Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2022 – 04:17 pm BST

PDB ID	:	7QIJ
Title	:	Complex of the Yersinia enterocolitica Type III secretion export gate YscV with substrate:chaperone complex YscX:YscY
Authors	:	Gilzer, D.; Niemann, H.H.
Deposited on	:	2021-12-15
Resolution	:	4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

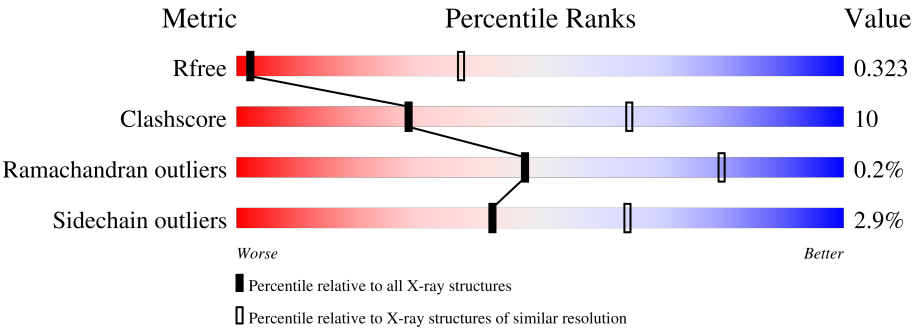
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	AA	350	67% 24% • 8%
1	BA	350	70% 23% • 5%
1	CA	350	68% 29% ••
1	DA	350	67% 25% • 7%
1	EA	350	69% 24% 6%
1	FA	350	72% 24% ••
1	GA	350	69% 28% •

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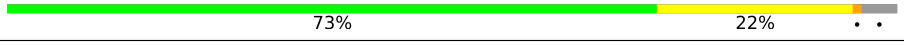
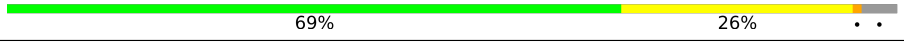
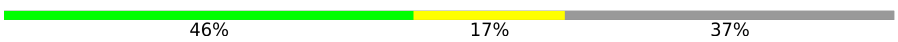
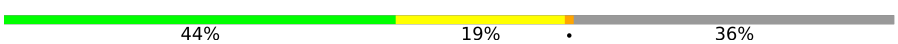
Mol	Chain	Length	Quality of chain
1	HA	350	
1	IA	350	
1	JA	350	
1	KA	350	
1	LA	350	
1	MA	350	
1	NA	350	
1	OA	350	
1	PA	350	
1	QA	350	
1	RA	350	
2	AB	95	
2	BB	95	
2	CB	95	
2	DB	95	
2	EB	95	
2	FB	95	
2	GB	95	
2	HB	95	
2	IB	95	
2	JB	95	
2	KB	95	
2	LB	95	
2	MB	95	
2	NB	95	

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Mol	Chain	Length	Quality of chain
2	OB	95	42% 29% 26%
2	PB	95	48% 20% 32%
2	QB	95	49% 17% 31%
2	RB	95	56% 18% 26%
3	AC	122	62% 12% 24%
3	BC	122	61% 15% 22%
3	CC	122	67% 21% 11%
3	DC	122	61% 20% 17%
3	EC	122	61% 18% 20%
3	FC	122	66% 20% 13%
3	GC	122	59% 28% 11%
3	HC	122	66% 16% 16%
3	IC	122	61% 12% 27%
3	JC	122	63% 24% 11%
3	KC	122	66% 24% 8%
3	LC	122	64% 20% 14%
3	MC	122	56% 22% 21%
3	NC	122	62% 21% 16%
3	OC	122	70% 19% 11%
3	PC	122	61% 27% 11%
3	QC	122	59% 16% 24%
3	RC	122	65% 24% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 73488 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Low calcium response locus protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	323	Total	C	N	O	S	0	0	0
			2628	1676	448	495	9			
1	BA	331	Total	C	N	O	S	0	0	0
			2688	1712	458	509	9			
1	CA	343	Total	C	N	O	S	0	0	0
			2792	1779	474	530	9			
1	DA	326	Total	C	N	O	S	0	0	0
			2661	1695	451	506	9			
1	EA	329	Total	C	N	O	S	0	0	0
			2684	1710	456	509	9			
1	FA	337	Total	C	N	O	S	0	0	0
			2736	1740	466	521	9			
1	GA	341	Total	C	N	O	S	0	0	0
			2772	1766	469	528	9			
1	HA	335	Total	C	N	O	S	0	0	0
			2727	1741	460	517	9			
1	IA	336	Total	C	N	O	S	0	0	0
			2731	1738	465	519	9			
1	JA	330	Total	C	N	O	S	0	0	0
			2689	1713	457	510	9			
1	KA	335	Total	C	N	O	S	0	0	0
			2736	1746	464	517	9			
1	LA	336	Total	C	N	O	S	0	0	0
			2734	1743	462	520	9			
1	MA	322	Total	C	N	O	S	0	0	0
			2632	1683	448	493	8			
1	NA	331	Total	C	N	O	S	0	0	0
			2698	1720	456	513	9			
1	OA	331	Total	C	N	O	S	0	0	0
			2694	1718	458	509	9			
1	PA	330	Total	C	N	O	S	0	0	0
			2688	1713	457	509	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	334	Total	C	N	O	S	0	0	0
			2713	1728	462	514	9			
1	RA	344	Total	C	N	O	S	0	0	0
			2798	1782	474	533	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	355	MET	-	initiating methionine	UNP P0C2V3
AA	621	ARG	GLY	variant	UNP P0C2V3
BA	355	MET	-	initiating methionine	UNP P0C2V3
BA	621	ARG	GLY	variant	UNP P0C2V3
CA	355	MET	-	initiating methionine	UNP P0C2V3
CA	621	ARG	GLY	variant	UNP P0C2V3
DA	355	MET	-	initiating methionine	UNP P0C2V3
DA	621	ARG	GLY	variant	UNP P0C2V3
EA	355	MET	-	initiating methionine	UNP P0C2V3
EA	621	ARG	GLY	variant	UNP P0C2V3
FA	355	MET	-	initiating methionine	UNP P0C2V3
FA	621	ARG	GLY	variant	UNP P0C2V3
GA	355	MET	-	initiating methionine	UNP P0C2V3
GA	621	ARG	GLY	variant	UNP P0C2V3
HA	355	MET	-	initiating methionine	UNP P0C2V3
HA	621	ARG	GLY	variant	UNP P0C2V3
IA	355	MET	-	initiating methionine	UNP P0C2V3
IA	621	ARG	GLY	variant	UNP P0C2V3
JA	355	MET	-	initiating methionine	UNP P0C2V3
JA	621	ARG	GLY	variant	UNP P0C2V3
KA	355	MET	-	initiating methionine	UNP P0C2V3
KA	621	ARG	GLY	variant	UNP P0C2V3
LA	355	MET	-	initiating methionine	UNP P0C2V3
LA	621	ARG	GLY	variant	UNP P0C2V3
MA	355	MET	-	initiating methionine	UNP P0C2V3
MA	621	ARG	GLY	variant	UNP P0C2V3
NA	355	MET	-	initiating methionine	UNP P0C2V3
NA	621	ARG	GLY	variant	UNP P0C2V3
OA	355	MET	-	initiating methionine	UNP P0C2V3
OA	621	ARG	GLY	variant	UNP P0C2V3
PA	355	MET	-	initiating methionine	UNP P0C2V3
PA	621	ARG	GLY	variant	UNP P0C2V3
QA	355	MET	-	initiating methionine	UNP P0C2V3
QA	621	ARG	GLY	variant	UNP P0C2V3

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Chain	Residue	Modelled	Actual	Comment	Reference
RA	355	MET	-	initiating methionine	UNP P0C2V3
RA	621	ARG	GLY	variant	UNP P0C2V3

- Molecule 2 is a protein called Yop proteins translocation protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CB	68	Total	C	N	O	S	0	0	0
			546	338	102	105	1			
2	JB	69	Total	C	N	O	S	0	0	0
			554	346	98	109	1			
2	KB	77	Total	C	N	O	S	0	0	0
			624	390	114	119	1			
2	RB	70	Total	C	N	O	S	0	0	0
			559	347	102	109	1			
2	GB	73	Total	C	N	O	S	0	0	0
			596	371	110	114	1			
2	LB	70	Total	C	N	O	S	0	1	0
			569	356	99	113	1			
2	NB	61	Total	C	N	O	S	0	0	0
			487	302	87	97	1			
2	OB	70	Total	C	N	O	S	0	0	0
			562	349	104	108	1			
2	PB	65	Total	C	N	O	S	0	0	0
			521	322	95	103	1			
2	EB	60	Total	C	N	O	S	0	0	0
			482	299	86	96	1			
2	FB	71	Total	C	N	O	S	3	1	0
			572	357	101	113	1			
2	HB	65	Total	C	N	O	S	1	0	0
			524	324	97	102	1			
2	IB	63	Total	C	N	O	S	0	0	0
			503	312	90	100	1			
2	AB	70	Total	C	N	O	S	0	0	0
			562	349	104	108	1			
2	BB	65	Total	C	N	O	S	0	0	0
			524	324	97	102	1			
2	DB	61	Total	C	N	O	S	0	0	0
			493	306	88	98	1			
2	MB	64	Total	C	N	O	S	0	0	0
			513	320	95	97	1			
2	QB	66	Total	C	N	O	S	0	0	0
			532	331	97	103	1			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CB	28	GLY	-	expression tag	UNP P0C2N4
CB	29	ALA	-	expression tag	UNP P0C2N4
CB	30	MET	-	expression tag	UNP P0C2N4
CB	31	GLY	-	expression tag	UNP P0C2N4
JB	28	GLY	-	expression tag	UNP P0C2N4
JB	29	ALA	-	expression tag	UNP P0C2N4
JB	30	MET	-	expression tag	UNP P0C2N4
JB	31	GLY	-	expression tag	UNP P0C2N4
KB	28	GLY	-	expression tag	UNP P0C2N4
KB	29	ALA	-	expression tag	UNP P0C2N4
KB	30	MET	-	expression tag	UNP P0C2N4
KB	31	GLY	-	expression tag	UNP P0C2N4
RB	28	GLY	-	expression tag	UNP P0C2N4
RB	29	ALA	-	expression tag	UNP P0C2N4
RB	30	MET	-	expression tag	UNP P0C2N4
RB	31	GLY	-	expression tag	UNP P0C2N4
GB	28	GLY	-	expression tag	UNP P0C2N4
GB	29	ALA	-	expression tag	UNP P0C2N4
GB	30	MET	-	expression tag	UNP P0C2N4
GB	31	GLY	-	expression tag	UNP P0C2N4
LB	28	GLY	-	expression tag	UNP P0C2N4
LB	29	ALA	-	expression tag	UNP P0C2N4
LB	30	MET	-	expression tag	UNP P0C2N4
LB	31	GLY	-	expression tag	UNP P0C2N4
NB	28	GLY	-	expression tag	UNP P0C2N4
NB	29	ALA	-	expression tag	UNP P0C2N4
NB	30	MET	-	expression tag	UNP P0C2N4
NB	31	GLY	-	expression tag	UNP P0C2N4
OB	28	GLY	-	expression tag	UNP P0C2N4
OB	29	ALA	-	expression tag	UNP P0C2N4
OB	30	MET	-	expression tag	UNP P0C2N4
OB	31	GLY	-	expression tag	UNP P0C2N4
PB	28	GLY	-	expression tag	UNP P0C2N4
PB	29	ALA	-	expression tag	UNP P0C2N4
PB	30	MET	-	expression tag	UNP P0C2N4
PB	31	GLY	-	expression tag	UNP P0C2N4
EB	28	GLY	-	expression tag	UNP P0C2N4
EB	29	ALA	-	expression tag	UNP P0C2N4
EB	30	MET	-	expression tag	UNP P0C2N4
EB	31	GLY	-	expression tag	UNP P0C2N4
FB	28	GLY	-	expression tag	UNP P0C2N4
FB	29	ALA	-	expression tag	UNP P0C2N4

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Chain	Residue	Modelled	Actual	Comment	Reference
FB	30	MET	-	expression tag	UNP P0C2N4
FB	31	GLY	-	expression tag	UNP P0C2N4
HB	28	GLY	-	expression tag	UNP P0C2N4
HB	29	ALA	-	expression tag	UNP P0C2N4
HB	30	MET	-	expression tag	UNP P0C2N4
HB	31	GLY	-	expression tag	UNP P0C2N4
IB	28	GLY	-	expression tag	UNP P0C2N4
IB	29	ALA	-	expression tag	UNP P0C2N4
IB	30	MET	-	expression tag	UNP P0C2N4
IB	31	GLY	-	expression tag	UNP P0C2N4
AB	28	GLY	-	expression tag	UNP P0C2N4
AB	29	ALA	-	expression tag	UNP P0C2N4
AB	30	MET	-	expression tag	UNP P0C2N4
AB	31	GLY	-	expression tag	UNP P0C2N4
BB	28	GLY	-	expression tag	UNP P0C2N4
BB	29	ALA	-	expression tag	UNP P0C2N4
BB	30	MET	-	expression tag	UNP P0C2N4
BB	31	GLY	-	expression tag	UNP P0C2N4
DB	28	GLY	-	expression tag	UNP P0C2N4
DB	29	ALA	-	expression tag	UNP P0C2N4
DB	30	MET	-	expression tag	UNP P0C2N4
DB	31	GLY	-	expression tag	UNP P0C2N4
MB	28	GLY	-	expression tag	UNP P0C2N4
MB	29	ALA	-	expression tag	UNP P0C2N4
MB	30	MET	-	expression tag	UNP P0C2N4
MB	31	GLY	-	expression tag	UNP P0C2N4
QB	28	GLY	-	expression tag	UNP P0C2N4
QB	29	ALA	-	expression tag	UNP P0C2N4
QB	30	MET	-	expression tag	UNP P0C2N4
QB	31	GLY	-	expression tag	UNP P0C2N4

- Molecule 3 is a protein called Chaperone protein YscY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CC	108	Total	C	N	O	S	0	0	0
			879	549	169	157	4			
3	JC	109	Total	C	N	O	S	2	0	0
			883	548	170	161	4			
3	KC	112	Total	C	N	O	S	0	0	0
			904	562	174	164	4			
3	RC	108	Total	C	N	O	S	0	1	0
			878	549	168	156	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	GC	108	Total	C	N	O	S	3	1	0
			878	549	168	156	5			
3	LC	105	Total	C	N	O	S	0	0	0
			851	533	162	152	4			
3	NC	102	Total	C	N	O	S	0	0	0
			826	515	159	148	4			
3	OC	108	Total	C	N	O	S	0	0	0
			875	543	169	159	4			
3	PC	109	Total	C	N	O	S	0	0	0
			883	551	170	158	4			
3	EC	98	Total	C	N	O	S	0	0	0
			800	499	155	142	4			
3	FC	106	Total	C	N	O	S	0	0	0
			858	536	165	153	4			
3	HC	102	Total	C	N	O	S	0	1	0
			830	519	160	147	4			
3	IC	89	Total	C	N	O	S	0	0	0
			732	460	142	126	4			
3	AC	93	Total	C	N	O	S	0	0	0
			754	473	142	136	3			
3	BC	95	Total	C	N	O	S	0	0	0
			771	482	144	141	4			
3	DC	101	Total	C	N	O	S	0	0	0
			817	513	156	144	4			
3	MC	96	Total	C	N	O	S	0	0	0
			784	489	153	138	4			
3	QC	93	Total	C	N	O	S	0	0	0
			761	477	147	133	4			

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	-7	MET	-	initiating methionine	UNP P0C2N2
CC	-6	GLY	-	expression tag	UNP P0C2N2
CC	-5	HIS	-	expression tag	UNP P0C2N2
CC	-4	HIS	-	expression tag	UNP P0C2N2
CC	-3	HIS	-	expression tag	UNP P0C2N2
CC	-2	HIS	-	expression tag	UNP P0C2N2
CC	-1	HIS	-	expression tag	UNP P0C2N2
CC	0	HIS	-	expression tag	UNP P0C2N2
CC	1	GLY	-	expression tag	UNP P0C2N2
JC	-7	MET	-	initiating methionine	UNP P0C2N2
JC	-6	GLY	-	expression tag	UNP P0C2N2

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Chain	Residue	Modelled	Actual	Comment	Reference
JC	-5	HIS	-	expression tag	UNP P0C2N2
JC	-4	HIS	-	expression tag	UNP P0C2N2
JC	-3	HIS	-	expression tag	UNP P0C2N2
JC	-2	HIS	-	expression tag	UNP P0C2N2
JC	-1	HIS	-	expression tag	UNP P0C2N2
JC	0	HIS	-	expression tag	UNP P0C2N2
JC	1	GLY	-	expression tag	UNP P0C2N2
KC	-7	MET	-	initiating methionine	UNP P0C2N2
KC	-6	GLY	-	expression tag	UNP P0C2N2
KC	-5	HIS	-	expression tag	UNP P0C2N2
KC	-4	HIS	-	expression tag	UNP P0C2N2
KC	-3	HIS	-	expression tag	UNP P0C2N2
KC	-2	HIS	-	expression tag	UNP P0C2N2
KC	-1	HIS	-	expression tag	UNP P0C2N2
KC	0	HIS	-	expression tag	UNP P0C2N2
KC	1	GLY	-	expression tag	UNP P0C2N2
RC	-7	MET	-	initiating methionine	UNP P0C2N2
RC	-6	GLY	-	expression tag	UNP P0C2N2
RC	-5	HIS	-	expression tag	UNP P0C2N2
RC	-4	HIS	-	expression tag	UNP P0C2N2
RC	-3	HIS	-	expression tag	UNP P0C2N2
RC	-2	HIS	-	expression tag	UNP P0C2N2
RC	-1	HIS	-	expression tag	UNP P0C2N2
RC	0	HIS	-	expression tag	UNP P0C2N2
RC	1	GLY	-	expression tag	UNP P0C2N2
GC	-7	MET	-	initiating methionine	UNP P0C2N2
GC	-6	GLY	-	expression tag	UNP P0C2N2
GC	-5	HIS	-	expression tag	UNP P0C2N2
GC	-4	HIS	-	expression tag	UNP P0C2N2
GC	-3	HIS	-	expression tag	UNP P0C2N2
GC	-2	HIS	-	expression tag	UNP P0C2N2
GC	-1	HIS	-	expression tag	UNP P0C2N2
GC	0	HIS	-	expression tag	UNP P0C2N2
GC	1	GLY	-	expression tag	UNP P0C2N2
LC	-7	MET	-	initiating methionine	UNP P0C2N2
LC	-6	GLY	-	expression tag	UNP P0C2N2
LC	-5	HIS	-	expression tag	UNP P0C2N2
LC	-4	HIS	-	expression tag	UNP P0C2N2
LC	-3	HIS	-	expression tag	UNP P0C2N2
LC	-2	HIS	-	expression tag	UNP P0C2N2
LC	-1	HIS	-	expression tag	UNP P0C2N2
LC	0	HIS	-	expression tag	UNP P0C2N2

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Chain	Residue	Modelled	Actual	Comment	Reference
LC	1	GLY	-	expression tag	UNP P0C2N2
NC	-7	MET	-	initiating methionine	UNP P0C2N2
NC	-6	GLY	-	expression tag	UNP P0C2N2
NC	-5	HIS	-	expression tag	UNP P0C2N2
NC	-4	HIS	-	expression tag	UNP P0C2N2
NC	-3	HIS	-	expression tag	UNP P0C2N2
NC	-2	HIS	-	expression tag	UNP P0C2N2
NC	-1	HIS	-	expression tag	UNP P0C2N2
NC	0	HIS	-	expression tag	UNP P0C2N2
NC	1	GLY	-	expression tag	UNP P0C2N2
OC	-7	MET	-	initiating methionine	UNP P0C2N2
OC	-6	GLY	-	expression tag	UNP P0C2N2
OC	-5	HIS	-	expression tag	UNP P0C2N2
OC	-4	HIS	-	expression tag	UNP P0C2N2
OC	-3	HIS	-	expression tag	UNP P0C2N2
OC	-2	HIS	-	expression tag	UNP P0C2N2
OC	-1	HIS	-	expression tag	UNP P0C2N2
OC	0	HIS	-	expression tag	UNP P0C2N2
OC	1	GLY	-	expression tag	UNP P0C2N2
PC	-7	MET	-	initiating methionine	UNP P0C2N2
PC	-6	GLY	-	expression tag	UNP P0C2N2
PC	-5	HIS	-	expression tag	UNP P0C2N2
PC	-4	HIS	-	expression tag	UNP P0C2N2
PC	-3	HIS	-	expression tag	UNP P0C2N2
PC	-2	HIS	-	expression tag	UNP P0C2N2
PC	-1	HIS	-	expression tag	UNP P0C2N2
PC	0	HIS	-	expression tag	UNP P0C2N2
PC	1	GLY	-	expression tag	UNP P0C2N2
EC	-7	MET	-	initiating methionine	UNP P0C2N2
EC	-6	GLY	-	expression tag	UNP P0C2N2
EC	-5	HIS	-	expression tag	UNP P0C2N2
EC	-4	HIS	-	expression tag	UNP P0C2N2
EC	-3	HIS	-	expression tag	UNP P0C2N2
EC	-2	HIS	-	expression tag	UNP P0C2N2
EC	-1	HIS	-	expression tag	UNP P0C2N2
EC	0	HIS	-	expression tag	UNP P0C2N2
EC	1	GLY	-	expression tag	UNP P0C2N2
FC	-7	MET	-	initiating methionine	UNP P0C2N2
FC	-6	GLY	-	expression tag	UNP P0C2N2
FC	-5	HIS	-	expression tag	UNP P0C2N2
FC	-4	HIS	-	expression tag	UNP P0C2N2
FC	-3	HIS	-	expression tag	UNP P0C2N2

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Chain	Residue	Modelled	Actual	Comment	Reference
FC	-2	HIS	-	expression tag	UNP P0C2N2
FC	-1	HIS	-	expression tag	UNP P0C2N2
FC	0	HIS	-	expression tag	UNP P0C2N2
FC	1	GLY	-	expression tag	UNP P0C2N2
HC	-7	MET	-	initiating methionine	UNP P0C2N2
HC	-6	GLY	-	expression tag	UNP P0C2N2
HC	-5	HIS	-	expression tag	UNP P0C2N2
HC	-4	HIS	-	expression tag	UNP P0C2N2
HC	-3	HIS	-	expression tag	UNP P0C2N2
HC	-2	HIS	-	expression tag	UNP P0C2N2
HC	-1	HIS	-	expression tag	UNP P0C2N2
HC	0	HIS	-	expression tag	UNP P0C2N2
HC	1	GLY	-	expression tag	UNP P0C2N2
IC	-7	MET	-	initiating methionine	UNP P0C2N2
IC	-6	GLY	-	expression tag	UNP P0C2N2
IC	-5	HIS	-	expression tag	UNP P0C2N2
IC	-4	HIS	-	expression tag	UNP P0C2N2
IC	-3	HIS	-	expression tag	UNP P0C2N2
IC	-2	HIS	-	expression tag	UNP P0C2N2
IC	-1	HIS	-	expression tag	UNP P0C2N2
IC	0	HIS	-	expression tag	UNP P0C2N2
IC	1	GLY	-	expression tag	UNP P0C2N2
AC	-7	MET	-	initiating methionine	UNP P0C2N2
AC	-6	GLY	-	expression tag	UNP P0C2N2
AC	-5	HIS	-	expression tag	UNP P0C2N2
AC	-4	HIS	-	expression tag	UNP P0C2N2
AC	-3	HIS	-	expression tag	UNP P0C2N2
AC	-2	HIS	-	expression tag	UNP P0C2N2
AC	-1	HIS	-	expression tag	UNP P0C2N2
AC	0	HIS	-	expression tag	UNP P0C2N2
AC	1	GLY	-	expression tag	UNP P0C2N2
BC	-7	MET	-	initiating methionine	UNP P0C2N2
BC	-6	GLY	-	expression tag	UNP P0C2N2
BC	-5	HIS	-	expression tag	UNP P0C2N2
BC	-4	HIS	-	expression tag	UNP P0C2N2
BC	-3	HIS	-	expression tag	UNP P0C2N2
BC	-2	HIS	-	expression tag	UNP P0C2N2
BC	-1	HIS	-	expression tag	UNP P0C2N2
BC	0	HIS	-	expression tag	UNP P0C2N2
BC	1	GLY	-	expression tag	UNP P0C2N2
DC	-7	MET	-	initiating methionine	UNP P0C2N2
DC	-6	GLY	-	expression tag	UNP P0C2N2

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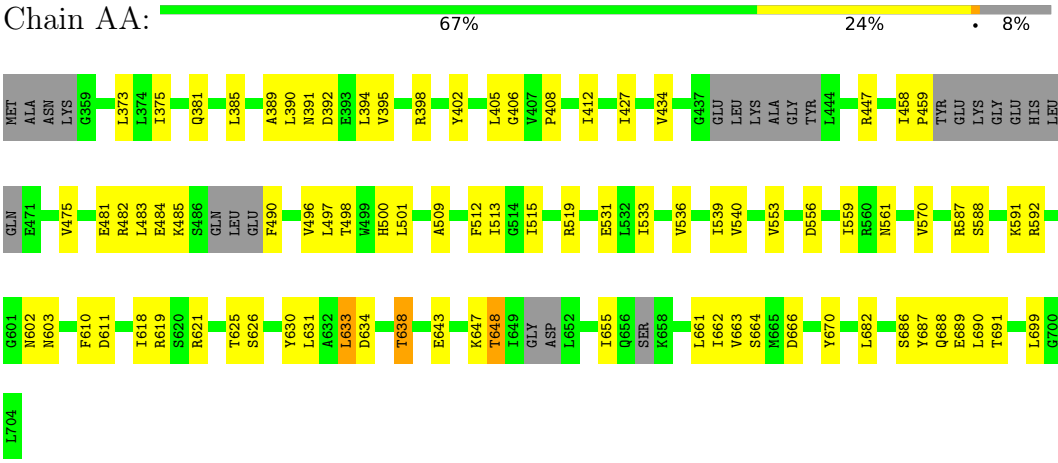
Chain	Residue	Modelled	Actual	Comment	Reference
DC	-5	HIS	-	expression tag	UNP P0C2N2
DC	-4	HIS	-	expression tag	UNP P0C2N2
DC	-3	HIS	-	expression tag	UNP P0C2N2
DC	-2	HIS	-	expression tag	UNP P0C2N2
DC	-1	HIS	-	expression tag	UNP P0C2N2
DC	0	HIS	-	expression tag	UNP P0C2N2
DC	1	GLY	-	expression tag	UNP P0C2N2
MC	-7	MET	-	initiating methionine	UNP P0C2N2
MC	-6	GLY	-	expression tag	UNP P0C2N2
MC	-5	HIS	-	expression tag	UNP P0C2N2
MC	-4	HIS	-	expression tag	UNP P0C2N2
MC	-3	HIS	-	expression tag	UNP P0C2N2
MC	-2	HIS	-	expression tag	UNP P0C2N2
MC	-1	HIS	-	expression tag	UNP P0C2N2
MC	0	HIS	-	expression tag	UNP P0C2N2
MC	1	GLY	-	expression tag	UNP P0C2N2
QC	-7	MET	-	initiating methionine	UNP P0C2N2
QC	-6	GLY	-	expression tag	UNP P0C2N2
QC	-5	HIS	-	expression tag	UNP P0C2N2
QC	-4	HIS	-	expression tag	UNP P0C2N2
QC	-3	HIS	-	expression tag	UNP P0C2N2
QC	-2	HIS	-	expression tag	UNP P0C2N2
QC	-1	HIS	-	expression tag	UNP P0C2N2
QC	0	HIS	-	expression tag	UNP P0C2N2
QC	1	GLY	-	expression tag	UNP P0C2N2

3 Residue-property plots (i)

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

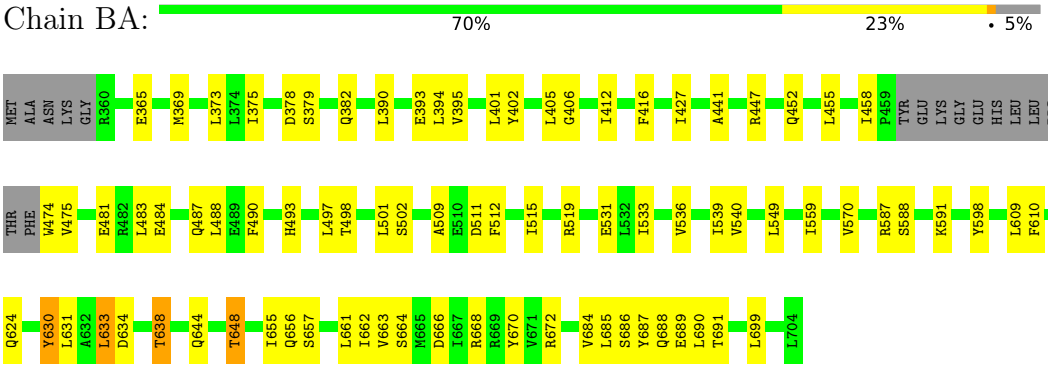
• Molecule 1: Low calcium response locus protein D

Chain AA:



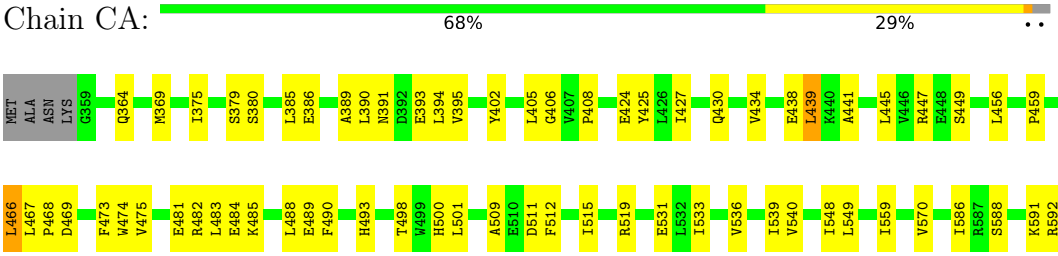
• Molecule 1: Low calcium response locus protein D

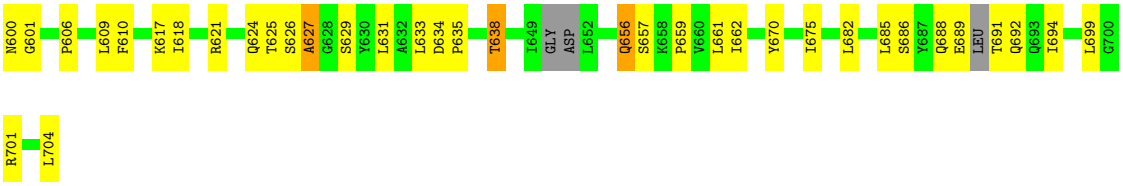
Chain BA:



• Molecule 1: Low calcium response locus protein D

Chain CA:



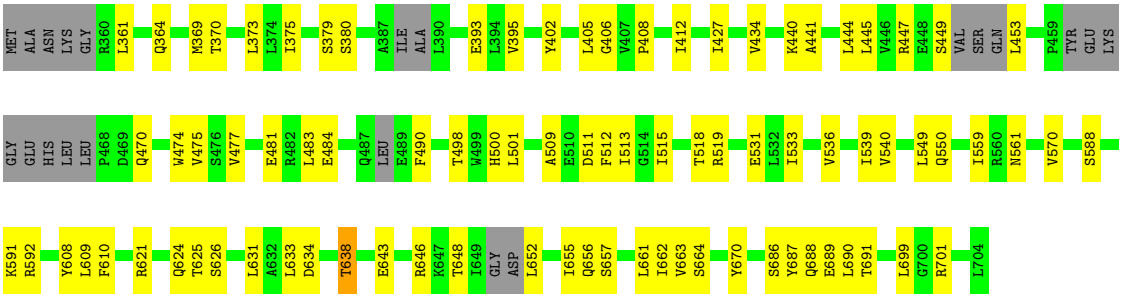


• Molecule 1: Low calcium response locus protein D

Chain DA:

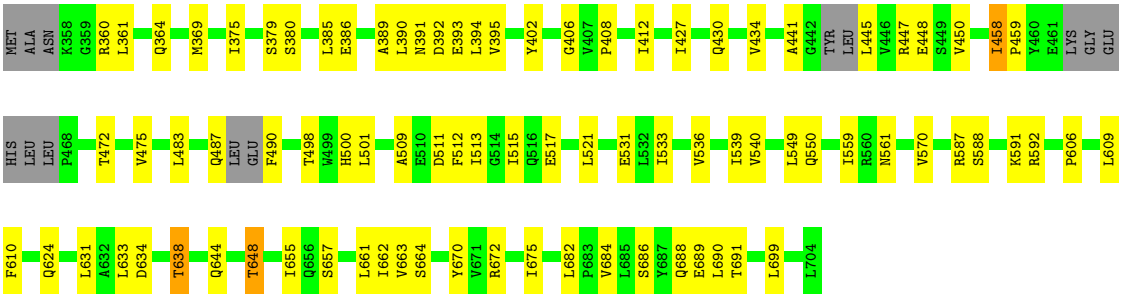
• Molecule 1: Low calcium response locus protein D

Chain EA:



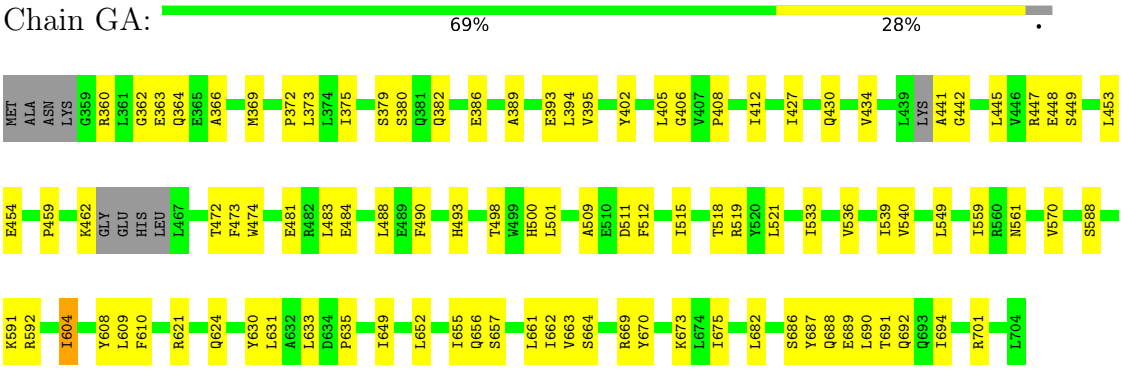
• Molecule 1: Low calcium response locus protein D

Chain FA:



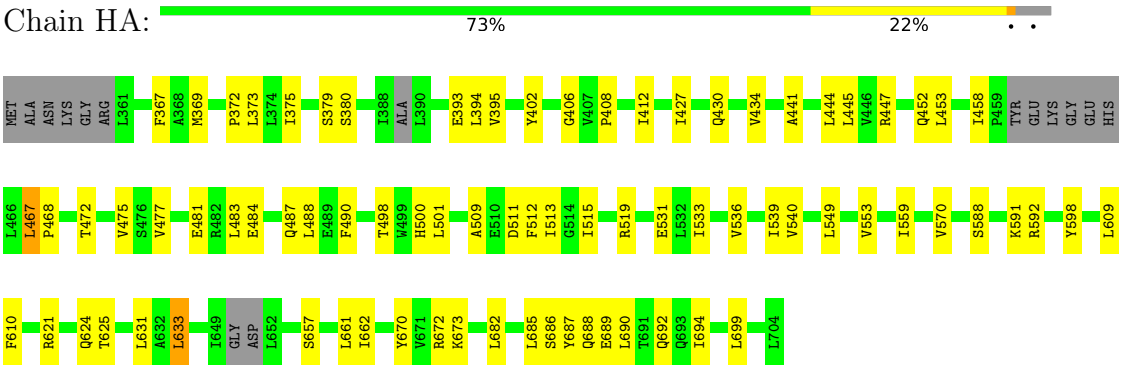
• Molecule 1: Low calcium response locus protein D

Chain GA:



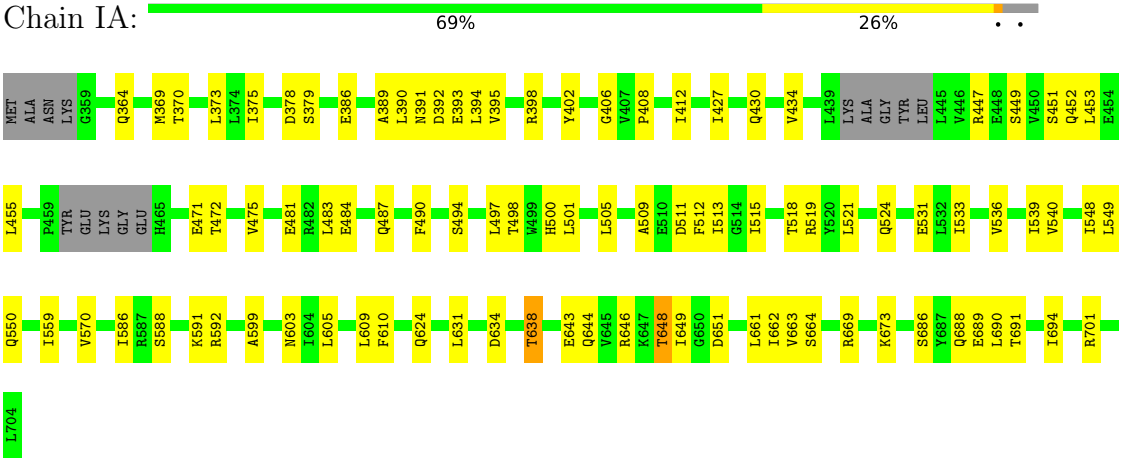
• Molecule 1: Low calcium response locus protein D

Chain HA:



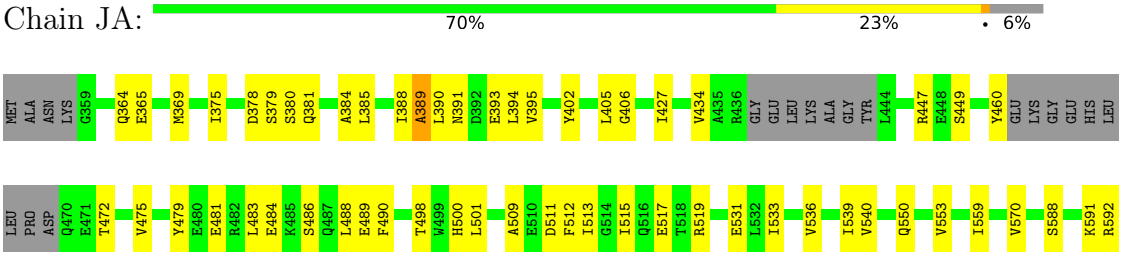
• Molecule 1: Low calcium response locus protein D

Chain IA:



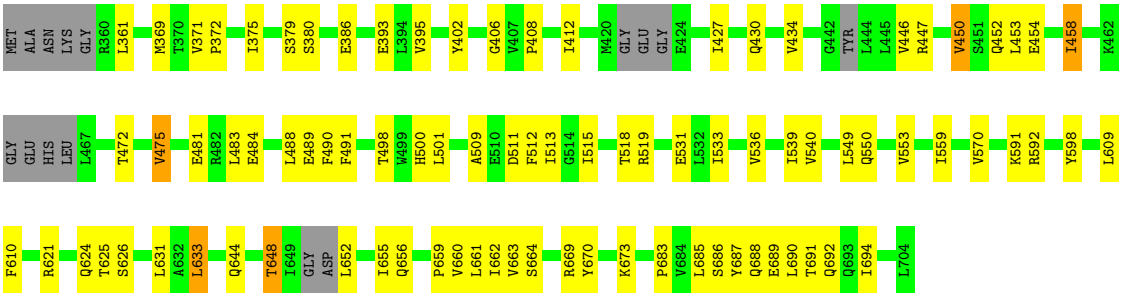
• Molecule 1: Low calcium response locus protein D

Chain JA:



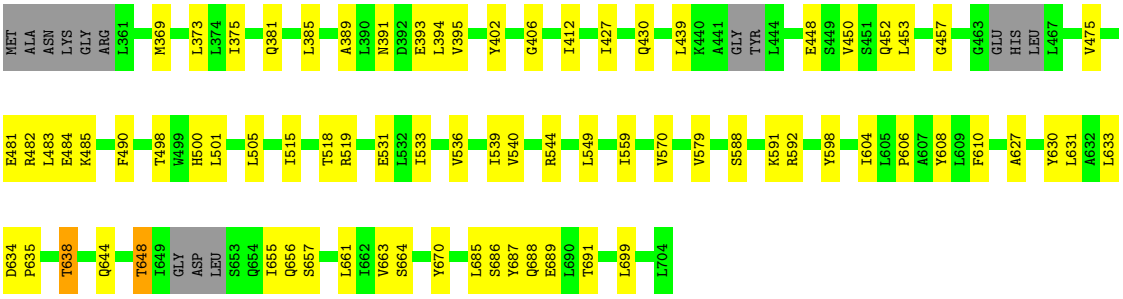
• Molecule 1: Low calcium response locus protein D

Chain KA:



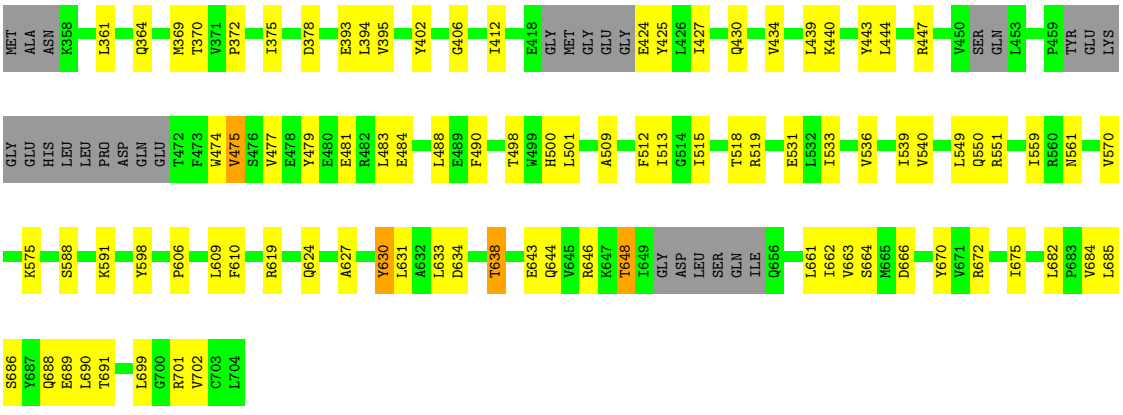
• Molecule 1: Low calcium response locus protein D

Chain LA:



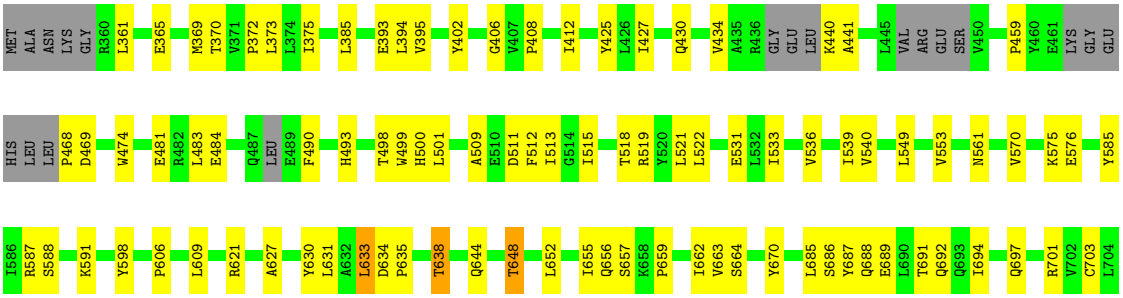
• Molecule 1: Low calcium response locus protein D

Chain MA:



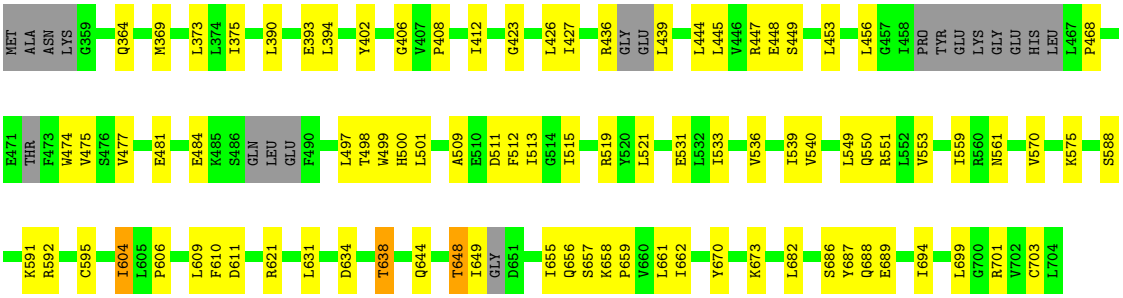
• Molecule 1: Low calcium response locus protein D

Chain NA:



• Molecule 1: Low calcium response locus protein D

Chain OA:

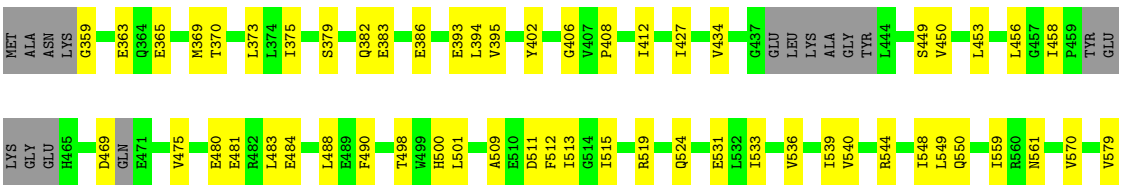


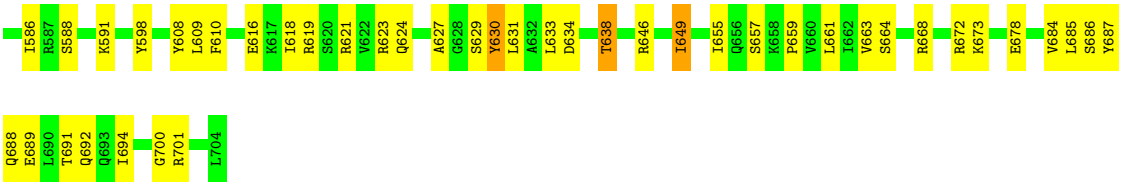
• Molecule 1: Low calcium response locus protein D

Chain PA:

• Molecule 1: Low calcium response locus protein D

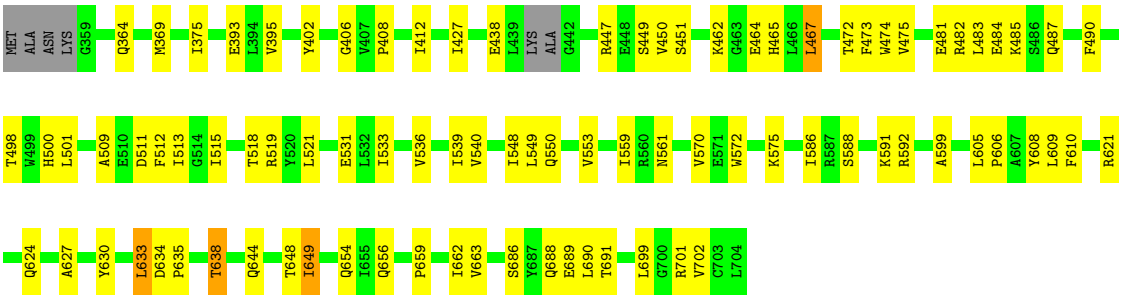
Chain QA:





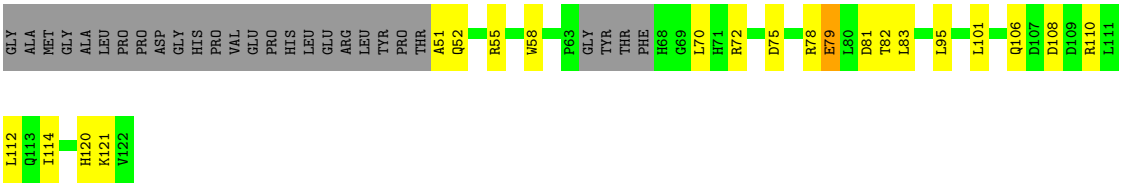
• Molecule 1: Low calcium response locus protein D

Chain RA:



• Molecule 2: Yop proteins translocation protein X

Chain CB:

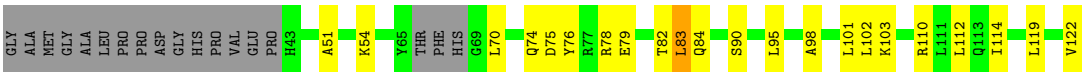


• Molecule 2: Yop proteins translocation protein X

Chain JB:

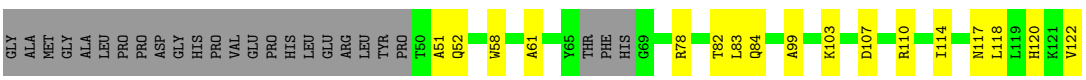
• Molecule 2: Yop proteins translocation protein X

Chain KB:



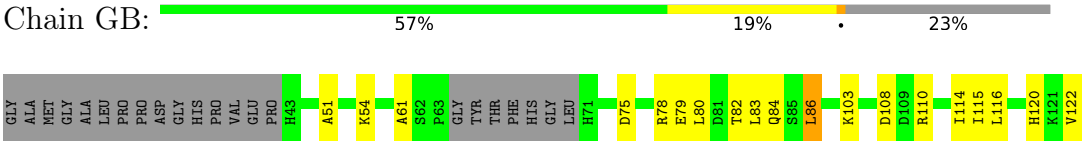
• Molecule 2: Yop proteins translocation protein X

Chain RB:



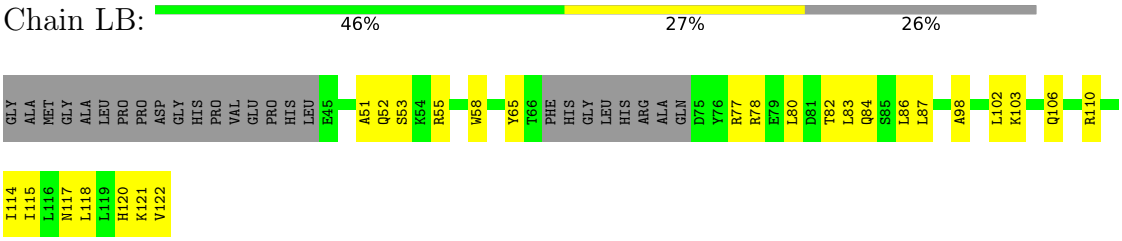
• Molecule 2: Yop proteins translocation protein X

Chain GB:



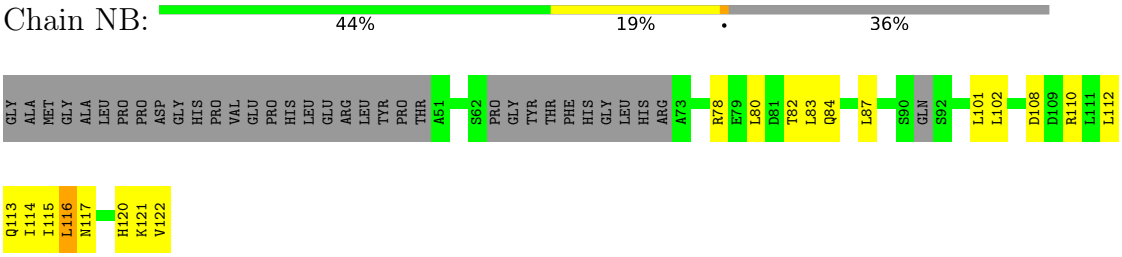
• Molecule 2: Yop proteins translocation protein X

Chain LB:



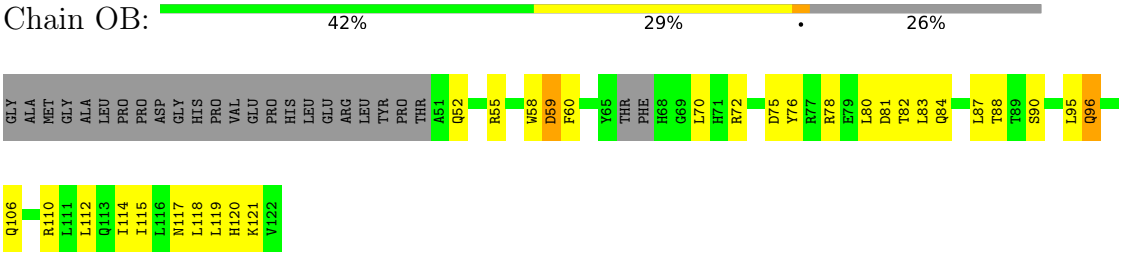
• Molecule 2: Yop proteins translocation protein X

Chain NB:



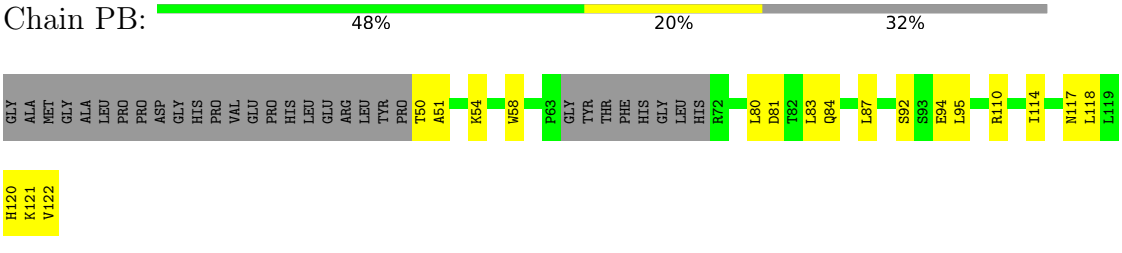
• Molecule 2: Yop proteins translocation protein X

Chain OB:



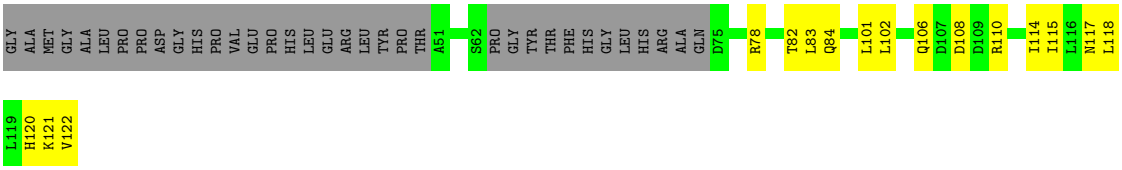
• Molecule 2: Yop proteins translocation protein X

Chain PB:



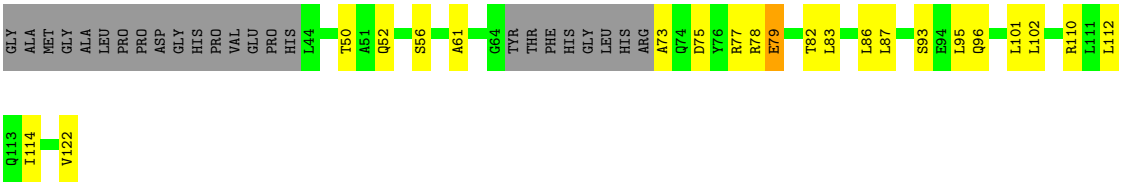
• Molecule 2: Yop proteins translocation protein X

Chain EB:



• Molecule 2: Yop proteins translocation protein X

Chain FB:

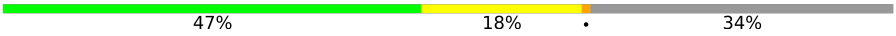


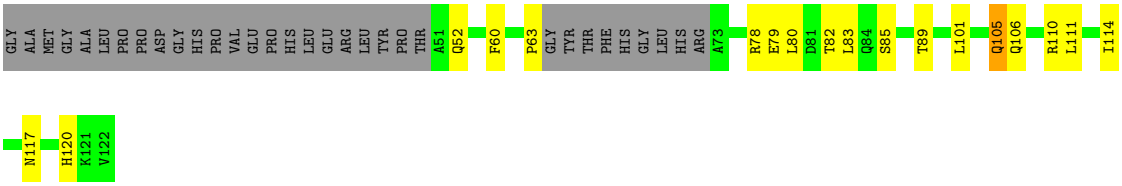
• Molecule 2: Yop proteins translocation protein X

Chain HB:

• Molecule 2: Yop proteins translocation protein X

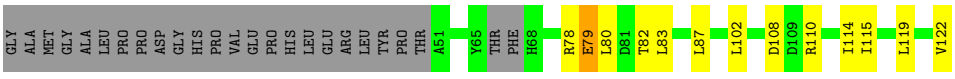
Chain IB:





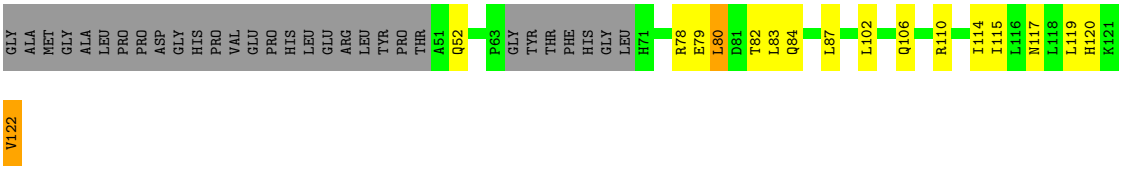
• Molecule 2: Yop proteins translocation protein X

Chain AB:



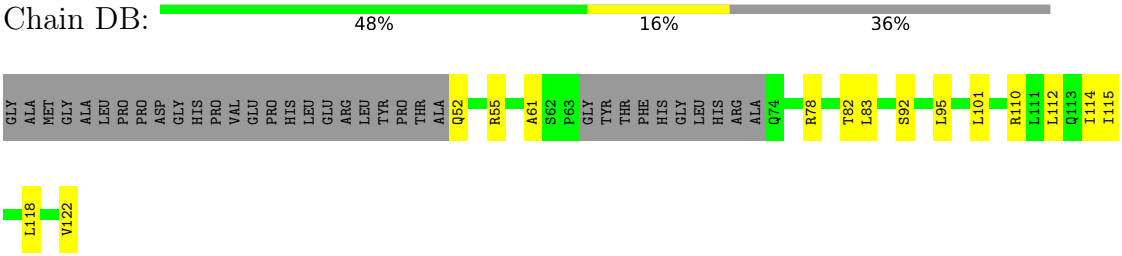
• Molecule 2: Yop proteins translocation protein X

Chain BB:



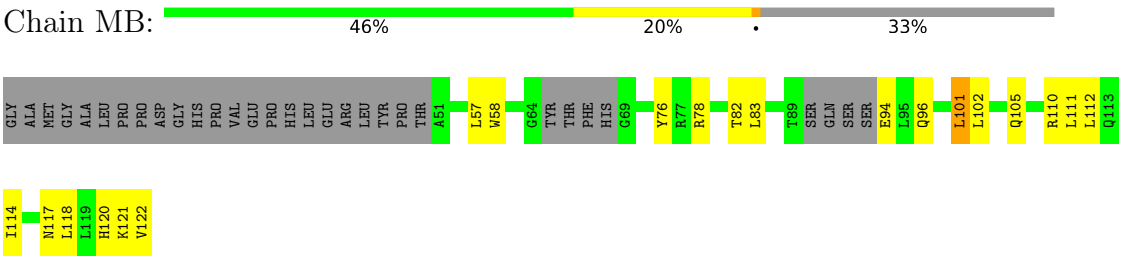
• Molecule 2: Yop proteins translocation protein X

Chain DB:



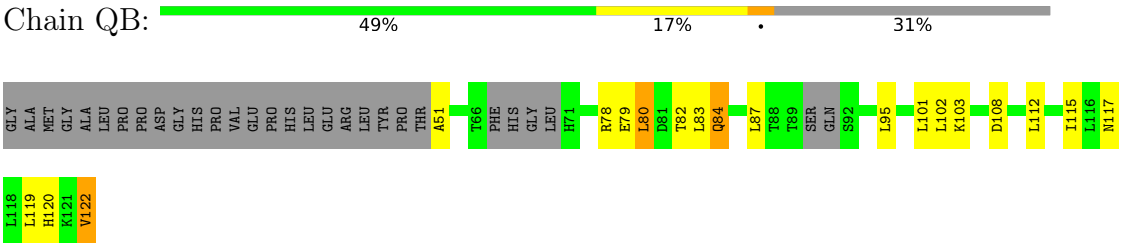
• Molecule 2: Yop proteins translocation protein X

Chain MB:



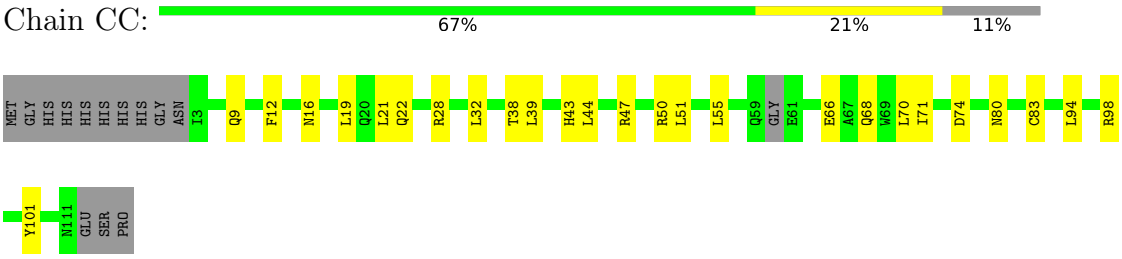
• Molecule 2: Yop proteins translocation protein X

Chain QB:



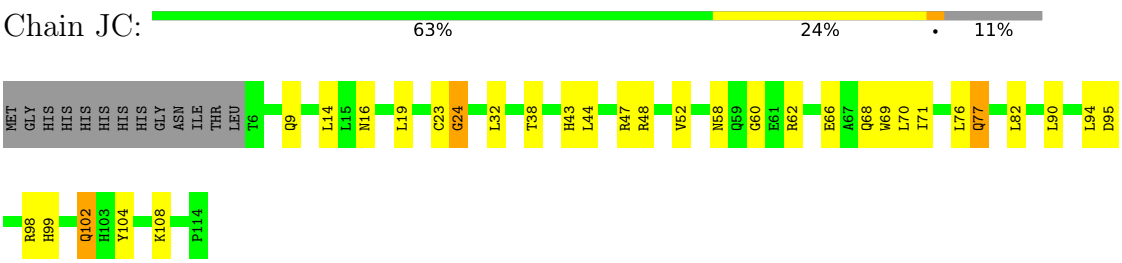
• Molecule 3: Chaperone protein YscY

Chain CC:



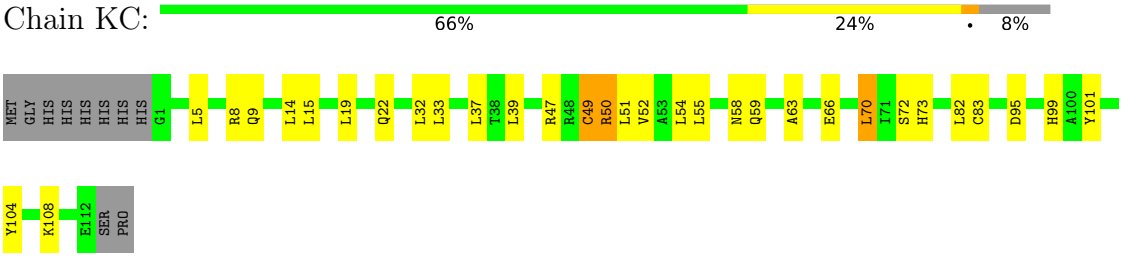
• Molecule 3: Chaperone protein YscY

Chain JC:



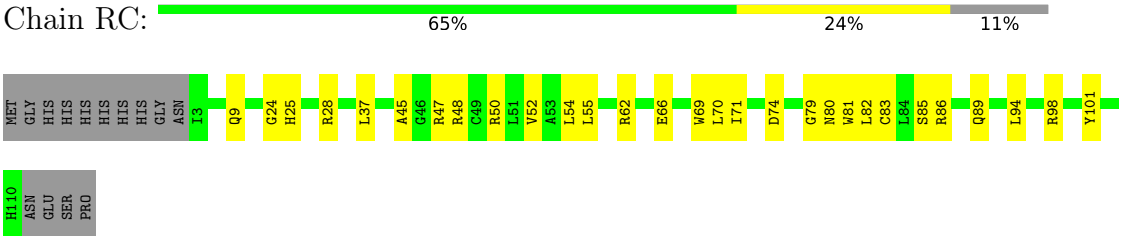
• Molecule 3: Chaperone protein YscY

Chain KC:



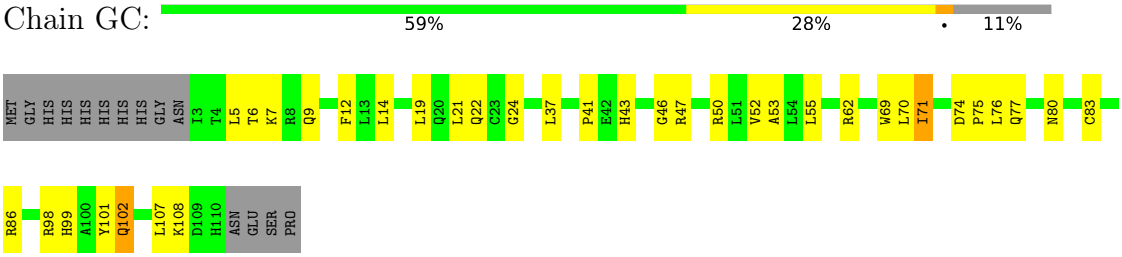
• Molecule 3: Chaperone protein YscY

Chain RC:



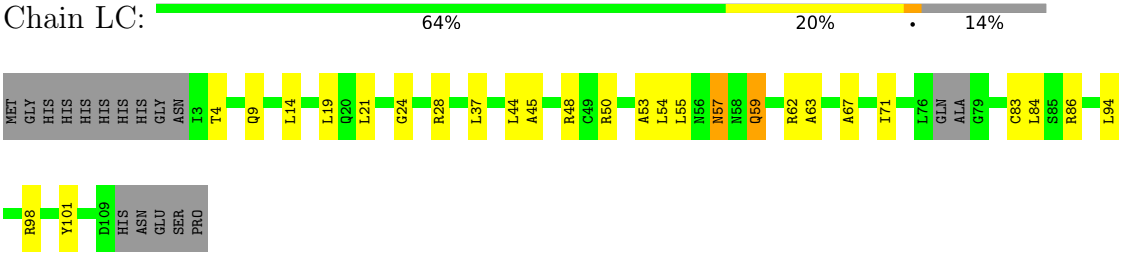
• Molecule 3: Chaperone protein YscY

Chain GC:



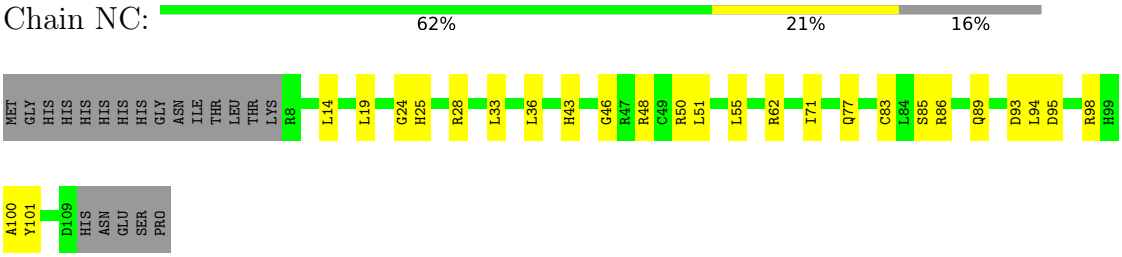
• Molecule 3: Chaperone protein YscY

Chain LC:



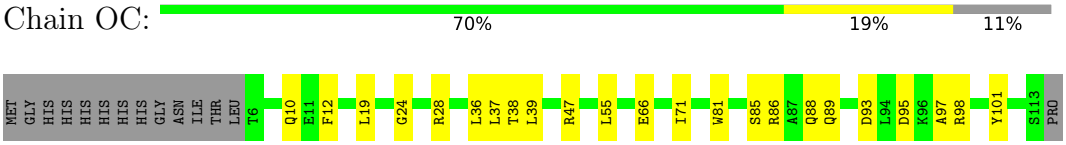
• Molecule 3: Chaperone protein YscY

Chain NC:



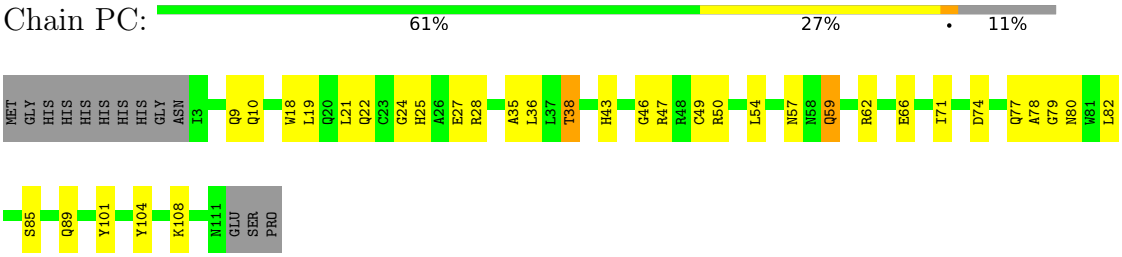
• Molecule 3: Chaperone protein YscY

Chain OC:



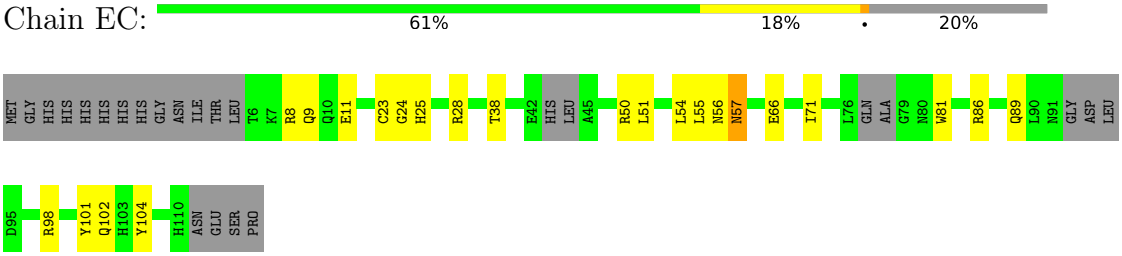
• Molecule 3: Chaperone protein YscY

Chain PC:



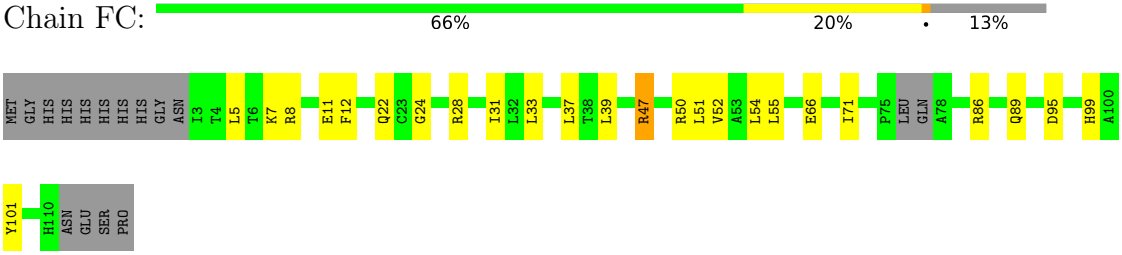
• Molecule 3: Chaperone protein YscY

Chain EC:



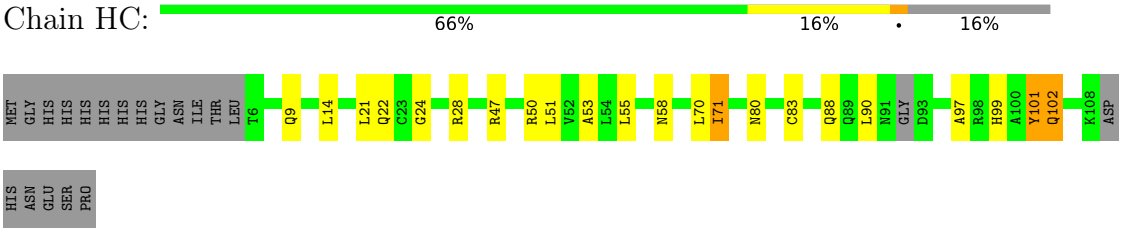
• Molecule 3: Chaperone protein YscY

Chain FC:



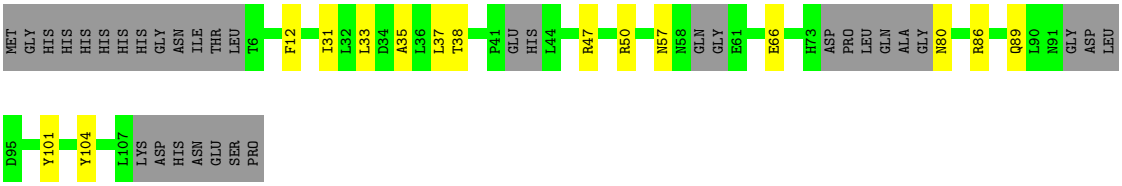
• Molecule 3: Chaperone protein YscY

Chain HC:



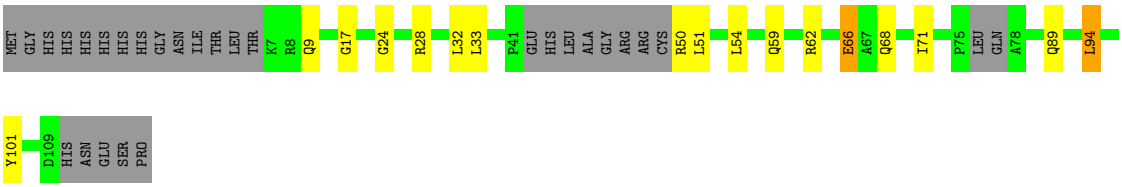
• Molecule 3: Chaperone protein YscY

Chain IC:



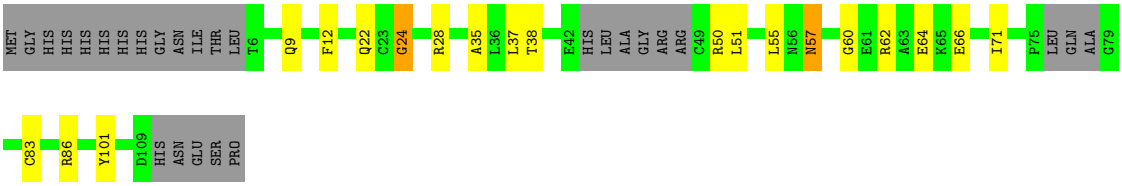
• Molecule 3: Chaperone protein YscY

Chain AC:



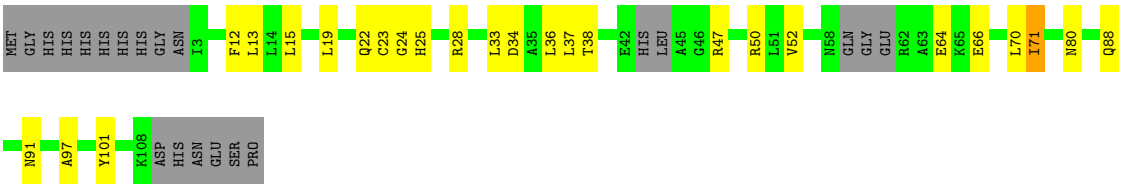
• Molecule 3: Chaperone protein YscY

Chain BC:



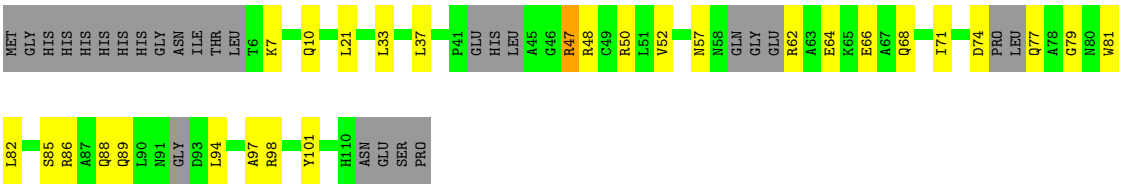
• Molecule 3: Chaperone protein YscY

Chain DC:



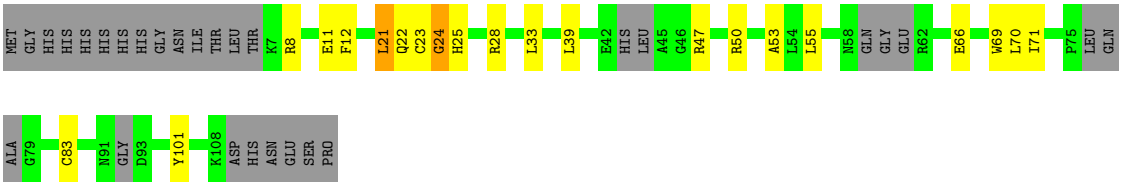
• Molecule 3: Chaperone protein YscY

Chain MC:



• Molecule 3: Chaperone protein YscY

Chain QC:


MET GLY HIS HIS HIS HIS HIS GLY ASN ILE THR LEU THR K7 R8 E11 F12 L21 Q22 C23 G24 H25 R28 L33 L39 E42 HIS LEU A45 G46 R47 R50 A53 L54 L55 N58 GLN GLY GLU R62 E66 W69 L70 I71 P75 LEU GLN
ALA G79 C83 N91 GLY D93 Y101 K108 ASP HIS ASN GLU SER PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	143.46Å 324.92Å 369.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 4.10 49.83 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.83-4.10) 91.0 (49.83-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.305 , 0.325 0.306 , 0.323	Depositor DCC
R_{free} test set	6770 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	153.2	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	73488	wwPDB-VP
Average B, all atoms (Å^2)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	AA	0.24	0/2667	0.49	0/3597
1	BA	0.24	0/2731	0.50	0/3689
1	CA	0.24	0/2838	0.51	0/3832
1	DA	0.24	0/2704	0.50	0/3652
1	EA	0.24	0/2725	0.49	0/3674
1	FA	0.24	0/2779	0.50	0/3749
1	GA	0.25	0/2817	0.52	0/3805
1	HA	0.24	0/2770	0.49	0/3741
1	IA	0.24	0/2775	0.50	0/3749
1	JA	0.24	0/2732	0.50	0/3690
1	KA	0.25	0/2778	0.50	0/3749
1	LA	0.24	0/2777	0.50	0/3749
1	MA	0.24	0/2673	0.51	0/3607
1	NA	0.24	0/2741	0.50	0/3699
1	OA	0.24	0/2734	0.50	0/3687
1	PA	0.24	0/2730	0.50	0/3687
1	QA	0.24	0/2756	0.50	0/3722
1	RA	0.25	0/2845	0.51	0/3844
2	AB	0.24	0/569	0.53	0/765
2	BB	0.24	0/529	0.57	0/711
2	CB	0.25	0/552	0.55	0/742
2	DB	0.24	0/497	0.53	0/668
2	EB	0.24	0/485	0.52	0/651
2	FB	0.25	0/581	0.57	0/783
2	GB	0.24	0/604	0.62	1/814 (0.1%)
2	HB	0.25	0/529	0.54	0/711
2	IB	0.25	0/507	0.54	0/682
2	JB	0.25	0/561	0.50	0/756
2	KB	0.25	0/633	0.60	1/853 (0.1%)
2	LB	0.26	0/579	0.59	0/781
2	MB	0.24	0/517	0.54	1/693 (0.1%)
2	NB	0.26	0/489	0.62	0/655
2	OB	0.24	0/569	0.56	0/765
2	PB	0.24	0/525	0.55	0/706

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	QB	0.25	0/537	0.55	0/721
2	RB	0.25	0/565	0.52	0/760
3	AC	0.23	0/766	0.48	0/1033
3	BC	0.23	0/783	0.47	0/1056
3	CC	0.23	0/894	0.49	0/1208
3	DC	0.23	0/829	0.50	0/1118
3	EC	0.22	0/812	0.48	0/1092
3	FC	0.23	0/873	0.49	0/1179
3	GC	0.23	0/897	0.50	0/1213
3	HC	0.24	0/844	0.50	0/1139
3	IC	0.23	0/741	0.50	0/995
3	JC	0.24	0/900	0.49	0/1216
3	KC	0.26	0/920	0.56	0/1244
3	LC	0.24	0/865	0.53	0/1168
3	MC	0.23	0/794	0.49	0/1066
3	NC	0.23	0/841	0.49	0/1137
3	OC	0.23	0/891	0.45	0/1204
3	PC	0.24	0/899	0.50	0/1216
3	QC	0.22	0/771	0.46	0/1035
3	RC	0.24	0/897	0.50	0/1213
All	All	0.24	0/74617	0.51	3/100671 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	GB	86	LEU	CA-CB-CG	6.65	130.60	115.30
2	MB	101	LEU	CA-CB-CG	5.39	127.70	115.30
2	KB	83	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

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	AA	2628	0	2660	58	0
1	BA	2688	0	2723	57	0
1	CA	2792	0	2814	73	0
1	DA	2661	0	2673	66	0
1	EA	2684	0	2705	54	0
1	FA	2736	0	2757	55	0
1	GA	2772	0	2792	67	0
1	HA	2727	0	2759	51	0
1	IA	2731	0	2754	63	0
1	JA	2689	0	2714	57	0
1	KA	2736	0	2772	63	0
1	LA	2734	0	2761	59	0
1	MA	2632	0	2673	59	0
1	NA	2698	0	2713	63	0
1	OA	2694	0	2723	63	0
1	PA	2688	0	2719	61	0
1	QA	2713	0	2739	73	0
1	RA	2798	0	2815	66	0
2	AB	562	0	560	11	0
2	BB	524	0	527	13	0
2	CB	546	0	548	18	0
2	DB	493	0	497	11	0
2	EB	482	0	487	14	0
2	FB	572	0	579	20	0
2	GB	596	0	598	10	0
2	HB	524	0	527	13	0
2	IB	503	0	507	13	0
2	JB	554	0	549	10	0
2	KB	624	0	624	20	0
2	LB	569	0	571	22	0
2	MB	513	0	520	13	0
2	NB	487	0	491	14	0
2	OB	562	0	560	23	0
2	PB	521	0	527	15	0
2	QB	532	0	532	15	0
2	RB	559	0	560	15	0
3	AC	754	0	744	11	0
3	BC	771	0	757	16	0
3	CC	879	0	873	18	0
3	DC	817	0	823	17	0
3	EC	800	0	790	17	0
3	FC	858	0	851	21	0
3	GC	878	0	876	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	HC	830	0	827	12	0
3	IC	732	0	734	10	0
3	JC	883	0	866	22	0
3	KC	904	0	895	24	0
3	LC	851	0	850	22	0
3	MC	784	0	776	19	0
3	NC	826	0	815	19	0
3	OC	875	0	859	15	0
3	PC	883	0	877	26	0
3	QC	761	0	758	14	0
3	RC	878	0	876	17	0
All	All	73488	0	73877	1436	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 10.

All (1436) 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:QA:687:TYR:HB3	2:QB:119:LEU:HD11	1.44	0.96
2:EB:84:GLN:HE22	2:EB:106:GLN:HB2	1.30	0.94
1:AA:687:TYR:HB3	2:AB:119:LEU:HD11	1.53	0.90
2:BB:87:LEU:HD12	2:BB:102:LEU:HD12	1.59	0.84
1:LA:627:ALA:HB2	1:MA:575:LYS:HD3	1.60	0.82
1:IA:649:ILE:HG22	1:IA:651:ASP:H	1.46	0.81
1:EA:655:ILE:HG12	3:EC:24:GLY:HA3	1.63	0.80
3:KC:37:LEU:HD12	3:KC:50:ARG:HD3	1.64	0.80
1:OA:631:LEU:HD22	1:OA:670:TYR:HB3	1.63	0.79
3:NC:33:LEU:HD22	3:NC:46:GLY:HA2	1.63	0.79
3:NC:55:LEU:HD13	3:NC:86:ARG:HD3	1.66	0.78
2:KB:84:GLN:HE22	2:KB:103:LYS:HE2	1.49	0.77
1:FA:655:ILE:HG12	3:FC:24:GLY:HA3	1.65	0.76
1:JA:604:ILE:HD13	3:JC:19:LEU:HD11	1.68	0.76
1:LA:655:ILE:HD13	3:LC:24:GLY:HA2	1.67	0.76
1:GA:655:ILE:HG21	3:GC:24:GLY:H	1.52	0.75
2:OB:96:GLN:HE22	2:FB:93:SER:HA	1.52	0.75
1:JA:655:ILE:HG12	3:JC:24:GLY:HA3	1.69	0.75
3:JC:47:ARG:HB3	3:JC:70:LEU:HD11	1.69	0.74
1:PA:364:GLN:HE22	1:QA:408:PRO:HB2	1.53	0.74
1:AA:630:TYR:HA	2:BB:122:VAL:HB	1.70	0.73
1:AA:631:LEU:HD22	1:AA:670:TYR:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:609:LEU:HD13	2:KB:112:LEU:HD21	1.69	0.73
1:LA:515:ILE:HD11	1:MA:570:VAL:HG11	1.70	0.73
2:NB:84:GLN:HB2	2:NB:102:LEU:HD22	1.69	0.73
1:PA:483:LEU:HB3	1:PA:490:PHE:HZ	1.54	0.73
1:QA:655:ILE:HG23	3:QC:23:CYS:HA	1.71	0.72
1:DA:487:GLN:O	2:DB:52:GLN:N	2.22	0.72
1:RA:447:ARG:HE	1:RA:472:THR:HG23	1.54	0.72
1:RA:450:VAL:HG21	2:RB:51:ALA:HB2	1.70	0.72
2:OB:72:ARG:HB3	2:OB:75:ASP:HB2	1.71	0.72
1:DA:609:LEU:HD13	2:DB:112:LEU:HD21	1.71	0.72
1:GA:360:ARG:HG2	1:GA:362:GLY:H	1.55	0.72
2:LB:51:ALA:HA	2:LB:55:ARG:HD3	1.72	0.71
3:MC:50:ARG:NH2	3:MC:66:GLU:OE1	2.21	0.71
3:GC:37:LEU:HD12	3:GC:50:ARG:HH11	1.54	0.71
1:FA:447:ARG:HE	1:FA:472:THR:HG23	1.54	0.71
1:JA:483:LEU:HD11	1:JA:488:LEU:HD12	1.71	0.70
1:LA:450:VAL:HG21	2:LB:52:GLN:HG2	1.73	0.70
1:DA:591:LYS:HB3	1:DA:691:THR:HB	1.72	0.70
2:OB:117:ASN:HA	2:OB:120:HIS:CD2	2.27	0.70
2:JB:83:LEU:HD21	3:JC:9:GLN:HG2	1.73	0.69
1:DA:386:GLU:HA	1:DA:390:LEU:HB2	1.74	0.69
2:DB:92:SER:HB3	2:DB:95:LEU:HD13	1.74	0.69
1:CA:657:SER:HB3	3:CC:22:GLN:HG2	1.74	0.69
2:JB:74:GLN:HG2	2:JB:77:ARG:HH21	1.58	0.69
3:OC:10:GLN:HG3	3:OC:36:LEU:HD11	1.73	0.69
2:NB:83:LEU:HB3	2:NB:102:LEU:HD11	1.74	0.69
2:OB:96:GLN:NE2	2:FB:96:GLN:OE1	2.25	0.69
1:GA:442:GLY:O	1:GA:493:HIS:NE2	2.26	0.69
1:IA:389:ALA:HB1	1:IA:392:ASP:HB2	1.74	0.68
1:LA:630:TYR:HB3	2:MB:121:LYS:HA	1.73	0.68
1:PA:515:ILE:HD11	1:QA:570:VAL:HG11	1.75	0.68
2:EB:84:GLN:NE2	2:EB:106:GLN:HB2	2.08	0.68
1:BA:655:ILE:HG12	3:BC:24:GLY:HA3	1.76	0.67
1:PA:699:LEU:O	3:PC:28:ARG:NH1	2.27	0.67
1:AA:655:ILE:HG12	3:AC:24:GLY:HA3	1.77	0.67
2:EB:78:ARG:O	2:EB:82:THR:HG23	1.94	0.67
3:DC:34:ASP:OD1	3:DC:50:ARG:NE	2.27	0.67
1:AA:570:VAL:HG11	1:IA:515:ILE:HD11	1.77	0.67
1:HA:657:SER:HB2	3:HC:22:GLN:O	1.94	0.67
2:KB:78:ARG:O	2:KB:82:THR:HG23	1.95	0.67
2:BB:84:GLN:OE1	2:BB:106:GLN:NE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:425:TYR:HE1	1:NA:440:LYS:HB2	1.61	0.66
1:QA:609:LEU:HD13	2:QB:112:LEU:HD21	1.75	0.66
1:OA:604:ILE:HD13	3:OC:19:LEU:HD21	1.76	0.66
1:PA:604:ILE:HD11	1:PA:697:GLN:HB2	1.75	0.66
1:CA:609:LEU:HD13	2:CB:112:LEU:HD21	1.76	0.66
1:OA:515:ILE:HD11	1:PA:570:VAL:HG11	1.77	0.66
1:BA:631:LEU:HD13	1:BA:670:TYR:HB3	1.76	0.66
1:MA:515:ILE:HD11	1:NA:570:VAL:HG11	1.77	0.66
2:RB:78:ARG:O	2:RB:82:THR:HG23	1.96	0.66
1:DA:412:ILE:HD13	1:DA:501:LEU:HD11	1.78	0.66
1:FA:513:ILE:O	1:FA:550:GLN:NE2	2.25	0.66
2:CB:52:GLN:OE1	2:CB:55:ARG:NH2	2.29	0.66
1:EA:515:ILE:HD11	1:FA:570:VAL:HG11	1.78	0.66
3:GC:47:ARG:HA	3:GC:50:ARG:HG2	1.78	0.66
1:FA:657:SER:HB3	3:FC:22:GLN:HG2	1.77	0.65
3:EC:23:CYS:O	3:EC:25:HIS:ND1	2.27	0.65
1:GA:483:LEU:HB3	1:GA:490:PHE:HZ	1.60	0.65
1:HA:515:ILE:HD11	1:IA:570:VAL:HG11	1.77	0.65
3:EC:55:LEU:HD13	3:EC:86:ARG:HD3	1.79	0.65
3:FC:51:LEU:HD13	3:FC:66:GLU:HB2	1.78	0.65
2:DB:78:ARG:O	2:DB:82:THR:HG23	1.96	0.65
1:OA:412:ILE:HD13	1:OA:501:LEU:HD11	1.79	0.65
1:FA:458:ILE:HG12	1:FA:459:PRO:HD2	1.79	0.65
1:JA:515:ILE:HD11	1:KA:570:VAL:HG11	1.79	0.65
1:PA:591:LYS:HB3	1:PA:691:THR:HB	1.78	0.65
1:MA:393:GLU:HG3	1:MA:498:THR:HG21	1.79	0.64
1:LA:393:GLU:HG3	1:LA:498:THR:HG21	1.80	0.64
2:CB:78:ARG:O	2:CB:82:THR:HG23	1.98	0.64
2:GB:78:ARG:O	2:GB:82:THR:HG23	1.98	0.64
2:DB:61:ALA:HB2	3:DC:52:VAL:HG21	1.77	0.64
2:MB:78:ARG:O	2:MB:82:THR:HG23	1.97	0.64
3:QC:47:ARG:NH1	3:QC:66:GLU:OE1	2.30	0.64
1:RA:699:LEU:O	3:RC:28:ARG:NH1	2.31	0.64
2:LB:78:ARG:O	2:LB:82:THR:HG23	1.97	0.64
2:FB:79:GLU:HG2	3:FC:12:PHE:HB2	1.80	0.64
3:CC:50:ARG:NH1	3:CC:66:GLU:OE2	2.31	0.64
1:GA:447:ARG:HH12	1:GA:449:SER:HB2	1.62	0.64
1:IA:539:ILE:HG22	1:IA:540:VAL:HG13	1.80	0.64
1:KA:375:ILE:HD11	1:KA:501:LEU:HD12	1.80	0.63
1:EA:631:LEU:HD22	1:EA:670:TYR:HB3	1.80	0.63
1:QA:375:ILE:HD11	1:QA:501:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:539:ILE:HG22	1:CA:540:VAL:HG13	1.80	0.63
1:LA:539:ILE:HG22	1:LA:540:VAL:HG13	1.80	0.63
1:QA:513:ILE:O	1:QA:550:GLN:NE2	2.28	0.63
1:AA:394:LEU:HD22	1:AA:501:LEU:HD13	1.80	0.63
1:BA:515:ILE:HD11	1:CA:570:VAL:HG11	1.79	0.63
2:OB:78:ARG:O	2:OB:82:THR:HG23	1.98	0.63
1:MA:609:LEU:HD13	2:MB:112:LEU:HD21	1.81	0.63
2:BB:78:ARG:O	2:BB:82:THR:HG23	1.99	0.63
1:FA:591:LYS:HB3	1:FA:691:THR:HB	1.80	0.63
1:JA:483:LEU:HB3	1:JA:490:PHE:HZ	1.64	0.63
3:GC:41:PRO:O	3:GC:47:ARG:NH2	2.32	0.63
1:JA:631:LEU:HD22	1:JA:670:TYR:HB3	1.81	0.63
2:NB:78:ARG:O	2:NB:82:THR:HG23	1.98	0.63
1:QA:515:ILE:HD11	1:RA:570:VAL:HG11	1.80	0.62
2:FB:87:LEU:HD12	2:FB:102:LEU:HD22	1.79	0.62
1:BA:699:LEU:O	3:BC:28:ARG:NH1	2.32	0.62
2:BB:83:LEU:HD11	3:BC:9:GLN:HG3	1.80	0.62
1:AA:395:VAL:HG23	1:AA:398:ARG:HH21	1.64	0.62
1:LA:699:LEU:O	3:LC:28:ARG:NH1	2.32	0.62
2:HB:78:ARG:O	2:HB:82:THR:HG23	2.00	0.62
1:QA:655:ILE:HG12	3:QC:24:GLY:HA3	1.80	0.62
2:JB:61:ALA:HB2	3:JC:52:VAL:HG21	1.81	0.62
3:NC:48:ARG:NH2	3:NC:77:GLN:OE1	2.32	0.62
3:HC:47:ARG:HA	3:HC:50:ARG:HG2	1.81	0.62
1:OA:539:ILE:HG22	1:OA:540:VAL:HG13	1.81	0.62
1:LA:610:PHE:HE1	1:LA:661:LEU:HD11	1.65	0.62
2:HB:77:ARG:HG2	2:HB:78:ARG:H	1.65	0.62
2:BB:110:ARG:O	2:BB:114:ILE:HG12	2.00	0.62
1:CA:656:GLN:H	1:CA:656:GLN:HE21	1.45	0.62
1:EA:444:LEU:HB3	1:EA:477:VAL:HG13	1.82	0.62
1:LA:373:LEU:HD22	1:LA:412:ILE:HG23	1.81	0.62
1:PA:485:LYS:O	3:PC:108:LYS:NZ	2.27	0.62
1:GA:363:GLU:OE2	1:GA:366:ALA:N	2.32	0.61
1:KA:483:LEU:HD11	1:KA:488:LEU:HD12	1.82	0.61
1:OA:699:LEU:O	3:OC:28:ARG:NH1	2.32	0.61
3:PC:57:ASN:OD1	3:PC:59:GLN:NE2	2.32	0.61
1:CA:634:ASP:O	1:CA:638:THR:HG23	2.00	0.61
1:HA:539:ILE:HG22	1:HA:540:VAL:HG13	1.81	0.61
1:AA:375:ILE:HD11	1:AA:501:LEU:HD12	1.82	0.61
1:AA:412:ILE:HD13	1:AA:501:LEU:HD11	1.82	0.61
1:CA:515:ILE:HD11	1:DA:570:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:600:ASN:OD1	1:CA:601:GLY:N	2.33	0.61
1:MA:591:LYS:HB3	1:MA:691:THR:HB	1.82	0.61
1:DA:402:TYR:O	1:DA:406:GLY:N	2.34	0.61
1:OA:364:GLN:NE2	1:PA:517:GLU:OE1	2.34	0.61
2:FB:61:ALA:HB2	3:FC:52:VAL:HG21	1.83	0.61
1:EA:364:GLN:NE2	1:FA:517:GLU:OE1	2.33	0.61
1:GA:462:LYS:HB2	1:GA:473:PHE:HB3	1.83	0.61
1:IA:375:ILE:HG12	1:IA:427:ILE:HG12	1.83	0.61
1:MA:440:LYS:HB2	1:MA:474:TRP:CD2	2.36	0.61
1:DA:515:ILE:HD11	1:EA:570:VAL:HG11	1.82	0.61
1:PA:656:GLN:HG3	2:PB:50:THR:HG21	1.82	0.61
1:AA:634:ASP:O	1:AA:638:THR:HG23	2.01	0.60
3:CC:44:LEU:HD23	3:CC:70:LEU:HD23	1.83	0.60
3:OC:55:LEU:HD13	3:OC:86:ARG:HD3	1.83	0.60
3:EC:51:LEU:HD13	3:EC:66:GLU:HB2	1.83	0.60
1:BA:483:LEU:HB3	1:BA:490:PHE:HZ	1.67	0.60
1:GA:539:ILE:HG22	1:GA:540:VAL:HG13	1.83	0.60
1:KA:687:TYR:HB3	2:KB:119:LEU:HD11	1.83	0.60
2:JB:110:ARG:O	2:JB:114:ILE:HG12	2.01	0.60
3:BC:55:LEU:HD13	3:BC:86:ARG:HD3	1.82	0.60
1:KA:483:LEU:HB3	1:KA:490:PHE:HZ	1.66	0.60
3:KC:33:LEU:HB2	3:KC:50:ARG:HG3	1.83	0.60
3:DC:47:ARG:HB3	3:DC:70:LEU:HD11	1.82	0.60
1:HA:519:ARG:HG2	1:IA:531:GLU:HG2	1.81	0.60
1:MA:662:ILE:HD13	1:MA:690:LEU:HD11	1.82	0.60
1:HA:511:ASP:OD2	1:IA:592:ARG:NH1	2.33	0.60
1:QA:591:LYS:HB3	1:QA:691:THR:HB	1.81	0.60
2:JB:78:ARG:O	2:JB:82:THR:HG23	2.01	0.60
3:IC:47:ARG:HG3	3:IC:50:ARG:HE	1.65	0.60
1:GA:604:ILE:HG21	3:GC:19:LEU:HD21	1.82	0.60
1:KA:450:VAL:HG21	2:KB:51:ALA:HB2	1.84	0.60
1:AA:531:GLU:HG2	1:IA:519:ARG:HG2	1.83	0.60
1:AA:686:SER:HB2	1:AA:689:GLU:HG3	1.84	0.60
1:FA:364:GLN:HE22	1:GA:408:PRO:HB2	1.66	0.60
2:IB:79:GLU:HG3	2:IB:83:LEU:HD23	1.84	0.60
1:GA:364:GLN:HE22	1:HA:408:PRO:HB2	1.66	0.60
1:DA:662:ILE:HD13	1:DA:690:LEU:HD11	1.84	0.59
1:KA:539:ILE:HG22	1:KA:540:VAL:HG13	1.83	0.59
2:OB:70:LEU:HB2	2:OB:72:ARG:HG3	1.84	0.59
1:DA:513:ILE:O	1:DA:550:GLN:NE2	2.32	0.59
1:AA:556:ASP:O	1:AA:597:LYS:NZ	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:539:ILE:HG22	1:DA:540:VAL:HG13	1.84	0.59
1:FA:441:ALA:HA	1:FA:445:LEU:HB3	1.84	0.59
1:HA:412:ILE:HD13	1:HA:501:LEU:HD11	1.82	0.59
1:JA:511:ASP:OD2	1:KA:592:ARG:NH1	2.34	0.59
1:KA:402:TYR:O	1:KA:406:GLY:N	2.35	0.59
1:PA:631:LEU:HD22	1:PA:670:TYR:HB3	1.84	0.59
1:NA:627:ALA:HB1	1:OA:575:LYS:HD3	1.83	0.59
2:CB:95:LEU:HD11	3:CC:39:LEU:HD21	1.82	0.59
2:FB:95:LEU:HD11	3:FC:39:LEU:HD21	1.84	0.59
1:OA:453:LEU:HA	1:OA:456:LEU:HB2	1.84	0.59
1:QA:402:TYR:O	1:QA:406:GLY:N	2.36	0.59
1:EA:375:ILE:HD11	1:EA:501:LEU:HD12	1.84	0.59
1:JA:393:GLU:HG3	1:JA:498:THR:HG21	1.84	0.59
2:RB:61:ALA:HB2	3:RC:52:VAL:HG21	1.85	0.59
1:BA:539:ILE:HG22	1:BA:540:VAL:HG13	1.85	0.59
1:BA:686:SER:HB2	1:BA:689:GLU:HG3	1.85	0.59
1:EA:662:ILE:HD13	1:EA:690:LEU:HD11	1.85	0.59
1:FA:393:GLU:HG3	1:FA:498:THR:HG21	1.84	0.59
1:IA:591:LYS:HB3	1:IA:691:THR:HB	1.85	0.59
1:JA:570:VAL:HG11	1:RA:515:ILE:HD11	1.83	0.59
1:NA:361:LEU:HD22	1:OA:412:ILE:HB	1.85	0.59
1:NA:402:TYR:O	1:NA:406:GLY:N	2.35	0.59
1:QA:412:ILE:HD13	1:QA:501:LEU:HD11	1.85	0.59
1:RA:656:GLN:HG3	2:RB:58:TRP:CE2	2.37	0.59
3:CC:47:ARG:HA	3:CC:50:ARG:HG2	1.85	0.59
2:LB:110:ARG:O	2:LB:114:ILE:HG13	2.03	0.59
1:GA:454:GLU:HG3	3:GC:86:ARG:HH11	1.66	0.58
1:NA:686:SER:HB2	1:NA:689:GLU:HG3	1.85	0.58
2:AB:87:LEU:HD12	2:AB:102:LEU:HD11	1.86	0.58
3:BC:51:LEU:HD13	3:BC:66:GLU:HB2	1.85	0.58
1:LA:402:TYR:O	1:LA:406:GLY:N	2.36	0.58
1:RA:648:THR:HG21	1:RA:702:VAL:HG22	1.84	0.58
1:DA:634:ASP:O	1:DA:638:THR:HG23	2.03	0.58
1:IA:497:LEU:HA	1:IA:500:HIS:NE2	2.17	0.58
3:CC:51:LEU:HD13	3:CC:66:GLU:HB2	1.85	0.58
2:NB:101:LEU:HD11	3:NC:28:ARG:HG3	1.83	0.58
2:IB:78:ARG:O	2:IB:82:THR:HG23	2.02	0.58
2:IB:79:GLU:HG2	3:IC:12:PHE:HB2	1.85	0.58
1:BA:662:ILE:HD13	1:BA:690:LEU:HD11	1.85	0.58
1:GA:604:ILE:HD13	3:GC:19:LEU:HD11	1.85	0.58
1:PA:539:ILE:HG22	1:PA:540:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:606:PRO:HB3	1:PA:699:LEU:HD11	1.83	0.58
3:JC:58:ASN:HA	3:JC:90:LEU:HD11	1.84	0.58
2:AB:83:LEU:HD11	3:AC:9:GLN:HB3	1.85	0.58
3:AC:59:GLN:HB3	3:AC:62:ARG:HB2	1.84	0.58
1:DA:381:GLN:HB3	1:DA:385:LEU:HD13	1.85	0.58
1:FA:511:ASP:OD2	1:GA:592:ARG:NH1	2.35	0.58
1:JA:610:PHE:HE1	1:JA:661:LEU:HD11	1.67	0.58
1:RA:539:ILE:HG22	1:RA:540:VAL:HG13	1.84	0.58
1:FA:515:ILE:HD11	1:GA:570:VAL:HG11	1.85	0.58
1:FA:539:ILE:HG22	1:FA:540:VAL:HG13	1.86	0.58
1:HA:447:ARG:HE	1:HA:472:THR:HG23	1.68	0.58
1:IA:389:ALA:O	1:IA:391:ASN:N	2.36	0.58
1:IA:673:LYS:HG3	2:AB:122:VAL:HA	1.86	0.58
2:LB:84:GLN:HE21	2:LB:103:LYS:HD3	1.68	0.58
1:EA:634:ASP:O	1:EA:638:THR:HG23	2.02	0.58
1:KA:631:LEU:HD22	1:KA:670:TYR:HB3	1.86	0.58
1:MA:539:ILE:HG22	1:MA:540:VAL:HG13	1.86	0.58
2:FB:86:LEU:HD13	3:FC:5:LEU:HD12	1.85	0.58
2:DB:101:LEU:HD13	3:DC:28:ARG:HD2	1.86	0.58
1:JA:634:ASP:O	1:JA:638:THR:HG23	2.03	0.58
1:OA:375:ILE:HD11	1:OA:501:LEU:HD12	1.86	0.58
1:PA:393:GLU:HG3	1:PA:498:THR:HG21	1.84	0.58
1:CA:375:ILE:HG12	1:CA:427:ILE:HG12	1.86	0.58
1:KA:686:SER:HB2	1:KA:689:GLU:HG3	1.84	0.58
1:NA:511:ASP:OD2	1:OA:592:ARG:NH1	2.36	0.58
1:QA:634:ASP:O	1:QA:638:THR:HG23	2.03	0.58
1:FA:402:TYR:O	1:FA:406:GLY:N	2.37	0.58
1:IA:634:ASP:O	1:IA:638:THR:HG23	2.04	0.58
1:NA:539:ILE:HG22	1:NA:540:VAL:HG13	1.86	0.58
1:NA:631:LEU:HD22	1:NA:670:TYR:HB3	1.86	0.58
2:FB:79:GLU:HG3	2:FB:83:LEU:HD23	1.86	0.58
1:CA:483:LEU:HB3	1:CA:490:PHE:HZ	1.68	0.57
1:GA:631:LEU:HD22	1:GA:670:TYR:HB3	1.85	0.57
1:PA:402:TYR:O	1:PA:406:GLY:N	2.37	0.57
1:GA:662:ILE:HD13	1:GA:690:LEU:HD11	1.86	0.57
1:KA:591:LYS:HB3	1:KA:691:THR:HB	1.86	0.57
1:NA:634:ASP:O	1:NA:638:THR:HG23	2.04	0.57
3:FC:47:ARG:HD2	3:FC:50:ARG:HH11	1.68	0.57
1:DA:631:LEU:HD22	1:DA:670:TYR:HB3	1.85	0.57
1:IA:395:VAL:HG23	1:IA:398:ARG:HH21	1.69	0.57
1:KA:515:ILE:HD11	1:LA:570:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:EC:25:HIS:HB3	3:EC:28:ARG:HB3	1.87	0.57
1:EA:686:SER:HB2	1:EA:689:GLU:HG3	1.86	0.57
1:RA:375:ILE:HD11	1:RA:501:LEU:HD12	1.87	0.57
1:RA:634:ASP:O	1:RA:638:THR:HG23	2.05	0.57
2:RB:110:ARG:O	2:RB:114:ILE:HG13	2.02	0.57
2:OB:95:LEU:HD11	3:OC:39:LEU:HD21	1.86	0.57
1:GA:515:ILE:HD11	1:HA:570:VAL:HG11	1.86	0.57
1:LA:375:ILE:HD11	1:LA:501:LEU:HD12	1.86	0.57
1:NA:655:ILE:HG12	3:NC:24:GLY:HA3	1.86	0.57
1:PA:519:ARG:HG2	1:QA:531:GLU:HG2	1.86	0.57
1:DA:609:LEU:HD23	1:DA:662:ILE:HB	1.85	0.57
1:LA:604:ILE:HD13	3:LC:19:LEU:HD11	1.87	0.57
2:CB:110:ARG:O	2:CB:114:ILE:HG13	2.04	0.57
3:KC:33:LEU:CB	3:KC:50:ARG:HG3	2.35	0.57
3:AC:17:GLY:HA3	3:AC:32:LEU:HD11	1.87	0.57
1:JA:517:GLU:OE1	1:RA:364:GLN:NE2	2.38	0.57
1:OA:393:GLU:HG3	1:OA:498:THR:HG21	1.85	0.57
3:LC:54:LEU:HD23	3:LC:63:ALA:HA	1.86	0.57
3:OC:47:ARG:NH1	3:OC:66:GLU:OE1	2.36	0.57
1:BA:483:LEU:HD11	1:BA:488:LEU:HD12	1.87	0.57
2:PB:58:TRP:HZ3	3:PC:21:LEU:HG	1.70	0.57
3:FC:33:LEU:O	3:FC:50:ARG:NH2	2.36	0.57
3:IC:50:ARG:NH2	3:IC:66:GLU:OE1	2.22	0.57
1:MA:631:LEU:HD22	1:MA:670:TYR:HB3	1.86	0.56
2:IB:110:ARG:O	2:IB:114:ILE:HG23	2.05	0.56
1:AA:390:LEU:HD11	1:AA:497:LEU:HD23	1.87	0.56
1:AA:408:PRO:HB2	1:IA:364:GLN:HE22	1.69	0.56
1:IA:686:SER:HB2	1:IA:689:GLU:HG3	1.87	0.56
1:NA:469:ASP:HB3	1:NA:499:TRP:HH2	1.69	0.56
2:LB:52:GLN:HG3	2:LB:53:SER:H	1.70	0.56
3:PC:10:GLN:HG3	3:PC:36:LEU:HD11	1.87	0.56
1:FA:686:SER:HB2	1:FA:689:GLU:HG3	1.88	0.56
1:IA:483:LEU:HB3	1:IA:490:PHE:HZ	1.70	0.56
1:JA:375:ILE:HD11	1:JA:501:LEU:HD12	1.86	0.56
1:JA:539:ILE:HG22	1:JA:540:VAL:HG13	1.86	0.56
1:MA:447:ARG:HB3	1:MA:474:TRP:CE3	2.40	0.56
1:QA:393:GLU:HG3	1:QA:498:THR:HG21	1.88	0.56
3:KC:58:ASN:O	3:KC:59:GLN:NE2	2.35	0.56
3:MC:7:LYS:HB2	3:MC:10:GLN:HG2	1.88	0.56
1:CA:631:LEU:HD22	1:CA:670:TYR:HB3	1.88	0.56
1:GA:445:LEU:HB3	1:GA:474:TRP:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:519:ARG:HG2	1:DA:531:GLU:HG2	1.87	0.56
1:FA:375:ILE:HG12	1:FA:427:ILE:HG12	1.87	0.56
1:BA:519:ARG:HG2	1:CA:531:GLU:HG2	1.87	0.56
1:GA:591:LYS:HB3	1:GA:691:THR:HB	1.87	0.56
1:IA:644:GLN:O	1:IA:648:THR:OG1	2.23	0.56
1:JA:402:TYR:O	1:JA:406:GLY:N	2.38	0.56
2:JB:88:THR:OG1	2:JB:103:LYS:NZ	2.38	0.56
2:FB:52:GLN:O	2:FB:56:SER:N	2.32	0.56
1:AA:539:ILE:HG22	1:AA:540:VAL:HG13	1.87	0.56
1:CA:402:TYR:O	1:CA:406:GLY:N	2.36	0.56
1:MA:634:ASP:O	1:MA:638:THR:HG23	2.06	0.56
1:QA:373:LEU:HD22	1:QA:412:ILE:HG23	1.88	0.56
1:QA:701:ARG:NE	2:QB:108:ASP:OD1	2.38	0.56
1:RA:393:GLU:HG3	1:RA:498:THR:HG21	1.87	0.56
3:LC:67:ALA:O	3:LC:71:ILE:HG12	2.06	0.56
1:BA:393:GLU:HG3	1:BA:498:THR:HG21	1.87	0.56
1:GA:686:SER:HB2	1:GA:689:GLU:HG3	1.86	0.56
3:GC:21:LEU:HD13	3:GC:53:ALA:HA	1.88	0.56
1:HA:375:ILE:HD11	1:HA:501:LEU:HD12	1.87	0.56
2:GB:83:LEU:HD21	3:GC:9:GLN:HB3	1.88	0.56
3:BC:37:LEU:HD11	3:BC:50:ARG:NE	2.21	0.56
1:BA:375:ILE:HG12	1:BA:427:ILE:HG12	1.87	0.55
1:EA:402:TYR:O	1:EA:406:GLY:N	2.40	0.55
1:HA:393:GLU:HG3	1:HA:498:THR:HG21	1.88	0.55
1:HA:631:LEU:HD22	1:HA:670:TYR:HB3	1.87	0.55
2:PB:110:ARG:O	2:PB:114:ILE:HG13	2.05	0.55
1:AA:402:TYR:O	1:AA:406:GLY:N	2.40	0.55
1:BA:657:SER:HB3	3:BC:22:GLN:HG2	1.88	0.55
1:MA:402:TYR:O	1:MA:406:GLY:N	2.37	0.55
1:DA:519:ARG:HG2	1:EA:531:GLU:HG2	1.88	0.55
1:EA:699:LEU:O	3:EC:28:ARG:NH1	2.39	0.55
1:KA:412:ILE:HD13	1:KA:501:LEU:HD11	1.88	0.55
1:PA:450:VAL:HG21	1:PA:488:LEU:HD22	1.88	0.55
1:RA:513:ILE:O	1:RA:550:GLN:NE2	2.28	0.55
3:AC:54:LEU:HD22	3:AC:59:GLN:HG3	1.87	0.55
1:GA:481:GLU:O	1:GA:484:GLU:HG3	2.07	0.55
1:HA:483:LEU:HD11	1:HA:488:LEU:HD12	1.89	0.55
1:QA:394:LEU:HD23	1:QA:498:THR:HG22	1.88	0.55
3:DC:19:LEU:HA	3:DC:22:GLN:HG2	1.87	0.55
1:AA:373:LEU:HD22	1:AA:412:ILE:HG23	1.87	0.55
1:EA:519:ARG:HG2	1:FA:531:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:686:SER:HB2	1:LA:689:GLU:HG3	1.87	0.55
1:QA:655:ILE:HG21	1:QA:659:PRO:HD3	1.89	0.55
1:HA:402:TYR:O	1:HA:406:GLY:N	2.40	0.55
1:JA:449:SER:HB3	1:JA:489:GLU:HG3	1.89	0.55
1:QA:539:ILE:HG22	1:QA:540:VAL:HG13	1.89	0.55
1:BA:634:ASP:O	1:BA:638:THR:HG23	2.06	0.55
1:GA:402:TYR:O	1:GA:406:GLY:N	2.39	0.55
1:JA:686:SER:HB2	1:JA:689:GLU:HG3	1.89	0.55
1:MA:375:ILE:HD11	1:MA:501:LEU:HD12	1.89	0.55
3:OC:81:TRP:O	3:OC:85:SER:OG	2.22	0.55
1:IA:375:ILE:HD11	1:IA:501:LEU:HD12	1.89	0.55
1:KA:447:ARG:NH1	1:KA:472:THR:OG1	2.40	0.55
1:QA:686:SER:HB2	1:QA:689:GLU:HG3	1.89	0.55
2:GB:110:ARG:O	2:GB:114:ILE:HG13	2.07	0.55
2:QB:79:GLU:HG3	2:QB:83:LEU:HD23	1.89	0.55
1:KA:458:ILE:HD11	3:KC:101:TYR:HE2	1.71	0.55
1:MA:364:GLN:HE22	1:NA:408:PRO:HB2	1.72	0.55
1:PA:634:ASP:O	1:PA:638:THR:HG23	2.06	0.55
1:QA:519:ARG:HG2	1:RA:531:GLU:HG2	1.88	0.55
1:QA:661:LEU:HD23	1:QA:684:VAL:HG13	1.87	0.55
1:EA:591:LYS:HB3	1:EA:691:THR:HB	1.89	0.55
1:HA:610:PHE:HE1	1:HA:661:LEU:HD11	1.72	0.55
1:MA:627:ALA:HB2	1:NA:575:LYS:HD3	1.89	0.55
1:GA:375:ILE:HD11	1:GA:501:LEU:HD12	1.89	0.54
1:PA:447:ARG:HE	1:PA:472:THR:HG23	1.71	0.54
3:HC:55:LEU:HD11	3:HC:83:CYS:HA	1.88	0.54
1:GA:375:ILE:HG12	1:GA:427:ILE:HG12	1.90	0.54
1:KA:393:GLU:HG3	1:KA:498:THR:HG21	1.90	0.54
1:KA:446:VAL:N	1:KA:475:VAL:O	2.40	0.54
1:MA:361:LEU:H	1:MA:361:LEU:HD23	1.71	0.54
1:MA:444:LEU:HB3	1:MA:477:VAL:HG13	1.89	0.54
1:QA:483:LEU:HB3	1:QA:490:PHE:HZ	1.71	0.54
3:RC:94:LEU:HD21	3:RC:98:ARG:HH21	1.72	0.54
1:GA:609:LEU:HD23	1:GA:662:ILE:HB	1.90	0.54
1:HA:483:LEU:HB3	1:HA:490:PHE:HZ	1.72	0.54
2:OB:81:ASP:HA	2:OB:84:GLN:HG2	1.89	0.54
3:FC:55:LEU:HD13	3:FC:86:ARG:HD3	1.89	0.54
1:BA:394:LEU:HD22	1:BA:501:LEU:HD13	1.90	0.54
1:CA:466:LEU:HD22	1:CA:466:LEU:H	1.72	0.54
1:DA:393:GLU:HG3	1:DA:498:THR:HG21	1.88	0.54
3:MC:48:ARG:NH2	3:MC:74:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:393:GLU:HG3	1:IA:498:THR:HG21	1.89	0.54
1:LA:634:ASP:O	1:LA:638:THR:HG23	2.07	0.54
2:MB:58:TRP:HZ3	3:MC:21:LEU:HG	1.71	0.54
1:AA:699:LEU:O	3:AC:28:ARG:NH1	2.40	0.54
1:FA:412:ILE:HD13	1:FA:501:LEU:HD11	1.90	0.54
1:JA:447:ARG:HE	1:JA:472:THR:HG23	1.73	0.54
1:LA:412:ILE:HD13	1:LA:501:LEU:HD11	1.88	0.54
1:RA:447:ARG:HH22	1:RA:449:SER:HA	1.72	0.54
1:GA:393:GLU:HG3	1:GA:498:THR:HG21	1.90	0.54
1:IA:402:TYR:O	1:IA:406:GLY:N	2.39	0.54
1:LA:483:LEU:HB3	1:LA:490:PHE:HZ	1.73	0.54
1:OA:402:TYR:O	1:OA:406:GLY:N	2.39	0.54
3:GC:71:ILE:HG13	3:GC:80:ASN:HB3	1.90	0.54
2:AB:110:ARG:O	2:AB:114:ILE:HG13	2.08	0.54
2:MB:83:LEU:HB3	2:MB:102:LEU:HD21	1.90	0.54
1:EA:539:ILE:HG22	1:EA:540:VAL:HG13	1.88	0.54
1:IA:447:ARG:NH2	1:IA:472:THR:OG1	2.40	0.54
1:BA:441:ALA:O	1:BA:493:HIS:NE2	2.39	0.54
1:CA:393:GLU:HG3	1:CA:498:THR:HG21	1.90	0.54
1:DA:375:ILE:HD11	1:DA:501:LEU:HD12	1.89	0.54
1:DA:657:SER:HB2	3:DC:22:GLN:HG3	1.90	0.54
1:MA:513:ILE:O	1:MA:550:GLN:NE2	2.32	0.54
1:PA:375:ILE:HG12	1:PA:427:ILE:HG12	1.90	0.54
1:LA:481:GLU:O	1:LA:484:GLU:HG3	2.08	0.54
1:MA:701:ARG:CZ	2:MB:111:LEU:HD23	2.38	0.54
1:EA:643:GLU:OE1	1:EA:646:ARG:NH2	2.39	0.53
1:GA:483:LEU:HD11	1:GA:488:LEU:HD12	1.89	0.53
1:LA:635:PRO:HD3	2:MB:118:LEU:HD21	1.90	0.53
3:RC:55:LEU:HD11	3:RC:83:CYS:HA	1.89	0.53
3:GC:77:GLN:H	3:GC:107:LEU:HD21	1.74	0.53
1:AA:515:ILE:HD11	1:BA:570:VAL:HG11	1.91	0.53
1:LA:457:GLY:O	3:LC:98:ARG:NH1	2.41	0.53
1:OA:610:PHE:HE1	1:OA:661:LEU:HD11	1.72	0.53
2:RB:120:HIS:O	2:RB:122:VAL:HG23	2.08	0.53
1:BA:511:ASP:OD2	1:CA:592:ARG:NH1	2.41	0.53
1:DA:481:GLU:O	1:DA:484:GLU:HG3	2.08	0.53
1:GA:412:ILE:HD13	1:GA:501:LEU:HD11	1.90	0.53
1:JA:513:ILE:O	1:JA:550:GLN:NE2	2.34	0.53
3:GC:14:LEU:HD11	3:GC:43:HIS:NE2	2.23	0.53
2:FB:79:GLU:HA	2:FB:82:THR:HG22	1.91	0.53
2:IB:85:SER:O	2:IB:89:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:381:GLN:HA	1:DA:384:ALA:HB3	1.90	0.53
1:OA:609:LEU:HD23	1:OA:662:ILE:HB	1.90	0.53
1:LA:604:ILE:HG21	3:LC:19:LEU:HD13	1.91	0.53
1:OA:448:GLU:HG2	1:OA:449:SER:H	1.74	0.53
1:OA:511:ASP:OD2	1:PA:592:ARG:NH1	2.36	0.53
3:LC:45:ALA:HA	3:LC:48:ARG:HE	1.73	0.53
3:PC:79:GLY:HA2	3:PC:82:LEU:HD23	1.90	0.53
1:BA:609:LEU:HD23	1:BA:662:ILE:HB	1.90	0.53
1:BA:644:GLN:O	1:BA:648:THR:OG1	2.26	0.53
1:EA:393:GLU:HG3	1:EA:498:THR:HG21	1.90	0.53
1:PA:609:LEU:HD23	1:PA:662:ILE:HB	1.89	0.53
2:HB:110:ARG:O	2:HB:114:ILE:HG13	2.09	0.53
3:HC:71:ILE:HG13	3:HC:80:ASN:HB3	1.90	0.53
2:MB:117:ASN:HA	2:MB:120:HIS:CE1	2.43	0.53
1:AA:610:PHE:HE1	1:AA:661:LEU:HD11	1.73	0.53
1:CA:688:GLN:N	1:CA:688:GLN:OE1	2.41	0.53
3:IC:37:LEU:HD11	3:IC:50:ARG:NE	2.23	0.53
1:AA:483:LEU:HB3	1:AA:490:PHE:HZ	1.73	0.53
1:CA:688:GLN:HE21	2:CB:121:LYS:HE3	1.74	0.53
1:HA:662:ILE:HD13	1:HA:690:LEU:HD11	1.89	0.53
1:OA:686:SER:HB2	1:OA:689:GLU:HG3	1.89	0.53
1:RA:686:SER:HB2	1:RA:689:GLU:HG3	1.90	0.53
3:GC:69:TRP:HE3	3:GC:70:LEU:HD12	1.74	0.53
1:CA:481:GLU:O	1:CA:484:GLU:HG3	2.09	0.53
1:CA:621:ARG:HG3	1:CA:633:LEU:HA	1.91	0.53
1:RA:402:TYR:O	1:RA:406:GLY:N	2.41	0.53
1:CA:385:LEU:HG	1:CA:386:GLU:H	1.74	0.53
1:GA:701:ARG:NH1	2:GB:108:ASP:OD1	2.38	0.53
1:MA:609:LEU:HD23	1:MA:662:ILE:HB	1.91	0.53
1:QA:511:ASP:OD2	1:RA:592:ARG:NH1	2.41	0.53
2:LB:52:GLN:CG	2:LB:53:SER:H	2.21	0.53
2:EB:83:LEU:HD21	3:EC:9:GLN:HB3	1.89	0.53
3:HC:58:ASN:HA	3:HC:90:LEU:HD13	1.89	0.53
1:DA:600:ASN:ND2	1:DA:657:SER:O	2.42	0.52
1:EA:511:ASP:OD2	1:FA:592:ARG:NH1	2.40	0.52
3:GC:76:LEU:HB3	3:GC:107:LEU:HD21	1.91	0.52
3:PC:19:LEU:HA	3:PC:22:GLN:HG2	1.91	0.52
3:DC:71:ILE:HG13	3:DC:80:ASN:HB3	1.90	0.52
1:DA:686:SER:HB2	1:DA:689:GLU:HG3	1.89	0.52
1:FA:688:GLN:OE1	1:FA:688:GLN:N	2.41	0.52
1:MA:643:GLU:OE1	1:MA:646:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:361:LEU:HD23	1:EA:361:LEU:H	1.74	0.52
1:IA:669:ARG:HE	1:IA:673:LYS:HE2	1.75	0.52
1:MA:475:VAL:HG22	1:MA:479:TYR:HD2	1.74	0.52
1:QA:449:SER:OG	1:QA:469:ASP:OD2	2.28	0.52
1:QA:481:GLU:O	1:QA:484:GLU:HG3	2.08	0.52
3:JC:60:GLY:H	3:JC:90:LEU:HD22	1.75	0.52
2:QB:95:LEU:HD11	3:QC:39:LEU:HD21	1.91	0.52
1:CA:375:ILE:HD11	1:CA:501:LEU:HD12	1.91	0.52
1:DA:688:GLN:N	1:DA:688:GLN:OE1	2.43	0.52
1:EA:624:GLN:OE1	1:EA:624:GLN:N	2.37	0.52
1:HA:686:SER:HB2	1:HA:689:GLU:HG3	1.91	0.52
1:IA:662:ILE:HD13	1:IA:690:LEU:HD11	1.91	0.52
1:RA:412:ILE:HD13	1:RA:501:LEU:HD11	1.91	0.52
3:FC:7:LYS:HG2	3:FC:8:ARG:H	1.73	0.52
2:IB:80:LEU:HD21	2:IB:105:GLN:HE21	1.74	0.52
1:CA:591:LYS:HB3	1:CA:691:THR:HB	1.92	0.52
1:HA:444:LEU:HD13	1:HA:477:VAL:HG11	1.92	0.52
1:IA:643:GLU:OE1	1:IA:646:ARG:NH2	2.42	0.52
1:QA:375:ILE:HG12	1:QA:427:ILE:HG12	1.91	0.52
3:KC:15:LEU:O	3:KC:19:LEU:HD23	2.10	0.52
1:FA:609:LEU:HD13	2:FB:112:LEU:HD21	1.92	0.52
1:IA:701:ARG:CZ	2:IB:111:LEU:HD23	2.40	0.52
1:KA:513:ILE:O	1:KA:550:GLN:NE2	2.36	0.52
1:RA:654:GLN:HB3	1:RA:656:GLN:HG2	1.92	0.52
3:JC:47:ARG:HG3	3:JC:69:TRP:HZ3	1.75	0.52
1:DA:604:ILE:HD13	3:DC:19:LEU:HD11	1.91	0.52
1:QA:549:LEU:HB3	1:QA:559:ILE:HD11	1.91	0.52
2:MB:110:ARG:O	2:MB:114:ILE:HG13	2.10	0.52
1:CA:483:LEU:HD11	1:CA:488:LEU:HD12	1.92	0.52
1:FA:375:ILE:HD11	1:FA:501:LEU:HD12	1.91	0.52
1:GA:655:ILE:HG22	1:GA:656:GLN:H	1.75	0.52
1:QA:673:LYS:HE2	2:RB:122:VAL:H	1.74	0.52
3:GC:47:ARG:HG3	3:GC:50:ARG:HD3	1.91	0.52
1:AA:662:ILE:HD13	1:AA:690:LEU:HD11	1.91	0.51
1:DA:483:LEU:HB3	1:DA:490:PHE:HZ	1.75	0.51
1:FA:379:SER:O	1:FA:380:SER:OG	2.23	0.51
1:FA:483:LEU:O	1:FA:487:GLN:N	2.42	0.51
1:GA:379:SER:O	1:GA:380:SER:OG	2.26	0.51
1:GA:610:PHE:HE1	1:GA:661:LEU:HD11	1.75	0.51
1:IA:481:GLU:O	1:IA:484:GLU:HG3	2.10	0.51
1:MA:551:ARG:HH12	2:NB:122:VAL:HG12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:373:LEU:HD22	1:OA:412:ILE:HG23	1.91	0.51
1:PA:509:ALA:HA	1:PA:512:PHE:HD2	1.75	0.51
2:IB:117:ASN:HA	2:IB:120:HIS:CE1	2.46	0.51
1:FA:430:GLN:OE1	1:GA:561:ASN:ND2	2.28	0.51
1:QA:657:SER:HB2	3:QC:22:GLN:HG2	1.90	0.51
1:RA:481:GLU:O	1:RA:484:GLU:HG3	2.10	0.51
1:RA:644:GLN:O	1:RA:648:THR:HG22	2.10	0.51
1:AA:561:ASN:ND2	1:IA:430:GLN:OE1	2.33	0.51
1:DA:511:ASP:OD2	1:EA:592:ARG:NH1	2.36	0.51
1:IA:513:ILE:O	1:IA:550:GLN:NE2	2.36	0.51
1:JA:609:LEU:HD23	1:JA:662:ILE:HB	1.92	0.51
1:NA:375:ILE:HD11	1:NA:501:LEU:HD12	1.93	0.51
1:RA:591:LYS:HB3	1:RA:691:THR:HB	1.92	0.51
2:GB:61:ALA:HB2	3:GC:52:VAL:HG21	1.93	0.51
2:EB:117:ASN:O	2:EB:120:HIS:NE2	2.44	0.51
2:BB:83:LEU:HD21	3:BC:9:GLN:HA	1.92	0.51
1:PA:361:LEU:H	1:PA:361:LEU:HD23	1.76	0.51
1:CA:462:LYS:HB2	1:CA:473:PHE:HB3	1.92	0.51
1:FA:609:LEU:HD23	1:FA:662:ILE:HB	1.92	0.51
1:JA:519:ARG:HG2	1:KA:531:GLU:HG2	1.91	0.51
1:LA:430:GLN:OE1	1:MA:561:ASN:ND2	2.31	0.51
1:MA:483:LEU:HB3	1:MA:490:PHE:HZ	1.74	0.51
1:PA:610:PHE:HE1	1:PA:661:LEU:HD11	1.76	0.51
1:AA:394:LEU:HD23	1:AA:498:THR:HG22	1.91	0.51
1:BA:610:PHE:HE1	1:BA:661:LEU:HD11	1.76	0.51
1:MA:481:GLU:O	1:MA:484:GLU:HG3	2.11	0.51
1:OA:609:LEU:HD13	2:OB:112:LEU:HD21	1.92	0.51
1:OA:611:ASP:OD1	1:OA:701:ARG:NH2	2.40	0.51
2:JB:87:LEU:O	2:JB:90:SER:HB3	2.10	0.51
3:LC:55:LEU:HD11	3:LC:83:CYS:HA	1.92	0.51
2:NB:87:LEU:HD12	2:NB:102:LEU:HD12	1.92	0.51
3:EC:81:TRP:HB2	3:EC:104:TYR:HB2	1.92	0.51
3:DC:64:GLU:OE1	3:DC:91:ASN:ND2	2.44	0.51
1:FA:386:GLU:HA	1:FA:390:LEU:HB2	1.92	0.51
1:FA:644:GLN:O	1:FA:648:THR:OG1	2.29	0.51
1:PA:375:ILE:HD11	1:PA:501:LEU:HD12	1.92	0.51
3:JC:82:LEU:HB2	3:JC:104:TYR:CE1	2.46	0.51
3:HC:21:LEU:HD21	3:HC:53:ALA:HA	1.92	0.51
1:JA:675:ILE:HD12	1:JA:682:LEU:HD23	1.93	0.51
1:KA:481:GLU:O	1:KA:484:GLU:HG3	2.10	0.51
3:KC:104:TYR:CZ	3:KC:108:LYS:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:634:ASP:O	1:OA:638:THR:HG23	2.10	0.51
2:FB:110:ARG:O	2:FB:114:ILE:HG13	2.11	0.51
1:CA:379:SER:O	1:CA:380:SER:OG	2.27	0.50
1:CA:699:LEU:O	3:CC:28:ARG:NH1	2.44	0.50
1:IA:688:GLN:N	1:IA:688:GLN:OE1	2.44	0.50
1:JA:591:LYS:HB3	1:JA:691:THR:HB	1.92	0.50
1:LA:375:ILE:HG12	1:LA:427:ILE:HG12	1.93	0.50
1:PA:390:LEU:O	1:PA:391:ASN:HB2	2.11	0.50
1:NA:375:ILE:HG12	1:NA:427:ILE:HG12	1.93	0.50
3:DC:47:ARG:NH2	3:DC:66:GLU:OE1	2.43	0.50
2:QB:78:ARG:O	2:QB:82:THR:HG23	2.11	0.50
1:AA:509:ALA:HA	1:AA:512:PHE:HD2	1.77	0.50
1:BA:591:LYS:HB3	1:BA:691:THR:HB	1.93	0.50
1:CA:364:GLN:HE22	1:DA:408:PRO:HB2	1.75	0.50
1:HA:487:GLN:O	2:HB:52:GLN:HB3	2.11	0.50
1:OA:549:LEU:HB3	1:OA:559:ILE:HD11	1.92	0.50
2:AB:79:GLU:HG3	2:AB:83:LEU:HD23	1.93	0.50
1:BA:481:GLU:O	1:BA:484:GLU:HG3	2.12	0.50
1:DA:587:ARG:NE	1:DA:689:GLU:OE2	2.41	0.50
1:PA:686:SER:HB2	1:PA:689:GLU:HG3	1.94	0.50
2:MB:76:TYR:OH	2:MB:105:GLN:OE1	2.29	0.50
1:GA:408:PRO:HG3	1:GA:521:LEU:HD21	1.93	0.50
1:HA:481:GLU:O	1:HA:484:GLU:HG3	2.11	0.50
1:MA:394:LEU:HD22	1:MA:501:LEU:HD13	1.94	0.50
1:RA:609:LEU:HD23	1:RA:662:ILE:HB	1.93	0.50
1:RA:662:ILE:HD13	1:RA:690:LEU:HD11	1.93	0.50
1:FA:634:ASP:O	1:FA:638:THR:HG23	2.12	0.50
1:HA:379:SER:O	1:HA:380:SER:OG	2.27	0.50
1:KA:610:PHE:HE1	1:KA:661:LEU:HD11	1.75	0.50
1:RA:606:PRO:HB3	1:RA:699:LEU:HD11	1.94	0.50
2:OB:59:ASP:OD1	2:OB:60:PHE:N	2.44	0.50
2:EB:110:ARG:O	2:EB:114:ILE:HG13	2.11	0.50
3:MC:37:LEU:HD11	3:MC:50:ARG:NE	2.26	0.50
1:AA:561:ASN:HD22	1:IA:370:THR:HG21	1.75	0.50
1:FA:610:PHE:HE1	1:FA:661:LEU:HD11	1.77	0.50
1:PA:394:LEU:HD22	1:PA:501:LEU:HD13	1.94	0.50
3:RC:45:ALA:O	3:RC:48:ARG:HG2	2.12	0.50
3:RC:81:TRP:O	3:RC:85:SER:OG	2.19	0.50
3:GC:55:LEU:HD11	3:GC:83:CYS:HA	1.94	0.50
1:CA:624:GLN:OE1	1:CA:624:GLN:N	2.36	0.50
1:EA:688:GLN:N	1:EA:688:GLN:OE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:549:LEU:HB3	1:IA:559:ILE:HD11	1.93	0.50
1:OA:688:GLN:N	1:OA:688:GLN:OE1	2.45	0.50
1:QA:649:ILE:HD12	1:QA:700:GLY:HA3	1.94	0.50
3:QC:23:CYS:O	3:QC:25:HIS:N	2.44	0.50
1:IA:509:ALA:HA	1:IA:512:PHE:HD2	1.77	0.50
1:JA:364:GLN:HE22	1:KA:408:PRO:HB2	1.77	0.50
2:LB:87:LEU:HD12	2:LB:102:LEU:HD11	1.93	0.50
1:EA:688:GLN:HG2	2:EB:121:LYS:HE3	1.93	0.49
1:FA:624:GLN:OE1	1:FA:624:GLN:N	2.39	0.49
1:NA:412:ILE:HD13	1:NA:501:LEU:HD11	1.94	0.49
1:QA:646:ARG:NH1	1:QA:678:GLU:OE1	2.45	0.49
1:EA:656:GLN:HG3	1:EA:657:SER:H	1.78	0.49
3:RC:69:TRP:HE3	3:RC:70:LEU:HD12	1.77	0.49
3:PC:74:ASP:OD1	3:PC:74:ASP:N	2.44	0.49
2:HB:84:GLN:HE22	2:HB:106:GLN:NE2	2.09	0.49
2:QB:117:ASN:HA	2:QB:120:HIS:CE1	2.46	0.49
1:AA:591:LYS:HB3	1:AA:691:THR:HB	1.93	0.49
1:BA:373:LEU:HD22	1:BA:412:ILE:HG23	1.93	0.49
1:BA:688:GLN:N	1:BA:688:GLN:OE1	2.45	0.49
1:DA:389:ALA:HB1	1:DA:392:ASP:H	1.77	0.49
1:GA:389:ALA:HB1	1:GA:393:GLU:HB2	1.94	0.49
1:JA:655:ILE:HG23	3:JC:23:CYS:HA	1.94	0.49
1:LA:518:THR:HG22	1:LA:549:LEU:HD12	1.95	0.49
1:NA:644:GLN:O	1:NA:648:THR:OG1	2.30	0.49
1:OA:644:GLN:O	1:OA:648:THR:OG1	2.29	0.49
1:OA:687:TYR:HB3	2:OB:119:LEU:HD11	1.94	0.49
1:CA:686:SER:HB2	1:CA:689:GLU:HG3	1.94	0.49
1:HA:588:SER:O	1:HA:591:LYS:HG3	2.13	0.49
1:KA:519:ARG:HG2	1:LA:531:GLU:HG2	1.93	0.49
1:MA:688:GLN:OE1	1:MA:688:GLN:N	2.45	0.49
3:KC:37:LEU:HD11	3:KC:47:ARG:HA	1.95	0.49
3:FC:86:ARG:HA	3:FC:89:GLN:HG2	1.94	0.49
2:HB:84:GLN:HG2	2:HB:102:LEU:HB3	1.94	0.49
1:CA:511:ASP:OD2	1:DA:592:ARG:NH1	2.36	0.49
1:HA:509:ALA:HA	1:HA:512:PHE:HD2	1.77	0.49
1:MA:630:TYR:HB3	2:NB:121:LYS:HA	1.94	0.49
1:OA:408:PRO:HG3	1:OA:521:LEU:HD21	1.95	0.49
2:KB:83:LEU:HD22	3:KC:9:GLN:OE1	2.12	0.49
3:LC:94:LEU:O	3:LC:98:ARG:HG3	2.12	0.49
2:DB:110:ARG:O	2:DB:114:ILE:HG13	2.13	0.49
3:MC:94:LEU:HD21	3:MC:98:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:513:ILE:O	1:EA:550:GLN:NE2	2.31	0.49
1:JA:375:ILE:HG12	1:JA:427:ILE:HG12	1.93	0.49
1:NA:630:TYR:HB3	2:OB:121:LYS:HA	1.94	0.49
1:PA:549:LEU:HB3	1:PA:559:ILE:HD11	1.95	0.49
3:PC:46:GLY:HA2	3:PC:49:CYS:SG	2.53	0.49
1:BA:365:GLU:HG2	1:CA:408:PRO:HA	1.94	0.49
1:BA:402:TYR:O	1:BA:406:GLY:N	2.45	0.49
1:FA:662:ILE:HD13	1:FA:690:LEU:HD11	1.93	0.49
1:GA:511:ASP:OD2	1:HA:592:ARG:NH1	2.44	0.49
1:LA:389:ALA:C	1:LA:391:ASN:H	2.16	0.49
1:LA:688:GLN:N	1:LA:688:GLN:OE1	2.43	0.49
1:RA:462:LYS:HE2	1:RA:473:PHE:HE2	1.78	0.49
2:RB:117:ASN:O	2:RB:120:HIS:CD2	2.66	0.49
3:GC:50:ARG:NH2	3:GC:62:ARG:HH21	2.10	0.49
3:QC:25:HIS:HB3	3:QC:28:ARG:HB3	1.93	0.49
1:CA:425:TYR:HE1	1:CA:439:LEU:HG	1.78	0.49
1:NA:394:LEU:HD22	1:NA:501:LEU:HD13	1.95	0.49
1:NA:481:GLU:O	1:NA:484:GLU:HG3	2.12	0.49
1:PA:451:SER:HA	1:PA:471:GLU:HB2	1.95	0.49
3:FC:47:ARG:HD2	3:FC:50:ARG:NH1	2.27	0.49
3:MC:37:LEU:HD11	3:MC:50:ARG:CZ	2.42	0.49
1:DA:389:ALA:C	1:DA:391:ASN:H	2.16	0.49
1:HA:373:LEU:HD22	1:HA:412:ILE:HG23	1.95	0.49
1:IA:497:LEU:HD12	1:IA:500:HIS:CE1	2.48	0.49
1:RA:462:LYS:HG2	1:RA:473:PHE:CE2	2.48	0.49
1:RA:621:ARG:HG3	1:RA:633:LEU:HA	1.94	0.49
1:AA:643:GLU:HG3	1:AA:647:LYS:HE2	1.95	0.49
1:JA:378:ASP:OD1	1:JA:379:SER:N	2.44	0.49
1:JA:621:ARG:HG3	1:JA:633:LEU:HA	1.93	0.49
1:JA:688:GLN:N	1:JA:688:GLN:OE1	2.46	0.49
1:LA:519:ARG:HG2	1:MA:531:GLU:HG2	1.95	0.49
1:MA:533:ILE:HA	1:MA:536:VAL:HG12	1.94	0.49
2:CB:75:ASP:O	2:CB:78:ARG:HG3	2.13	0.49
2:RB:83:LEU:HD21	3:RC:9:GLN:HB3	1.94	0.49
3:RC:79:GLY:HA2	3:RC:82:LEU:HD23	1.95	0.49
2:NB:110:ARG:O	2:NB:114:ILE:HG13	2.13	0.49
1:FA:394:LEU:HD22	1:FA:501:LEU:HD13	1.95	0.48
1:JA:592:ARG:NH1	1:RA:511:ASP:OD2	2.42	0.48
1:OA:655:ILE:HG13	3:OC:24:GLY:HA2	1.94	0.48
1:RA:599:ALA:HB2	1:RA:605:LEU:HD13	1.95	0.48
3:AC:68:GLN:HA	3:AC:71:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:587:ARG:NE	1:AA:689:GLU:OE2	2.40	0.48
1:EA:533:ILE:HA	1:EA:536:VAL:HG12	1.95	0.48
1:HA:533:ILE:HA	1:HA:536:VAL:HG12	1.96	0.48
1:IA:603:ASN:HB2	1:IA:694:ILE:HA	1.94	0.48
1:LA:655:ILE:HG23	2:LB:58:TRP:HH2	1.78	0.48
1:NA:688:GLN:N	1:NA:688:GLN:OE1	2.45	0.48
1:EA:412:ILE:HD13	1:EA:501:LEU:HD11	1.94	0.48
1:GA:459:PRO:HD3	3:GC:98:ARG:HH12	1.77	0.48
1:HA:367:PHE:HD2	1:IA:524:GLN:HG2	1.78	0.48
1:IA:533:ILE:HA	1:IA:536:VAL:HG12	1.94	0.48
1:MA:610:PHE:CE1	1:MA:661:LEU:HD11	2.48	0.48
1:NA:373:LEU:HD22	1:NA:412:ILE:HG23	1.96	0.48
1:PA:449:SER:OG	1:PA:470:GLN:OE1	2.30	0.48
2:KB:110:ARG:O	2:KB:114:ILE:HG13	2.12	0.48
3:KC:95:ASP:O	3:KC:99:HIS:ND1	2.41	0.48
2:OB:110:ARG:O	2:OB:114:ILE:HG13	2.13	0.48
1:IA:373:LEU:HD22	1:IA:412:ILE:HG23	1.96	0.48
1:IA:497:LEU:HD12	1:IA:500:HIS:NE2	2.28	0.48
1:OA:481:GLU:O	1:OA:484:GLU:HG3	2.13	0.48
1:RA:487:GLN:O	2:RB:52:GLN:HB2	2.14	0.48
2:JB:117:ASN:O	2:JB:120:HIS:NE2	2.46	0.48
3:RC:74:ASP:O	3:RC:80:ASN:ND2	2.46	0.48
3:GC:43:HIS:CD2	3:GC:46:GLY:H	2.32	0.48
3:OC:86:ARG:HA	3:OC:89:GLN:HG2	1.95	0.48
1:DA:606:PRO:HB3	1:DA:699:LEU:HD11	1.96	0.48
1:MA:610:PHE:HE1	1:MA:661:LEU:HD11	1.78	0.48
1:MA:619:ARG:NE	1:MA:666:ASP:OD2	2.41	0.48
1:NA:609:LEU:HD23	1:NA:662:ILE:HB	1.95	0.48
1:CA:465:HIS:CD2	1:CA:474:TRP:HE1	2.32	0.48
1:DA:464:GLU:HB2	1:DA:467:LEU:HD13	1.96	0.48
1:GA:509:ALA:HA	1:GA:512:PHE:HD2	1.79	0.48
3:RC:50:ARG:O	3:RC:54:LEU:HD23	2.14	0.48
2:OB:84:GLN:HE22	2:OB:106:GLN:HG2	1.79	0.48
3:FC:8:ARG:O	3:FC:11:GLU:N	2.47	0.48
1:AA:533:ILE:HA	1:AA:536:VAL:HG12	1.95	0.48
1:EA:483:LEU:HB3	1:EA:490:PHE:HZ	1.78	0.48
1:GA:454:GLU:HG3	3:GC:86:ARG:NH1	2.28	0.48
1:HA:375:ILE:HG12	1:HA:427:ILE:HG12	1.96	0.48
1:KA:533:ILE:HA	1:KA:536:VAL:HG12	1.96	0.48
1:QA:533:ILE:HA	1:QA:536:VAL:HG12	1.96	0.48
3:GC:47:ARG:HB3	3:GC:70:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:79:GLU:HG2	3:QC:12:PHE:HB2	1.95	0.48
2:QB:84:GLN:HG3	2:QB:103:LYS:HG2	1.94	0.48
1:CA:405:LEU:O	1:CA:559:ILE:N	2.47	0.48
1:CA:675:ILE:HD12	1:CA:682:LEU:HD23	1.95	0.48
1:DA:610:PHE:HE1	1:DA:661:LEU:HD11	1.79	0.48
1:EA:375:ILE:HG12	1:EA:427:ILE:HG12	1.95	0.48
1:OA:394:LEU:HD22	1:OA:501:LEU:HD13	1.96	0.48
1:OA:445:LEU:HG	1:OA:474:TRP:HB3	1.94	0.48
1:PA:588:SER:O	1:PA:591:LYS:HG3	2.14	0.48
2:CB:70:LEU:HG	2:CB:72:ARG:H	1.78	0.48
1:CA:609:LEU:HD23	1:CA:662:ILE:HB	1.96	0.48
1:MA:378:ASP:OD2	1:MA:424:GLU:N	2.47	0.48
1:OA:390:LEU:HD11	1:OA:497:LEU:HD23	1.94	0.48
3:RC:37:LEU:HD11	3:RC:47:ARG:HG2	1.96	0.48
3:GC:19:LEU:HA	3:GC:22:GLN:HG2	1.94	0.48
2:OB:115:ILE:O	2:OB:118:LEU:HG	2.14	0.48
3:OC:88:GLN:HG3	3:OC:97:ALA:HB2	1.95	0.48
3:EC:56:ASN:OD1	3:EC:86:ARG:NH2	2.46	0.48
2:FB:101:LEU:HD11	3:FC:28:ARG:NE	2.28	0.48
1:CA:466:LEU:O	1:CA:468:PRO:HD3	2.14	0.47
1:CA:588:SER:O	1:CA:591:LYS:HG3	2.14	0.47
1:CA:606:PRO:HB2	1:CA:659:PRO:HA	1.96	0.47
1:DA:619:ARG:NE	1:DA:666:ASP:OD2	2.45	0.47
1:FA:385:LEU:HG	1:FA:386:GLU:H	1.78	0.47
1:GA:372:PRO:O	1:GA:430:GLN:N	2.38	0.47
1:HA:688:GLN:N	1:HA:688:GLN:OE1	2.46	0.47
1:FA:483:LEU:HB3	1:FA:490:PHE:HZ	1.78	0.47
1:MA:483:LEU:HD11	1:MA:488:LEU:HD12	1.96	0.47
1:QA:509:ALA:HA	1:QA:512:PHE:HD2	1.79	0.47
3:JC:69:TRP:HE3	3:JC:70:LEU:HD12	1.79	0.47
3:KC:82:LEU:HD11	3:KC:104:TYR:CD1	2.49	0.47
3:RC:62:ARG:O	3:RC:66:GLU:HG2	2.14	0.47
1:CA:489:GLU:HG3	2:CB:51:ALA:HB1	1.95	0.47
1:DA:365:GLU:HG2	1:EA:408:PRO:HA	1.95	0.47
1:DA:375:ILE:HG12	1:DA:427:ILE:HG12	1.96	0.47
1:GA:405:LEU:O	1:GA:559:ILE:N	2.47	0.47
1:RA:375:ILE:HG12	1:RA:427:ILE:HG12	1.96	0.47
1:RA:688:GLN:OE1	1:RA:688:GLN:N	2.46	0.47
2:KB:51:ALA:HB3	2:KB:54:LYS:HG3	1.96	0.47
3:KC:5:LEU:HD11	3:KC:39:LEU:HD13	1.96	0.47
1:QA:394:LEU:HD22	1:QA:501:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:598:TYR:HE2	1:QA:685:LEU:HD21	1.79	0.47
1:QA:627:ALA:HA	1:RA:575:LYS:HD3	1.96	0.47
3:AC:17:GLY:HA2	3:AC:32:LEU:HD21	1.97	0.47
1:JA:365:GLU:HG2	1:KA:408:PRO:HA	1.97	0.47
1:PA:548:ILE:HG21	1:PA:586:ILE:HD12	1.95	0.47
2:CB:81:ASP:HA	2:CB:106:GLN:NE2	2.29	0.47
1:CA:549:LEU:HB3	1:CA:559:ILE:HD11	1.97	0.47
1:MA:425:TYR:CD1	1:MA:439:LEU:HD23	2.50	0.47
1:MA:644:GLN:O	1:MA:648:THR:OG1	2.33	0.47
1:OA:447:ARG:HB3	1:OA:474:TRP:CE3	2.49	0.47
1:OA:657:SER:OG	1:OA:658:LYS:N	2.46	0.47
1:QA:370:THR:HG21	1:RA:561:ASN:HD22	1.78	0.47
2:IB:111:LEU:O	2:IB:114:ILE:HG12	2.13	0.47
1:CA:364:GLN:NE2	1:DA:408:PRO:O	2.47	0.47
1:FA:360:ARG:HG2	1:FA:361:LEU:H	1.80	0.47
1:FA:610:PHE:HB2	1:FA:663:VAL:HG23	1.97	0.47
1:JA:486:SER:O	3:JC:108:LYS:NZ	2.47	0.47
1:JA:670:TYR:CE1	2:KB:122:VAL:HG11	2.50	0.47
1:QA:588:SER:O	1:QA:591:LYS:HG3	2.14	0.47
1:QA:688:GLN:N	1:QA:688:GLN:OE1	2.45	0.47
1:RA:549:LEU:HB3	1:RA:559:ILE:HD11	1.95	0.47
1:RA:648:THR:HG23	1:RA:649:ILE:H	1.80	0.47
3:LC:44:LEU:O	3:LC:48:ARG:HG3	2.15	0.47
2:PB:83:LEU:HD21	3:PC:9:GLN:HB3	1.95	0.47
3:PC:82:LEU:HD21	3:PC:104:TYR:CD1	2.50	0.47
2:FB:78:ARG:NH1	2:FB:79:GLU:OE1	2.47	0.47
3:HC:99:HIS:O	3:HC:102:GLN:HG3	2.14	0.47
3:MC:33:LEU:HD13	3:MC:50:ARG:HB3	1.96	0.47
1:CA:610:PHE:HE1	1:CA:661:LEU:HD11	1.80	0.47
1:DA:588:SER:O	1:DA:591:LYS:HG3	2.15	0.47
1:FA:389:ALA:C	1:FA:391:ASN:H	2.18	0.47
1:FA:631:LEU:HD22	1:FA:670:TYR:HB3	1.96	0.47
1:JA:533:ILE:HA	1:JA:536:VAL:HG12	1.97	0.47
1:JA:624:GLN:OE1	1:JA:624:GLN:N	2.38	0.47
1:LA:373:LEU:HD13	1:LA:412:ILE:HG12	1.97	0.47
1:QA:483:LEU:HD11	1:QA:488:LEU:HD12	1.96	0.47
2:LB:117:ASN:HA	2:LB:120:HIS:NE2	2.29	0.47
2:BB:83:LEU:HG	3:BC:12:PHE:CD1	2.50	0.47
3:MC:86:ARG:O	3:MC:89:GLN:HG2	2.15	0.47
1:CA:617:LYS:HE3	1:CA:704:LEU:HD11	1.97	0.47
1:CA:701:ARG:NE	2:CB:108:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MA:412:ILE:HD13	1:MA:501:LEU:HD11	1.96	0.47
1:OA:423:GLY:O	1:OA:439:LEU:N	2.48	0.47
1:RA:513:ILE:HB	1:RA:550:GLN:HG2	1.97	0.47
2:FB:83:LEU:HB3	2:FB:102:LEU:HD21	1.95	0.47
3:MC:77:GLN:HG3	3:MC:79:GLY:H	1.80	0.47
1:HA:609:LEU:HD23	1:HA:662:ILE:HB	1.96	0.47
1:HA:687:TYR:CE2	2:HB:115:ILE:HG21	2.50	0.47
1:KA:662:ILE:HD13	1:KA:690:LEU:HD11	1.96	0.47
1:NA:459:PRO:HD3	3:NC:98:ARG:HH12	1.79	0.47
3:GC:19:LEU:HD23	3:GC:22:GLN:OE1	2.14	0.47
2:PB:117:ASN:O	2:PB:120:HIS:HD2	1.98	0.47
2:BB:80:LEU:HD22	3:BC:12:PHE:HE2	1.80	0.47
1:CA:441:ALA:HB3	1:CA:493:HIS:NE2	2.31	0.46
1:IA:394:LEU:HD22	1:IA:501:LEU:HD13	1.96	0.46
1:KA:644:GLN:O	1:KA:648:THR:OG1	2.32	0.46
1:KA:655:ILE:HG21	1:KA:659:PRO:HD3	1.97	0.46
1:KA:673:LYS:NZ	2:LB:122:VAL:O	2.43	0.46
1:KA:688:GLN:OE1	1:KA:688:GLN:N	2.47	0.46
1:LA:549:LEU:HB3	1:LA:559:ILE:HD11	1.97	0.46
1:PA:412:ILE:HD13	1:PA:501:LEU:HD11	1.96	0.46
2:LB:86:LEU:HD13	3:LC:4:THR:HG21	1.97	0.46
3:IC:47:ARG:HA	3:IC:50:ARG:HG2	1.97	0.46
3:IC:86:ARG:NH1	3:IC:89:GLN:OE1	2.49	0.46
3:AC:33:LEU:HD13	3:AC:50:ARG:HA	1.98	0.46
1:AA:392:ASP:HA	1:AA:395:VAL:HG12	1.97	0.46
1:AA:687:TYR:CZ	2:AB:115:ILE:HD13	2.50	0.46
1:FA:447:ARG:HH21	1:FA:472:THR:HA	1.81	0.46
1:QA:608:TYR:HE2	1:QA:659:PRO:HB2	1.80	0.46
2:DB:115:ILE:O	2:DB:118:LEU:HG	2.16	0.46
1:FA:587:ARG:NE	1:FA:689:GLU:OE2	2.46	0.46
1:IA:609:LEU:HD23	1:IA:662:ILE:HB	1.98	0.46
1:JA:405:LEU:O	1:JA:559:ILE:N	2.49	0.46
1:PA:394:LEU:HD23	1:PA:498:THR:HG22	1.98	0.46
3:OC:37:LEU:HD13	3:OC:47:ARG:CZ	2.46	0.46
1:BA:452:GLN:H	1:BA:455:LEU:HD23	1.80	0.46
1:EA:373:LEU:HD22	1:EA:412:ILE:HG23	1.97	0.46
1:EA:449:SER:OG	1:EA:470:GLN:OE1	2.28	0.46
1:OA:610:PHE:CE1	1:OA:661:LEU:HD11	2.49	0.46
1:OA:661:LEU:HB2	1:OA:682:LEU:HD21	1.97	0.46
1:RA:533:ILE:HA	1:RA:536:VAL:HG12	1.97	0.46
3:RC:94:LEU:HG	3:RC:98:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HB:87:LEU:HD22	2:HB:95:LEU:HD22	1.96	0.46
2:DB:83:LEU:HD21	3:DC:13:LEU:HD21	1.97	0.46
1:AA:661:LEU:HB2	1:AA:682:LEU:HD21	1.97	0.46
1:AA:688:GLN:OE1	1:AA:688:GLN:N	2.46	0.46
1:BA:687:TYR:CZ	2:BB:115:ILE:HD13	2.50	0.46
1:GA:441:ALA:HA	1:GA:445:LEU:HB2	1.97	0.46
1:LA:533:ILE:HA	1:LA:536:VAL:HG12	1.98	0.46
1:MA:606:PRO:HB3	1:MA:699:LEU:HD11	1.98	0.46
1:NA:598:TYR:CE2	1:NA:685:LEU:HD21	2.50	0.46
1:OA:513:ILE:O	1:OA:550:GLN:NE2	2.30	0.46
1:QA:608:TYR:HB2	1:QA:661:LEU:HD12	1.98	0.46
3:CC:47:ARG:HG3	3:CC:50:ARG:HE	1.79	0.46
1:BA:624:GLN:OE1	1:BA:624:GLN:N	2.38	0.46
1:FA:606:PRO:HB3	1:FA:699:LEU:HD11	1.97	0.46
1:GA:624:GLN:OE1	1:GA:624:GLN:N	2.39	0.46
1:PA:367:PHE:HD2	1:QA:524:GLN:HG2	1.80	0.46
1:RA:624:GLN:OE1	1:RA:624:GLN:N	2.40	0.46
3:IC:33:LEU:HD13	3:IC:50:ARG:HB3	1.96	0.46
1:BA:390:LEU:HD11	1:BA:497:LEU:HD23	1.98	0.46
1:GA:610:PHE:CE1	1:GA:661:LEU:HD11	2.51	0.46
1:MA:394:LEU:HD23	1:MA:498:THR:HG22	1.98	0.46
1:RA:635:PRO:HG3	2:JB:118:LEU:HD21	1.97	0.46
2:IB:60:PHE:O	2:IB:63:PRO:HD2	2.15	0.46
1:CA:389:ALA:C	1:CA:391:ASN:H	2.19	0.46
1:CA:635:PRO:HG2	2:DB:114:ILE:HG23	1.98	0.46
1:DA:482:ARG:HA	1:DA:485:LYS:HD2	1.96	0.46
1:DA:549:LEU:HB3	1:DA:559:ILE:HD11	1.96	0.46
1:DA:673:LYS:NZ	2:EB:122:VAL:O	2.44	0.46
1:HA:692:GLN:O	1:HA:694:ILE:HG13	2.16	0.46
1:KA:489:GLU:HB3	1:KA:491:PHE:HE1	1.81	0.46
1:KA:610:PHE:CE1	1:KA:661:LEU:HD11	2.50	0.46
1:MA:686:SER:HB2	1:MA:689:GLU:HG3	1.97	0.46
1:PA:688:GLN:OE1	1:PA:688:GLN:N	2.46	0.46
1:QA:610:PHE:HB2	1:QA:663:VAL:HG23	1.98	0.46
2:GB:80:LEU:HD12	3:GC:12:PHE:CZ	2.50	0.46
2:LB:84:GLN:NE2	2:LB:103:LYS:HD3	2.30	0.46
3:OC:88:GLN:HB2	3:OC:93:ASP:HB2	1.96	0.46
1:CA:656:GLN:H	1:CA:656:GLN:NE2	2.12	0.46
1:IA:599:ALA:HB2	1:IA:605:LEU:HD13	1.98	0.46
1:NA:468:PRO:HB2	1:NA:469:ASP:H	1.62	0.46
1:NA:591:LYS:HB3	1:NA:691:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:611:ASP:OD2	1:OA:703:CYS:HA	2.16	0.46
1:OA:656:GLN:HG3	1:OA:657:SER:H	1.81	0.46
1:PA:655:ILE:HG21	3:PC:24:GLY:H	1.80	0.46
1:QA:608:TYR:CE2	1:QA:659:PRO:HB2	2.51	0.46
1:QA:621:ARG:HB2	1:QA:633:LEU:HG	1.97	0.46
2:CB:58:TRP:HZ3	3:CC:21:LEU:HD22	1.80	0.46
3:KC:50:ARG:HH22	3:KC:66:GLU:CD	2.20	0.46
3:KC:54:LEU:HB3	3:KC:63:ALA:HB2	1.98	0.46
3:PC:78:ALA:HB1	3:PC:104:TYR:HD1	1.81	0.46
1:AA:481:GLU:O	1:AA:484:GLU:HG3	2.16	0.46
1:DA:533:ILE:HA	1:DA:536:VAL:HG12	1.97	0.46
1:DA:655:ILE:HG23	3:DC:23:CYS:HA	1.98	0.46
1:IA:610:PHE:HE1	1:IA:661:LEU:HD11	1.81	0.46
1:NA:609:LEU:HD13	2:NB:112:LEU:HD21	1.98	0.46
2:CB:79:GLU:HG3	2:CB:83:LEU:HD23	1.98	0.46
3:LC:57:ASN:O	3:LC:57:ASN:ND2	2.43	0.46
1:BA:533:ILE:HA	1:BA:536:VAL:HG12	1.98	0.45
1:GA:519:ARG:HG2	1:HA:531:GLU:HG2	1.97	0.45
1:JA:481:GLU:O	1:JA:484:GLU:HG3	2.16	0.45
1:LA:610:PHE:CE1	1:LA:661:LEU:HD11	2.48	0.45
1:LA:644:GLN:O	1:LA:648:THR:OG1	2.34	0.45
1:PA:456:LEU:HD11	3:PC:101:TYR:CG	2.51	0.45
1:QA:365:GLU:HG2	1:RA:408:PRO:HA	1.98	0.45
1:RA:465:HIS:HD2	1:RA:467:LEU:HD23	1.81	0.45
2:HB:83:LEU:HD11	3:HC:9:GLN:HB3	1.97	0.45
1:EA:701:ARG:NH1	2:EB:108:ASP:OD1	2.37	0.45
1:JA:644:GLN:O	1:JA:648:THR:OG1	2.34	0.45
3:CC:55:LEU:HD11	3:CC:83:CYS:HA	1.97	0.45
3:DC:88:GLN:HG3	3:DC:97:ALA:HB2	1.97	0.45
1:HA:610:PHE:CE1	1:HA:661:LEU:HD11	2.51	0.45
1:KA:549:LEU:HB3	1:KA:559:ILE:HD11	1.98	0.45
1:LA:630:TYR:HA	2:MB:122:VAL:HG23	1.99	0.45
1:MA:375:ILE:HG12	1:MA:427:ILE:HG12	1.98	0.45
1:RA:656:GLN:HG3	2:RB:58:TRP:CZ2	2.51	0.45
2:LB:80:LEU:HD21	2:LB:106:GLN:HA	1.98	0.45
2:NB:117:ASN:O	2:NB:120:HIS:CD2	2.70	0.45
3:HC:51:LEU:HD12	3:HC:70:LEU:HD22	1.98	0.45
1:EA:441:ALA:HA	1:EA:445:LEU:HB3	1.98	0.45
1:GA:373:LEU:HD22	1:GA:412:ILE:HG23	1.98	0.45
1:GA:533:ILE:HA	1:GA:536:VAL:HG12	1.99	0.45
1:GA:675:ILE:HD12	1:GA:682:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:372:PRO:O	1:HA:430:GLN:N	2.38	0.45
1:JA:588:SER:O	1:JA:591:LYS:HG3	2.16	0.45
1:JA:673:LYS:HD2	2:KB:122:VAL:HA	1.98	0.45
3:JC:47:ARG:HG3	3:JC:69:TRP:CZ3	2.50	0.45
2:PB:81:ASP:HA	2:PB:84:GLN:HG2	1.97	0.45
2:PB:92:SER:O	2:PB:94:GLU:N	2.48	0.45
1:GA:382:GLN:O	1:GA:386:GLU:HB2	2.16	0.45
1:NA:656:GLN:O	1:NA:657:SER:OG	2.30	0.45
3:KC:51:LEU:HD11	3:KC:83:CYS:HB3	1.99	0.45
3:HC:88:GLN:HG3	3:HC:97:ALA:HB2	1.98	0.45
3:AC:51:LEU:HD13	3:AC:66:GLU:HB3	1.98	0.45
1:CA:456:LEU:HA	1:CA:459:PRO:HB3	1.98	0.45
1:EA:370:THR:HG21	1:FA:561:ASN:HD22	1.82	0.45
1:EA:610:PHE:HE1	1:EA:661:LEU:HD11	1.81	0.45
1:HA:441:ALA:HA	1:HA:445:LEU:HB3	1.97	0.45
1:JA:509:ALA:HA	1:JA:512:PHE:HD2	1.82	0.45
1:NA:652:LEU:HD12	1:NA:655:ILE:HD12	1.98	0.45
1:QA:627:ALA:HB1	1:RA:572:TRP:HZ3	1.81	0.45
2:RB:84:GLN:HG3	2:RB:103:LYS:HG2	1.97	0.45
3:PC:35:ALA:O	3:PC:38:THR:HG22	2.17	0.45
1:AA:389:ALA:C	1:AA:391:ASN:H	2.20	0.45
1:BA:447:ARG:HB3	1:BA:474:TRP:CE3	2.52	0.45
1:EA:609:LEU:HD23	1:EA:662:ILE:HB	1.98	0.45
1:KA:372:PRO:O	1:KA:430:GLN:N	2.38	0.45
3:BC:57:ASN:O	3:BC:57:ASN:ND2	2.44	0.45
1:CA:424:GLU:HA	1:CA:438:GLU:HA	1.98	0.45
1:FA:549:LEU:HB3	1:FA:559:ILE:HD11	1.99	0.45
1:LA:655:ILE:HG23	2:LB:58:TRP:CH2	2.52	0.45
1:RA:465:HIS:HB2	1:RA:474:TRP:HE1	1.81	0.45
2:QB:101:LEU:HD11	3:QC:28:ARG:NE	2.31	0.45
1:KA:379:SER:O	1:KA:380:SER:OG	2.28	0.45
1:KA:518:THR:HG22	1:KA:549:LEU:HD12	1.99	0.45
1:KA:687:TYR:HB3	2:KB:119:LEU:CD1	2.47	0.45
3:PC:74:ASP:O	3:PC:80:ASN:ND2	2.50	0.45
2:EB:117:ASN:O	2:EB:120:HIS:CD2	2.70	0.45
3:AC:89:GLN:HA	3:AC:94:LEU:HB3	1.97	0.45
1:CA:618:ILE:HA	1:CA:633:LEU:HD21	1.99	0.45
1:DA:372:PRO:O	1:DA:430:GLN:N	2.40	0.45
1:DA:509:ALA:HA	1:DA:512:PHE:HD2	1.81	0.45
1:DA:644:GLN:O	1:DA:648:THR:OG1	2.35	0.45
1:FA:509:ALA:HA	1:FA:512:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:688:GLN:OE1	1:GA:688:GLN:N	2.48	0.45
1:IA:452:GLN:HG3	1:IA:453:LEU:H	1.82	0.45
1:OA:426:LEU:HA	1:OA:436:ARG:HA	1.98	0.45
1:BA:598:TYR:CE2	1:BA:685:LEU:HD21	2.52	0.44
1:DA:624:GLN:OE1	1:DA:624:GLN:N	2.39	0.44
1:JA:379:SER:O	1:JA:380:SER:OG	2.26	0.44
1:KA:450:VAL:HG13	2:KB:54:LYS:HE3	1.98	0.44
1:MA:648:THR:HG21	1:MA:702:VAL:HA	2.00	0.44
1:NA:509:ALA:HA	1:NA:512:PHE:HD2	1.82	0.44
1:NA:576:GLU:HG3	1:NA:585:TYR:HE2	1.82	0.44
1:NA:635:PRO:HG3	2:OB:114:ILE:HG23	1.99	0.44
1:OA:468:PRO:HB2	1:OA:499:TRP:CZ3	2.52	0.44
1:PA:533:ILE:HA	1:PA:536:VAL:HG12	1.98	0.44
1:QA:673:LYS:HD3	2:RB:122:VAL:HG22	1.99	0.44
1:RA:464:GLU:HB3	1:RA:473:PHE:CE1	2.53	0.44
2:KB:101:LEU:HD23	3:KC:32:LEU:HD21	1.99	0.44
3:LC:37:LEU:HD12	3:LC:50:ARG:HH11	1.81	0.44
3:MC:81:TRP:O	3:MC:85:SER:OG	2.25	0.44
2:QB:87:LEU:HD12	2:QB:102:LEU:HD12	1.98	0.44
1:BA:587:ARG:NE	1:BA:689:GLU:OE2	2.48	0.44
1:EA:481:GLU:O	1:EA:484:GLU:HG3	2.18	0.44
1:FA:588:SER:O	1:FA:591:LYS:HG3	2.17	0.44
1:GA:656:GLN:HG2	1:GA:657:SER:H	1.82	0.44
1:IA:378:ASP:OD1	1:IA:379:SER:N	2.49	0.44
3:NC:51:LEU:O	3:NC:55:LEU:HG	2.17	0.44
2:PB:58:TRP:HB3	3:PC:18:TRP:HH2	1.82	0.44
1:AA:611:ASP:CG	1:AA:701:ARG:HH21	2.20	0.44
1:DA:394:LEU:HD23	1:DA:498:THR:HG22	1.98	0.44
1:JA:385:LEU:HD12	1:JA:388:ILE:HD12	2.00	0.44
1:JA:610:PHE:CE1	1:JA:661:LEU:HD11	2.50	0.44
1:KA:669:ARG:HE	1:KA:673:LYS:HE3	1.83	0.44
1:NA:621:ARG:HB2	1:NA:633:LEU:HG	1.99	0.44
1:NA:701:ARG:NE	2:NB:108:ASP:OD1	2.50	0.44
1:RA:483:LEU:HB3	1:RA:490:PHE:HZ	1.81	0.44
1:RA:610:PHE:HB2	1:RA:663:VAL:HG23	1.99	0.44
1:BA:375:ILE:HD11	1:BA:501:LEU:HD12	1.98	0.44
1:IA:631:LEU:H	2:AB:122:VAL:HG21	1.82	0.44
1:KA:624:GLN:OE1	1:KA:624:GLN:N	2.40	0.44
1:LA:482:ARG:HA	1:LA:485:LYS:HD2	2.00	0.44
1:MA:372:PRO:O	1:MA:430:GLN:N	2.38	0.44
3:FC:37:LEU:HB2	3:FC:50:ARG:CZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:592:ARG:NH1	1:IA:511:ASP:OD2	2.42	0.44
1:DA:657:SER:HB2	3:DC:22:GLN:HE21	1.82	0.44
1:FA:533:ILE:HA	1:FA:536:VAL:HG12	2.00	0.44
1:GA:588:SER:O	1:GA:591:LYS:HG3	2.17	0.44
1:HA:624:GLN:OE1	1:HA:624:GLN:N	2.37	0.44
1:MA:588:SER:O	1:MA:591:LYS:HG3	2.16	0.44
3:JC:62:ARG:O	3:JC:66:GLU:HG2	2.17	0.44
1:BA:656:GLN:HG3	1:BA:657:SER:H	1.83	0.44
1:CA:394:LEU:HD23	1:CA:498:THR:HG22	1.99	0.44
1:CA:625:THR:OG1	1:CA:626:SER:N	2.51	0.44
1:GA:621:ARG:HG3	1:GA:633:LEU:HD13	1.99	0.44
1:JA:624:GLN:HA	1:JA:629:SER:HA	1.99	0.44
1:QA:548:ILE:HG21	1:QA:586:ILE:HD12	2.00	0.44
3:RC:47:ARG:HA	3:RC:50:ARG:HG2	1.98	0.44
2:HB:98:ALA:O	2:HB:102:LEU:HG	2.18	0.44
1:AA:625:THR:OG1	1:AA:626:SER:N	2.50	0.44
1:FA:389:ALA:HB1	1:FA:392:ASP:H	1.82	0.44
1:FA:408:PRO:HG3	1:FA:521:LEU:HD21	2.00	0.44
1:HA:394:LEU:HD22	1:HA:501:LEU:HD13	1.98	0.44
1:KA:361:LEU:HG	1:LA:412:ILE:HB	2.00	0.44
1:KA:625:THR:OG1	1:KA:626:SER:N	2.51	0.44
1:OA:588:SER:O	1:OA:591:LYS:HG3	2.18	0.44
2:CB:79:GLU:HG2	3:CC:12:PHE:HB2	2.00	0.44
3:JC:14:LEU:HD22	3:JC:43:HIS:HE1	1.83	0.44
2:OB:72:ARG:O	2:OB:76:TYR:N	2.46	0.44
2:OB:83:LEU:HD12	3:OC:12:PHE:HD2	1.83	0.44
3:QC:21:LEU:HD21	3:QC:53:ALA:HB2	2.00	0.44
1:AA:458:ILE:HA	1:AA:459:PRO:HD2	1.79	0.44
1:KA:509:ALA:HA	1:KA:512:PHE:HD2	1.83	0.44
1:KA:690:LEU:HD23	1:KA:690:LEU:HA	1.87	0.44
1:RA:701:ARG:HD2	1:RA:701:ARG:HA	1.75	0.44
3:NC:86:ARG:HA	3:NC:89:GLN:HG2	1.99	0.44
1:CA:447:ARG:HB3	1:CA:474:TRP:CZ3	2.53	0.44
1:HA:631:LEU:H	1:HA:673:LYS:NZ	2.16	0.44
1:JA:389:ALA:C	1:JA:391:ASN:H	2.21	0.44
1:JA:513:ILE:HD11	1:JA:553:VAL:HG21	1.98	0.44
1:MA:519:ARG:HG2	1:NA:531:GLU:HG2	1.99	0.44
1:MA:549:LEU:HB3	1:MA:559:ILE:HD11	1.99	0.44
1:OA:394:LEU:HD23	1:OA:498:THR:HG22	2.00	0.44
1:OA:519:ARG:HG2	1:PA:531:GLU:HG2	1.99	0.44
2:RB:99:ALA:O	2:RB:103:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:RB:114:ILE:O	2:RB:118:LEU:HG	2.18	0.44
2:OB:80:LEU:O	2:OB:84:GLN:HG2	2.17	0.44
2:HB:84:GLN:HG2	2:HB:102:LEU:CB	2.48	0.44
3:MC:94:LEU:HG	3:MC:98:ARG:HE	1.83	0.44
1:BA:401:LEU:HD11	1:BA:502:SER:HA	1.99	0.43
1:DA:669:ARG:NE	1:DA:673:LYS:HE3	2.32	0.43
1:JA:460:TYR:HB3	1:JA:479:TYR:CG	2.53	0.43
1:KA:598:TYR:HE2	1:KA:685:LEU:HD21	1.83	0.43
1:NA:518:THR:HG22	1:NA:549:LEU:HD12	1.99	0.43
1:QA:623:ARG:HB2	1:QA:630:TYR:O	2.17	0.43
2:GB:75:ASP:O	2:GB:79:GLU:HG3	2.18	0.43
3:OC:95:ASP:OD1	3:OC:95:ASP:N	2.51	0.43
2:AB:78:ARG:O	2:AB:82:THR:HG23	2.18	0.43
1:CA:394:LEU:HD22	1:CA:501:LEU:HD13	2.00	0.43
1:EA:518:THR:HG22	1:EA:549:LEU:HD12	1.99	0.43
1:GA:448:GLU:O	1:GA:472:THR:HA	2.18	0.43
1:OA:375:ILE:HG12	1:OA:427:ILE:HG12	2.00	0.43
3:JC:99:HIS:O	3:JC:102:GLN:HG3	2.18	0.43
2:GB:84:GLN:HG3	2:GB:103:LYS:HG2	1.99	0.43
3:LC:59:GLN:HG3	3:LC:62:ARG:HD2	2.01	0.43
3:OC:95:ASP:HA	3:OC:98:ARG:HE	1.82	0.43
3:BC:35:ALA:O	3:BC:38:THR:HG22	2.17	0.43
3:MC:79:GLY:HA2	3:MC:82:LEU:HD23	1.99	0.43
1:BA:378:ASP:OD1	1:BA:379:SER:N	2.49	0.43
1:BA:588:SER:O	1:BA:591:LYS:HG3	2.19	0.43
1:EA:588:SER:O	1:EA:591:LYS:HG3	2.18	0.43
1:GA:635:PRO:HG3	2:HB:114:ILE:HG23	1.98	0.43
1:IA:548:ILE:HG21	1:IA:586:ILE:HD12	2.00	0.43
1:NA:483:LEU:HB3	1:NA:490:PHE:HZ	1.84	0.43
1:OA:444:LEU:HB3	1:OA:477:VAL:CG1	2.48	0.43
1:PA:382:GLN:HG2	1:PA:416:PHE:CD1	2.53	0.43
1:QA:610:PHE:HE1	1:QA:661:LEU:HD11	1.82	0.43
1:QA:621:ARG:HG3	1:QA:633:LEU:HA	2.00	0.43
2:OB:87:LEU:O	2:OB:90:SER:HB3	2.17	0.43
1:AA:375:ILE:HG12	1:AA:427:ILE:HG12	1.99	0.43
1:AA:381:GLN:HB3	1:AA:385:LEU:HB2	2.01	0.43
1:DA:430:GLN:OE1	1:EA:561:ASN:ND2	2.32	0.43
1:IA:408:PRO:HG3	1:IA:521:LEU:HD21	1.99	0.43
1:JA:598:TYR:CE2	1:JA:685:LEU:HD21	2.53	0.43
1:KA:669:ARG:NE	1:KA:673:LYS:HE3	2.33	0.43
1:NA:441:ALA:HB2	1:NA:474:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:GC:5:LEU:HD22	3:GC:7:LYS:HE3	2.01	0.43
3:PC:85:SER:O	3:PC:89:GLN:N	2.46	0.43
1:CA:509:ALA:HA	1:CA:512:PHE:HD2	1.83	0.43
1:CA:627:ALA:O	1:CA:629:SER:N	2.45	0.43
1:EA:509:ALA:HA	1:EA:512:PHE:HD2	1.83	0.43
1:GA:394:LEU:HD23	1:GA:498:THR:HG22	1.99	0.43
1:JA:606:PRO:HB3	1:JA:699:LEU:HD11	2.00	0.43
1:KA:511:ASP:OD2	1:LA:592:ARG:NH1	2.52	0.43
1:NA:644:GLN:HG2	1:NA:703:CYS:O	2.19	0.43
1:PA:675:ILE:HD12	1:PA:682:LEU:HD23	1.99	0.43
1:RA:699:LEU:HB3	3:RC:25:HIS:CE1	2.54	0.43
3:JC:44:LEU:O	3:JC:48:ARG:HG3	2.18	0.43
2:GB:51:ALA:O	2:GB:54:LYS:N	2.51	0.43
1:HA:549:LEU:HB3	1:HA:559:ILE:HD11	2.01	0.43
1:IA:395:VAL:HG23	1:IA:398:ARG:NH2	2.34	0.43
1:IA:624:GLN:OE1	1:IA:624:GLN:N	2.38	0.43
1:JA:394:LEU:HD22	1:JA:501:LEU:HD13	1.99	0.43
1:KA:621:ARG:HG3	1:KA:633:LEU:HA	2.01	0.43
1:LA:608:TYR:HB2	1:LA:661:LEU:HD12	2.01	0.43
1:OA:444:LEU:HB3	1:OA:477:VAL:HG11	2.00	0.43
1:RA:509:ALA:HA	1:RA:512:PHE:HD2	1.82	0.43
3:JC:94:LEU:O	3:JC:98:ARG:HG2	2.18	0.43
2:KB:74:GLN:C	2:KB:76:TYR:H	2.21	0.43
3:GC:43:HIS:HD2	3:GC:46:GLY:H	1.65	0.43
3:GC:99:HIS:O	3:GC:102:GLN:HG3	2.18	0.43
2:LB:65:TYR:OH	3:LC:14:LEU:HB3	2.18	0.43
3:LC:55:LEU:HD22	3:LC:86:ARG:HB2	2.00	0.43
2:NB:113:GLN:HA	2:NB:116:LEU:HD23	2.00	0.43
2:OB:52:GLN:OE1	2:OB:55:ARG:NH2	2.52	0.43
1:BA:487:GLN:HB2	2:BB:52:GLN:OE1	2.18	0.43
1:CA:430:GLN:OE1	1:DA:561:ASN:ND2	2.31	0.43
1:DA:518:THR:HG22	1:DA:549:LEU:HD12	2.00	0.43
1:EA:405:LEU:O	1:EA:559:ILE:N	2.52	0.43
1:EA:447:ARG:HB3	1:EA:474:TRP:CE3	2.54	0.43
1:GA:608:TYR:CD1	1:GA:649:ILE:HG12	2.54	0.43
1:HA:452:GLN:CD	1:HA:453:LEU:H	2.21	0.43
1:KA:687:TYR:CB	2:KB:119:LEU:HD11	2.49	0.43
1:NA:515:ILE:HD11	1:OA:570:VAL:HG11	1.99	0.43
1:QA:453:LEU:HD12	1:QA:456:LEU:HB2	2.01	0.43
2:CB:78:ARG:NH1	2:CB:79:GLU:OE1	2.52	0.43
3:LC:50:ARG:O	3:LC:54:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:84:GLN:HG2	2:EB:102:LEU:HB3	2.00	0.43
1:DA:610:PHE:HB2	1:DA:663:VAL:HG23	2.00	0.43
1:JA:488:LEU:HD23	1:JA:488:LEU:HA	1.80	0.43
1:KA:452:GLN:OE1	1:KA:454:GLU:N	2.51	0.43
1:PA:456:LEU:HD21	3:PC:101:TYR:HB3	2.00	0.43
1:PA:673:LYS:HG3	2:QB:122:VAL:HA	2.00	0.43
3:CC:94:LEU:O	3:CC:98:ARG:HG3	2.19	0.43
2:KB:98:ALA:O	2:KB:102:LEU:HG	2.19	0.43
2:PB:114:ILE:O	2:PB:118:LEU:HG	2.19	0.43
3:EC:57:ASN:O	3:EC:57:ASN:ND2	2.43	0.43
2:QB:112:LEU:HD23	2:QB:115:ILE:HD12	1.99	0.43
1:EA:379:SER:O	1:EA:380:SER:OG	2.28	0.43
1:FA:609:LEU:HD22	2:FB:112:LEU:HD21	2.01	0.43
1:IA:451:SER:HA	1:IA:455:LEU:HD23	2.01	0.43
1:MA:624:GLN:OE1	1:MA:624:GLN:N	2.37	0.43
1:NA:522:LEU:HD22	1:NA:533:ILE:HG23	1.99	0.43
1:NA:663:VAL:HG22	1:NA:664:SER:H	1.84	0.43
1:QA:450:VAL:HG21	2:QB:51:ALA:HB2	2.00	0.43
3:QC:8:ARG:O	3:QC:11:GLU:N	2.50	0.43
3:QC:69:TRP:HE3	3:QC:70:LEU:HD12	1.84	0.43
1:AA:602:ASN:CG	1:AA:603:ASN:H	2.21	0.43
1:BA:668:ARG:HD3	1:BA:686:SER:OG	2.19	0.43
1:CA:386:GLU:HA	1:CA:390:LEU:HB2	2.00	0.43
1:EA:625:THR:OG1	1:EA:626:SER:N	2.52	0.43
1:LA:394:LEU:HD22	1:LA:501:LEU:HD13	2.01	0.43
1:LA:448:GLU:OE2	1:LA:450:VAL:N	2.45	0.43
1:LA:452:GLN:HG3	1:LA:453:LEU:H	1.84	0.43
1:LA:544:ARG:HD2	1:LA:579:VAL:HG22	2.01	0.43
2:CB:72:ARG:HH12	3:CC:19:LEU:HD11	1.83	0.43
2:CB:83:LEU:HD21	3:CC:9:GLN:HB3	2.00	0.43
3:CC:74:ASP:O	3:CC:80:ASN:ND2	2.52	0.43
3:PC:77:GLN:HB2	3:PC:80:ASN:ND2	2.34	0.43
2:MB:57:LEU:HD22	3:MC:52:VAL:HG22	2.01	0.43
1:EA:440:LYS:HB3	1:EA:474:TRP:CE2	2.53	0.42
1:GA:549:LEU:HB3	1:GA:559:ILE:HD11	2.00	0.42
1:JA:662:ILE:HD13	1:JA:690:LEU:HD11	1.99	0.42
1:NA:697:GLN:OE1	3:NC:19:LEU:HD13	2.19	0.42
1:OA:595:CYS:HB2	1:OA:694:ILE:HD11	2.00	0.42
1:OA:649:ILE:HD11	1:OA:682:LEU:HD22	2.00	0.42
1:RA:438:GLU:HB2	1:RA:465:HIS:HE2	1.84	0.42
3:NC:89:GLN:HA	3:NC:93:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:NC:94:LEU:O	3:NC:98:ARG:HG3	2.18	0.42
2:DB:52:GLN:O	2:DB:55:ARG:HB2	2.19	0.42
1:BA:610:PHE:CE1	1:BA:661:LEU:HD11	2.54	0.42
1:DA:669:ARG:HE	1:DA:673:LYS:HE3	1.84	0.42
1:HA:458:ILE:HD11	3:HC:101:TYR:CE2	2.54	0.42
1:HA:621:ARG:HG3	1:HA:633:LEU:HA	2.01	0.42
1:OA:509:ALA:HA	1:OA:512:PHE:HD2	1.83	0.42
1:OA:533:ILE:HA	1:OA:536:VAL:HG12	2.00	0.42
1:PA:688:GLN:HG2	2:PB:121:LYS:HE3	2.00	0.42
3:BC:55:LEU:HD11	3:BC:83:CYS:HA	2.01	0.42
1:DA:609:LEU:H	1:DA:609:LEU:HG	1.56	0.42
1:EA:610:PHE:CE1	1:EA:661:LEU:HD11	2.55	0.42
1:KA:488:LEU:HD23	1:KA:488:LEU:HA	1.92	0.42
1:MA:370:THR:HG21	1:NA:561:ASN:HA	2.01	0.42
1:PA:408:PRO:HG3	1:PA:521:LEU:HD21	2.00	0.42
1:PA:655:ILE:HG21	3:PC:24:GLY:N	2.34	0.42
2:LB:83:LEU:HA	2:LB:83:LEU:HD23	1.73	0.42
2:FB:78:ARG:HH22	3:FC:8:ARG:HD3	1.84	0.42
3:DC:37:LEU:HD12	3:DC:50:ARG:HD3	2.02	0.42
3:QC:55:LEU:HD11	3:QC:83:CYS:HA	2.00	0.42
1:CA:447:ARG:HH12	1:CA:449:SER:HB2	1.84	0.42
1:GA:364:GLN:NE2	1:HA:408:PRO:O	2.52	0.42
1:IA:451:SER:HB3	1:IA:471:GLU:HG3	2.01	0.42
1:IA:610:PHE:CE1	1:IA:661:LEU:HD11	2.54	0.42
1:PA:544:ARG:HD2	1:PA:579:VAL:HG22	2.01	0.42
1:RA:518:THR:HG22	1:RA:549:LEU:HD12	2.01	0.42
2:NB:80:LEU:HD12	2:NB:102:LEU:CD2	2.48	0.42
3:NC:51:LEU:HD22	3:NC:83:CYS:HB3	2.01	0.42
2:BB:119:LEU:O	2:BB:120:HIS:C	2.58	0.42
1:AA:611:ASP:OD1	1:AA:701:ARG:NH2	2.52	0.42
1:BA:631:LEU:HD23	1:BA:631:LEU:H	1.85	0.42
1:GA:669:ARG:HE	1:GA:673:LYS:HE3	1.84	0.42
1:KA:371:VAL:O	1:KA:430:GLN:HA	2.19	0.42
1:MA:509:ALA:HA	1:MA:512:PHE:HD2	1.84	0.42
1:MA:672:ARG:HA	1:MA:684:VAL:HG21	2.00	0.42
3:KC:72:SER:HG	3:KC:73:HIS:HD1	1.67	0.42
3:RC:86:ARG:O	3:RC:89:GLN:HG2	2.18	0.42
3:NC:95:ASP:HA	3:NC:98:ARG:HD2	2.01	0.42
3:DC:33:LEU:HD23	3:DC:36:LEU:HD12	2.00	0.42
1:AA:618:ILE:HA	1:AA:633:LEU:HD21	2.01	0.42
1:AA:648:THR:HG21	1:AA:702:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:412:ILE:HD13	1:BA:501:LEU:HD11	2.00	0.42
1:BA:663:VAL:HG22	1:BA:664:SER:H	1.84	0.42
1:HA:631:LEU:H	1:HA:673:LYS:HZ1	1.67	0.42
1:HA:672:ARG:NH1	1:HA:682:LEU:O	2.53	0.42
1:IA:487:GLN:NE2	2:IB:52:GLN:OE1	2.46	0.42
1:IA:663:VAL:HG22	1:IA:664:SER:H	1.85	0.42
1:LA:394:LEU:HD23	1:LA:498:THR:HG22	2.02	0.42
1:LA:687:TYR:CE2	2:LB:115:ILE:HG21	2.55	0.42
1:LA:688:GLN:HG3	2:LB:121:LYS:HD3	2.01	0.42
1:QA:598:TYR:CE2	1:QA:685:LEU:HD21	2.55	0.42
1:QA:624:GLN:HA	1:QA:629:SER:HB3	2.02	0.42
2:KB:90:SER:OG	2:KB:95:LEU:HD12	2.20	0.42
3:KC:55:LEU:HD11	3:KC:83:CYS:SG	2.58	0.42
3:LC:71:ILE:HD11	3:LC:84:LEU:HB2	2.02	0.42
3:FC:86:ARG:O	3:FC:89:GLN:HG2	2.19	0.42
3:MC:64:GLU:O	3:MC:68:GLN:HG3	2.19	0.42
1:BA:549:LEU:HB3	1:BA:559:ILE:HD11	2.02	0.42
1:NA:365:GLU:HG2	1:OA:408:PRO:HA	2.01	0.42
1:OA:621:ARG:O	1:OA:631:LEU:HD12	2.20	0.42
1:RA:465:HIS:HB2	1:RA:474:TRP:NE1	2.34	0.42
1:RA:482:ARG:HA	1:RA:485:LYS:HD2	2.01	0.42
2:LB:83:LEU:HD11	3:LC:9:GLN:HG3	2.01	0.42
3:PC:50:ARG:O	3:PC:54:LEU:HD13	2.18	0.42
1:AA:513:ILE:HD11	1:AA:553:VAL:HG21	2.00	0.42
1:AA:621:ARG:HB2	1:AA:633:LEU:HG	2.02	0.42
1:CA:439:LEU:HD22	1:CA:465:HIS:CE1	2.54	0.42
1:IA:447:ARG:HH22	1:IA:449:SER:HB2	1.83	0.42
1:KA:609:LEU:HD23	1:KA:662:ILE:HB	2.01	0.42
1:KA:663:VAL:HG22	1:KA:664:SER:H	1.85	0.42
1:LA:655:ILE:HG21	3:LC:21:LEU:O	2.19	0.42
1:NA:652:LEU:HA	1:NA:655:ILE:HG13	2.02	0.42
1:RA:621:ARG:HB2	1:RA:633:LEU:HG	2.01	0.42
1:AA:373:LEU:HD13	1:AA:412:ILE:HG12	2.01	0.42
1:AA:447:ARG:HE	1:AA:496:VAL:HB	1.85	0.42
1:BA:690:LEU:HD23	1:BA:690:LEU:HA	1.90	0.42
1:IA:588:SER:O	1:IA:591:LYS:HG3	2.19	0.42
1:PA:669:ARG:HE	1:PA:673:LYS:HE2	1.85	0.42
3:IC:80:ASN:N	3:IC:104:TYR:HD1	2.17	0.42
1:BA:382:GLN:HA	1:BA:416:PHE:CE1	2.55	0.42
1:FA:663:VAL:HG22	1:FA:664:SER:H	1.85	0.42
1:FA:672:ARG:HA	1:FA:684:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:382:GLN:HG3	1:QA:383:GLU:H	1.85	0.42
1:RA:548:ILE:HG21	1:RA:586:ILE:HD12	2.02	0.42
3:CC:68:GLN:O	3:CC:71:ILE:HG22	2.20	0.42
3:EC:25:HIS:O	3:EC:28:ARG:N	2.52	0.42
2:BB:117:ASN:HA	2:BB:120:HIS:NE2	2.35	0.42
3:MC:86:ARG:HA	3:MC:89:GLN:HG2	2.01	0.42
1:AA:519:ARG:HG2	1:BA:531:GLU:HG2	2.00	0.41
1:DA:373:LEU:HD22	1:DA:412:ILE:HG23	2.01	0.41
1:JA:381:GLN:HA	1:JA:384:ALA:HB3	2.02	0.41
1:JA:598:TYR:HE2	1:JA:685:LEU:HD21	1.85	0.41
1:KA:652:LEU:HD12	1:KA:655:ILE:HD12	2.02	0.41
1:LA:591:LYS:HB3	1:LA:691:THR:HB	2.02	0.41
1:LA:606:PRO:HB3	1:LA:699:LEU:HD11	2.02	0.41
1:NA:370:THR:HG21	1:OA:561:ASN:HD22	1.84	0.41
1:OA:673:LYS:NZ	2:PB:120:HIS:O	2.49	0.41
1:RA:588:SER:O	1:RA:591:LYS:HG3	2.20	0.41
3:JC:76:LEU:HG	3:JC:77:GLN:H	1.85	0.41
3:PC:25:HIS:HB3	3:PC:28:ARG:HD3	2.02	0.41
3:EC:8:ARG:O	3:EC:11:GLU:N	2.52	0.41
1:DA:437:GLY:HA2	1:DA:464:GLU:HB3	2.01	0.41
1:EA:453:LEU:HD11	3:EC:89:GLN:HB2	2.01	0.41
1:LA:381:GLN:HB3	1:LA:385:LEU:HD13	2.01	0.41
1:PA:373:LEU:HD22	1:PA:412:ILE:HG23	2.02	0.41
1:QA:359:GLY:HA3	1:QA:363:GLU:HG2	2.01	0.41
1:QA:663:VAL:HG22	1:QA:664:SER:H	1.86	0.41
1:RA:451:SER:HB3	1:RA:473:PHE:CE2	2.56	0.41
1:RA:608:TYR:CE2	1:RA:699:LEU:HD12	2.55	0.41
3:NC:14:LEU:HD21	3:NC:43:HIS:NE2	2.35	0.41
3:NC:85:SER:HB3	3:NC:100:ALA:HB3	2.01	0.41
1:AA:619:ARG:NE	1:AA:666:ASP:OD2	2.47	0.41
1:GA:687:TYR:CE2	2:GB:115:ILE:HG21	2.56	0.41
1:GA:692:GLN:O	1:GA:694:ILE:HG13	2.21	0.41
1:IA:392:ASP:HA	1:IA:395:VAL:HG12	2.01	0.41
1:LA:631:LEU:HD22	1:LA:670:TYR:HB3	2.03	0.41
1:NA:372:PRO:O	1:NA:430:GLN:N	2.41	0.41
1:QA:692:GLN:O	1:QA:694:ILE:HG13	2.20	0.41
2:PB:80:LEU:O	2:PB:84:GLN:HG2	2.21	0.41
2:IB:101:LEU:HD22	3:IC:31:ILE:HD11	2.03	0.41
1:GA:518:THR:HG22	1:GA:549:LEU:HD12	2.02	0.41
1:HA:467:LEU:HD23	1:HA:468:PRO:HD2	2.02	0.41
1:LA:655:ILE:HG22	1:LA:656:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:385:LEU:HD23	1:NA:385:LEU:HA	1.91	0.41
1:PA:598:TYR:HE2	1:PA:685:LEU:HD21	1.85	0.41
1:QA:618:ILE:HA	1:QA:633:LEU:HD21	2.01	0.41
1:QA:668:ARG:HD3	1:QA:686:SER:OG	2.21	0.41
1:RA:408:PRO:HG3	1:RA:521:LEU:HD21	2.02	0.41
2:PB:51:ALA:HB3	2:PB:54:LYS:HD2	2.02	0.41
2:IB:80:LEU:HD22	2:IB:106:GLN:CG	2.51	0.41
2:AB:87:LEU:HD12	2:AB:102:LEU:CD1	2.50	0.41
1:CA:385:LEU:O	1:CA:386:GLU:HB2	2.21	0.41
1:CA:482:ARG:HA	1:CA:485:LYS:HD2	2.01	0.41
1:DA:394:LEU:HD22	1:DA:501:LEU:HD13	2.02	0.41
1:KA:692:GLN:O	1:KA:694:ILE:HG13	2.21	0.41
1:NA:393:GLU:HG3	1:NA:498:THR:HG21	2.02	0.41
1:QA:672:ARG:HA	1:QA:684:VAL:HG21	2.03	0.41
3:CC:16:ASN:HB3	3:CC:32:LEU:HD13	2.03	0.41
3:JC:43:HIS:O	3:JC:47:ARG:HG2	2.19	0.41
3:KC:33:LEU:CD1	3:KC:49:CYS:HB3	2.50	0.41
3:PC:47:ARG:HG3	3:PC:66:GLU:OE2	2.19	0.41
2:FB:75:ASP:O	2:FB:78:ARG:HG3	2.21	0.41
1:AA:482:ARG:HA	1:AA:485:LYS:HD2	2.03	0.41
1:AA:588:SER:O	1:AA:591:LYS:HG3	2.20	0.41
1:BA:509:ALA:HA	1:BA:512:PHE:HD2	1.85	0.41
1:DA:385:LEU:C	1:DA:387:ALA:H	2.24	0.41
1:DA:467:LEU:O	1:DA:469:ASP:N	2.52	0.41
1:JA:531:GLU:HG2	1:RA:519:ARG:HG2	2.02	0.41
1:NA:519:ARG:HG2	1:OA:531:GLU:HG2	2.02	0.41
1:QA:379:SER:O	1:QA:382:GLN:HG2	2.20	0.41
3:KC:52:VAL:HA	3:KC:55:LEU:HD12	2.03	0.41
3:GC:108:LYS:HD3	3:GC:108:LYS:HA	1.93	0.41
2:LB:114:ILE:O	2:LB:118:LEU:HG	2.21	0.41
2:PB:87:LEU:HD22	2:PB:95:LEU:HD22	2.02	0.41
2:EB:101:LEU:HD11	3:EC:28:ARG:NE	2.35	0.41
2:QB:80:LEU:HD13	2:QB:80:LEU:HA	1.92	0.41
3:QC:33:LEU:HD13	3:QC:50:ARG:HB2	2.03	0.41
1:BA:405:LEU:O	1:BA:559:ILE:N	2.54	0.41
1:CA:441:ALA:HA	1:CA:474:TRP:CZ3	2.56	0.41
1:JA:389:ALA:O	1:JA:390:LEU:HB2	2.21	0.41
1:KA:660:VAL:HG12	1:KA:683:PRO:HG2	2.01	0.41
1:MA:440:LYS:HB2	1:MA:474:TRP:CE2	2.56	0.41
1:MA:518:THR:HG22	1:MA:549:LEU:HD12	2.03	0.41
1:NA:687:TYR:CZ	2:NB:115:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:655:ILE:HG23	2:OB:58:TRP:CH2	2.56	0.41
1:RA:513:ILE:HD11	1:RA:553:VAL:HG21	2.03	0.41
2:KB:75:ASP:HA	2:KB:78:ARG:HG2	2.03	0.41
3:FC:50:ARG:O	3:FC:54:LEU:HD13	2.20	0.41
3:DC:12:PHE:O	3:DC:15:LEU:HG	2.21	0.41
3:MC:47:ARG:HD3	3:MC:50:ARG:NH2	2.36	0.41
1:CA:598:TYR:HE2	1:CA:685:LEU:HD21	1.85	0.41
1:EA:663:VAL:HG22	1:EA:664:SER:H	1.85	0.41
1:FA:675:ILE:HD12	1:FA:682:LEU:HD23	2.03	0.41
1:HA:598:TYR:HD2	1:HA:685:LEU:HD11	1.86	0.41
1:LA:598:TYR:CE2	1:LA:685:LEU:HD21	2.55	0.41
1:NA:513:ILE:HD11	1:NA:553:VAL:HG21	2.03	0.41
1:PA:621:ARG:HB2	1:PA:633:LEU:HG	2.01	0.41
3:JC:16:ASN:HB3	3:JC:32:LEU:HD13	2.02	0.41
2:LB:98:ALA:O	2:LB:102:LEU:HG	2.20	0.41
3:EC:98:ARG:NH1	3:EC:102:GLN:OE1	2.53	0.41
1:CA:692:GLN:O	1:CA:694:ILE:HG13	2.21	0.41
1:DA:635:PRO:HD3	2:EB:118:LEU:HD21	2.02	0.41
1:EA:687:TYR:CE2	2:EB:115:ILE:HG21	2.56	0.41
1:FA:448:GLU:HG3	1:FA:450:VAL:H	1.86	0.41
1:IA:373:LEU:HD11	1:IA:505:LEU:HD21	2.01	0.41
1:IA:393:GLU:HG2	1:IA:494:SER:HB2	2.02	0.41
1:KA:375:ILE:HG12	1:KA:427:ILE:HG12	2.03	0.41
1:MA:598:TYR:CE2	1:MA:685:LEU:HD21	2.55	0.41
1:MA:663:VAL:HG22	1:MA:664:SER:H	1.86	0.41
1:NA:408:PRO:HG3	1:NA:521:LEU:HD21	2.02	0.41
1:NA:533:ILE:HA	1:NA:536:VAL:HG12	2.03	0.41
1:NA:692:GLN:O	1:NA:694:ILE:HG13	2.21	0.41
1:OA:513:ILE:HD11	1:OA:553:VAL:HG21	2.02	0.41
1:OA:606:PRO:HB2	1:OA:659:PRO:HA	2.02	0.41
1:QA:509:ALA:HA	1:QA:512:PHE:CD2	2.55	0.41
1:QA:544:ARG:HD2	1:QA:579:VAL:HG22	2.03	0.41
2:KB:70:LEU:HD12	3:KC:8:ARG:HG2	2.03	0.41
2:KB:79:GLU:OE2	3:KC:8:ARG:HB3	2.21	0.41
3:KC:66:GLU:O	3:KC:70:LEU:HD12	2.20	0.41
3:LC:53:ALA:O	3:LC:57:ASN:HB2	2.20	0.41
3:NC:50:ARG:NH2	3:NC:62:ARG:HD3	2.36	0.41
3:EC:50:ARG:O	3:EC:54:LEU:HD13	2.20	0.41
3:BC:60:GLY:O	3:BC:64:GLU:HG3	2.21	0.41
3:BC:62:ARG:O	3:BC:66:GLU:HG2	2.21	0.41
1:BA:619:ARG:NE	1:BA:666:ASP:OD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:672:ARG:HA	1:BA:684:VAL:HG21	2.03	0.41
1:CA:533:ILE:HA	1:CA:536:VAL:HG12	2.02	0.41
1:EA:621:ARG:HB2	1:EA:633:LEU:HG	2.03	0.41
1:KA:513:ILE:HD11	1:KA:553:VAL:HG21	2.03	0.41
1:LA:656:GLN:O	1:LA:657:SER:OG	2.32	0.41
1:OA:551:ARG:HH12	2:PB:122:VAL:HG22	1.85	0.41
1:PA:692:GLN:O	1:PA:694:ILE:HG13	2.21	0.41
2:JB:111:LEU:HD23	2:JB:111:LEU:HA	1.96	0.41
3:NC:25:HIS:O	3:NC:28:ARG:N	2.55	0.41
2:OB:84:GLN:O	2:OB:88:THR:OG1	2.29	0.41
3:FC:95:ASP:O	3:FC:99:HIS:ND1	2.34	0.41
3:IC:35:ALA:O	3:IC:38:THR:HG22	2.20	0.41
1:CA:548:ILE:HG21	1:CA:586:ILE:HD12	2.01	0.40
1:GA:483:LEU:HB3	1:GA:490:PHE:CZ	2.48	0.40
1:HA:513:ILE:HD11	1:HA:553:VAL:HG21	2.02	0.40
1:KA:598:TYR:CE2	1:KA:685:LEU:HD21	2.55	0.40
1:MA:440:LYS:HD2	1:MA:474:TRP:CD1	2.55	0.40
1:NA:425:TYR:CE1	1:NA:440:LYS:HB2	2.48	0.40
1:NA:588:SER:O	1:NA:591:LYS:HG3	2.20	0.40
1:NA:606:PRO:HB2	1:NA:659:PRO:HA	2.03	0.40
1:RA:606:PRO:HB2	1:RA:659:PRO:HA	2.03	0.40
2:HB:96:GLN:OE1	2:MB:96:GLN:HB2	2.21	0.40
3:MC:88:GLN:HG3	3:MC:97:ALA:HB2	2.03	0.40
1:CA:441:ALA:O	1:CA:445:LEU:N	2.55	0.40
1:LA:588:SER:O	1:LA:591:LYS:HG3	2.21	0.40
1:NA:459:PRO:HG3	3:NC:98:ARG:HH12	1.86	0.40
1:PA:644:GLN:O	1:PA:648:THR:OG1	2.37	0.40
3:NC:36:LEU:HD22	3:NC:46:GLY:HA3	2.02	0.40
2:FB:73:ALA:C	2:FB:77:ARG:HH21	2.25	0.40
2:FB:101:LEU:HD22	3:FC:31:ILE:HD11	2.02	0.40
1:BA:623:ARG:HB2	1:BA:630:TYR:O	2.20	0.40
1:BA:655:ILE:CG1	3:BC:24:GLY:HA3	2.49	0.40
1:CA:438:GLU:HB2	1:CA:466:LEU:HD21	2.03	0.40
1:GA:394:LEU:HD22	1:GA:501:LEU:HD13	2.03	0.40
1:IA:518:THR:HG22	1:IA:549:LEU:HD12	2.04	0.40
1:KA:656:GLN:OE1	3:KC:22:GLN:NE2	2.53	0.40
1:LA:663:VAL:HG22	1:LA:664:SER:H	1.86	0.40
1:NA:587:ARG:NE	1:NA:689:GLU:OE2	2.49	0.40
3:JC:95:ASP:N	3:JC:95:ASP:OD1	2.54	0.40
3:GC:74:ASP:OD1	3:GC:75:PRO:HD2	2.21	0.40
1:AA:405:LEU:O	1:AA:559:ILE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:663:VAL:HG22	1:AA:664:SER:H	1.85	0.40
1:BA:633:LEU:HB2	1:BA:634:ASP:H	1.73	0.40
1:LA:373:LEU:HD11	1:LA:505:LEU:HD21	2.03	0.40
1:PA:480:GLU:HA	1:PA:490:PHE:HE2	1.86	0.40
1:PA:513:ILE:HD11	1:PA:553:VAL:HG21	2.03	0.40
1:PA:591:LYS:HE2	1:PA:688:GLN:O	2.21	0.40
1:QA:616:GLU:OE1	1:QA:619:ARG:NH1	2.55	0.40
1:AA:701:ARG:HD3	2:AB:108:ASP:OD1	2.21	0.40
1:DA:663:VAL:HG22	1:DA:664:SER:H	1.85	0.40
1:EA:608:TYR:OH	3:EC:25:HIS:HE1	2.05	0.40
1:GA:663:VAL:HG22	1:GA:664:SER:H	1.86	0.40
1:HA:699:LEU:O	3:HC:28:ARG:NH1	2.55	0.40
1:MA:675:ILE:HD12	1:MA:682:LEU:HD23	2.02	0.40
1:PA:430:GLN:OE1	1:QA:561:ASN:ND2	2.25	0.40
1:PA:699:LEU:HB3	3:PC:25:HIS:NE2	2.37	0.40
1:QA:480:GLU:HG2	1:QA:490:PHE:CE1	2.56	0.40
1:QA:609:LEU:H	1:QA:609:LEU:HG	1.62	0.40
2:CB:101:LEU:HD11	3:CC:28:ARG:NE	2.36	0.40
3:PC:50:ARG:HH21	3:PC:62:ARG:NH2	2.19	0.40
3:MC:62:ARG:O	3:MC:66:GLU:HG2	2.22	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 X-ray entries followed by that with respect to entries of similar resolution.

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	AA	311/350 (89%)	283 (91%)	27 (9%)	1 (0%)	41 75
1	BA	327/350 (93%)	302 (92%)	25 (8%)	0	100 100
1	CA	337/350 (96%)	294 (87%)	41 (12%)	2 (1%)	25 63
1	DA	318/350 (91%)	288 (91%)	30 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EA	317/350 (91%)	289 (91%)	28 (9%)	0	100	100
1	FA	329/350 (94%)	299 (91%)	30 (9%)	0	100	100
1	GA	335/350 (96%)	298 (89%)	37 (11%)	0	100	100
1	HA	327/350 (93%)	294 (90%)	33 (10%)	0	100	100
1	IA	330/350 (94%)	296 (90%)	32 (10%)	2 (1%)	25	63
1	JA	324/350 (93%)	289 (89%)	34 (10%)	1 (0%)	41	75
1	KA	325/350 (93%)	296 (91%)	27 (8%)	2 (1%)	25	63
1	LA	328/350 (94%)	298 (91%)	30 (9%)	0	100	100
1	MA	312/350 (89%)	276 (88%)	36 (12%)	0	100	100
1	NA	321/350 (92%)	290 (90%)	31 (10%)	0	100	100
1	OA	319/350 (91%)	284 (89%)	35 (11%)	0	100	100
1	PA	322/350 (92%)	284 (88%)	37 (12%)	1 (0%)	41	75
1	QA	326/350 (93%)	292 (90%)	33 (10%)	1 (0%)	41	75
1	RA	340/350 (97%)	299 (88%)	40 (12%)	1 (0%)	41	75
2	AB	66/95 (70%)	61 (92%)	5 (8%)	0	100	100
2	BB	61/95 (64%)	57 (93%)	4 (7%)	0	100	100
2	CB	64/95 (67%)	59 (92%)	4 (6%)	1 (2%)	9	43
2	DB	57/95 (60%)	55 (96%)	2 (4%)	0	100	100
2	EB	56/95 (59%)	54 (96%)	2 (4%)	0	100	100
2	FB	68/95 (72%)	64 (94%)	4 (6%)	0	100	100
2	GB	69/95 (73%)	66 (96%)	3 (4%)	0	100	100
2	HB	61/95 (64%)	54 (88%)	7 (12%)	0	100	100
2	IB	59/95 (62%)	57 (97%)	2 (3%)	0	100	100
2	JB	65/95 (68%)	62 (95%)	3 (5%)	0	100	100
2	KB	73/95 (77%)	67 (92%)	6 (8%)	0	100	100
2	LB	67/95 (70%)	55 (82%)	11 (16%)	1 (2%)	10	44
2	MB	58/95 (61%)	54 (93%)	4 (7%)	0	100	100
2	NB	55/95 (58%)	53 (96%)	2 (4%)	0	100	100
2	OB	66/95 (70%)	63 (96%)	3 (4%)	0	100	100
2	PB	61/95 (64%)	54 (88%)	7 (12%)	0	100	100
2	QB	60/95 (63%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	RB	66/95 (70%)	63 (96%)	3 (4%)	0	100	100
3	AC	87/122 (71%)	80 (92%)	7 (8%)	0	100	100
3	BC	89/122 (73%)	84 (94%)	4 (4%)	1 (1%)	14	50
3	CC	104/122 (85%)	100 (96%)	4 (4%)	0	100	100
3	DC	95/122 (78%)	89 (94%)	5 (5%)	1 (1%)	14	50
3	EC	90/122 (74%)	84 (93%)	6 (7%)	0	100	100
3	FC	102/122 (84%)	93 (91%)	9 (9%)	0	100	100
3	GC	107/122 (88%)	97 (91%)	10 (9%)	0	100	100
3	HC	98/122 (80%)	90 (92%)	7 (7%)	1 (1%)	15	52
3	IC	79/122 (65%)	74 (94%)	5 (6%)	0	100	100
3	JC	107/122 (88%)	99 (92%)	7 (6%)	1 (1%)	17	54
3	KC	110/122 (90%)	105 (96%)	5 (4%)	0	100	100
3	LC	101/122 (83%)	95 (94%)	6 (6%)	0	100	100
3	MC	86/122 (70%)	82 (95%)	4 (5%)	0	100	100
3	NC	100/122 (82%)	93 (93%)	7 (7%)	0	100	100
3	OC	106/122 (87%)	98 (92%)	8 (8%)	0	100	100
3	PC	107/122 (88%)	99 (92%)	8 (8%)	0	100	100
3	QC	83/122 (68%)	78 (94%)	4 (5%)	1 (1%)	13	48
3	RC	107/122 (88%)	100 (94%)	6 (6%)	1 (1%)	17	54
All	All	8738/10206 (86%)	7947 (91%)	772 (9%)	19 (0%)	47	80

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CA	469	ASP
1	CA	627	ALA
1	PA	391	ASN
2	CB	120	HIS
2	LB	77	ARG
1	RA	627	ALA
3	QC	24	GLY
1	QA	386	GLU
1	AA	600	ASN
1	JA	389	ALA
1	IA	386	GLU

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Mol	Chain	Res	Type
1	KA	386	GLU
1	IA	390	LEU
3	JC	24	GLY
3	BC	24	GLY
3	DC	24	GLY
1	KA	450	VAL
3	RC	24	GLY
3	HC	24	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AA	290/312 (93%)	284 (98%)	6 (2%)	53	72
1	BA	296/312 (95%)	288 (97%)	8 (3%)	44	66
1	CA	307/312 (98%)	297 (97%)	10 (3%)	38	62
1	DA	294/312 (94%)	284 (97%)	10 (3%)	37	61
1	EA	296/312 (95%)	288 (97%)	8 (3%)	44	66
1	FA	301/312 (96%)	292 (97%)	9 (3%)	41	64
1	GA	305/312 (98%)	297 (97%)	8 (3%)	46	67
1	HA	302/312 (97%)	294 (97%)	8 (3%)	46	67
1	IA	302/312 (97%)	297 (98%)	5 (2%)	60	78
1	JA	297/312 (95%)	288 (97%)	9 (3%)	41	64
1	KA	303/312 (97%)	294 (97%)	9 (3%)	41	64
1	LA	302/312 (97%)	294 (97%)	8 (3%)	46	67
1	MA	290/312 (93%)	280 (97%)	10 (3%)	37	61
1	NA	297/312 (95%)	289 (97%)	8 (3%)	44	66
1	OA	297/312 (95%)	291 (98%)	6 (2%)	55	73
1	PA	298/312 (96%)	288 (97%)	10 (3%)	37	61
1	QA	300/312 (96%)	290 (97%)	10 (3%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	RA	308/312 (99%)	299 (97%)	9 (3%)	42	64
2	AB	61/81 (75%)	59 (97%)	2 (3%)	38	62
2	BB	58/81 (72%)	55 (95%)	3 (5%)	23	51
2	CB	60/81 (74%)	59 (98%)	1 (2%)	60	78
2	DB	56/81 (69%)	55 (98%)	1 (2%)	59	77
2	EB	54/81 (67%)	54 (100%)	0	100	100
2	FB	64/81 (79%)	61 (95%)	3 (5%)	26	53
2	GB	66/81 (82%)	62 (94%)	4 (6%)	18	47
2	HB	58/81 (72%)	58 (100%)	0	100	100
2	IB	56/81 (69%)	55 (98%)	1 (2%)	59	77
2	JB	61/81 (75%)	61 (100%)	0	100	100
2	KB	68/81 (84%)	68 (100%)	0	100	100
2	LB	64/81 (79%)	64 (100%)	0	100	100
2	MB	55/81 (68%)	53 (96%)	2 (4%)	35	60
2	NB	54/81 (67%)	53 (98%)	1 (2%)	57	75
2	OB	61/81 (75%)	59 (97%)	2 (3%)	38	62
2	PB	58/81 (72%)	58 (100%)	0	100	100
2	QB	58/81 (72%)	55 (95%)	3 (5%)	23	51
2	RB	61/81 (75%)	60 (98%)	1 (2%)	62	78
3	AC	78/103 (76%)	75 (96%)	3 (4%)	33	59
3	BC	81/103 (79%)	78 (96%)	3 (4%)	34	59
3	CC	92/103 (89%)	89 (97%)	3 (3%)	38	62
3	DC	85/103 (82%)	81 (95%)	4 (5%)	26	53
3	EC	83/103 (81%)	79 (95%)	4 (5%)	25	53
3	FC	89/103 (86%)	86 (97%)	3 (3%)	37	61
3	GC	92/103 (89%)	88 (96%)	4 (4%)	29	56
3	HC	86/103 (84%)	82 (95%)	4 (5%)	26	53
3	IC	76/103 (74%)	74 (97%)	2 (3%)	46	67
3	JC	92/103 (89%)	87 (95%)	5 (5%)	22	50
3	KC	94/103 (91%)	90 (96%)	4 (4%)	29	56
3	LC	89/103 (86%)	86 (97%)	3 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	MC	81/103 (79%)	77 (95%)	4 (5%)	25 52
3	NC	85/103 (82%)	83 (98%)	2 (2%)	49 69
3	OC	91/103 (88%)	88 (97%)	3 (3%)	38 62
3	PC	92/103 (89%)	87 (95%)	5 (5%)	22 50
3	QC	79/103 (77%)	76 (96%)	3 (4%)	33 59
3	RC	92/103 (89%)	90 (98%)	2 (2%)	52 71
All	All	8015/8928 (90%)	7779 (97%)	236 (3%)	42 64

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	434	VAL
1	AA	475	VAL
1	AA	500	HIS
1	AA	633	LEU
1	AA	638	THR
1	AA	648	THR
1	BA	369	MET
1	BA	395	VAL
1	BA	458	ILE
1	BA	475	VAL
1	BA	630	TYR
1	BA	633	LEU
1	BA	638	THR
1	BA	648	THR
1	CA	369	MET
1	CA	395	VAL
1	CA	434	VAL
1	CA	439	LEU
1	CA	466	LEU
1	CA	467	LEU
1	CA	475	VAL
1	CA	500	HIS
1	CA	638	THR
1	CA	656	GLN
1	DA	369	MET
1	DA	395	VAL
1	DA	434	VAL
1	DA	472	THR
1	DA	475	VAL

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Mol	Chain	Res	Type
1	DA	500	HIS
1	DA	604	ILE
1	DA	630	TYR
1	DA	638	THR
1	DA	648	THR
1	EA	369	MET
1	EA	395	VAL
1	EA	434	VAL
1	EA	475	VAL
1	EA	500	HIS
1	EA	638	THR
1	EA	648	THR
1	EA	652	LEU
1	FA	369	MET
1	FA	395	VAL
1	FA	434	VAL
1	FA	458	ILE
1	FA	475	VAL
1	FA	500	HIS
1	FA	633	LEU
1	FA	638	THR
1	FA	648	THR
1	GA	369	MET
1	GA	395	VAL
1	GA	434	VAL
1	GA	453	LEU
1	GA	500	HIS
1	GA	604	ILE
1	GA	630	TYR
1	GA	652	LEU
1	HA	369	MET
1	HA	395	VAL
1	HA	434	VAL
1	HA	467	LEU
1	HA	475	VAL
1	HA	500	HIS
1	HA	625	THR
1	HA	633	LEU
1	IA	369	MET
1	IA	434	VAL
1	IA	475	VAL
1	IA	638	THR

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Mol	Chain	Res	Type
1	IA	648	THR
1	JA	369	MET
1	JA	395	VAL
1	JA	434	VAL
1	JA	475	VAL
1	JA	500	HIS
1	JA	604	ILE
1	JA	633	LEU
1	JA	638	THR
1	JA	648	THR
1	KA	369	MET
1	KA	395	VAL
1	KA	434	VAL
1	KA	453	LEU
1	KA	458	ILE
1	KA	475	VAL
1	KA	500	HIS
1	KA	633	LEU
1	KA	648	THR
1	LA	369	MET
1	LA	395	VAL
1	LA	439	LEU
1	LA	475	VAL
1	LA	500	HIS
1	LA	633	LEU
1	LA	638	THR
1	LA	648	THR
1	MA	369	MET
1	MA	395	VAL
1	MA	434	VAL
1	MA	443	TYR
1	MA	475	VAL
1	MA	500	HIS
1	MA	630	TYR
1	MA	633	LEU
1	MA	638	THR
1	MA	648	THR
1	NA	369	MET
1	NA	395	VAL
1	NA	434	VAL
1	NA	493	HIS
1	NA	500	HIS

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Mol	Chain	Res	Type
1	NA	633	LEU
1	NA	638	THR
1	NA	648	THR
1	OA	369	MET
1	OA	475	VAL
1	OA	500	HIS
1	OA	604	ILE
1	OA	638	THR
1	OA	648	THR
1	PA	369	MET
1	PA	395	VAL
1	PA	455	LEU
1	PA	458	ILE
1	PA	475	VAL
1	PA	482	ARG
1	PA	500	HIS
1	PA	633	LEU
1	PA	638	THR
1	PA	648	THR
1	QA	369	MET
1	QA	395	VAL
1	QA	434	VAL
1	QA	458	ILE
1	QA	475	VAL
1	QA	500	HIS
1	QA	630	TYR
1	QA	631	LEU
1	QA	638	THR
1	QA	649	ILE
1	RA	369	MET
1	RA	395	VAL
1	RA	467	LEU
1	RA	475	VAL
1	RA	500	HIS
1	RA	630	TYR
1	RA	633	LEU
1	RA	638	THR
1	RA	649	ILE
2	CB	79	GLU
3	CC	38	THR
3	CC	43	HIS
3	CC	101	TYR

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Mol	Chain	Res	Type
3	JC	38	THR
3	JC	68	GLN
3	JC	71	ILE
3	JC	77	GLN
3	JC	102	GLN
3	KC	14	LEU
3	KC	49	CYS
3	KC	50	ARG
3	KC	70	LEU
2	RB	107	ASP
3	RC	71	ILE
3	RC	101	TYR
2	GB	86	LEU
2	GB	116	LEU
2	GB	120	HIS
2	GB	122	VAL
3	GC	6	THR
3	GC	71	ILE
3	GC	101	TYR
3	GC	102	GLN
3	LC	57	ASN
3	LC	59	GLN
3	LC	101	TYR
2	NB	116	LEU
3	NC	71	ILE
3	NC	101	TYR
2	OB	59	ASP
2	OB	96	GLN
3	OC	38	THR
3	OC	71	ILE
3	OC	101	TYR
3	PC	27	GLU
3	PC	38	THR
3	PC	43	HIS
3	PC	59	GLN
3	PC	71	ILE
3	EC	38	THR
3	EC	57	ASN
3	EC	71	ILE
3	EC	101	TYR
2	FB	50	THR
2	FB	79	GLU

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Mol	Chain	Res	Type
2	FB	122	VAL
3	FC	47	ARG
3	FC	71	ILE
3	FC	101	TYR
3	HC	14	LEU
3	HC	71	ILE
3	HC	101	TYR
3	HC	102	GLN
2	IB	105	GLN
3	IC	57	ASN
3	IC	101	TYR
2	AB	79	GLU
2	AB	80	LEU
3	AC	66	GLU
3	AC	94	LEU
3	AC	101	TYR
2	BB	79	GLU
2	BB	80	LEU
2	BB	122	VAL
3	BC	57	ASN
3	BC	71	ILE
3	BC	101	TYR
2	DB	122	VAL
3	DC	25	HIS
3	DC	38	THR
3	DC	71	ILE
3	DC	101	TYR
2	MB	94	GLU
2	MB	101	LEU
3	MC	47	ARG
3	MC	57	ASN
3	MC	71	ILE
3	MC	101	TYR
2	QB	80	LEU
2	QB	84	GLN
2	QB	122	VAL
3	QC	21	LEU
3	QC	71	ILE
3	QC	101	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	CA	465	HIS
1	CA	656	GLN
1	EA	697	GLN
1	PA	364	GLN
1	RA	654	GLN
2	JB	84	GLN
2	JB	106	GLN
2	KB	84	GLN
3	RC	25	HIS
3	RC	56	ASN
2	LB	84	GLN
2	OB	96	GLN
2	OB	120	HIS
2	EB	84	GLN
2	FB	106	GLN
2	HB	106	GLN
2	IB	105	GLN
2	BB	106	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.