0.45
1:WC:169:GLN:NE2	1:WC:170:LYS:O	2.44	0.45
1:WH:167:ARG:HH22	4:J:162:PRO:HG2	1.80	0.45
1:WK:193:ALA:HB1	1:WL:213:VAL:HG11	1.98	0.45
1:WL:145:GLU:O	1:WL:146:THR:C	2.53	0.45
1:WS:219:LEU:HG	1:WS:221:THR:H	1.82	0.45
1:WV:164:LEU:HB3	4:G:152:ARG:HH12	1.82	0.45
2:D:60:ILE:O	2:D:64:VAL:HG22	2.17	0.45
4:J:239:LEU:HD12	4:J:239:LEU:HA	1.84	0.45
1:9:235:LEU:HD13	1:0:244:ARG:HH22	1.81	0.45
1:UL:129:GLN:O	1:UL:133:GLN:N	2.29	0.45
1:UM:80:ALA:N	1:UM:85:ALA:O	2.49	0.45
1:UP:167:ARG:HH11	1:8:236:LYS:CE	2.29	0.45
1:WB:113:PHE:CE2	1:WB:139:GLU:HG3	2.52	0.45
1:WB:114:GLU:O	1:WB:115:LEU:C	2.55	0.45
1:WE:164:LEU:CD2	4:I:159:LEU:HD22	2.46	0.45
1:WG:206:PRO:O	1:WG:207:PRO:C	2.56	0.45
1:WO:206:PRO:O	1:WO:207:PRO:C	2.56	0.45
1:WU:164:LEU:CA	4:G:152:ARG:HG3	2.47	0.45
2:A:10:GLY:O	2:A:14:MET:HG2	2.16	0.45
4:H:90:LEU:HG	5:M:104:VAL:CG2	2.47	0.45
1:AF:235:LEU:HD13	1:AG:244:ARG:HH22	1.81	0.45
1:UM:98:LEU:HD11	1:UM:143:THR:O	2.16	0.45
1:UN:80:ALA:N	1:UN:85:ALA:O	2.49	0.45
1:UO:164:LEU:HD22	1:UO:164:LEU:H	1.82	0.45
1:WE:206:PRO:O	1:WE:207:PRO:C	2.56	0.45
1:WF:135:ALA:O	1:WF:139:GLU:HG2	2.16	0.45
1:WO:219:LEU:HG	1:WO:221:THR:H	1.82	0.45
3:E:8:GLN:O	3:E:12:TRP:HD1	2.00	0.45
3:E:144:LEU:HB3	4:J:149:LEU:HD22	1.98	0.45
4:J:114:GLN:HB3	4:J:115:PRO:HD3	1.99	0.45
6:Q:30:ILE:HG23	6:Q:102:MET:HE1	1.99	0.45
1:AM:235:LEU:HD13	1:AN:244:ARG:HH22	1.81	0.45
1:WH:135:ALA:O	1:WH:139:GLU:HG2	2.16	0.44
1:WI:165:PHE:CE2	4:J:162:PRO:HA	2.53	0.44
1:WQ:206:PRO:O	1:WQ:207:PRO:C	2.56	0.44
1:WU:135:ALA:O	1:WU:139:GLU:HG2	2.16	0.44
1:WW:192:SER:O	1:WW:195:VAL:HB	2.17	0.44
2:C:27:VAL:HG22	2:C:57:ALA:HB1	1.99	0.44
6:S:31:ALA:HB1	7:X:13:ALA:HB2	1.98	0.44
6:S:73:ILE:HD12	1:AD:363:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:86:ASP:OD1	7:W:86:ASP:N	2.41	0.44
1:UI:103:GLN:NE2	1:WB:182:PRO:HB3	2.32	0.44
1:UJ:55:PHE:O	1:UJ:85:ALA:HA	2.18	0.44
1:UJ:103:GLN:OE1	1:WD:182:PRO:CG	2.65	0.44
1:UN:98:LEU:HD11	1:UN:143:THR:O	2.16	0.44
1:WB:166:VAL:O	4:H:152:ARG:CD	2.63	0.44
1:WC:131:ASN:O	1:WC:134:ARG:N	2.51	0.44
1:WE:161:LYS:H	1:WE:161:LYS:HD3	1.82	0.44
1:WL:159:MET:HE3	1:WL:159:MET:HB2	1.94	0.44
1:WV:187:ASP:N	1:WV:190:GLN:HB2	2.31	0.44
1:WW:206:PRO:O	1:WW:207:PRO:C	2.56	0.44
2:B:2:THR:HG23	2:B:5:SER:H	1.82	0.44
2:B:20:LEU:HD11	2:B:73:LEU:HD13	2.00	0.44
5:K:15:GLN:HG3	5:K:16:ALA:N	2.30	0.44
5:L:7:ILE:CG1	1:AI:370:ARG:HH21	2.26	0.44
5:M:70:ASP:OD1	6:S:13:GLN:NE2	2.50	0.44
6:S:65:LEU:HD11	1:AD:365:ASN:ND2	2.32	0.44
6:S:73:ILE:HD13	1:AE:297:GLN:CB	2.35	0.44
6:S:109:PHE:CZ	7:X:118:VAL:HG13	2.53	0.44
1:4:235:LEU:HD13	1:5:244:ARG:HH22	1.81	0.44
1:AP:235:LEU:HD13	1:AQ:244:ARG:HH22	1.81	0.44
1:UI:98:LEU:HD11	1:UI:143:THR:O	2.16	0.44
1:UK:164:LEU:H	1:UK:164:LEU:HD22	1.82	0.44
1:UL:55:PHE:O	1:UL:85:ALA:HA	2.18	0.44
1:UM:75:ILE:HG21	1:UM:96:LEU:HD11	2.00	0.44
1:UN:164:LEU:H	1:UN:164:LEU:HD22	1.82	0.44
1:WH:206:PRO:O	1:WH:207:PRO:C	2.55	0.44
1:WJ:206:PRO:O	1:WJ:207:PRO:C	2.56	0.44
1:WP:186:LEU:HA	1:WP:190:GLN:OE1	2.17	0.44
1:WR:142:ARG:O	1:WR:146:THR:HG23	2.16	0.44
3:E:75:MET:O	3:E:79:LEU:HG	2.17	0.44
4:G:57:ILE:O	4:G:61:MET:HB2	2.17	0.44
4:J:204:LEU:HD11	4:J:217:ILE:HD12	1.99	0.44
6:Q:23:GLN:HE22	7:V:125:MET:HE1	1.82	0.44
1:UJ:94:HIS:HB2	1:UJ:146:THR:HG21	1.97	0.44
1:UK:98:LEU:HD12	1:UK:146:THR:HG1	1.79	0.44
1:WD:206:PRO:O	1:WD:207:PRO:C	2.56	0.44
1:WF:166:VAL:HG22	1:WF:168:GLU:H	1.82	0.44
1:WO:190:GLN:NE2	1:WP:216:SER:O	2.50	0.44
1:WQ:187:ASP:OD1	1:WQ:188:GLU:N	2.51	0.44
1:WR:135:ALA:O	1:WR:139:GLU:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WS:206:PRO:O	1:WS:207:PRO:C	2.56	0.44
1:WT:134:ARG:HH21	1:WT:134:ARG:HB3	1.83	0.44
1:WU:158:ALA:O	1:WU:160:PRO:HD3	2.18	0.44
1:WU:206:PRO:O	1:WU:207:PRO:C	2.55	0.44
6:S:72:HIS:CA	1:AE:295:SER:HB3	2.45	0.44
1:UM:160:PRO:HG2	1:UM:170:LYS:HB3	2.00	0.44
1:WA:196:HIS:NE2	1:WB:219:LEU:HD22	2.33	0.44
1:WF:206:PRO:O	1:WF:207:PRO:C	2.56	0.44
1:WI:206:PRO:O	1:WI:207:PRO:C	2.56	0.44
1:WQ:171:SER:HB3	1:WQ:206:PRO:HD3	2.00	0.44
1:WS:197:LEU:CD1	1:WT:175:SER:OG	2.64	0.44
1:WT:128:GLU:CG	1:WU:126:PHE:CD2	2.99	0.44
4:H:127:LEU:HD23	4:H:127:LEU:HA	1.88	0.44
5:M:21:ALA:HB3	1:O:278:THR:HG21	1.97	0.44
1:AD:235:LEU:HD13	1:AE:244:ARG:HH22	1.81	0.44
1:UI:55:PHE:O	1:UI:85:ALA:HA	2.18	0.44
1:UJ:100:LEU:HD23	1:UJ:103:GLN:HE21	1.83	0.44
1:UK:55:PHE:O	1:UK:85:ALA:HA	2.18	0.44
1:UN:75:ILE:HG21	1:UN:96:LEU:HD11	2.00	0.44
1:UP:80:ALA:N	1:UP:85:ALA:O	2.49	0.44
1:WF:148:GLY:N	1:WG:215:GLN:O	2.39	0.44
1:WI:167:ARG:CG	4:J:160:GLN:O	2.65	0.44
3:E:123:PRO:HB2	3:E:126:ALA:HB3	1.99	0.44
4:F:213:PRO:HA	4:F:214:PRO:HD3	1.91	0.44
4:I:147:LEU:HD21	4:I:165:VAL:HG11	2.00	0.44
6:Q:49:LEU:O	6:Q:53:MET:HG2	2.17	0.44
1:UL:160:PRO:HG2	1:UL:170:LYS:HB3	2.00	0.44
1:WB:113:PHE:HB3	1:WC:134:ARG:CZ	2.48	0.44
1:WB:142:ARG:O	1:WB:146:THR:HG23	2.17	0.44
1:WD:191:ILE:O	1:WD:195:VAL:HG23	2.17	0.44
1:WE:200:SER:O	1:WF:158:ALA:HB3	2.18	0.44
1:WH:219:LEU:HG	1:WH:221:THR:H	1.82	0.44
1:WJ:145:GLU:HG2	1:WJ:153:ALA:N	2.33	0.44
1:WN:219:LEU:HG	1:WN:221:THR:H	1.82	0.44
1:WP:196:HIS:CD2	1:WQ:219:LEU:HD13	2.52	0.44
1:WS:168:GLU:O	1:WS:169:GLN:HB3	2.18	0.44
1:WT:206:PRO:O	1:WT:207:PRO:C	2.56	0.44
1:UL:94:HIS:HB2	1:UL:146:THR:HG21	1.97	0.44
1:UO:55:PHE:O	1:UO:85:ALA:HA	2.18	0.44
1:UO:75:ILE:HG21	1:UO:96:LEU:HD11	2.00	0.44
1:WA:206:PRO:O	1:WA:207:PRO:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WC:130:VAL:HG12	1:WC:134:ARG:HD2	1.99	0.44
1:WC:200:SER:O	1:WD:158:ALA:HB3	2.14	0.44
1:WE:164:LEU:HD13	1:WE:165:PHE:H	1.82	0.44
1:WG:164:LEU:HD13	1:WG:164:LEU:HA	1.80	0.44
1:WS:125:GLN:CB	2:A:4:GLU:HB2	2.40	0.44
1:WW:134:ARG:HH21	1:WW:134:ARG:CB	2.30	0.44
4:I:161:GLY:C	4:I:163:GLU:H	2.20	0.44
4:I:212:VAL:HG21	4:I:217:ILE:HD11	2.00	0.44
5:N:21:ALA:HB3	1:4:278:THR:CG2	2.31	0.44
6:S:72:HIS:ND1	1:AD:365:ASN:CG	2.70	0.44
1:AP:429:THR:OG1	1:AQ:418:GLU:OE2	2.36	0.44
1:UI:80:ALA:N	1:UI:85:ALA:O	2.49	0.44
1:UK:160:PRO:HG2	1:UK:170:LYS:HB3	2.00	0.44
1:UM:55:PHE:O	1:UM:85:ALA:HA	2.18	0.44
1:UO:160:PRO:HG2	1:UO:170:LYS:HB3	2.00	0.44
1:UP:55:PHE:O	1:UP:85:ALA:HA	2.18	0.44
1:WJ:125:GLN:HB3	3:E:242:HIS:HB2	1.97	0.44
1:WL:219:LEU:HG	1:WL:221:THR:H	1.82	0.44
1:WM:187:ASP:OD1	1:WM:190:GLN:N	2.44	0.44
1:WR:190:GLN:HG2	1:WS:217:GLY:HA3	2.00	0.44
1:WS:193:ALA:HB1	1:WT:213:VAL:CG1	2.48	0.44
6:S:67:LEU:HD21	6:S:74:PRO:HA	2.00	0.44
7:Z:97:ASP:O	7:Z:101:GLU:HG2	2.18	0.44
1:3:429:THR:OG1	1:4:418:GLU:OE2	2.36	0.44
1:AC:429:THR:OG1	1:AD:418:GLU:OE2	2.36	0.44
1:UI:160:PRO:HG2	1:UI:170:LYS:HB3	2.00	0.43
1:UI:164:LEU:HD22	1:UI:164:LEU:H	1.82	0.43
1:UP:75:ILE:HG21	1:UP:96:LEU:HD11	2.00	0.43
1:UP:164:LEU:H	1:UP:164:LEU:HD22	1.81	0.43
1:WE:167:ARG:HH21	4:I:162:PRO:CD	2.30	0.43
1:WK:206:PRO:O	1:WK:207:PRO:C	2.55	0.43
1:WM:219:LEU:HG	1:WM:221:THR:H	1.82	0.43
1:WT:192:SER:O	1:WT:195:VAL:HB	2.18	0.43
1:WV:117:ASP:OD1	1:WW:120:LYS:NZ	2.51	0.43
1:WV:192:SER:O	1:WV:195:VAL:HB	2.18	0.43
3:E:251:LEU:HD23	3:E:251:LEU:HA	1.84	0.43
4:J:80:THR:CB	4:J:83:ALA:HB2	2.48	0.43
5:N:14:LEU:HD11	1:6:370:ARG:NH2	2.32	0.43
5:P:11:ILE:HD11	1:AQ:276:GLU:CD	2.38	0.43
6:S:88:ARG:HH12	6:S:108:GLN:HG3	1.83	0.43
6:U:73:ILE:HG13	1:2:295:SER:CB	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UJ:160:PRO:HG2	1:UJ:170:LYS:HB3	2.00	0.43
1:UN:160:PRO:HG2	1:UN:170:LYS:HB3	2.00	0.43
1:UO:98:LEU:HD12	1:UO:146:THR:HG1	1.80	0.43
1:WB:145:GLU:C	1:WB:147:LEU:H	2.22	0.43
1:WH:139:GLU:HB3	1:WI:154:ARG:NH2	2.33	0.43
1:WM:206:PRO:O	1:WM:207:PRO:C	2.56	0.43
2:D:52:ILE:HD13	2:D:52:ILE:HA	1.83	0.43
4:J:195:ILE:O	4:J:199:VAL:HG13	2.18	0.43
1:UJ:103:GLN:CB	1:WD:182:PRO:HA	2.48	0.43
1:UJ:167:ARG:NH1	1:2:236:LYS:NZ	2.60	0.43
1:UM:129:GLN:O	1:UM:133:GLN:N	2.29	0.43
1:UN:218:HIS:NE2	1:AB:265:GLN:NE2	2.65	0.43
1:UO:98:LEU:HD11	1:UO:143:THR:O	2.16	0.43
1:UP:129:GLN:O	1:UP:133:GLN:N	2.29	0.43
1:WB:206:PRO:O	1:WB:207:PRO:C	2.56	0.43
1:WM:142:ARG:O	1:WM:146:THR:HG23	2.18	0.43
1:WS:113:PHE:HB3	1:WT:134:ARG:CZ	2.49	0.43
2:A:37:ILE:HD13	2:B:44:ILE:HD11	2.00	0.43
4:J:124:GLN:H	4:J:124:GLN:HG2	1.67	0.43
5:L:84:MET:HE2	5:L:84:MET:HB2	1.91	0.43
6:R:68:THR:CG2	1:AJ:294:ARG:HD2	2.49	0.43
1:2:429:THR:OG1	1:3:418:GLU:OE2	2.36	0.43
1:AA:429:THR:OG1	1:AB:418:GLU:OE2	2.36	0.43
1:AE:429:THR:OG1	1:AF:418:GLU:OE2	2.36	0.43
1:AF:429:THR:OG1	1:AG:418:GLU:OE2	2.36	0.43
1:UK:129:GLN:O	1:UK:133:GLN:N	2.29	0.43
1:UO:80:ALA:N	1:UO:85:ALA:O	2.49	0.43
1:WC:206:PRO:O	1:WC:207:PRO:C	2.56	0.43
1:WD:172:PRO:HD2	1:WD:204:GLY:O	2.18	0.43
1:WP:145:GLU:C	1:WP:147:LEU:N	2.72	0.43
2:C:77:VAL:HG12	4:I:229:VAL:HG11	2.00	0.43
3:E:179:ILE:H	3:E:179:ILE:HG13	1.69	0.43
3:E:205:ASN:HB3	4:F:209:MET:HG3	2.00	0.43
5:N:7:ILE:HD11	1:7:370:ARG:NE	2.32	0.43
1:UJ:164:LEU:HD22	1:UJ:164:LEU:H	1.81	0.43
1:UP:160:PRO:HG2	1:UP:170:LYS:HB3	2.00	0.43
1:WC:190:GLN:C	1:WC:192:SER:N	2.72	0.43
1:WD:193:ALA:HB1	1:WE:213:VAL:HG21	2.00	0.43
1:WE:132:TYR:HB2	1:WF:126:PHE:HZ	1.83	0.43
1:WL:172:PRO:HD2	1:WL:204:GLY:O	2.19	0.43
1:WR:206:PRO:O	1:WR:207:PRO:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WT:131:ASN:HA	1:WT:134:ARG:HD3	1.99	0.43
1:WU:128:GLU:HG2	1:WV:126:PHE:CD2	2.48	0.43
4:H:143:ARG:HH22	4:H:177:SER:HA	1.83	0.43
6:T:19:ARG:NH2	6:T:115:LYS:HD3	2.33	0.43
6:T:117:GLN:HE22	7:Y:125:MET:CG	2.32	0.43
1:AH:429:THR:OG1	1:AI:418:GLU:OE2	2.36	0.43
1:AM:429:THR:OG1	1:AN:418:GLU:OE2	2.36	0.43
1:UL:75:ILE:HG21	1:UL:96:LEU:HD11	2.00	0.43
1:UN:129:GLN:O	1:UN:133:GLN:N	2.29	0.43
1:WD:197:LEU:HD11	1:WE:156:HIS:HD2	1.84	0.43
1:WT:145:GLU:C	1:WT:147:LEU:N	2.72	0.43
1:WV:113:PHE:HB3	1:WW:134:ARG:NH1	2.33	0.43
1:WV:200:SER:O	1:WW:158:ALA:HB3	2.16	0.43
2:D:29:LEU:HD12	3:E:216:ILE:HG13	2.01	0.43
4:F:63:SER:HB2	4:F:66:ARG:HH21	1.84	0.43
4:F:99:PHE:C	4:F:99:PHE:CD2	2.91	0.43
4:G:119:GLN:HE22	6:R:4:ARG:HG2	1.84	0.43
4:G:217:ILE:O	4:G:220:PRO:HD2	2.18	0.43
4:H:121:ILE:HD12	4:H:121:ILE:HA	1.89	0.43
6:T:11:PHE:CD1	6:T:53:MET:HE2	2.53	0.43
1:AN:429:THR:OG1	1:AO:418:GLU:OE2	2.36	0.43
1:UI:75:ILE:HG21	1:UI:96:LEU:HD11	2.00	0.43
1:UN:55:PHE:O	1:UN:85:ALA:HA	2.18	0.43
1:WG:166:VAL:HG12	1:WG:168:GLU:H	1.83	0.43
1:WH:166:VAL:HG12	4:J:147:LEU:HD12	2.00	0.43
1:WP:166:VAL:HG21	4:F:160:GLN:HB3	1.82	0.43
1:WP:206:PRO:O	1:WP:207:PRO:C	2.56	0.43
1:WR:192:SER:O	1:WR:195:VAL:HB	2.19	0.43
3:E:224:VAL:O	3:E:228:LEU:HB2	2.18	0.43
4:H:114:GLN:O	4:H:118:GLU:HG2	2.19	0.43
1:1:429:THR:OG1	1:2:418:GLU:OE2	2.36	0.43
1:UJ:102:GLN:CG	1:UJ:193:ALA:HB2	2.49	0.43
1:UL:103:GLN:HG2	1:WH:182:PRO:CB	2.46	0.43
1:WE:164:LEU:HD21	4:I:159:LEU:HD22	2.00	0.43
1:WH:186:LEU:HD22	1:WH:190:GLN:HG2	2.00	0.43
1:WH:200:SER:O	1:WI:158:ALA:HB3	2.13	0.43
1:WM:172:PRO:HD2	1:WM:204:GLY:O	2.18	0.43
1:WN:206:PRO:O	1:WN:207:PRO:C	2.56	0.43
1:WS:142:ARG:O	1:WS:146:THR:HG23	2.17	0.43
1:WV:206:PRO:O	1:WV:207:PRO:C	2.56	0.43
4:F:147:LEU:HD23	4:F:147:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:190:PHE:CD1	4:H:220:PRO:HG3	2.54	0.43
4:H:141:GLN:NE2	4:H:243:PHE:HA	2.33	0.43
5:K:11:ILE:CD1	1:AL:276:GLU:CD	2.87	0.43
6:T:68:THR:HG21	1:7:294:ARG:HD2	2.01	0.43
6:T:68:THR:CG2	1:7:294:ARG:HD2	2.48	0.43
7:W:7:PHE:CD2	7:W:119:LEU:HD11	2.54	0.43
7:W:82:ASN:HD22	7:W:91:VAL:HG21	1.83	0.43
1:5:429:THR:OG1	1:6:418:GLU:OE2	2.36	0.43
1:0:429:THR:OG1	1:AA:418:GLU:OE2	2.36	0.43
1:AJ:429:THR:OG1	1:AK:418:GLU:OE2	2.36	0.43
1:AO:429:THR:OG1	1:AP:418:GLU:OE2	2.36	0.43
1:UJ:80:ALA:N	1:UJ:85:ALA:O	2.49	0.43
1:WA:187:ASP:OD1	1:WA:190:GLN:N	2.42	0.43
1:WB:166:VAL:CG2	1:WB:169:GLN:HA	2.49	0.43
1:WG:165:PHE:HE1	4:J:240:ALA:CB	2.18	0.43
1:WN:172:PRO:HD2	1:WN:204:GLY:O	2.18	0.43
1:WT:161:LYS:CB	1:WT:162:PRO:HD2	2.49	0.43
1:WV:130:VAL:HG12	1:WV:134:ARG:HD2	1.99	0.43
1:WV:164:LEU:O	1:WV:166:VAL:N	2.49	0.43
1:WW:112:GLY:HA3	1:WW:135:ALA:HA	2.00	0.43
4:F:97:THR:HA	4:F:100:ILE:HG22	2.00	0.43
4:I:106:ASP:OD2	5:N:32:VAL:HG23	2.19	0.43
5:N:14:LEU:HD23	1:5:278:THR:CG2	2.49	0.43
7:V:122:VAL:O	7:V:126:MET:HG2	2.18	0.43
1:6:429:THR:OG1	1:7:418:GLU:OE2	2.36	0.43
1:9:429:THR:OG1	1:0:418:GLU:OE2	2.36	0.43
1:AD:429:THR:OG1	1:AE:418:GLU:OE2	2.36	0.43
1:AG:429:THR:OG1	1:AH:418:GLU:OE2	2.36	0.43
1:WA:190:GLN:O	1:WA:191:ILE:C	2.57	0.43
1:WJ:197:LEU:HD13	1:WK:175:SER:OG	2.09	0.43
1:WT:124:SER:OG	2:A:4:GLU:OE2	2.33	0.43
1:WW:115:LEU:O	1:WW:116:LEU:C	2.57	0.43
3:E:88:MET:HA	3:E:247:ILE:HG21	1.99	0.43
5:K:74:ASP:N	5:K:74:ASP:OD2	2.52	0.43
5:O:4:ILE:HG12	1:1:372:ILE:HB	2.00	0.43
6:S:65:LEU:HD23	6:S:75:ALA:CB	2.49	0.43
1:4:290:LYS:HE3	1:4:290:LYS:HB2	1.93	0.43
1:4:421:GLY:O	1:4:426:ARG:NH2	2.51	0.43
1:UJ:52:ARG:O	1:UJ:88:VAL:N	2.38	0.42
1:UK:94:HIS:HB2	1:UK:146:THR:HG21	1.97	0.42
1:UK:102:GLN:CG	1:UK:193:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UL:102:GLN:CG	1:UL:193:ALA:HB2	2.49	0.42
1:WC:142:ARG:O	1:WC:146:THR:HG23	2.18	0.42
1:WC:145:GLU:O	1:WC:146:THR:C	2.56	0.42
1:WI:161:LYS:HA	1:WI:162:PRO:HD3	1.89	0.42
1:WI:201:ALA:C	1:WJ:158:ALA:HB2	2.39	0.42
1:WL:206:PRO:O	1:WL:207:PRO:C	2.56	0.42
1:WQ:124:SER:CB	2:A:75:ASP:OD1	2.67	0.42
1:WQ:124:SER:HA	2:A:75:ASP:OD1	2.19	0.42
1:WQ:193:ALA:CB	1:WR:217:GLY:O	2.67	0.42
2:D:45:ASN:OD1	2:D:45:ASN:N	2.49	0.42
5:P:15:GLN:HB2	1:AQ:374:HIS:CG	2.53	0.42
1:3:421:GLY:O	1:3:426:ARG:NH2	2.51	0.42
1:AB:429:THR:OG1	1:AC:418:GLU:OE2	2.36	0.42
1:UK:75:ILE:HG21	1:UK:96:LEU:HD11	2.00	0.42
1:WI:191:ILE:O	1:WI:195:VAL:HG23	2.19	0.42
1:WJ:160:PRO:HG2	1:WJ:170:LYS:O	2.18	0.42
1:WU:192:SER:O	1:WU:195:VAL:HB	2.19	0.42
4:F:63:SER:O	4:F:67:ILE:HD12	2.19	0.42
4:J:82:SER:OG	4:J:82:SER:O	2.37	0.42
6:Q:77:ALA:HB3	1:AP:297:GLN:HE22	1.84	0.42
6:U:31:ALA:HB1	7:Z:13:ALA:HB2	2.00	0.42
7:Z:3:LEU:HD12	7:Z:3:LEU:HA	1.92	0.42
1:2:421:GLY:O	1:2:426:ARG:NH2	2.51	0.42
1:5:421:GLY:O	1:5:426:ARG:NH2	2.51	0.42
1:8:429:THR:OG1	1:9:418:GLU:OE2	2.36	0.42
1:UN:99:ARG:O	1:UN:103:GLN:HG3	2.18	0.42
1:UP:98:LEU:CD1	1:UP:146:THR:HG1	2.31	0.42
1:WA:113:PHE:CE2	1:WA:139:GLU:HG3	2.54	0.42
1:WF:140:LEU:O	1:WF:144:ILE:HG13	2.19	0.42
1:WG:122:GLY:O	1:WG:123:ILE:C	2.58	0.42
1:WK:128:GLU:OE1	1:WL:126:PHE:CE2	2.73	0.42
1:WS:140:LEU:O	1:WS:144:ILE:HG13	2.20	0.42
1:WT:140:LEU:O	1:WT:144:ILE:HG13	2.20	0.42
2:C:84:LEU:HD21	4:I:185:ILE:HG23	2.01	0.42
3:E:243:LEU:HD23	3:E:243:LEU:HA	1.81	0.42
4:G:114:GLN:HB3	4:G:115:PRO:HD3	2.01	0.42
5:N:7:ILE:CB	1:6:278:THR:HG21	2.50	0.42
5:O:4:ILE:CD1	1:1:374:HIS:HB2	2.50	0.42
6:Q:114:LEU:HD21	7:W:123:LYS:HG3	2.00	0.42
6:R:69:SER:OG	1:AK:294:ARG:HD3	2.19	0.42
7:V:13:ALA:HA	7:V:62:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:429:THR:OG1	1:5:418:GLU:OE2	2.36	0.42
1:6:421:GLY:O	1:6:426:ARG:NH2	2.51	0.42
1:AJ:290:LYS:HE3	1:AJ:290:LYS:HB2	1.93	0.42
1:AP:296:ARG:HG2	1:AP:296:ARG:NH1	2.35	0.42
1:UL:73:MET:HE3	1:UL:99:ARG:CD	2.44	0.42
1:UL:80:ALA:N	1:UL:85:ALA:O	2.49	0.42
1:WI:142:ARG:O	1:WI:146:THR:HG23	2.19	0.42
1:WI:164:LEU:HD22	4:J:148:ALA:HA	2.01	0.42
1:WN:140:LEU:O	1:WN:144:ILE:HG13	2.20	0.42
1:WQ:124:SER:OG	2:A:75:ASP:OD1	2.33	0.42
1:WR:165:PHE:O	1:WR:166:VAL:HG22	2.19	0.42
1:WT:113:PHE:CE1	1:WU:134:ARG:HG2	2.54	0.42
5:L:7:ILE:HG22	1:AH:278:THR:HG21	2.01	0.42
6:S:103:ASP:OD1	7:Y:112:TYR:OH	2.36	0.42
1:5:296:ARG:HG2	1:5:296:ARG:NH1	2.35	0.42
1:AQ:296:ARG:HG2	1:AQ:296:ARG:NH1	2.35	0.42
1:UN:69:GLN:HG3	1:UN:103:GLN:OE1	2.19	0.42
1:UP:94:HIS:HB2	1:UP:146:THR:HG21	1.97	0.42
1:WA:140:LEU:O	1:WA:144:ILE:HG13	2.19	0.42
1:WB:135:ALA:O	1:WB:139:GLU:HG2	2.18	0.42
1:WC:120:LYS:HE2	1:WC:120:LYS:HA	2.00	0.42
1:WC:191:ILE:O	1:WC:195:VAL:HG23	2.20	0.42
1:WD:190:GLN:HA	1:WE:217:GLY:O	2.19	0.42
1:WE:140:LEU:O	1:WE:144:ILE:HG13	2.20	0.42
1:WH:140:LEU:O	1:WH:144:ILE:HG13	2.20	0.42
1:WK:149:PRO:HD2	1:WK:190:GLN:HE22	1.84	0.42
1:WM:190:GLN:HA	1:WN:217:GLY:HA3	2.00	0.42
1:WQ:140:LEU:O	1:WQ:144:ILE:HG13	2.20	0.42
1:WR:140:LEU:O	1:WR:144:ILE:HG13	2.20	0.42
1:WT:196:HIS:HB3	1:WU:211:THR:CG2	2.30	0.42
1:WW:169:GLN:NE2	1:WW:170:LYS:O	2.53	0.42
2:C:52:ILE:O	2:C:55:ILE:HG22	2.18	0.42
3:E:125:LEU:O	3:E:129:MET:HG3	2.20	0.42
3:E:167:ASN:ND2	3:E:174:ARG:HH12	2.18	0.42
4:F:214:PRO:HG2	4:G:212:VAL:HG22	2.01	0.42
4:I:171:LEU:HB3	4:I:172:PRO:HD3	2.01	0.42
5:M:7:ILE:HD11	1:AC:370:ARG:NE	2.23	0.42
5:M:9:GLY:O	5:M:13:GLN:HG3	2.18	0.42
5:O:73:ALA:HB1	6:U:13:GLN:NE2	2.33	0.42
7:Y:112:TYR:CE2	7:Y:116:ILE:HD11	2.55	0.42
1:4:296:ARG:HG2	1:4:296:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:296:ARG:HG2	1:6:296:ARG:NH1	2.35	0.42
1:0:296:ARG:HG2	1:0:296:ARG:NH1	2.35	0.42
1:AA:296:ARG:HG2	1:AA:296:ARG:NH1	2.35	0.42
1:AB:296:ARG:HG2	1:AB:296:ARG:NH1	2.35	0.42
1:AK:429:THR:OG1	1:AL:418:GLU:OE2	2.36	0.42
1:UM:73:MET:HE1	1:UM:99:ARG:HD2	1.98	0.42
1:WB:164:LEU:O	4:H:152:ARG:HG3	2.18	0.42
1:WI:165:PHE:O	1:WI:165:PHE:CG	2.73	0.42
1:WJ:140:LEU:O	1:WJ:144:ILE:HG13	2.20	0.42
1:WJ:164:LEU:HD23	3:E:144:LEU:HB2	1.98	0.42
1:WL:214:ASP:OD1	1:WL:218:HIS:N	2.49	0.42
1:WT:142:ARG:O	1:WT:146:THR:HG23	2.20	0.42
1:WV:114:GLU:O	1:WV:118:GLN:HG3	2.20	0.42
1:WV:187:ASP:O	1:WV:190:GLN:HB2	2.20	0.42
4:H:59:LEU:O	4:H:65:THR:OG1	2.30	0.42
4:J:121:ILE:HG23	4:J:125:GLU:HB3	2.02	0.42
5:M:4:ILE:CD1	1:AC:374:HIS:CB	2.93	0.42
6:Q:85:LEU:HA	6:Q:85:LEU:HD23	1.81	0.42
1:AL:429:THR:OG1	1:AM:418:GLU:OE2	2.36	0.42
1:UJ:75:ILE:HG21	1:UJ:96:LEU:HD11	2.00	0.42
1:WA:115:LEU:HD22	1:WA:134:ARG:HD2	2.01	0.42
1:WA:126:PHE:HD2	1:WW:128:GLU:HG2	1.84	0.42
1:WG:140:LEU:O	1:WG:144:ILE:HG13	2.20	0.42
1:WJ:164:LEU:CD1	3:E:145:TRP:HA	2.50	0.42
1:WK:165:PHE:O	1:WK:166:VAL:HB	2.19	0.42
1:WP:140:LEU:O	1:WP:144:ILE:HG13	2.20	0.42
1:WP:147:LEU:O	1:WP:148:GLY:C	2.58	0.42
1:WR:192:SER:O	1:WR:195:VAL:N	2.53	0.42
1:WW:172:PRO:HD2	1:WW:204:GLY:O	2.19	0.42
3:E:122:MET:HG3	4:J:214:PRO:HG2	2.01	0.42
4:F:162:PRO:CD	4:F:163:GLU:N	2.82	0.42
4:G:121:ILE:HG12	4:G:125:GLU:HB3	2.02	0.42
4:H:86:ASN:HD22	5:M:103:GLN:HA	1.83	0.42
4:H:138:MET:HE2	4:H:170:LEU:HG	2.01	0.42
4:J:66:ARG:HA	4:J:182:ALA:HB2	2.02	0.42
6:T:68:THR:HG22	1:7:294:ARG:HD3	2.01	0.42
1:1:421:GLY:O	1:1:426:ARG:NH2	2.51	0.42
1:AC:296:ARG:HG2	1:AC:296:ARG:NH1	2.35	0.42
1:AO:296:ARG:HG2	1:AO:296:ARG:NH1	2.35	0.42
1:UI:102:GLN:CG	1:UI:193:ALA:HB2	2.49	0.42
1:UM:207:PRO:HD2	1:WP:187:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WE:113:PHE:CE2	1:WE:139:GLU:HG3	2.54	0.42
1:WG:166:VAL:CG1	1:WG:168:GLU:HB3	2.49	0.42
1:WI:129:GLN:HE22	1:WI:132:TYR:HD2	1.68	0.42
1:WI:140:LEU:O	1:WI:144:ILE:HG13	2.20	0.42
1:WJ:172:PRO:HD2	1:WJ:204:GLY:O	2.19	0.42
1:WO:140:LEU:O	1:WO:144:ILE:HG13	2.20	0.42
1:WO:214:ASP:OD1	1:WO:218:HIS:N	2.49	0.42
1:WQ:196:HIS:HB3	1:WR:211:THR:HG21	2.02	0.42
1:WW:140:LEU:O	1:WW:144:ILE:HG13	2.19	0.42
3:E:175:ALA:HA	3:E:178:LEU:HD23	2.02	0.42
3:E:254:ILE:HD13	3:E:254:ILE:HA	1.86	0.42
4:F:171:LEU:HB3	4:F:172:PRO:HD3	2.01	0.42
4:J:92:LEU:HD12	4:J:92:LEU:HA	1.78	0.42
5:L:48:ARG:HH22	6:R:6:ASP:CG	2.22	0.42
1:2:296:ARG:HG2	1:2:296:ARG:NH1	2.35	0.42
1:7:421:GLY:O	1:7:426:ARG:NH2	2.51	0.42
1:UM:102:GLN:CG	1:UM:193:ALA:HB2	2.49	0.42
1:WD:113:PHE:HB3	1:WE:134:ARG:NH1	2.34	0.42
1:WD:140:LEU:O	1:WD:144:ILE:HG13	2.19	0.42
1:WE:166:VAL:HG23	4:I:160:GLN:HA	1.84	0.42
1:WF:187:ASP:H	1:WF:190:GLN:CD	2.22	0.42
1:WH:200:SER:OG	1:WI:175:SER:CB	2.54	0.42
1:WU:140:LEU:O	1:WU:144:ILE:HG13	2.20	0.42
1:WW:147:LEU:O	1:WW:148:GLY:C	2.59	0.42
2:C:54:LYS:HB3	2:C:54:LYS:HE2	1.84	0.42
5:O:69:ASN:OD1	5:O:69:ASN:N	2.52	0.42
5:O:84:MET:SD	6:U:134:LEU:HD21	2.59	0.42
1:1:296:ARG:HG2	1:1:296:ARG:NH1	2.35	0.42
1:9:296:ARG:HG2	1:9:296:ARG:NH1	2.35	0.42
1:AK:296:ARG:HG2	1:AK:296:ARG:NH1	2.35	0.42
1:WE:164:LEU:HD13	1:WE:165:PHE:N	2.35	0.42
1:WK:145:GLU:O	1:WK:146:THR:C	2.58	0.42
1:WP:165:PHE:CA	4:F:160:GLN:O	2.68	0.42
1:WQ:121:PHE:HZ	2:A:15:LYS:HD3	1.85	0.42
1:WV:140:LEU:O	1:WV:144:ILE:HG13	2.20	0.42
4:J:189:ILE:O	4:J:192:PRO:HD2	2.19	0.42
7:W:10:ALA:HB3	7:W:119:LEU:HD13	2.02	0.42
1:O:290:LYS:HE3	1:O:290:LYS:HB2	1.93	0.42
1:AI:429:THR:OG1	1:AJ:418:GLU:OE2	2.36	0.42
1:AO:290:LYS:HE3	1:AO:290:LYS:HB2	1.93	0.42
1:UO:102:GLN:CG	1:UO:193:ALA:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UO:214:ASP:OD2	1:UO:218:HIS:HB2	2.20	0.41
1:WC:140:LEU:O	1:WC:144:ILE:HG13	2.20	0.41
1:WI:145:GLU:C	1:WI:147:LEU:N	2.74	0.41
1:WU:164:LEU:HA	4:G:152:ARG:NH2	2.35	0.41
1:7:296:ARG:HG2	1:7:296:ARG:NH1	2.35	0.41
1:8:421:GLY:O	1:8:426:ARG:NH2	2.51	0.41
1:AD:296:ARG:HG2	1:AD:296:ARG:NH1	2.35	0.41
1:AL:296:ARG:HG2	1:AL:296:ARG:NH1	2.35	0.41
1:WH:190:GLN:HG3	1:WI:217:GLY:HA3	2.02	0.41
1:WR:145:GLU:O	1:WR:146:THR:C	2.59	0.41
1:WS:125:GLN:N	2:A:4:GLU:HB3	2.34	0.41
1:WS:214:ASP:OD1	1:WS:218:HIS:N	2.49	0.41
4:J:129:LYS:HB3	4:J:129:LYS:HE3	1.87	0.41
4:J:225:LEU:HD12	4:J:229:VAL:HG22	2.01	0.41
6:T:39:GLN:HA	6:T:99:THR:HB	2.02	0.41
1:3:296:ARG:HG2	1:3:296:ARG:NH1	2.35	0.41
1:7:429:THR:OG1	1:8:418:GLU:OE2	2.36	0.41
1:AE:296:ARG:HG2	1:AE:296:ARG:NH1	2.35	0.41
1:UP:102:GLN:CG	1:UP:193:ALA:HB2	2.49	0.41
1:UP:214:ASP:OD2	1:UP:218:HIS:HB2	2.20	0.41
1:WB:114:GLU:O	1:WB:117:ASP:N	2.54	0.41
1:WK:140:LEU:O	1:WK:144:ILE:HG13	2.20	0.41
1:WN:145:GLU:C	1:WN:147:LEU:N	2.74	0.41
1:WV:128:GLU:CG	1:WW:126:PHE:CE2	3.03	0.41
4:I:190:PHE:CG	4:J:220:PRO:HG3	2.55	0.41
4:J:217:ILE:O	4:J:220:PRO:HD2	2.20	0.41
6:R:29:ASN:ND2	6:R:40:ALA:HA	2.35	0.41
1:AF:296:ARG:HG2	1:AF:296:ARG:NH1	2.35	0.41
1:WI:162:PRO:HG2	1:WJ:165:PHE:HZ	1.86	0.41
1:WP:164:LEU:O	4:F:159:LEU:O	2.38	0.41
1:WR:128:GLU:HB3	1:WS:126:PHE:CE2	2.55	0.41
1:WR:165:PHE:O	1:WR:167:ARG:N	2.53	0.41
1:WR:197:LEU:HA	1:WS:175:SER:CB	2.50	0.41
3:E:176:GLY:HA2	3:E:179:ILE:CD1	2.49	0.41
4:J:83:ALA:O	4:J:85:PRO:N	2.54	0.41
5:M:80:VAL:HG22	6:S:131:MET:HG2	2.01	0.41
7:Z:119:LEU:HA	7:Z:119:LEU:HD23	1.67	0.41
1:AG:296:ARG:HG2	1:AG:296:ARG:NH1	2.35	0.41
1:AM:296:ARG:HG2	1:AM:296:ARG:NH1	2.35	0.41
1:UI:214:ASP:OD2	1:UI:218:HIS:HB2	2.20	0.41
1:UK:207:PRO:CA	1:WE:187:ASP:OD1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WA:196:HIS:CD2	1:WB:219:LEU:HD13	2.56	0.41
1:WB:140:LEU:O	1:WB:144:ILE:HG13	2.20	0.41
1:WB:147:LEU:O	1:WB:148:GLY:C	2.58	0.41
1:WB:166:VAL:HG21	1:WB:169:GLN:HA	2.01	0.41
1:WB:196:HIS:HB3	1:WC:211:THR:HG21	2.01	0.41
1:WJ:125:GLN:HG3	3:E:242:HIS:CG	2.54	0.41
1:WK:190:GLN:CG	1:WL:217:GLY:HA3	2.51	0.41
1:WK:190:GLN:HA	1:WL:217:GLY:O	2.20	0.41
2:A:18:LEU:HD12	2:A:18:LEU:HA	1.91	0.41
2:D:7:MET:HE1	3:E:236:ILE:HD11	2.01	0.41
4:F:217:ILE:HD13	4:F:217:ILE:HA	1.89	0.41
5:M:3:ALA:HA	1:AC:372:ILE:HD13	2.02	0.41
5:N:4:ILE:HG12	1:7:372:ILE:HG21	2.02	0.41
1:AJ:296:ARG:HG2	1:AJ:296:ARG:NH1	2.35	0.41
1:AN:296:ARG:HG2	1:AN:296:ARG:NH1	2.35	0.41
1:AP:421:GLY:O	1:AP:426:ARG:NH2	2.51	0.41
1:UI:98:LEU:HD12	1:UI:146:THR:HG1	1.83	0.41
1:UN:94:HIS:HB2	1:UN:146:THR:HG21	1.97	0.41
1:WG:214:ASP:OD1	1:WG:218:HIS:N	2.51	0.41
1:WH:145:GLU:O	1:WH:146:THR:C	2.57	0.41
1:WI:135:ALA:O	1:WI:139:GLU:HG2	2.21	0.41
1:WT:128:GLU:HG3	1:WU:126:PHE:CE2	2.55	0.41
4:G:171:LEU:HD23	4:H:95:PHE:CZ	2.55	0.41
4:G:194:LEU:HD23	4:G:194:LEU:HA	1.83	0.41
4:I:52:THR:HG23	5:O:97:GLN:HE21	1.85	0.41
5:M:7:ILE:CD1	1:AC:370:ARG:HE	2.24	0.41
6:S:16:LEU:HD11	6:S:120:LEU:HG	2.02	0.41
1:AE:290:LYS:HE3	1:AE:290:LYS:HB2	1.93	0.41
1:AH:296:ARG:HG2	1:AH:296:ARG:NH1	2.35	0.41
1:WG:193:ALA:HB1	1:WH:213:VAL:CG1	2.48	0.41
1:WI:144:ILE:O	1:WI:147:LEU:HB2	2.20	0.41
1:WI:181:GLU:CB	1:WI:184:ARG:CG	2.85	0.41
1:WL:140:LEU:O	1:WL:144:ILE:HG13	2.20	0.41
1:WL:190:GLN:HG2	1:WM:216:SER:O	2.21	0.41
1:WM:140:LEU:O	1:WM:144:ILE:HG13	2.20	0.41
1:WO:181:GLU:CB	1:WO:184:ARG:CG	2.85	0.41
1:WT:165:PHE:HZ	4:G:144:GLU:HG2	1.86	0.41
1:WW:131:ASN:HA	1:WW:134:ARG:HD3	2.01	0.41
4:F:194:LEU:HD12	4:G:220:PRO:HG2	2.03	0.41
1:AE:235:LEU:HB3	1:AF:244:ARG:NH2	2.36	0.41
1:UN:214:ASP:OD2	1:UN:218:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WA:168:GLU:OE1	1:WW:169:GLN:HB2	2.21	0.41
1:WH:166:VAL:HG11	4:J:147:LEU:HD11	2.01	0.41
1:WL:196:HIS:HB3	1:WM:211:THR:HG21	2.03	0.41
1:WM:181:GLU:CB	1:WM:184:ARG:CG	2.85	0.41
1:WQ:186:LEU:HD23	1:WQ:186:LEU:HA	1.92	0.41
1:WR:165:PHE:CE2	4:F:153:LEU:HD23	2.55	0.41
2:A:52:ILE:N	2:A:52:ILE:HD12	2.35	0.41
2:B:51:PHE:CE2	2:B:55:ILE:HD11	2.56	0.41
3:E:231:ALA:O	3:E:234:PRO:HD2	2.21	0.41
4:F:175:VAL:O	4:F:179:LEU:HG	2.20	0.41
4:G:234:LEU:HD12	4:G:234:LEU:HA	1.92	0.41
1:8:296:ARG:HG2	1:8:296:ARG:NH1	2.35	0.41
1:9:235:LEU:HB3	1:0:244:ARG:NH2	2.36	0.41
1:UJ:263:ASP:OD2	1:UJ:267:HIS:HB2	2.20	0.41
1:WA:213:VAL:HG11	1:WW:193:ALA:CB	2.48	0.41
1:WB:190:GLN:CG	1:WC:216:SER:O	2.67	0.41
1:WG:121:PHE:CE2	1:WG:123:ILE:HA	2.55	0.41
1:WI:147:LEU:O	1:WI:148:GLY:C	2.60	0.41
1:WK:181:GLU:CB	1:WK:184:ARG:CG	2.85	0.41
1:WO:186:LEU:HA	1:WO:190:GLN:OE1	2.21	0.41
1:WP:190:GLN:C	1:WP:192:SER:N	2.73	0.41
1:WQ:164:LEU:CD2	4:F:149:LEU:HD13	2.51	0.41
1:WQ:164:LEU:HD21	4:F:149:LEU:HD13	2.02	0.41
1:WU:163:SER:O	1:WU:166:VAL:HG22	2.20	0.41
1:WU:193:ALA:HB1	1:WV:213:VAL:HG11	2.03	0.41
1:WV:145:GLU:O	1:WV:147:LEU:N	2.54	0.41
2:B:39:GLN:NE2	2:B:49:LEU:HD12	2.31	0.41
2:B:59:PHE:CZ	4:G:198:LEU:HD21	2.55	0.41
4:G:171:LEU:O	4:G:175:VAL:HG23	2.21	0.41
4:G:204:LEU:HD11	4:G:217:ILE:HD12	2.01	0.41
4:I:187:PHE:CD2	4:J:224:MET:HB2	2.56	0.41
4:J:213:PRO:HA	4:J:214:PRO:HD3	1.91	0.41
6:Q:60:THR:O	1:AO:297:GLN:NE2	2.52	0.41
6:R:29:ASN:HD22	6:R:38:TYR:HE2	1.68	0.41
6:U:72:HIS:CE1	1:1:366:TYR:O	2.74	0.41
7:Z:126:MET:O	7:Z:129:THR:HG22	2.21	0.41
1:6:235:LEU:HB3	1:7:244:ARG:NH2	2.36	0.41
1:8:235:LEU:HB3	1:9:244:ARG:NH2	2.36	0.41
1:9:290:LYS:HE3	1:9:290:LYS:HB2	1.93	0.41
1:9:421:GLY:O	1:9:426:ARG:NH2	2.51	0.41
1:AB:235:LEU:HB3	1:AC:244:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:235:LEU:HB3	1:AI:244:ARG:NH2	2.36	0.41
1:AI:296:ARG:HG2	1:AI:296:ARG:NH1	2.35	0.41
1:AK:235:LEU:HB3	1:AL:244:ARG:NH2	2.36	0.41
1:AO:421:GLY:O	1:AO:426:ARG:NH2	2.51	0.41
1:WE:197:LEU:HA	1:WF:175:SER:OG	2.21	0.41
1:WH:149:PRO:CD	1:WH:190:GLN:HE22	2.33	0.41
1:WK:167:ARG:CB	3:E:156:THR:HG22	2.50	0.41
1:WU:145:GLU:O	1:WU:147:LEU:N	2.54	0.41
2:D:35:ILE:HD13	2:D:35:ILE:HA	1.98	0.41
6:U:68:THR:HG22	1:1:294:ARG:CD	2.36	0.41
1:UL:69:GLN:NE2	1:WH:182:PRO:CG	2.84	0.40
1:WJ:165:PHE:N	4:J:152:ARG:HH22	2.18	0.40
1:WJ:181:GLU:O	1:WJ:182:PRO:C	2.60	0.40
1:WK:181:GLU:O	1:WK:182:PRO:C	2.60	0.40
1:WM:181:GLU:O	1:WM:182:PRO:C	2.60	0.40
1:WS:115:LEU:HA	1:WS:118:GLN:OE1	2.21	0.40
1:WT:181:GLU:CB	1:WT:184:ARG:CG	2.85	0.40
1:WU:181:GLU:O	1:WU:182:PRO:C	2.60	0.40
2:D:77:VAL:HG11	4:J:225:LEU:HD11	2.03	0.40
4:F:187:PHE:CZ	4:F:191:ILE:HD11	2.56	0.40
4:H:189:ILE:HD13	4:H:235:LEU:HD11	2.03	0.40
5:O:7:ILE:O	5:O:11:ILE:HG23	2.21	0.40
5:P:69:ASN:OD1	7:V:112:TYR:OH	2.11	0.40
1:3:290:LYS:HE3	1:3:290:LYS:HB2	1.93	0.40
1:5:235:LEU:HB3	1:6:244:ARG:NH2	2.36	0.40
1:AO:425:LYS:HE3	1:AO:425:LYS:HB3	1.96	0.40
1:UI:98:LEU:CD1	1:UI:146:THR:HG1	2.32	0.40
1:UJ:88:VAL:O	1:UJ:89:PRO:C	2.60	0.40
1:UK:214:ASP:OD2	1:UK:218:HIS:HB2	2.20	0.40
1:UL:51:TYR:HB2	1:UL:78:ARG:CZ	2.51	0.40
1:UN:102:GLN:CG	1:UN:193:ALA:HB2	2.49	0.40
1:WC:125:GLN:O	1:WC:128:GLU:HG2	2.20	0.40
1:WD:145:GLU:C	1:WD:147:LEU:N	2.74	0.40
1:WL:181:GLU:O	1:WL:182:PRO:C	2.60	0.40
1:WM:193:ALA:CB	1:WN:213:VAL:CG1	2.94	0.40
1:WR:193:ALA:HB1	1:WS:213:VAL:HG21	2.03	0.40
3:E:4:VAL:HB	5:P:44:ARG:HH12	1.86	0.40
4:G:75:ARG:HB2	4:G:83:ALA:CB	2.52	0.40
5:K:68:LEU:H	5:K:68:LEU:HD12	1.85	0.40
6:Q:96:ASP:N	6:Q:96:ASP:OD1	2.53	0.40
6:Q:128:LYS:HD2	6:Q:128:LYS:HA	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:235:LEU:HB3	1:4:244:ARG:NH2	2.36	0.40
1:AA:235:LEU:HB3	1:AB:244:ARG:NH2	2.36	0.40
1:AH:360:ARG:NH1	1:AH:362:GLU:OE1	2.55	0.40
1:AN:421:GLY:O	1:AN:426:ARG:NH2	2.51	0.40
1:UI:52:ARG:O	1:UI:88:VAL:N	2.38	0.40
1:UI:88:VAL:O	1:UI:89:PRO:C	2.60	0.40
1:UJ:51:TYR:HB2	1:UJ:78:ARG:CZ	2.51	0.40
1:UJ:54:LEU:HG	1:UJ:55:PHE:CD2	2.57	0.40
1:UJ:261:LEU:HG	1:UJ:269:LEU:HD12	2.04	0.40
1:UM:212:LEU:HG	1:UM:220:LEU:HD12	2.04	0.40
1:UM:214:ASP:OD2	1:UM:218:HIS:HB2	2.20	0.40
1:UO:54:LEU:HG	1:UO:55:PHE:CD2	2.57	0.40
1:WC:131:ASN:O	1:WC:132:TYR:C	2.60	0.40
1:WQ:181:GLU:O	1:WQ:182:PRO:C	2.60	0.40
1:WR:181:GLU:O	1:WR:182:PRO:C	2.60	0.40
1:WT:181:GLU:O	1:WT:182:PRO:C	2.60	0.40
2:A:15:LYS:HE2	2:A:15:LYS:HB3	1.88	0.40
2:A:50:SER:OG	2:B:46:GLU:OE2	2.25	0.40
2:B:84:LEU:HD22	4:H:185:ILE:HG23	2.03	0.40
2:C:49:LEU:HD23	2:C:49:LEU:HA	1.94	0.40
4:F:153:LEU:HD23	4:F:153:LEU:HA	1.91	0.40
4:H:71:PHE:HD1	4:H:71:PHE:HA	1.80	0.40
4:H:189:ILE:O	4:H:192:PRO:HD2	2.21	0.40
4:I:132:GLN:HB2	4:I:133:PRO:HD3	2.04	0.40
1:AB:360:ARG:NH1	1:AB:362:GLU:OE1	2.55	0.40
1:AG:360:ARG:NH1	1:AG:362:GLU:OE1	2.55	0.40
1:AK:360:ARG:NH1	1:AK:362:GLU:OE1	2.55	0.40
1:AO:360:ARG:NH1	1:AO:362:GLU:OE1	2.55	0.40
1:UM:51:TYR:HB2	1:UM:78:ARG:CZ	2.52	0.40
1:UM:54:LEU:HG	1:UM:55:PHE:CD2	2.57	0.40
1:UO:88:VAL:O	1:UO:89:PRO:C	2.60	0.40
1:WD:129:GLN:O	1:WD:130:VAL:C	2.60	0.40
1:WD:193:ALA:HB1	1:WE:213:VAL:CG2	2.50	0.40
1:WF:124:SER:O	1:WF:125:GLN:C	2.59	0.40
1:WG:120:LYS:HA	1:WG:120:LYS:HE2	2.03	0.40
1:WP:181:GLU:O	1:WP:182:PRO:C	2.60	0.40
1:WR:139:GLU:HB3	1:WS:156:HIS:HE1	1.87	0.40
1:WR:181:GLU:CB	1:WR:184:ARG:CG	2.85	0.40
1:WS:197:LEU:HA	1:WT:175:SER:CB	2.52	0.40
5:L:4:ILE:HA	1:AI:372:ILE:HD12	2.03	0.40
5:L:7:ILE:O	5:L:11:ILE:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:7:ILE:HB	1:6:278:THR:HG21	2.02	0.40
1:AD:360:ARG:NH1	1:AD:362:GLU:OE1	2.55	0.40
1:AE:360:ARG:NH1	1:AE:362:GLU:OE1	2.55	0.40
1:AN:360:ARG:NH1	1:AN:362:GLU:OE1	2.55	0.40
1:WC:163:SER:OG	1:WC:166:VAL:O	2.38	0.40
1:WF:120:LYS:HB3	1:WF:121:PHE:H	1.66	0.40
1:WG:124:SER:O	1:WG:127:SER:N	2.55	0.40
1:WG:181:GLU:O	1:WG:182:PRO:C	2.60	0.40
1:WG:187:ASP:HB3	1:WG:190:GLN:H	1.87	0.40
1:WH:181:GLU:O	1:WH:182:PRO:C	2.60	0.40
1:WJ:144:ILE:O	1:WJ:147:LEU:HB2	2.21	0.40
1:WL:191:ILE:HG23	1:WL:212:LEU:HD23	2.03	0.40
1:WN:181:GLU:O	1:WN:182:PRO:C	2.60	0.40
1:WQ:214:ASP:OD1	1:WQ:218:HIS:N	2.49	0.40
1:WW:181:GLU:O	1:WW:182:PRO:C	2.60	0.40
3:E:6:SER:OG	3:E:7:GLU:N	2.55	0.40
3:E:146:LEU:HD23	3:E:146:LEU:HA	1.80	0.40
5:M:3:ALA:C	1:AC:372:ILE:HD12	2.42	0.40
5:P:77:LYS:HE2	7:V:7:PHE:HB3	2.04	0.40
6:U:72:HIS:HA	1:2:295:SER:HB3	2.02	0.40
7:Y:119:LEU:HD12	7:Y:119:LEU:HA	1.84	0.40
1:AD:235:LEU:HB3	1:AE:244:ARG:NH2	2.36	0.40
1:AN:235:LEU:HB3	1:AO:244:ARG:NH2	2.36	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	0	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	1	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	3	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	4	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	5	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	6	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	7	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	8	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	9	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AA	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AB	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AC	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AD	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AE	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AF	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AG	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AH	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AI	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AJ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AK	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AL	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AM	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AN	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AO	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AP	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AQ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	10	39
1	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	27
1	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	19
1	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	45
1	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	19
1	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	23
1	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	27
1	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	34
1	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	30
1	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	14
1	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	13	44
1	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	25
1	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	28
1	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	28
1	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	21
1	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	32
1	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	17
1	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	22
1	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	14
1	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	16
1	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	14
1	WU	110/560 (20%)	101 (92%)	8 (7%)	1 (1%)	14	45
1	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	33
1	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	19
1	b	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
1	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
1	d	18/560 (3%)	18 (100%)	0	0	100	100
1	e	14/560 (2%)	14 (100%)	0	0	100	100
1	f	19/560 (3%)	19 (100%)	0	0	100	100
1	g	14/560 (2%)	12 (86%)	2 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	19/560 (3%)	19 (100%)	0	0	100	100
1	i	14/560 (2%)	14 (100%)	0	0	100	100
1	j	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
1	k	14/560 (2%)	14 (100%)	0	0	100	100
1	l	19/560 (3%)	19 (100%)	0	0	100	100
1	t	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	u	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	v	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	w	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	x	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	y	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	z	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
2	A	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
2	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
2	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
2	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
3	E	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	5	29
4	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
4	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	44
4	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
4	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	58
4	J	207/245 (84%)	201 (97%)	4 (2%)	2 (1%)	13	44
5	K	55/104 (53%)	53 (96%)	2 (4%)	0	100	100
5	L	87/104 (84%)	87 (100%)	0	0	100	100
5	M	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
5	N	89/104 (86%)	89 (100%)	0	0	100	100
5	O	89/104 (86%)	89 (100%)	0	0	100	100
5	P	88/104 (85%)	88 (100%)	0	0	100	100
6	Q	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
6	R	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
6	S	119/138 (86%)	116 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
6	U	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
7	V	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
7	W	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
7	X	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
7	Y	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
7	Z	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	49
7	a	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
All	All	12674/46523 (27%)	12203 (96%)	362 (3%)	109 (1%)	17	45

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	WO	168	GLU
1	WR	123	ILE
1	WR	165	PHE
1	WR	166	VAL
1	WS	187	ASP
3	E	188	LEU
3	E	190	VAL
4	J	83	ALA
1	WB	148	GLY
1	WB	163	SER
1	WD	146	THR
1	WD	148	GLY
1	WF	118	GLN
1	WI	146	THR
1	WI	160	PRO
1	WI	170	LYS
1	WK	166	VAL
1	WM	148	GLY
1	WN	146	THR
1	WN	148	GLY
1	WP	146	THR
1	WQ	146	THR
1	WQ	148	GLY
1	WQ	169	GLN
1	WS	146	THR
1	WT	146	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	WT	162	PRO
1	WW	146	THR
1	WW	148	GLY
3	E	167	ASN
3	E	213	ILE
4	G	83	ALA
4	I	160	GLN
1	UI	162	PRO
1	UJ	162	PRO
1	UK	162	PRO
1	UL	162	PRO
1	UM	162	PRO
1	UN	162	PRO
1	UO	162	PRO
1	UP	162	PRO
1	WB	146	THR
1	WB	164	LEU
1	WD	118	GLN
1	WE	160	PRO
1	WE	162	PRO
1	WI	148	GLY
1	WP	148	GLY
1	WS	118	GLN
1	WS	169	GLN
1	WT	165	PHE
1	WW	118	GLN
1	WW	168	GLU
3	E	189	PRO
1	UI	163	SER
1	UJ	163	SER
1	UK	163	SER
1	UL	163	SER
1	UM	163	SER
1	UN	163	SER
1	UO	163	SER
1	UP	163	SER
1	WA	182	PRO
1	WB	182	PRO
1	WD	165	PHE
1	WD	182	PRO
1	WE	182	PRO
1	WF	182	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	WG	182	PRO
1	WH	165	PHE
1	WH	182	PRO
1	WI	169	GLN
1	WI	182	PRO
1	WJ	182	PRO
1	WK	182	PRO
1	WL	182	PRO
1	WM	182	PRO
1	WN	182	PRO
1	WO	182	PRO
1	WP	182	PRO
1	WQ	182	PRO
1	WR	112	GLY
1	WR	182	PRO
1	WS	182	PRO
1	WT	182	PRO
1	WU	182	PRO
1	WV	148	GLY
1	WV	182	PRO
1	WW	182	PRO
1	WK	168	GLU
1	WR	121	PHE
1	WT	163	SER
4	G	162	PRO
1	WC	182	PRO
1	WE	221	THR
1	WG	163	SER
3	E	187	ALA
7	Z	58	ALA
1	WA	160	PRO
1	WF	162	PRO
1	WL	148	GLY
1	WS	148	GLY
1	WT	148	GLY
1	WA	148	GLY
1	WP	123	ILE
1	WR	148	GLY
1	WP	160	PRO
1	WT	161	LYS
4	J	229	VAL



### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	1	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	2	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	3	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	4	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	5	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	6	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	7	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	8	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	9	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AA	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AB	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AC	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AD	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AE	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AF	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AG	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AH	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AI	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AJ	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AK	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AL	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AM	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AN	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AO	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AP	141/467 (30%)	134 (95%)	7 (5%)	20	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AQ	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	UI	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UJ	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UK	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UL	128/467 (27%)	122 (95%)	6 (5%)	22	46
1	UM	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UN	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UO	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UP	128/467 (27%)	122 (95%)	6 (5%)	22	46
1	WA	95/467 (20%)	91 (96%)	4 (4%)	25	49
1	WB	93/467 (20%)	87 (94%)	6 (6%)	14	39
1	WC	91/467 (20%)	83 (91%)	8 (9%)	8	30
1	WD	92/467 (20%)	88 (96%)	4 (4%)	25	49
1	WE	94/467 (20%)	87 (93%)	7 (7%)	11	35
1	WF	93/467 (20%)	86 (92%)	7 (8%)	11	35
1	WG	94/467 (20%)	87 (93%)	7 (7%)	11	35
1	WH	79/467 (17%)	75 (95%)	4 (5%)	20	45
1	WI	79/467 (17%)	73 (92%)	6 (8%)	11	34
1	WJ	83/467 (18%)	79 (95%)	4 (5%)	21	46
1	WK	82/467 (18%)	77 (94%)	5 (6%)	15	41
1	WL	69/467 (15%)	66 (96%)	3 (4%)	25	49
1	WM	66/467 (14%)	65 (98%)	1 (2%)	60	74
1	WN	68/467 (15%)	66 (97%)	2 (3%)	37	58
1	WO	80/467 (17%)	76 (95%)	4 (5%)	20	45
1	WP	83/467 (18%)	77 (93%)	6 (7%)	12	36
1	WQ	93/467 (20%)	91 (98%)	2 (2%)	47	64
1	WR	93/467 (20%)	86 (92%)	7 (8%)	11	35
1	WS	93/467 (20%)	87 (94%)	6 (6%)	14	39
1	WT	93/467 (20%)	86 (92%)	7 (8%)	11	35
1	WU	94/467 (20%)	90 (96%)	4 (4%)	25	49
1	WV	92/467 (20%)	83 (90%)	9 (10%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	WW	93/467 (20%)	85 (91%)	8 (9%)	8	31
1	b	8/467 (2%)	8 (100%)	0	100	100
1	c	11/467 (2%)	10 (91%)	1 (9%)	7	28
1	d	14/467 (3%)	12 (86%)	2 (14%)	2	16
1	e	11/467 (2%)	11 (100%)	0	100	100
1	f	15/467 (3%)	15 (100%)	0	100	100
1	g	11/467 (2%)	11 (100%)	0	100	100
1	h	15/467 (3%)	15 (100%)	0	100	100
1	i	11/467 (2%)	11 (100%)	0	100	100
1	j	14/467 (3%)	13 (93%)	1 (7%)	12	36
1	k	11/467 (2%)	11 (100%)	0	100	100
1	l	15/467 (3%)	14 (93%)	1 (7%)	13	38
1	t	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	u	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	v	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	w	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	x	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	y	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	z	141/467 (30%)	134 (95%)	7 (5%)	20	45
2	A	74/74 (100%)	73 (99%)	1 (1%)	62	75
2	B	74/74 (100%)	73 (99%)	1 (1%)	62	75
2	C	74/74 (100%)	74 (100%)	0	100	100
2	D	74/74 (100%)	73 (99%)	1 (1%)	62	75
3	E	210/221 (95%)	204 (97%)	6 (3%)	37	58
4	F	177/204 (87%)	170 (96%)	7 (4%)	27	50
4	G	179/204 (88%)	173 (97%)	6 (3%)	32	55
4	H	178/204 (87%)	173 (97%)	5 (3%)	38	59
4	I	178/204 (87%)	172 (97%)	6 (3%)	32	55
4	J	179/204 (88%)	175 (98%)	4 (2%)	47	64
5	K	45/79 (57%)	40 (89%)	5 (11%)	5	21
5	L	68/79 (86%)	64 (94%)	4 (6%)	16	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	70/79 (89%)	65 (93%)	5 (7%)	12	36
5	N	70/79 (89%)	66 (94%)	4 (6%)	17	43
5	O	70/79 (89%)	66 (94%)	4 (6%)	17	43
5	P	69/79 (87%)	65 (94%)	4 (6%)	17	42
6	Q	110/113 (97%)	106 (96%)	4 (4%)	30	54
6	R	101/113 (89%)	99 (98%)	2 (2%)	50	68
6	S	103/113 (91%)	96 (93%)	7 (7%)	13	38
6	T	104/113 (92%)	102 (98%)	2 (2%)	52	69
6	U	102/113 (90%)	96 (94%)	6 (6%)	16	41
7	V	104/105 (99%)	104 (100%)	0	100	100
7	W	104/105 (99%)	103 (99%)	1 (1%)	73	80
7	X	104/105 (99%)	104 (100%)	0	100	100
7	Y	104/105 (99%)	102 (98%)	2 (2%)	52	69
7	Z	104/105 (99%)	101 (97%)	3 (3%)	37	58
7	a	104/105 (99%)	100 (96%)	4 (4%)	28	52
All	All	10879/38698 (28%)	10379 (95%)	500 (5%)	25	47

All (500) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UI	98	LEU
1	UI	127	SER
1	UI	154	ARG
1	UI	159	MET
1	UI	165	PHE
1	UJ	98	LEU
1	UJ	127	SER
1	UJ	154	ARG
1	UJ	159	MET
1	UJ	165	PHE
1	UK	98	LEU
1	UK	127	SER
1	UK	154	ARG
1	UK	159	MET
1	UK	165	PHE
1	UL	98	LEU
1	UL	127	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	UL	154	ARG
1	UL	159	MET
1	UL	165	PHE
1	UL	167	ARG
1	UM	98	LEU
1	UM	127	SER
1	UM	154	ARG
1	UM	159	MET
1	UM	165	PHE
1	UN	98	LEU
1	UN	127	SER
1	UN	154	ARG
1	UN	159	MET
1	UN	165	PHE
1	UO	98	LEU
1	UO	127	SER
1	UO	154	ARG
1	UO	159	MET
1	UO	165	PHE
1	UP	98	LEU
1	UP	127	SER
1	UP	154	ARG
1	UP	159	MET
1	UP	165	PHE
1	UP	167	ARG
1	WA	114	GLU
1	WA	128	GLU
1	WA	167	ARG
1	WA	170	LYS
1	WB	121	PHE
1	WB	128	GLU
1	WB	134	ARG
1	WB	137	GLU
1	WB	164	LEU
1	WB	169	GLN
1	WC	115	LEU
1	WC	120	LYS
1	WC	128	GLU
1	WC	134	ARG
1	WC	164	LEU
1	WC	166	VAL
1	WC	168	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	WC	170	LYS
1	WD	114	GLU
1	WD	115	LEU
1	WD	167	ARG
1	WD	170	LYS
1	WE	114	GLU
1	WE	128	GLU
1	WE	134	ARG
1	WE	160	PRO
1	WE	161	LYS
1	WE	164	LEU
1	WE	170	LYS
1	WF	111	VAL
1	WF	113	PHE
1	WF	120	LYS
1	WF	121	PHE
1	WF	128	GLU
1	WF	134	ARG
1	WF	142	ARG
1	WG	111	VAL
1	WG	114	GLU
1	WG	115	LEU
1	WG	120	LYS
1	WG	134	ARG
1	WG	164	LEU
1	WG	187	ASP
1	WH	128	GLU
1	WH	134	ARG
1	WH	168	GLU
1	WH	221	THR
1	WI	128	GLU
1	WI	134	ARG
1	WI	165	PHE
1	WI	168	GLU
1	WI	169	GLN
1	WI	170	LYS
1	WJ	128	GLU
1	WJ	165	PHE
1	WJ	167	ARG
1	WJ	169	GLN
1	WK	164	LEU
1	WK	165	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	WK	167	ARG
1	WK	170	LYS
1	WK	187	ASP
1	WL	128	GLU
1	WL	159	MET
1	WL	221	THR
1	WM	221	THR
1	WN	128	GLU
1	WN	221	THR
1	WO	128	GLU
1	WO	169	GLN
1	WO	170	LYS
1	WO	221	THR
1	WP	128	GLU
1	WP	154	ARG
1	WP	161	LYS
1	WP	165	PHE
1	WP	169	GLN
1	WP	170	LYS
1	WQ	114	GLU
1	WQ	128	GLU
1	WR	114	GLU
1	WR	117	ASP
1	WR	119	GLU
1	WR	128	GLU
1	WR	164	LEU
1	WR	166	VAL
1	WR	169	GLN
1	WS	114	GLU
1	WS	128	GLU
1	WS	134	ARG
1	WS	170	LYS
1	WS	187	ASP
1	WS	221	THR
1	WT	119	GLU
1	WT	123	ILE
1	WT	128	GLU
1	WT	134	ARG
1	WT	159	MET
1	WT	165	PHE
1	WT	167	ARG
1	WU	114	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	WU	128	GLU
1	WU	134	ARG
1	WU	161	LYS
1	WV	114	GLU
1	WV	117	ASP
1	WV	120	LYS
1	WV	128	GLU
1	WV	134	ARG
1	WV	164	LEU
1	WV	166	VAL
1	WV	169	GLN
1	WV	187	ASP
1	WW	114	GLU
1	WW	115	LEU
1	WW	128	GLU
1	WW	134	ARG
1	WW	167	ARG
1	WW	168	GLU
1	WW	169	GLN
1	WW	221	THR
2	A	7	MET
2	B	47	MET
2	D	9	MET
3	E	36	ARG
3	E	86	PHE
3	E	185	MET
3	E	214	PHE
3	E	227	MET
3	E	229	MET
4	F	38	TRP
4	F	123	MET
4	F	129	LYS
4	F	155	ASN
4	F	160	GLN
4	F	190	PHE
4	F	213	PRO
4	G	75	ARG
4	G	106	ASP
4	G	116	PHE
4	G	140	ARG
4	G	160	GLN
4	G	162	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	H	143	ARG
4	H	152	ARG
4	H	177	SER
4	H	187	PHE
4	H	190	PHE
4	I	113	TYR
4	I	143	ARG
4	I	187	PHE
4	I	205	MET
4	I	238	SER
4	I	241	GLN
4	J	117	SER
4	J	190	PHE
4	J	224	MET
4	J	230	ASP
5	K	15	GLN
5	K	19	MET
5	K	74	ASP
5	K	79	SER
5	K	101	SER
5	L	15	GLN
5	L	19	MET
5	L	75	MET
5	L	84	MET
5	M	7	ILE
5	M	11	ILE
5	M	14	LEU
5	M	15	GLN
5	M	70	ASP
5	N	15	GLN
5	N	19	MET
5	N	33	SER
5	N	81	SER
5	O	15	GLN
5	O	19	MET
5	O	101	SER
5	O	102	MET
5	P	15	GLN
5	P	19	MET
5	P	57	GLU
5	P	91	LYS
6	Q	34	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Q	101	ASP
6	Q	113	SER
6	Q	125	SER
6	R	47	SER
6	R	55	ARG
6	S	48	GLU
6	S	65	LEU
6	S	69	SER
6	S	71	HIS
6	S	72	HIS
6	S	91	ASP
6	S	128	LYS
6	T	47	SER
6	T	76	GLN
6	U	4	ARG
6	U	18	LEU
6	U	65	LEU
6	U	104	ARG
6	U	113	SER
6	U	125	SER
7	W	123	LYS
7	Y	30	ASN
7	Y	120	ASN
7	Z	20	ARG
7	Z	52	ASP
7	Z	84	LEU
7	a	86	ASP
7	a	88	ASN
7	a	125	MET
7	a	127	LEU
1	c	324	ASN
1	d	318	ASN
1	d	319	GLN
1	j	319	GLN
1	l	318	ASN
1	t	274	ASN
1	t	294	ARG
1	t	359	GLN
1	t	377	MET
1	t	381	ASP
1	t	417	ARG
1	t	424	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	u	274	ASN
1	u	294	ARG
1	u	359	GLN
1	u	377	MET
1	u	381	ASP
1	u	417	ARG
1	u	424	ASP
1	v	274	ASN
1	v	294	ARG
1	v	359	GLN
1	v	377	MET
1	v	381	ASP
1	v	417	ARG
1	v	424	ASP
1	w	274	ASN
1	w	294	ARG
1	w	359	GLN
1	w	377	MET
1	w	381	ASP
1	w	417	ARG
1	w	424	ASP
1	x	274	ASN
1	x	294	ARG
1	x	359	GLN
1	x	377	MET
1	x	381	ASP
1	x	417	ARG
1	x	424	ASP
1	y	274	ASN
1	y	294	ARG
1	y	359	GLN
1	y	377	MET
1	y	381	ASP
1	y	417	ARG
1	y	424	ASP
1	z	274	ASN
1	z	294	ARG
1	z	359	GLN
1	z	377	MET
1	z	381	ASP
1	z	417	ARG
1	z	424	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	274	ASN
1	1	294	ARG
1	1	359	GLN
1	1	377	MET
1	1	381	ASP
1	1	417	ARG
1	1	424	ASP
1	2	274	ASN
1	2	294	ARG
1	2	359	GLN
1	2	377	MET
1	2	381	ASP
1	2	417	ARG
1	2	424	ASP
1	3	274	ASN
1	3	294	ARG
1	3	359	GLN
1	3	377	MET
1	3	381	ASP
1	3	417	ARG
1	3	424	ASP
1	4	274	ASN
1	4	294	ARG
1	4	359	GLN
1	4	377	MET
1	4	381	ASP
1	4	417	ARG
1	4	424	ASP
1	5	274	ASN
1	5	294	ARG
1	5	359	GLN
1	5	377	MET
1	5	381	ASP
1	5	417	ARG
1	5	424	ASP
1	6	274	ASN
1	6	294	ARG
1	6	359	GLN
1	6	377	MET
1	6	381	ASP
1	6	417	ARG
1	6	424	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	7	274	ASN
1	7	294	ARG
1	7	359	GLN
1	7	377	MET
1	7	381	ASP
1	7	417	ARG
1	7	424	ASP
1	8	274	ASN
1	8	294	ARG
1	8	359	GLN
1	8	377	MET
1	8	381	ASP
1	8	417	ARG
1	8	424	ASP
1	9	274	ASN
1	9	294	ARG
1	9	359	GLN
1	9	377	MET
1	9	381	ASP
1	9	417	ARG
1	9	424	ASP
1	0	274	ASN
1	0	294	ARG
1	0	359	GLN
1	0	377	MET
1	0	381	ASP
1	0	417	ARG
1	0	424	ASP
1	AA	274	ASN
1	AA	294	ARG
1	AA	359	GLN
1	AA	377	MET
1	AA	381	ASP
1	AA	417	ARG
1	AA	424	ASP
1	AB	274	ASN
1	AB	294	ARG
1	AB	359	GLN
1	AB	377	MET
1	AB	381	ASP
1	AB	417	ARG
1	AB	424	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AC	274	ASN
1	AC	294	ARG
1	AC	359	GLN
1	AC	377	MET
1	AC	381	ASP
1	AC	417	ARG
1	AC	424	ASP
1	AD	274	ASN
1	AD	294	ARG
1	AD	359	GLN
1	AD	377	MET
1	AD	381	ASP
1	AD	417	ARG
1	AD	424	ASP
1	AE	274	ASN
1	AE	294	ARG
1	AE	359	GLN
1	AE	377	MET
1	AE	381	ASP
1	AE	417	ARG
1	AE	424	ASP
1	AF	274	ASN
1	AF	294	ARG
1	AF	359	GLN
1	AF	377	MET
1	AF	381	ASP
1	AF	417	ARG
1	AF	424	ASP
1	AG	274	ASN
1	AG	294	ARG
1	AG	359	GLN
1	AG	377	MET
1	AG	381	ASP
1	AG	417	ARG
1	AG	424	ASP
1	AH	274	ASN
1	AH	294	ARG
1	AH	359	GLN
1	AH	377	MET
1	AH	381	ASP
1	AH	417	ARG
1	AH	424	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AI	274	ASN
1	AI	294	ARG
1	AI	359	GLN
1	AI	377	MET
1	AI	381	ASP
1	AI	417	ARG
1	AI	424	ASP
1	AJ	274	ASN
1	AJ	294	ARG
1	AJ	359	GLN
1	AJ	377	MET
1	AJ	381	ASP
1	AJ	417	ARG
1	AJ	424	ASP
1	AK	274	ASN
1	AK	294	ARG
1	AK	359	GLN
1	AK	377	MET
1	AK	381	ASP
1	AK	417	ARG
1	AK	424	ASP
1	AL	274	ASN
1	AL	294	ARG
1	AL	359	GLN
1	AL	377	MET
1	AL	381	ASP
1	AL	417	ARG
1	AL	424	ASP
1	AM	274	ASN
1	AM	294	ARG
1	AM	359	GLN
1	AM	377	MET
1	AM	381	ASP
1	AM	417	ARG
1	AM	424	ASP
1	AN	274	ASN
1	AN	294	ARG
1	AN	359	GLN
1	AN	377	MET
1	AN	381	ASP
1	AN	417	ARG
1	AN	424	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AO	274	ASN
1	AO	294	ARG
1	AO	359	GLN
1	AO	377	MET
1	AO	381	ASP
1	AO	417	ARG
1	AO	424	ASP
1	AP	274	ASN
1	AP	294	ARG
1	AP	359	GLN
1	AP	377	MET
1	AP	381	ASP
1	AP	417	ARG
1	AP	424	ASP
1	AQ	274	ASN
1	AQ	294	ARG
1	AQ	359	GLN
1	AQ	377	MET
1	AQ	381	ASP
1	AQ	417	ARG
1	AQ	424	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	UI	196	HIS
1	UJ	245	HIS
1	UK	196	HIS
1	UL	69	GLN
1	UL	196	HIS
1	UM	196	HIS
1	UN	69	GLN
1	UN	196	HIS
1	UO	196	HIS
1	UP	196	HIS
1	WB	169	GLN
1	WE	156	HIS
1	WE	209	ASN
1	WF	118	GLN
1	WH	156	HIS
1	WI	129	GLN
1	WI	156	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	WJ	169	GLN
1	WJ	209	ASN
1	WO	209	ASN
1	WP	209	ASN
1	WV	169	GLN
1	WW	169	GLN
2	D	39	GLN
3	E	162	ASN
3	E	182	ASN
3	E	205	ASN
4	F	119	GLN
4	F	141	GLN
4	H	36	GLN
4	H	160	GLN
4	H	233	GLN
4	I	160	GLN
4	I	184	GLN
4	J	114	GLN
4	J	155	ASN
5	K	103	GLN
5	L	15	GLN
5	L	90	ASN
5	M	83	GLN
5	M	103	GLN
5	N	87	GLN
5	O	39	HIS
5	O	55	GLN
5	O	97	GLN
5	P	76	GLN
6	Q	17	ASN
6	Q	23	GLN
6	R	23	GLN
6	R	29	ASN
6	R	92	GLN
6	R	117	GLN
6	S	32	ASN
6	S	76	GLN
6	S	92	GLN
6	S	135	GLN
6	T	17	ASN
6	T	21	GLN
6	T	32	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	T	72	HIS
6	T	76	GLN
6	T	117	GLN
6	U	13	GLN
6	U	72	HIS
6	U	76	GLN
6	U	92	GLN
6	U	112	ASN
7	V	30	ASN
7	X	50	GLN
7	X	57	GLN
7	X	134	GLN
7	Z	17	GLN
7	a	5	ASN
7	a	57	GLN
7	a	115	ASN
1	b	319	GLN
1	j	318	ASN
1	l	318	ASN
1	t	303	GLN
1	t	374	HIS
1	u	303	GLN
1	u	374	HIS
1	v	303	GLN
1	v	374	HIS
1	w	303	GLN
1	w	374	HIS
1	x	303	GLN
1	x	374	HIS
1	y	374	HIS
1	z	297	GLN
1	z	303	GLN
1	z	374	HIS
1	1	297	GLN
1	1	299	ASN
1	1	303	GLN
1	1	374	HIS
1	2	303	GLN
1	2	374	HIS
1	3	303	GLN
1	3	374	HIS
1	4	303	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	4	374	HIS
1	5	299	ASN
1	5	303	GLN
1	5	374	HIS
1	6	303	GLN
1	6	374	HIS
1	7	299	ASN
1	7	303	GLN
1	7	374	HIS
1	8	303	GLN
1	8	374	HIS
1	9	303	GLN
1	9	374	HIS
1	0	303	GLN
1	0	374	HIS
1	AA	303	GLN
1	AB	265	GLN
1	AB	303	GLN
1	AB	374	HIS
1	AC	303	GLN
1	AC	374	HIS
1	AD	297	GLN
1	AD	303	GLN
1	AD	365	ASN
1	AD	374	HIS
1	AE	297	GLN
1	AE	303	GLN
1	AE	374	HIS
1	AF	303	GLN
1	AF	374	HIS
1	AG	303	GLN
1	AG	374	HIS
1	AG	434	ASN
1	AH	303	GLN
1	AH	374	HIS
1	AH	434	ASN
1	AI	303	GLN
1	AI	374	HIS
1	AI	434	ASN
1	AJ	303	GLN
1	AJ	374	HIS
1	AJ	434	ASN

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Mol	Chain	Res	Type
1	AK	303	GLN
1	AK	374	HIS
1	AK	434	ASN
1	AL	303	GLN
1	AL	374	HIS
1	AL	434	ASN
1	AM	303	GLN
1	AM	374	HIS
1	AM	434	ASN
1	AN	374	HIS
1	AN	434	ASN
1	AO	297	GLN
1	AO	303	GLN
1	AO	374	HIS
1	AO	434	ASN
1	AP	297	GLN
1	AP	303	GLN
1	AP	359	GLN
1	AP	374	HIS
1	AP	434	ASN
1	AQ	303	GLN
1	AQ	374	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

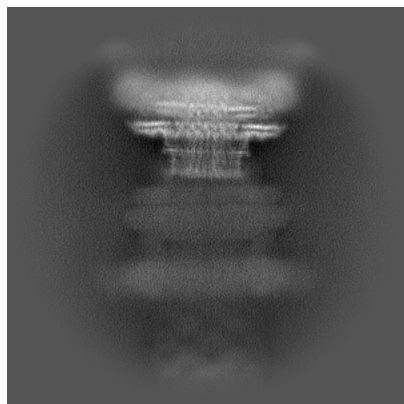
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37605. These allow visual inspection of the internal detail of the map and identification of artifacts.

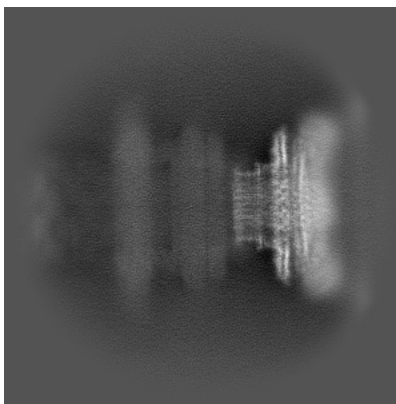
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

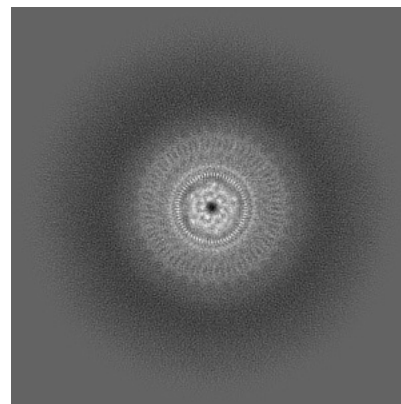
#### 6.1.1 Primary map



X

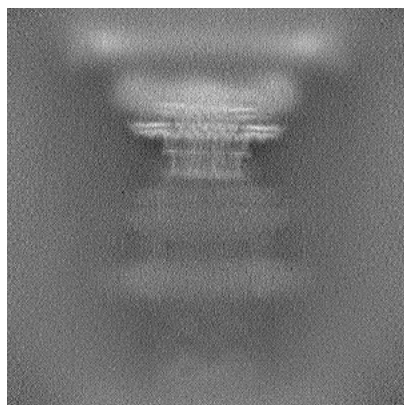


Y

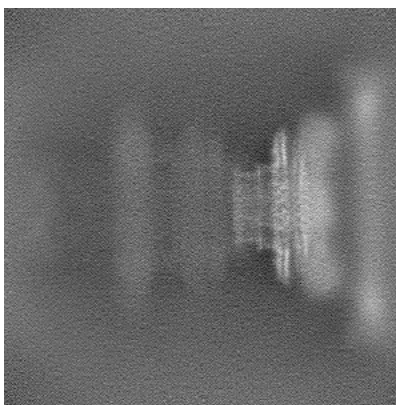


Z

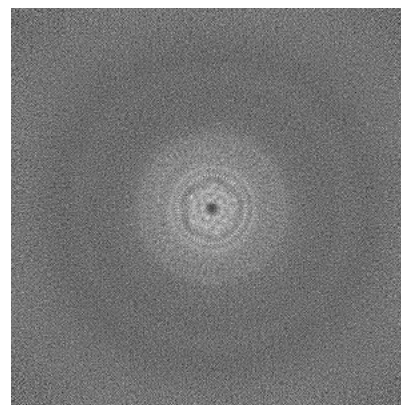
#### 6.1.2 Raw map



X



Y

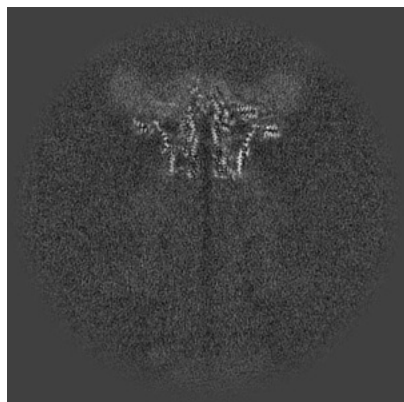


Z

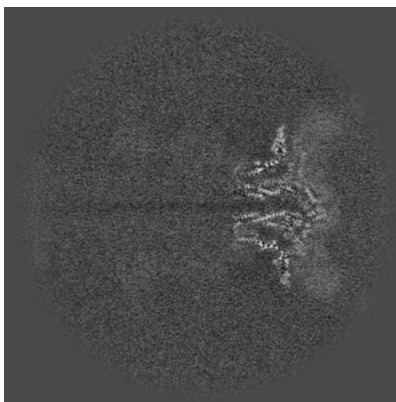
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

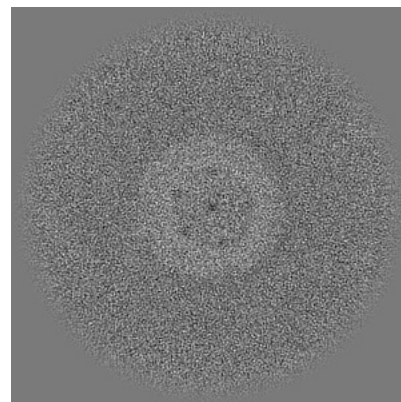
### 6.2.1 Primary map



X Index: 256



Y Index: 256

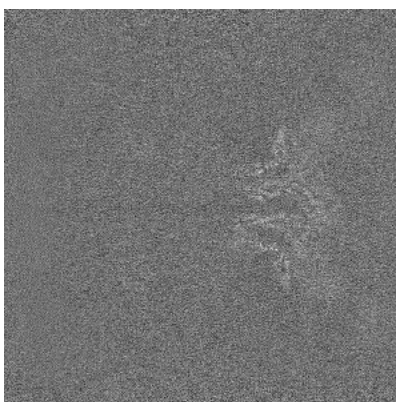


Z Index: 256

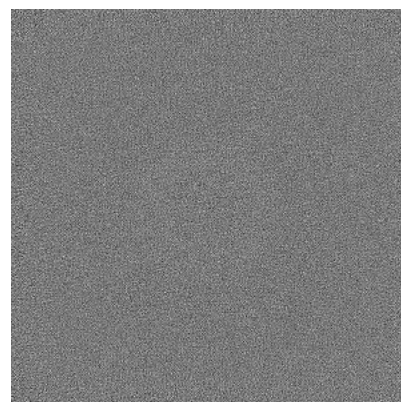
### 6.2.2 Raw map



X Index: 256



Y Index: 256



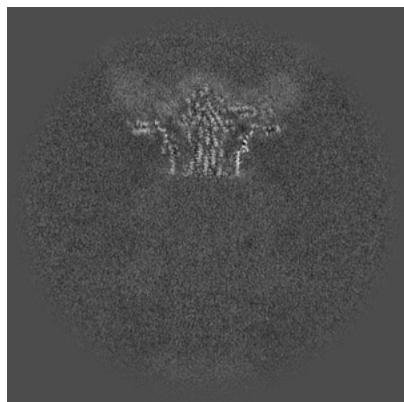
Z Index: 256

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

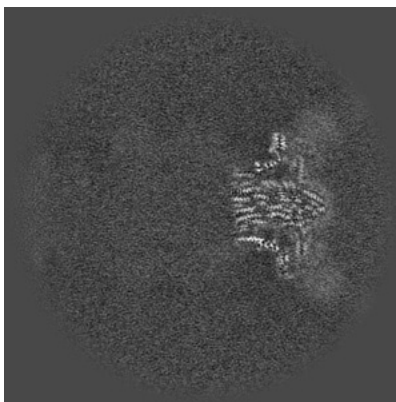


## 6.3 Largest variance slices [i](#)

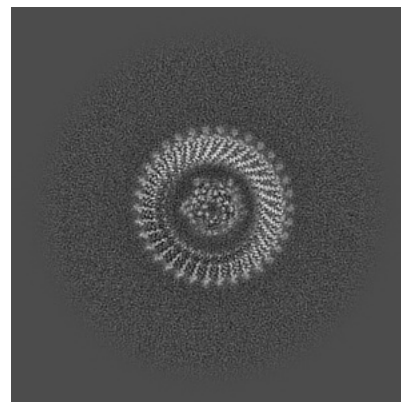
### 6.3.1 Primary map



X Index: 244

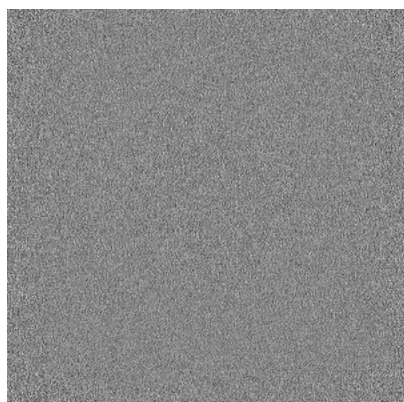


Y Index: 265

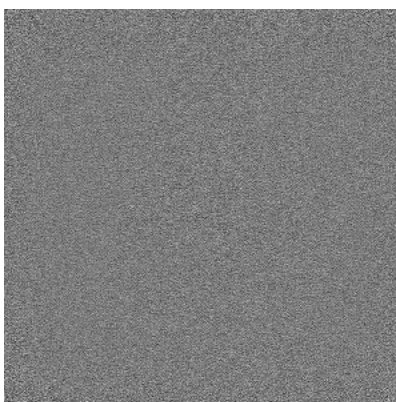


Z Index: 358

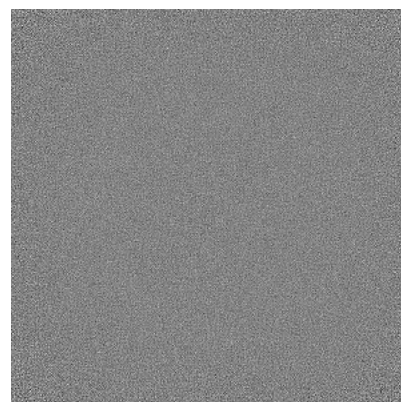
### 6.3.2 Raw map



X Index: 0



Y Index: 0



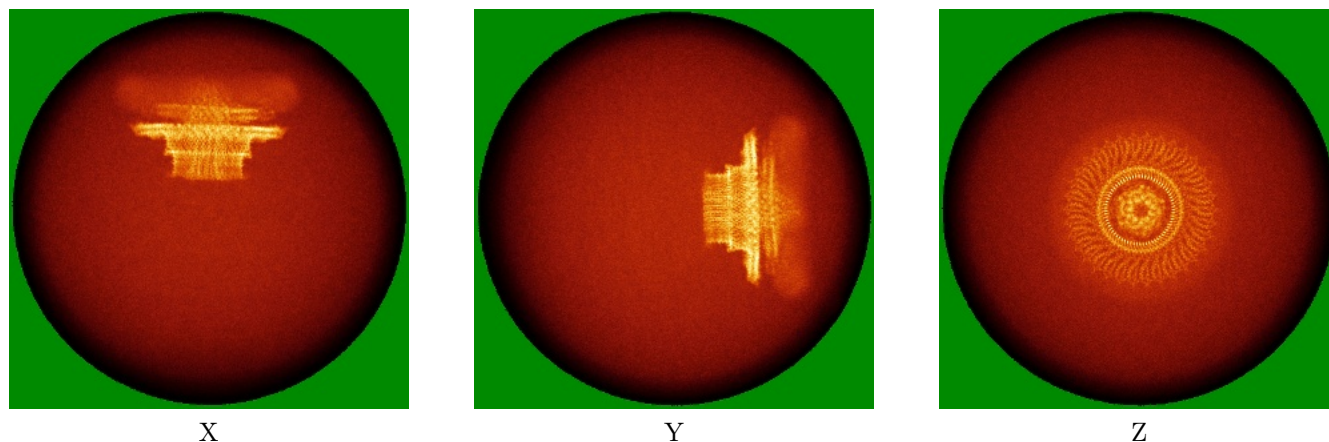
Z Index: 0

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

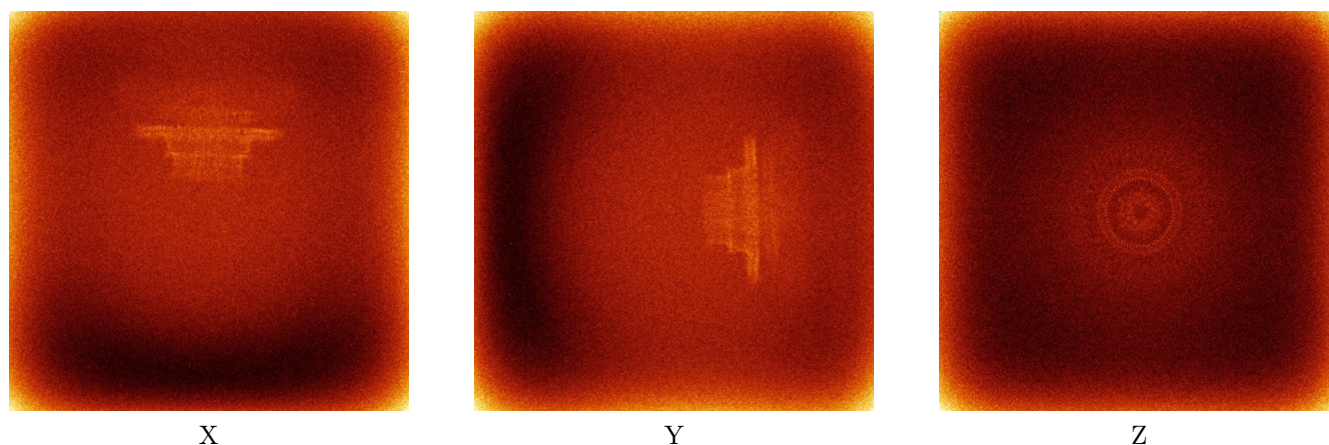


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



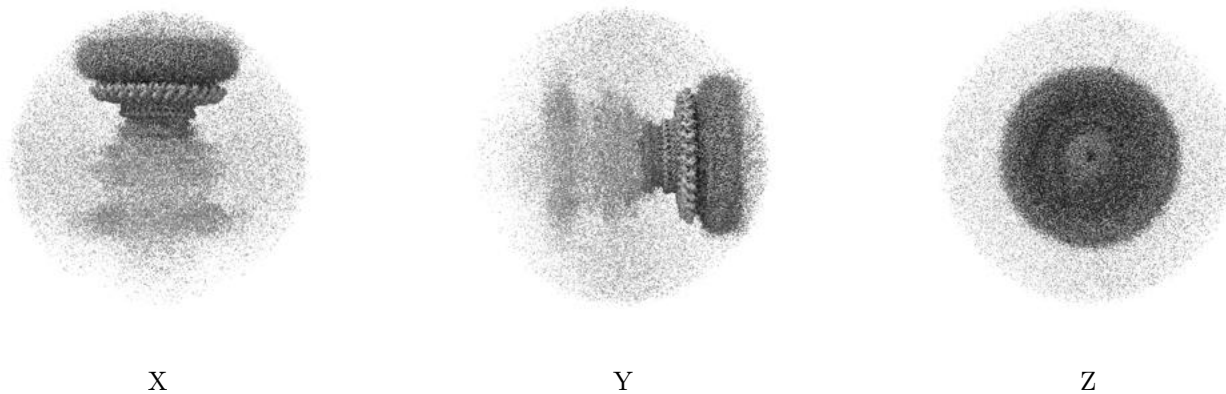
### 6.4.2 Raw map



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.

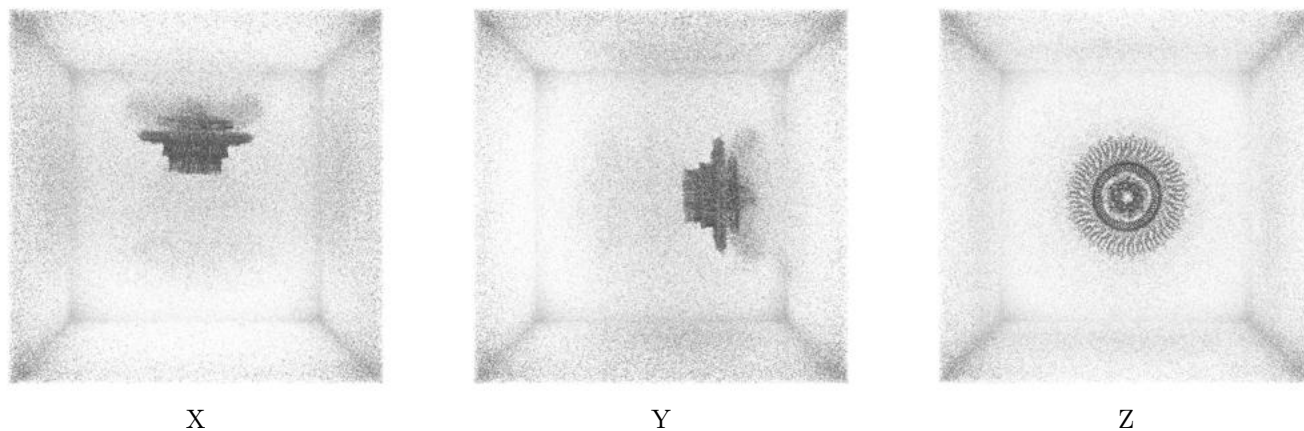
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

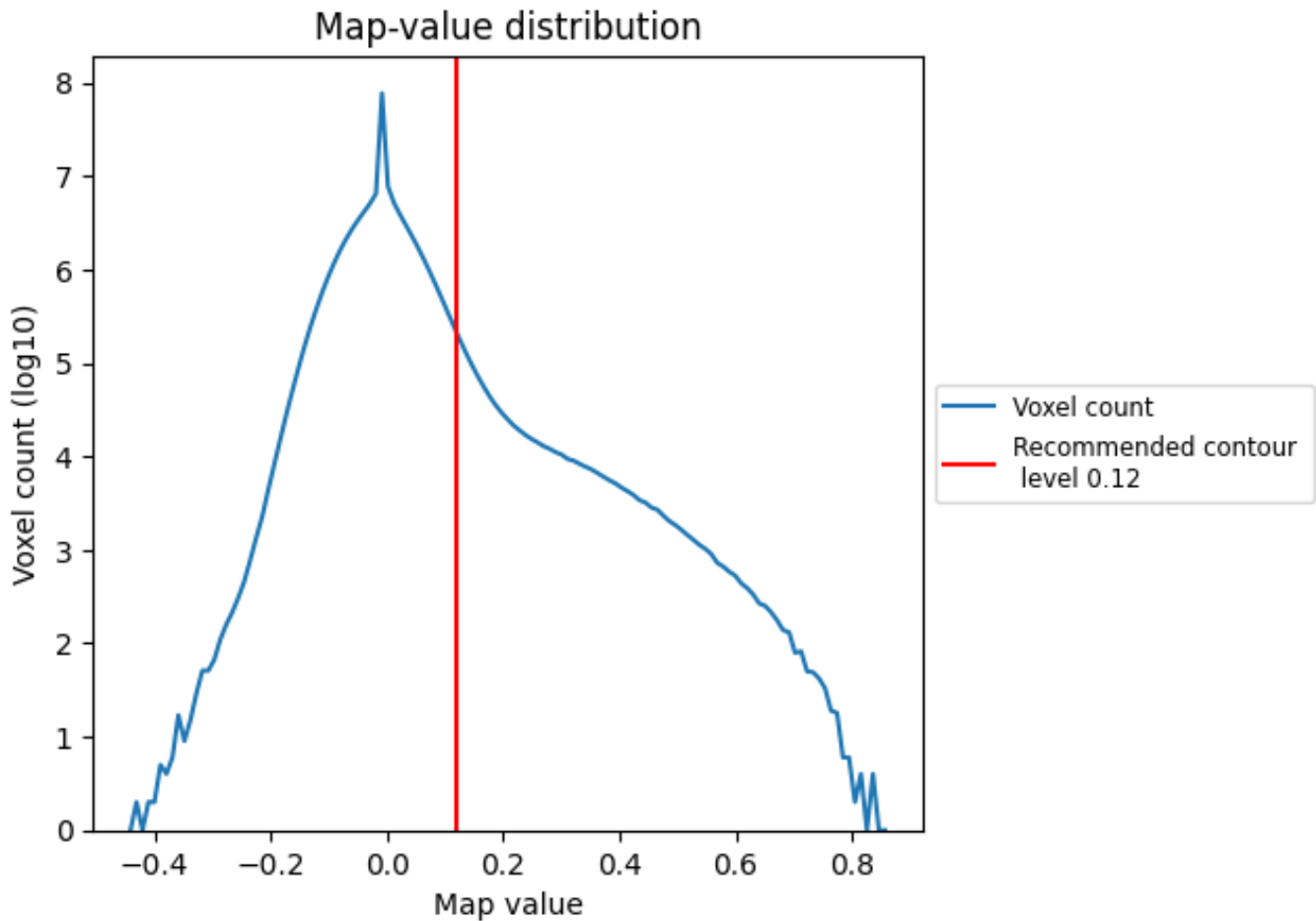
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

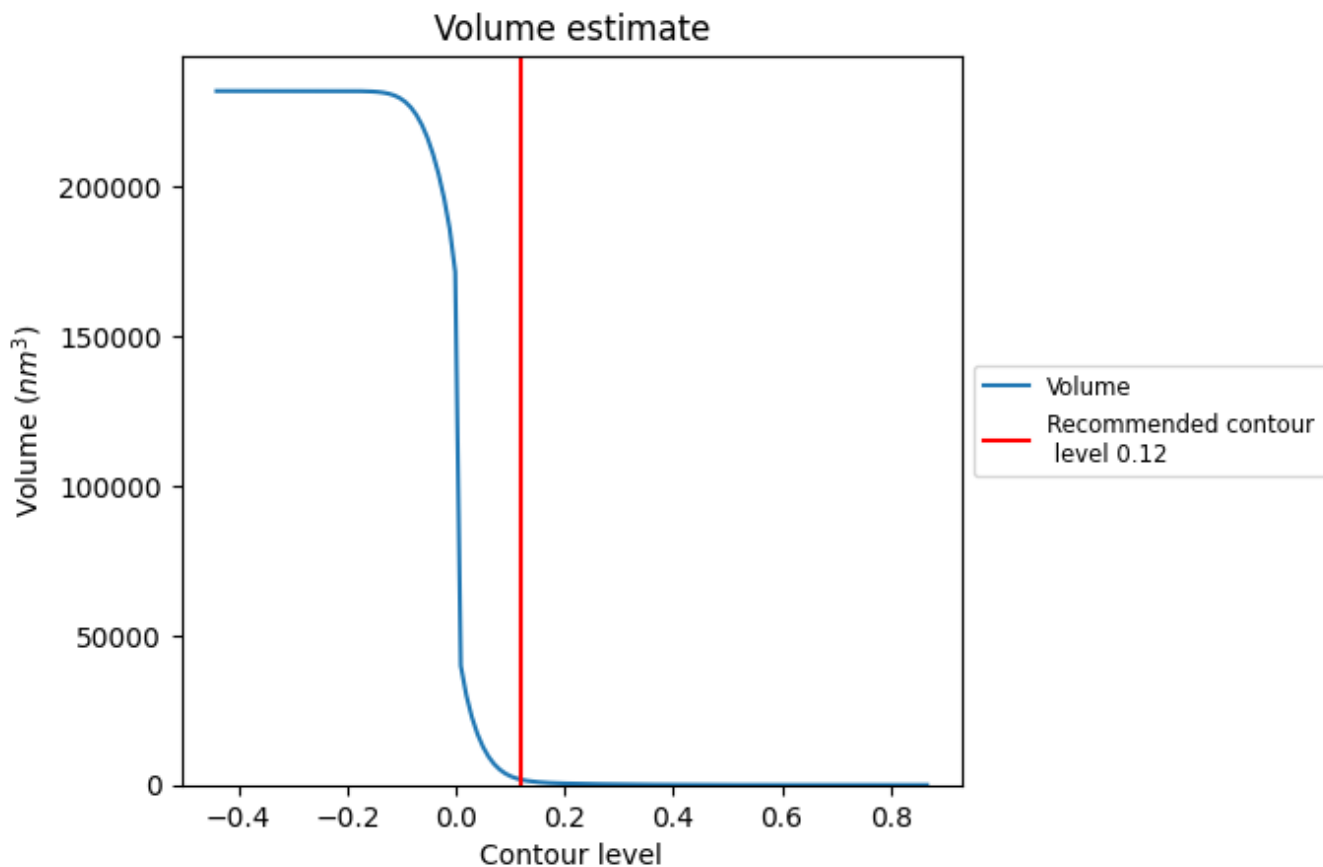
This section contains the results of statistical analysis of the map.

### 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.

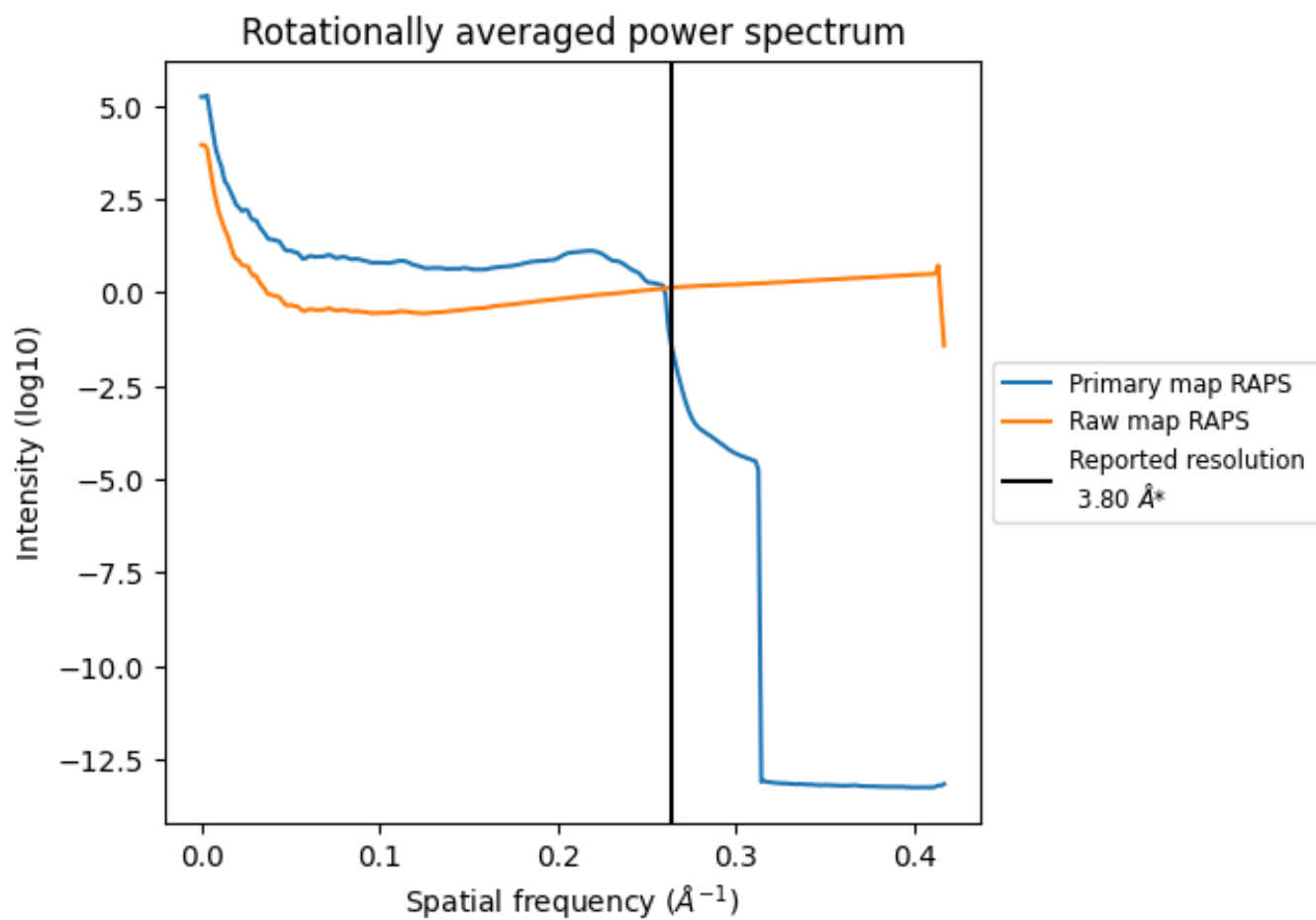
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1782  $\text{nm}^3$ ; this corresponds to an approximate mass of 1610 kDa.

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

### 7.3 Rotationally averaged power spectrum i

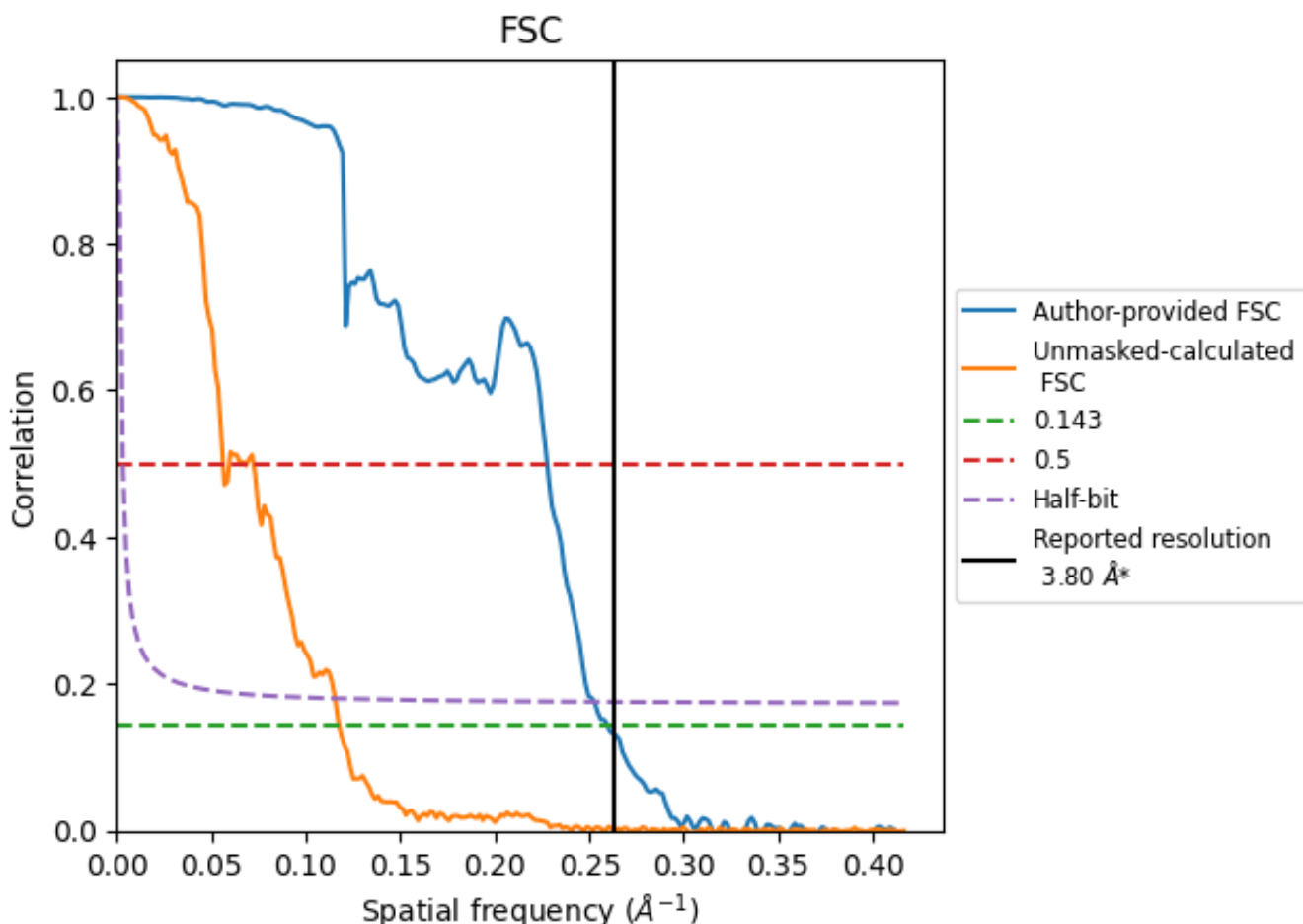


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

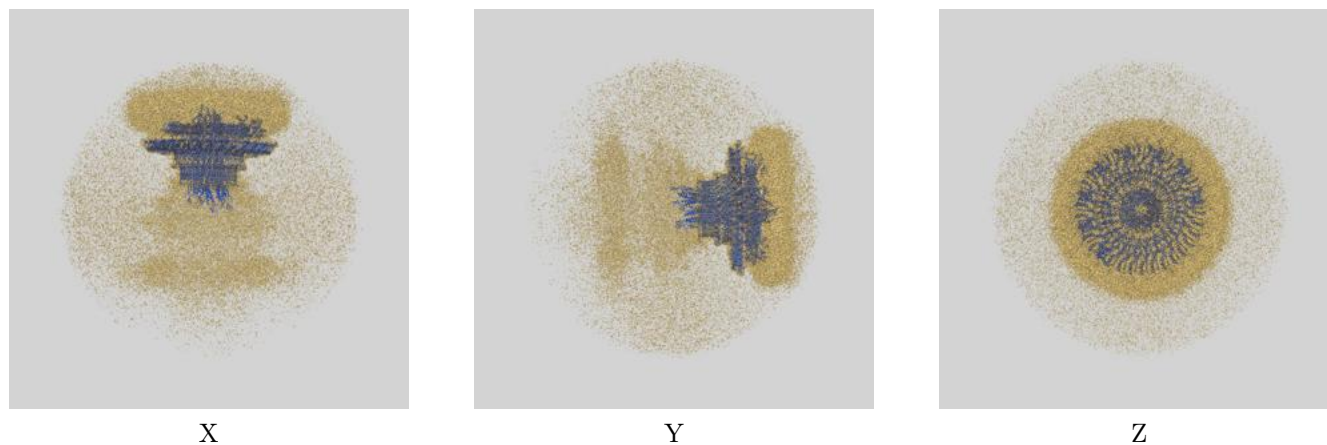
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.85	4.39	3.96
Unmasked-calculated*	8.49	17.76	8.65

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.49 differs from the reported value 3.8 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37605 and PDB model 8WKQ. Per-residue inclusion information can be found in section 3 on page 13.

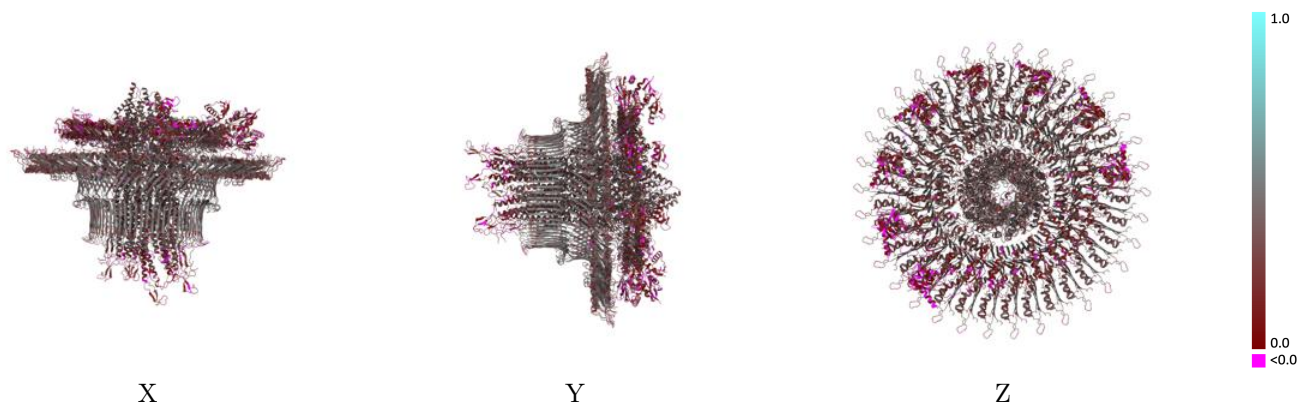
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

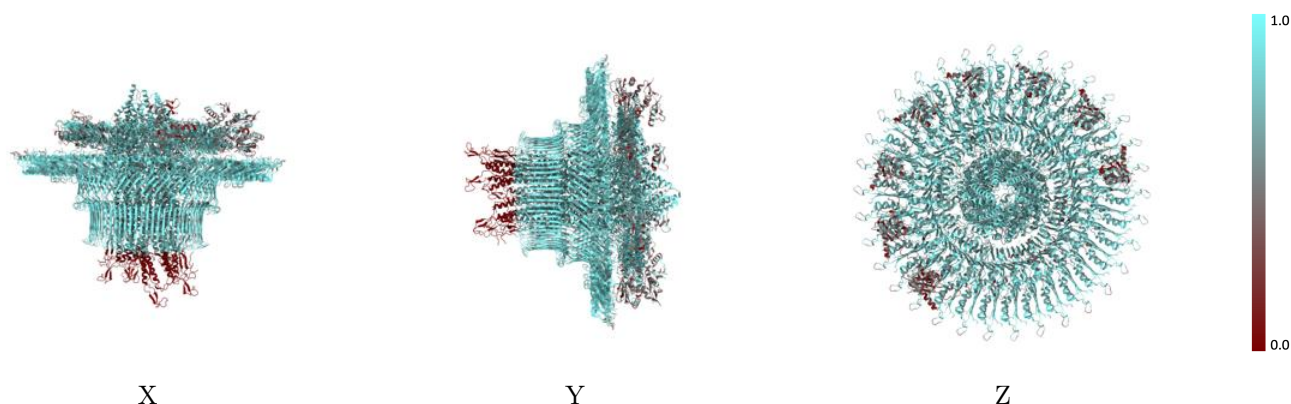


## 9.2 Q-score mapped to coordinate model [i](#)



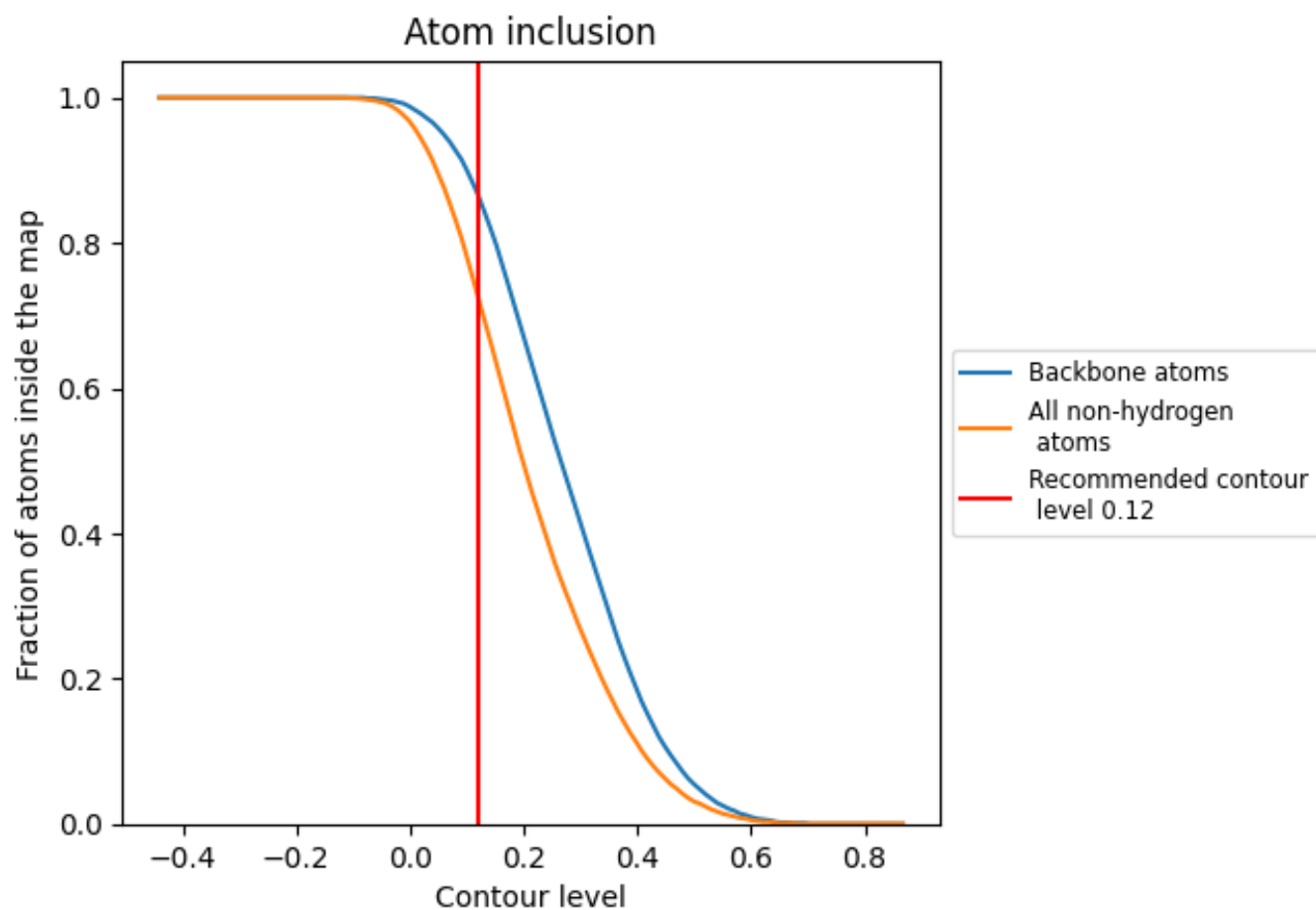
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.3190
0	 0.8170	 0.3700
1	 0.8140	 0.3590
2	 0.8250	 0.3680
3	 0.8290	 0.3720
4	 0.8250	 0.3740
5	 0.8190	 0.3730
6	 0.8280	 0.3770
7	 0.8200	 0.3750
8	 0.8340	 0.3860
9	 0.8330	 0.3850
A	 0.7670	 0.3160
AA	 0.8140	 0.3660
AB	 0.8210	 0.3660
AC	 0.8210	 0.3690
AD	 0.8240	 0.3640
AE	 0.8180	 0.3720
AF	 0.8290	 0.3590
AG	 0.8120	 0.3470
AH	 0.8200	 0.3540
AI	 0.8010	 0.3490
AJ	 0.8220	 0.3610
AK	 0.8270	 0.3650
AL	 0.8140	 0.3620
AM	 0.8110	 0.3650
AN	 0.8040	 0.3640
AO	 0.8250	 0.3750
AP	 0.8220	 0.3740
AQ	 0.8160	 0.3700
B	 0.8150	 0.3480
C	 0.8200	 0.3510
D	 0.8090	 0.3460
E	 0.7840	 0.3500
F	 0.7940	 0.3610
G	 0.8120	 0.3750

























































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Chain	Atom inclusion	Q-score
H	 0.7990	 0.3690
I	 0.7870	 0.3680
J	 0.7640	 0.3640
K	 0.7300	 0.3590
L	 0.7890	 0.3540
M	 0.7750	 0.3500
N	 0.7680	 0.3580
O	 0.7610	 0.3430
P	 0.7660	 0.3520
Q	 0.7750	 0.3790
R	 0.7740	 0.3690
S	 0.7420	 0.3670
T	 0.7260	 0.3610
U	 0.6610	 0.3390
UI	 0.5160	 0.2040
UJ	 0.4890	 0.1640
UK	 0.4160	 0.1540
UL	 0.3670	 0.1180
UM	 0.2850	 0.0510
UN	 0.3590	 0.0800
UO	 0.4200	 0.1310
UP	 0.4760	 0.1390
V	 0.5020	 0.3110
W	 0.4120	 0.2850
WA	 0.7920	 0.3380
WB	 0.7910	 0.3290
WC	 0.8040	 0.3460
WD	 0.7890	 0.3400
WE	 0.7680	 0.3210
WF	 0.7780	 0.3230
WG	 0.7460	 0.2860
WH	 0.7690	 0.2810
WI	 0.7200	 0.2360
WJ	 0.6920	 0.2170
WK	 0.6500	 0.1970
WL	 0.6770	 0.1880
WM	 0.7090	 0.2250
WN	 0.6880	 0.1660
WO	 0.6630	 0.1650
WP	 0.7480	 0.2330
WQ	 0.7300	 0.2510
WR	 0.7300	 0.2820

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Chain	Atom inclusion	Q-score
WS	 0.7870	 0.2910
WT	 0.7950	 0.3240
WU	 0.7600	 0.2930
WV	 0.7590	 0.2860
WW	 0.7790	 0.3220
X	 0.3500	 0.2540
Y	 0.2900	 0.2230
Z	 0.2590	 0.2420
a	 0.2050	 0.2240
b	 0.6670	 0.3370
c	 0.5050	 0.3570
d	 0.5640	 0.3320
e	 0.2430	 0.2510
f	 0.4930	 0.2610
g	 0.0870	 0.1150
h	 0.4360	 0.2610
i	 0.0680	 0.1250
j	 0.4510	 0.2720
k	 0.0780	 0.1940
l	 0.3360	 0.2730
t	 0.8270	 0.3780
u	 0.8270	 0.3630
v	 0.8240	 0.3710
w	 0.8280	 0.3750
x	 0.8300	 0.3680
y	 0.8260	 0.3730
z	 0.8250	 0.3740