



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:01 AM GMT

PDB ID : 3QA8
Title : Crystal Structure of inhibitor of kappa B kinase beta
Authors : Xu, G.; Lo, Y.C.; Li, Q.; Napolitano, G.; Wu, X.; Jiang, X.; Dreano, M.;
Karin, M.; Wu, H.
Deposited on : 2011-01-10
Resolution : 3.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

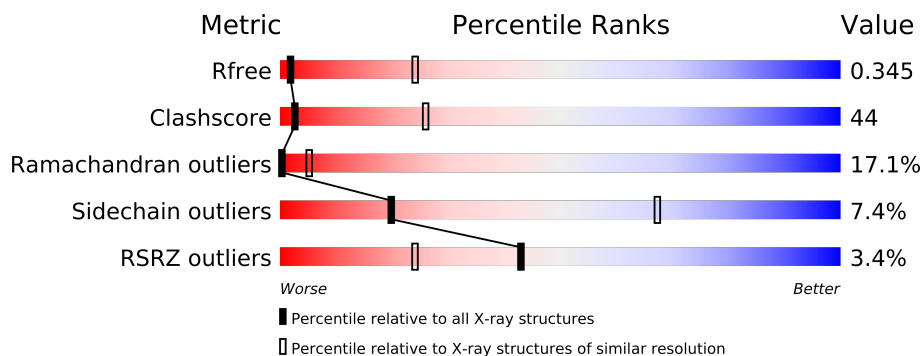
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.60 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}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	676	
1	B	676	
1	C	676	
1	D	676	
1	E	676	
1	F	676	
1	G	676	
1	H	676	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39026 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MGC80376 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	B	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	C	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	D	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	E	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	F	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	G	541	Total	C	N	O	S	0	0	0
			4369	2764	779	800	26			
1	H	541	Total	C	N	O	S	0	0	0
			4369	2764	779	800	26			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
A	4	SER	-	EXPRESSION TAG	UNP Q6INT1
A	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
A	6	SER	-	EXPRESSION TAG	UNP Q6INT1
A	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
A	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
A	9	THR	-	EXPRESSION TAG	UNP Q6INT1
A	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
A	11	THR	-	EXPRESSION TAG	UNP Q6INT1
A	12	CYS	-	EXPRESSION TAG	UNP Q6INT1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
A	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
A	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
A	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
A	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
B	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
B	4	SER	-	EXPRESSION TAG	UNP Q6INT1
B	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
B	6	SER	-	EXPRESSION TAG	UNP Q6INT1
B	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
B	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
B	9	THR	-	EXPRESSION TAG	UNP Q6INT1
B	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
B	11	THR	-	EXPRESSION TAG	UNP Q6INT1
B	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
B	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
B	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
B	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
B	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
B	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
C	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
C	4	SER	-	EXPRESSION TAG	UNP Q6INT1
C	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
C	6	SER	-	EXPRESSION TAG	UNP Q6INT1
C	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
C	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
C	9	THR	-	EXPRESSION TAG	UNP Q6INT1
C	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
C	11	THR	-	EXPRESSION TAG	UNP Q6INT1
C	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
C	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
C	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
C	16	GLU	-	EXPRESSION TAG	UNP Q6INT1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
C	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
D	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
D	4	SER	-	EXPRESSION TAG	UNP Q6INT1
D	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
D	6	SER	-	EXPRESSION TAG	UNP Q6INT1
D	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
D	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
D	9	THR	-	EXPRESSION TAG	UNP Q6INT1
D	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
D	11	THR	-	EXPRESSION TAG	UNP Q6INT1
D	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
D	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
D	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
D	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
D	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
D	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
E	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
E	4	SER	-	EXPRESSION TAG	UNP Q6INT1
E	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
E	6	SER	-	EXPRESSION TAG	UNP Q6INT1
E	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
E	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
E	9	THR	-	EXPRESSION TAG	UNP Q6INT1
E	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
E	11	THR	-	EXPRESSION TAG	UNP Q6INT1
E	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
E	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
E	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
E	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
E	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
E	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
F	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
F	1	GLY	-	EXPRESSION TAG	UNP Q6INT1

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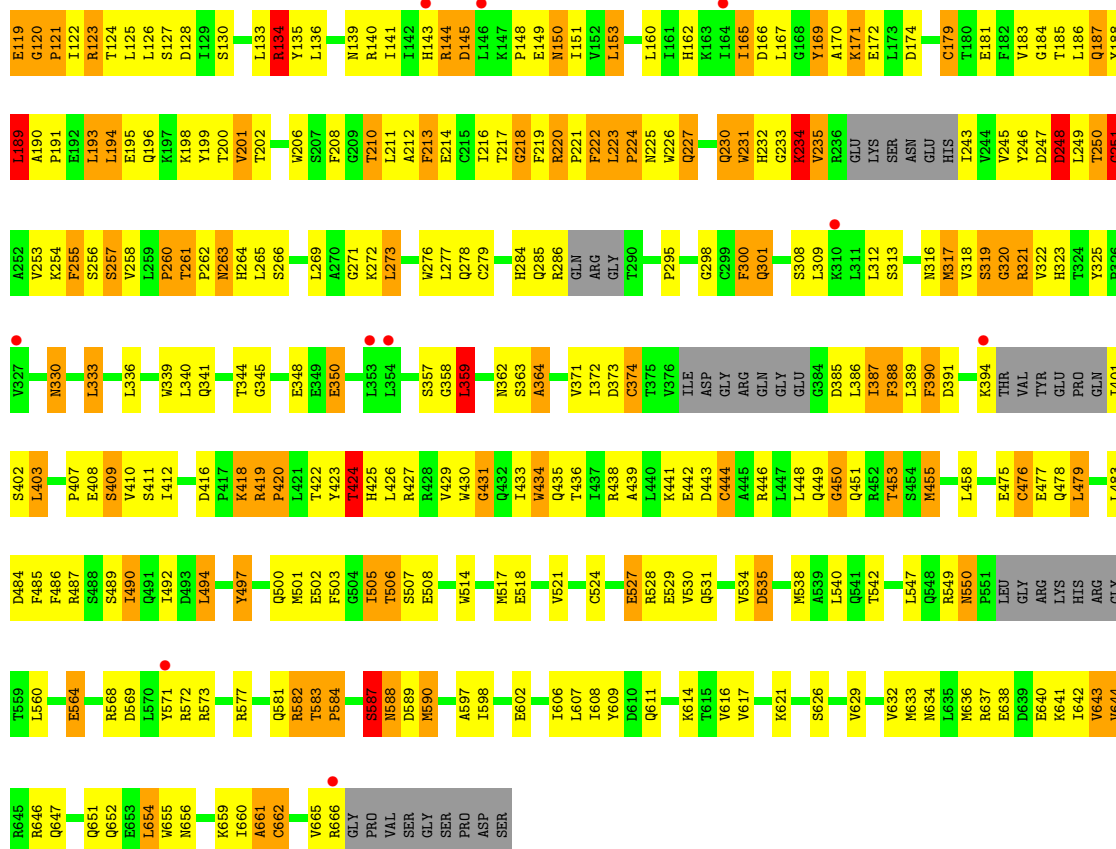
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Chain	Residue	Modelled	Actual	Comment	Reference
F	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
F	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
F	4	SER	-	EXPRESSION TAG	UNP Q6INT1
F	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
F	6	SER	-	EXPRESSION TAG	UNP Q6INT1
F	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
F	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
F	9	THR	-	EXPRESSION TAG	UNP Q6INT1
F	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
F	11	THR	-	EXPRESSION TAG	UNP Q6INT1
F	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
F	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
F	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
F	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
F	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
F	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
F	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
G	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
G	4	SER	-	EXPRESSION TAG	UNP Q6INT1
G	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
G	6	SER	-	EXPRESSION TAG	UNP Q6INT1
G	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
G	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
G	9	THR	-	EXPRESSION TAG	UNP Q6INT1
G	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
G	11	THR	-	EXPRESSION TAG	UNP Q6INT1
G	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
G	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
G	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
G	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
G	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
G	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
H	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
H	4	SER	-	EXPRESSION TAG	UNP Q6INT1
H	5	PRO	-	EXPRESSION TAG	UNP Q6INT1

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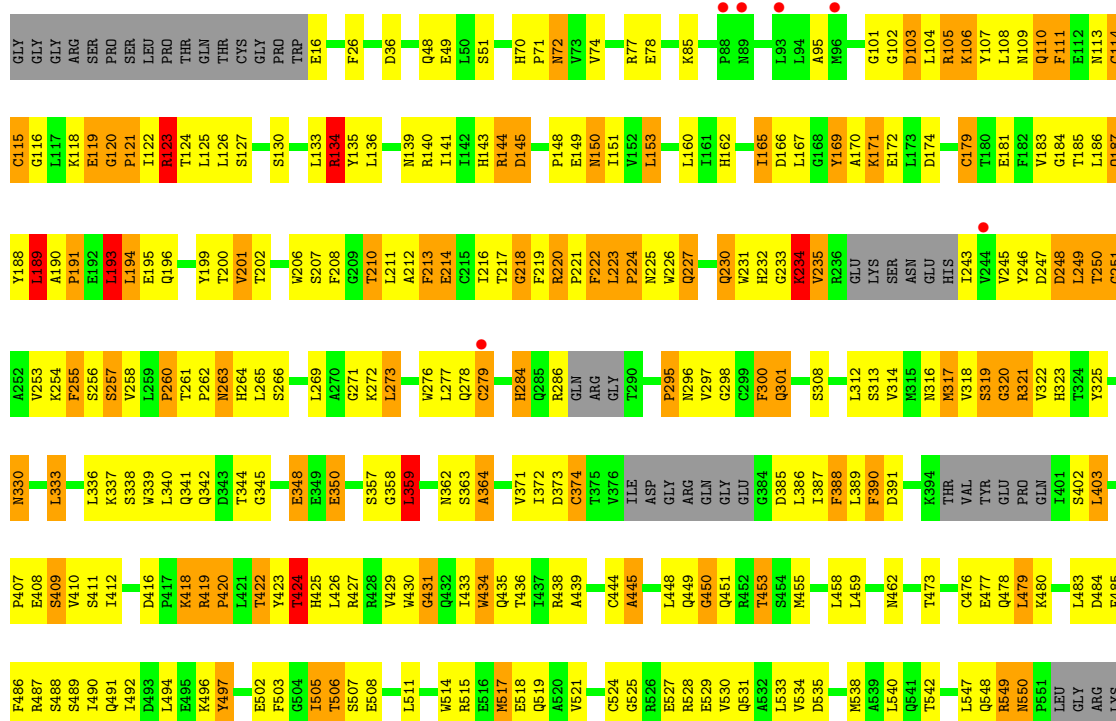
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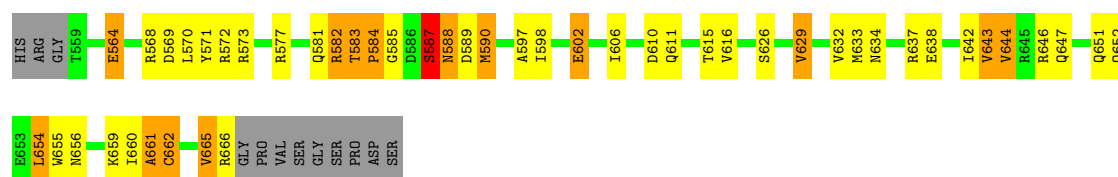
Chain	Residue	Modelled	Actual	Comment	Reference
H	6	SER	-	EXPRESSION TAG	UNP Q6INT1
H	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
H	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
H	9	THR	-	EXPRESSION TAG	UNP Q6INT1
H	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
H	11	THR	-	EXPRESSION TAG	UNP Q6INT1
H	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
H	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
H	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
H	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
H	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
H	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1



• Molecule 1: MGC80376 protein

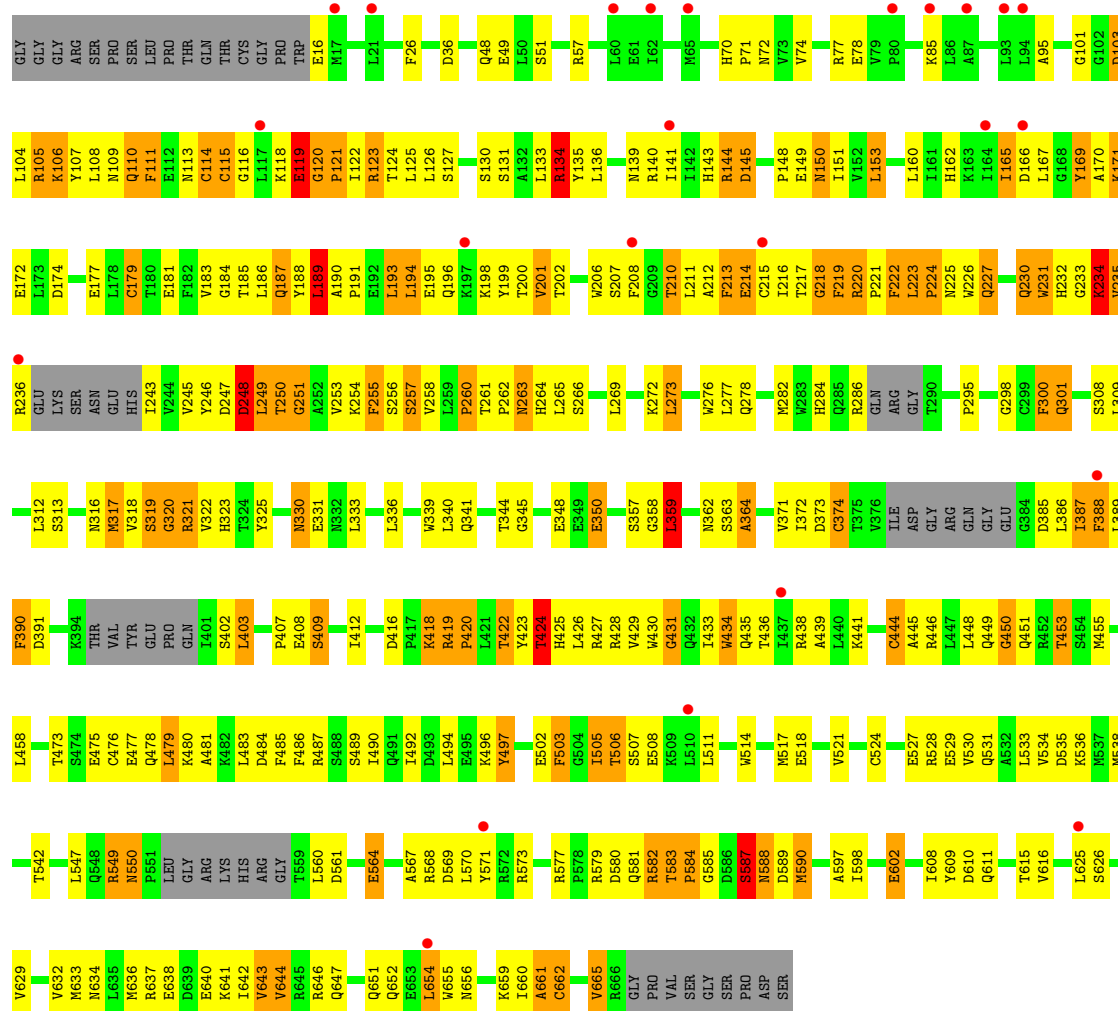
Chain C:





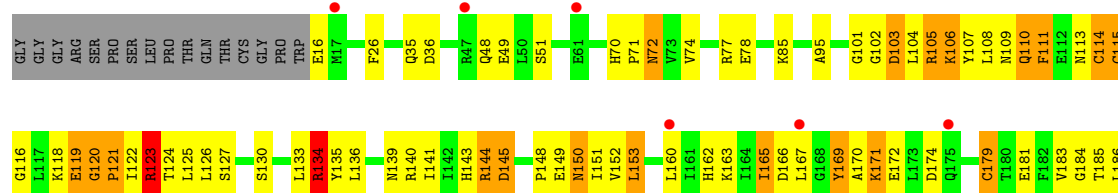
• Molecule 1: MGC80376 protein

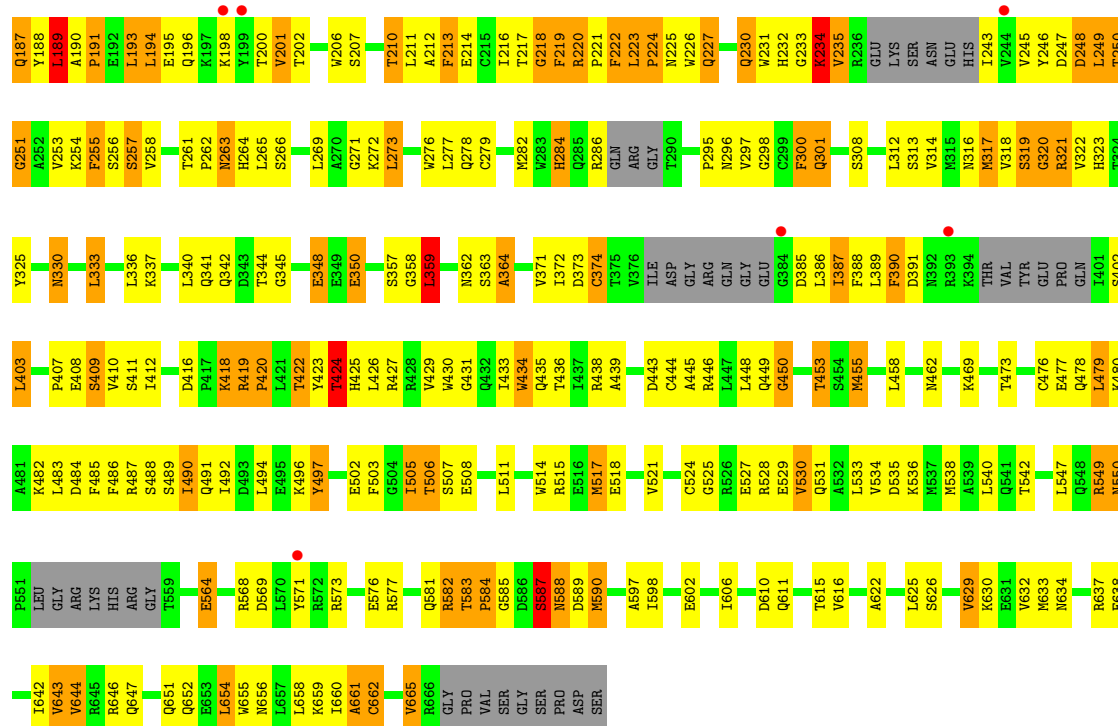
Chain D:



• Molecule 1: MGC80376 protein

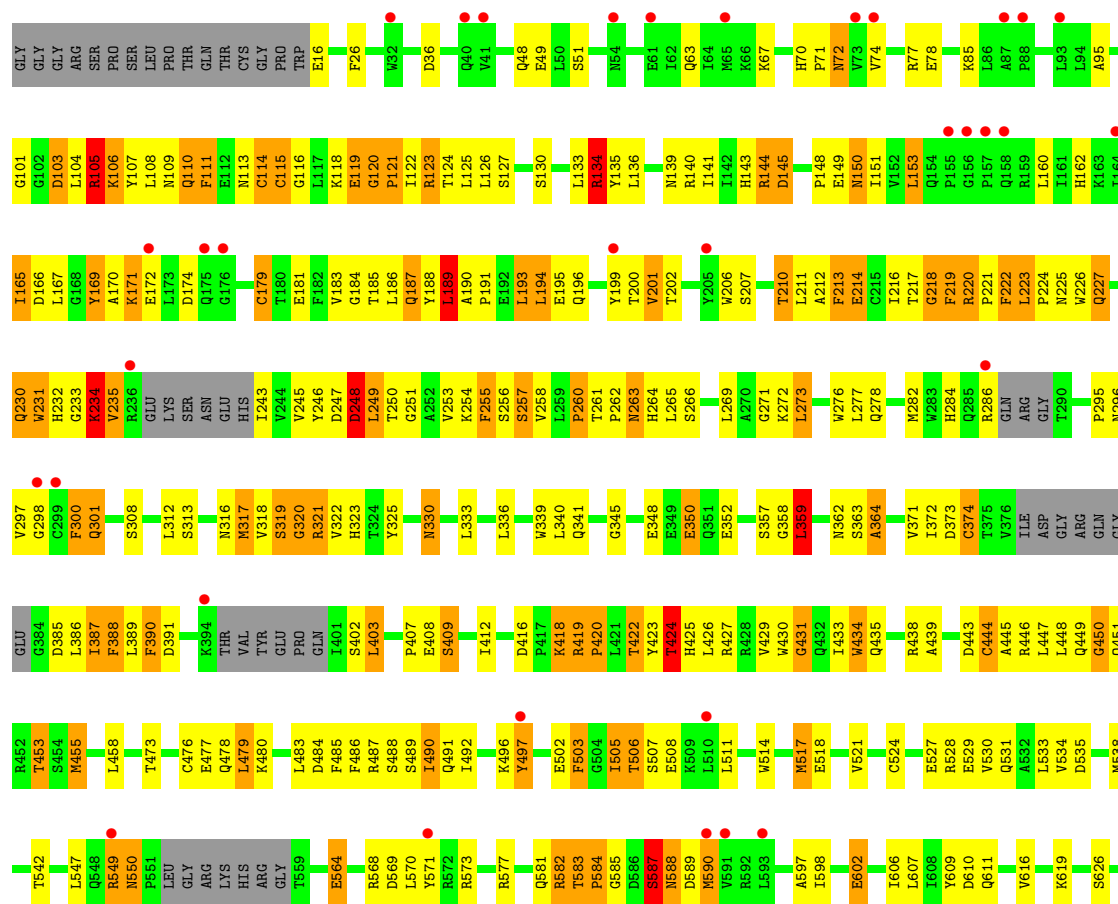
Chain E:

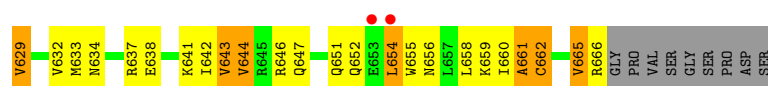




• Molecule 1: MGC80376 protein

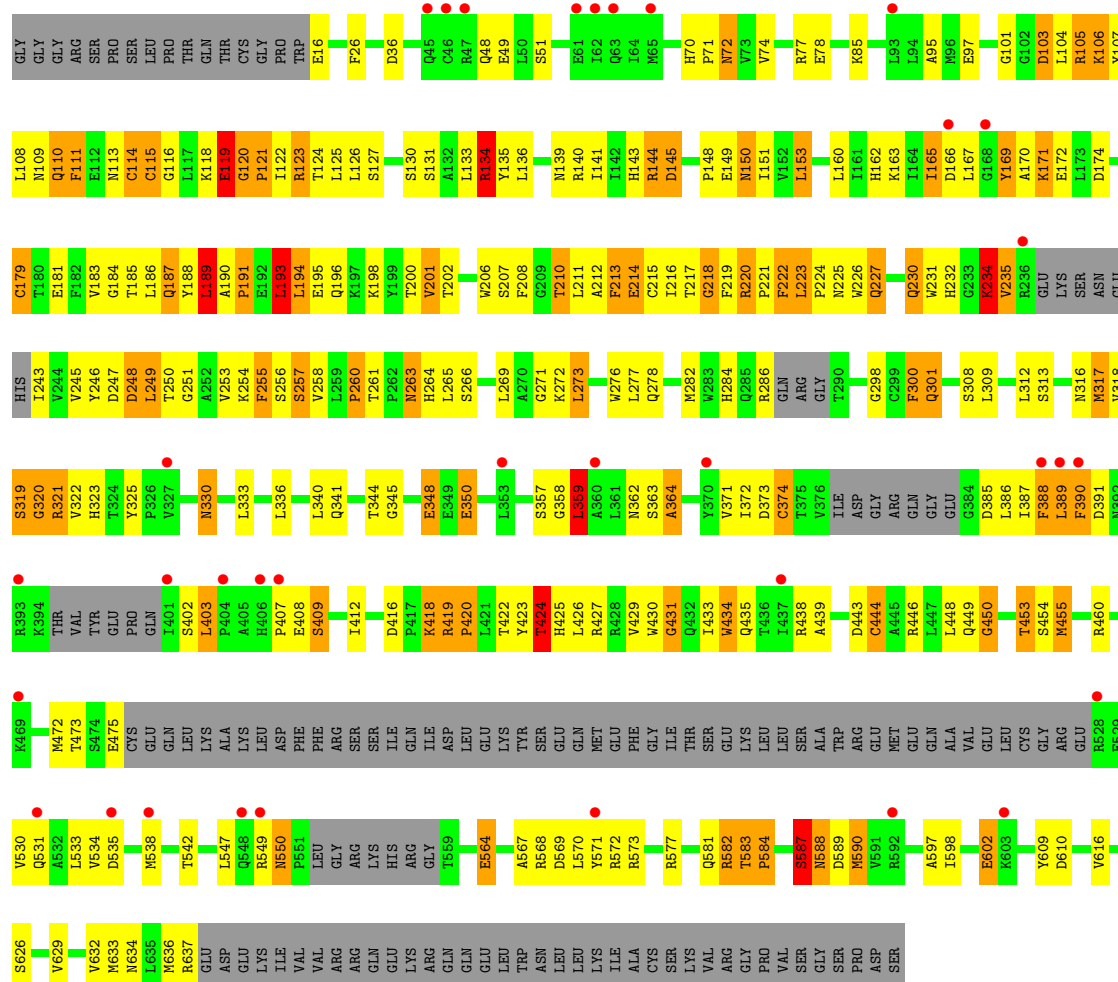
Chain F:





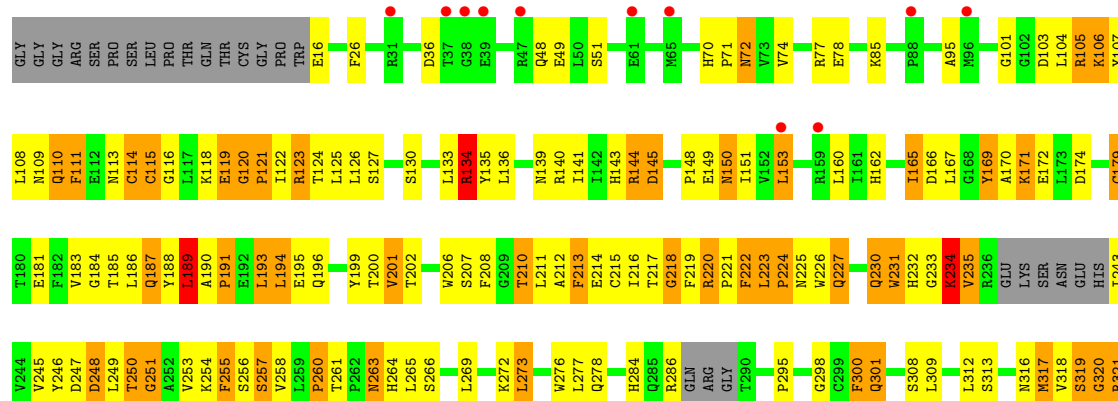
• Molecule 1: MGC80376 protein

Chain G:



• Molecule 1: MGC80376 protein

Chain H:



V322	S402	L401	LEU	Q541	ASP	GLU	GLU	LYS	ILE	VAL	ARG	GLN	GLY	T559	L563	GLU	ASN	LEU	LEU	LEU	LEU	LYS	ILE	ALA	CYS	SER	LYS	VAL	ARG	GLY	PRO	VAL	SER	GLY	SER	PRO	ASP	SER	L596	A597	I598	E602	Y609	D610	Q611	V616	S626	V629	V632										
H323	L403	L401	ALA	T542	ASP	GLU	GLU	LYS	ILE	VAL	ARG	GLN	GLY	T559	L563	GLU	ASN	LEU	LEU	LEU	LEU	LYS	ILE	ALA	CYS	SER	LYS	VAL	ARG	GLY	PRO	VAL	SER	GLY	SER	PRO	ASP	SER	L596	A597	I598	E602	Y609	D610	Q611	V616	S626	V629	V632										
T324	Y325	P407	ASP	S544	ASP	GLU	GLU	LYS	ILE	VAL	ARG	GLN	GLY	T559	L563	GLU	ASN	LEU	LEU	LEU	LEU	LYS	ILE	ALA	CYS	SER	LYS	VAL	ARG	GLY	PRO	VAL	SER	GLY	SER	PRO	ASP	SER	L596	A597	I598	E602	Y609	D610	Q611	V616	S626	V629	V632										
N330	L333	S409	PHE	L547	PHE	ARG	SER	ILE	GLN	ILE	ASP	LEU	GLU	GLY	T559	GLU	TYR	SER	GLU	GLN	MET	GLU	PHE	GLY	ILE	THR	SER	GLU	LYS	LEU	LEU	SER	ALA	TRP	C444	ARG	GLU	MET	GLU	GLN	ALA	VAL	GLU	LEU	CYS	GLY	ARG	GLU	R528	E529	V530	Q531	A532	I533	V534	D535	K536	M537	M538
L336	K337	D416	ARG	R549	ARG	SER	SER	ILE	GLN	ILE	ASP	LEU	GLU	GLY	T559	GLU	TYR	SER	GLU	GLN	MET	GLU	PHE	GLY	ILE	THR	SER	GLU	LYS	LEU	LEU	SER	ALA	TRP	C444	ARG	GLU	MET	GLU	GLN	ALA	VAL	GLU	LEU	CYS	GLY	ARG	GLU	R528	E529	V530	Q531	A532	I533	V534	D535	K536	M537	M538
S338	W339	P417	ARG	P551	ARG	SER	SER	ILE	GLN	ILE	ASP	LEU	GLU	GLY	T559	GLU	TYR	SER	GLU	GLN	MET	GLU	PHE	GLY	ILE	THR	SER	GLU	LYS	LEU	LEU	SER	ALA	TRP	C444	ARG	GLU	MET	GLU	GLN	ALA	VAL	GLU	LEU	CYS	GLY	ARG	GLU	R528	E529	V530	Q531	A532	I533	V534	D535	K536	M537	M538
L340	Q341	R419	ILE	ARG	LYS	HIS	ARG	GLY	GLN	GLY	ASP	LEU	GLU	GLY	T559	GLU	TYR	SER	GLU	GLN	MET	GLU	PHE	GLY	ILE	THR	SER	GLU	LYS	LEU	LEU	SER	ALA	TRP	C444	ARG	GLU	MET	GLU	GLN	ALA	VAL	GLU	LEU	CYS	GLY	ARG	GLU	R528	E529	V530	Q531	A532	I533	V534	D535	K536	M537	M538
T344	G345	L421	ASP	L547	PHE	ARG	SER	ILE	GLN	ILE	ASP	LEU	GLU	GLY	T559	GLU	TYR	SER	GLU	GLN	MET	GLU	PHE	GLY	ILE	THR	SER	GLU	LYS	LEU	LEU	SER	ALA	TRP	C444	ARG	GLU	MET	GLU	GLN	ALA	VAL	GLU	LEU	CYS	GLY	ARG	GLU	R528	E529	V530	Q531	A532	I533	V534	D535	K536	M537	M538
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C374	T375	V376	ILE	ASP	GLY	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN					
E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	D373	C3																																															

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.17Å 140.34Å 161.17Å 71.28° 79.56° 86.04°	Depositor
Resolution (Å)	15.00 – 3.60 48.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	78.7 (15.00-3.60) 76.9 (48.67-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.308 , 0.344 0.308 , 0.345	Depositor DCC
R_{free} test set	4124 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 97.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 96343 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	39026	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.74	0/5136	0.97	9/6931 (0.1%)
1	B	0.76	0/5136	0.97	10/6931 (0.1%)
1	C	0.78	1/5136 (0.0%)	0.98	11/6931 (0.2%)
1	D	0.74	2/5136 (0.0%)	0.96	10/6931 (0.1%)
1	E	0.77	1/5136 (0.0%)	0.98	10/6931 (0.1%)
1	F	0.75	0/5136	0.96	10/6931 (0.1%)
1	G	0.74	1/4448 (0.0%)	0.96	7/6012 (0.1%)
1	H	0.75	0/4448	0.97	8/6012 (0.1%)
All	All	0.75	5/39712 (0.0%)	0.97	75/53610 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	11
1	C	0	10
1	D	0	11
1	E	0	10
1	F	0	11
1	G	0	11
1	H	0	11
All	All	0	86

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	279	CYS	CB-SG	-6.95	1.70	1.82
1	C	279	CYS	CB-SG	-5.47	1.73	1.81
1	G	119	GLU	CG-CD	5.22	1.59	1.51
1	D	119	GLU	CG-CD	5.14	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	331	GLU	CG-CD	5.14	1.59	1.51

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	153	LEU	CA-CB-CG	6.42	130.08	115.30
1	A	153	LEU	CA-CB-CG	6.28	129.73	115.30
1	C	153	LEU	CA-CB-CG	6.27	129.72	115.30
1	D	153	LEU	CA-CB-CG	6.27	129.71	115.30
1	B	153	LEU	CA-CB-CG	6.23	129.62	115.30
1	F	153	LEU	CA-CB-CG	6.15	129.44	115.30
1	G	153	LEU	CA-CB-CG	6.15	129.44	115.30
1	D	189	LEU	CA-CB-CG	-6.14	101.17	115.30
1	H	193	LEU	N-CA-C	-6.13	94.44	111.00
1	C	189	LEU	CA-CB-CG	-6.06	101.36	115.30
1	A	193	LEU	N-CA-C	-6.00	94.81	111.00
1	G	193	LEU	N-CA-C	-6.00	94.81	111.00
1	H	153	LEU	CA-CB-CG	5.99	129.07	115.30
1	D	193	LEU	N-CA-C	-5.97	94.88	111.00
1	E	193	LEU	N-CA-C	-5.94	94.96	111.00
1	C	256	SER	N-CA-C	5.94	127.03	111.00
1	C	193	LEU	N-CA-C	-5.94	94.97	111.00
1	B	193	LEU	N-CA-C	-5.93	94.98	111.00
1	A	189	LEU	CA-CB-CG	-5.88	101.77	115.30
1	F	193	LEU	N-CA-C	-5.86	95.17	111.00
1	E	256	SER	N-CA-C	5.86	126.82	111.00
1	G	194	LEU	CA-CB-CG	5.84	128.74	115.30
1	H	256	SER	N-CA-C	5.81	126.68	111.00
1	A	194	LEU	CA-CB-CG	5.78	128.60	115.30
1	D	256	SER	N-CA-C	5.75	126.54	111.00
1	C	249	LEU	CA-CB-CG	5.75	128.52	115.30
1	E	189	LEU	CA-CB-CG	-5.75	102.08	115.30
1	F	194	LEU	CA-CB-CG	5.70	128.40	115.30
1	H	194	LEU	CA-CB-CG	5.70	128.40	115.30
1	D	194	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	194	LEU	CA-CB-CG	5.67	128.34	115.30
1	G	189	LEU	CA-CB-CG	-5.67	102.26	115.30
1	E	194	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	189	LEU	CA-CB-CG	-5.64	102.32	115.30
1	C	123	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	256	SER	N-CA-C	5.64	126.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	LEU	CA-CB-CG	5.61	128.20	115.30
1	C	359	LEU	CA-CB-CG	5.61	128.20	115.30
1	G	256	SER	N-CA-C	5.60	126.12	111.00
1	B	359	LEU	CA-CB-CG	5.60	128.18	115.30
1	G	359	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	256	SER	N-CA-C	5.57	126.05	111.00
1	F	256	SER	N-CA-C	5.56	126.02	111.00
1	H	359	LEU	CA-CB-CG	5.55	128.06	115.30
1	E	359	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	458	LEU	CA-CB-CG	5.52	127.99	115.30
1	F	458	LEU	CA-CB-CG	5.46	127.87	115.30
1	H	189	LEU	CA-CB-CG	-5.46	102.74	115.30
1	F	189	LEU	CA-CB-CG	-5.42	102.83	115.30
1	C	445	ALA	O-C-N	-5.42	114.04	122.70
1	C	458	LEU	CA-CB-CG	5.40	127.71	115.30
1	D	458	LEU	CA-CB-CG	5.39	127.69	115.30
1	E	458	LEU	CA-CB-CG	5.38	127.68	115.30
1	F	359	LEU	CA-CB-CG	5.36	127.64	115.30
1	D	248	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	458	LEU	CA-CB-CG	5.34	127.59	115.30
1	H	458	LEU	CA-CB-CG	5.28	127.45	115.30
1	E	224	PRO	N-CA-C	-5.28	98.39	112.10
1	F	249	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	248	ASP	CB-CG-OD1	5.26	123.03	118.30
1	F	105	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	249	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	359	LEU	CA-CB-CG	5.23	127.32	115.30
1	D	359	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	224	PRO	N-CA-C	-5.21	98.55	112.10
1	A	249	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	224	PRO	N-CA-C	-5.19	98.61	112.10
1	C	224	PRO	N-CA-C	-5.16	98.68	112.10
1	G	249	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	249	LEU	CA-CB-CG	5.13	127.10	115.30
1	H	224	PRO	N-CA-C	-5.10	98.85	112.10
1	B	251	GLY	N-CA-C	-5.07	100.42	113.10
1	F	248	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	224	PRO	N-CA-C	-5.05	98.98	112.10

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLU	Peptide
1	A	120	GLY	Peptide
1	A	169	TYR	Peptide
1	A	221	PRO	Peptide
1	A	223	LEU	Peptide
1	A	247	ASP	Peptide
1	A	255	PHE	Peptide
1	A	257	SER	Peptide
1	A	260	PRO	Peptide
1	A	389	LEU	Peptide
1	A	587	SER	Peptide
1	B	119	GLU	Peptide
1	B	120	GLY	Peptide
1	B	169	TYR	Peptide
1	B	221	PRO	Peptide
1	B	223	LEU	Peptide
1	B	247	ASP	Peptide
1	B	255	PHE	Peptide
1	B	257	SER	Peptide
1	B	389	LEU	Peptide
1	B	527	GLU	Mainchain
1	B	587	SER	Peptide
1	C	119	GLU	Peptide
1	C	120	GLY	Peptide
1	C	169	TYR	Peptide
1	C	221	PRO	Peptide
1	C	223	LEU	Peptide
1	C	247	ASP	Peptide
1	C	255	PHE	Peptide
1	C	257	SER	Peptide
1	C	389	LEU	Peptide
1	C	587	SER	Peptide
1	D	119	GLU	Peptide
1	D	120	GLY	Peptide
1	D	169	TYR	Peptide
1	D	221	PRO	Peptide
1	D	223	LEU	Peptide
1	D	247	ASP	Peptide
1	D	255	PHE	Peptide
1	D	257	SER	Peptide
1	D	260	PRO	Peptide
1	D	389	LEU	Peptide
1	D	587	SER	Peptide

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Mol	Chain	Res	Type	Group
1	E	119	GLU	Peptide
1	E	120	GLY	Peptide
1	E	169	TYR	Peptide
1	E	221	PRO	Peptide
1	E	223	LEU	Peptide
1	E	247	ASP	Peptide
1	E	255	PHE	Peptide
1	E	257	SER	Peptide
1	E	389	LEU	Peptide
1	E	587	SER	Peptide
1	F	119	GLU	Peptide
1	F	120	GLY	Peptide
1	F	169	TYR	Peptide
1	F	221	PRO	Peptide
1	F	223	LEU	Peptide
1	F	247	ASP	Peptide
1	F	255	PHE	Peptide
1	F	257	SER	Peptide
1	F	260	PRO	Peptide
1	F	389	LEU	Peptide
1	F	587	SER	Peptide
1	G	119	GLU	Peptide
1	G	120	GLY	Peptide
1	G	169	TYR	Peptide
1	G	221	PRO	Peptide
1	G	223	LEU	Peptide
1	G	247	ASP	Peptide
1	G	255	PHE	Peptide
1	G	257	SER	Peptide
1	G	260	PRO	Peptide
1	G	389	LEU	Peptide
1	G	587	SER	Peptide
1	H	119	GLU	Peptide
1	H	120	GLY	Peptide
1	H	169	TYR	Peptide
1	H	221	PRO	Peptide
1	H	223	LEU	Peptide
1	H	247	ASP	Peptide
1	H	255	PHE	Peptide
1	H	257	SER	Peptide
1	H	260	PRO	Peptide
1	H	389	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	H	587	SER	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5048	0	0	226	3
1	B	5048	0	0	239	2
1	C	5048	0	0	255	4
1	D	5048	0	0	256	0
1	E	5048	0	0	241	2
1	F	5048	0	0	219	0
1	G	4369	0	0	182	0
1	H	4369	0	0	180	1
All	All	39026	0	0	1733	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (1733) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:547:LEU:CD1	1:E:615:THR:CG2	1.86	1.51
1:A:230:GLN:O	1:A:232:HIS:N	1.66	1.28
1:D:230:GLN:O	1:D:232:HIS:N	1.67	1.27
1:G:230:GLN:O	1:G:232:HIS:N	1.68	1.26
1:B:230:GLN:O	1:B:232:HIS:N	1.67	1.26
1:C:230:GLN:O	1:C:232:HIS:N	1.68	1.26
1:F:230:GLN:O	1:F:232:HIS:N	1.69	1.23
1:E:230:GLN:O	1:E:232:HIS:N	1.70	1.23
1:H:230:GLN:O	1:H:232:HIS:N	1.69	1.21
1:C:496:LYS:CB	1:D:655:TRP:NE1	2.09	1.14
1:A:476:CYS:SG	1:A:477:GLU:OE2	2.06	1.14
1:B:527:GLU:O	1:B:529:GLU:N	1.82	1.13
1:D:476:CYS:SG	1:D:477:GLU:OE2	2.06	1.12
1:C:476:CYS:SG	1:C:477:GLU:OE2	2.09	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:219:PHE:O	1:C:220:ARG:CG	2.00	1.09
1:C:654:LEU:CD2	1:D:654:LEU:CD2	2.28	1.09
1:D:219:PHE:O	1:D:220:ARG:CG	2.01	1.09
1:F:219:PHE:O	1:F:220:ARG:CG	2.01	1.09
1:B:219:PHE:O	1:B:220:ARG:CG	2.01	1.08
1:E:219:PHE:O	1:E:220:ARG:CG	2.03	1.06
1:B:476:CYS:SG	1:B:477:GLU:OE2	2.13	1.06
1:A:524:CYS:SG	1:A:643:VAL:CG1	2.43	1.06
1:H:219:PHE:O	1:H:220:ARG:CG	2.05	1.05
1:A:219:PHE:O	1:A:220:ARG:CG	2.04	1.04
1:F:476:CYS:SG	1:F:477:GLU:OE2	2.15	1.04
1:A:655:TRP:CE3	1:B:654:LEU:CD1	2.41	1.03
1:H:226:TRP:CD1	1:H:227:GLN:N	2.28	1.02
1:H:26:PHE:CE2	1:H:181:GLU:CD	2.33	1.02
1:A:654:LEU:CD2	1:B:654:LEU:CD2	2.38	1.01
1:E:476:CYS:SG	1:E:477:GLU:OE2	2.19	1.01
1:G:219:PHE:O	1:G:220:ARG:CG	2.07	1.01
1:F:226:TRP:CD1	1:F:227:GLN:N	2.28	1.01
1:C:226:TRP:CD1	1:C:227:GLN:N	2.29	1.00
1:C:573:ARG:NH1	1:D:573:ARG:NH2	2.10	1.00
1:D:226:TRP:CD1	1:D:227:GLN:N	2.30	0.99
1:B:226:TRP:CD1	1:B:227:GLN:N	2.31	0.99
1:C:492:ILE:CG2	1:D:651:GLN:NE2	2.26	0.99
1:E:226:TRP:CD1	1:E:227:GLN:N	2.30	0.99
1:E:654:LEU:CD1	1:F:655:TRP:CE3	2.47	0.97
1:G:226:TRP:CD1	1:G:227:GLN:N	2.33	0.97
1:A:226:TRP:CD1	1:A:227:GLN:N	2.33	0.96
1:D:434:TRP:CZ3	1:D:568:ARG:CA	2.49	0.95
1:B:434:TRP:CZ3	1:B:568:ARG:CA	2.52	0.92
1:A:486:PHE:CZ	1:A:517:MET:CE	2.52	0.92
1:B:550:ASN:ND2	1:B:611:GLN:CD	2.25	0.90
1:B:550:ASN:ND2	1:B:611:GLN:OE1	2.05	0.90
1:E:654:LEU:CD2	1:F:654:LEU:CD2	2.50	0.90
1:A:527:GLU:O	1:A:529:GLU:N	2.05	0.90
1:C:651:GLN:NE2	1:D:492:ILE:CG2	2.35	0.90
1:E:118:LYS:CG	1:E:264:HIS:O	2.18	0.89
1:E:655:TRP:NE1	1:F:496:LYS:CB	2.37	0.88
1:C:118:LYS:CG	1:C:264:HIS:O	2.21	0.88
1:A:576:GLU:OE2	1:B:573:ARG:NH2	2.06	0.88
1:C:547:LEU:CD1	1:C:615:THR:CG2	2.51	0.88
1:B:494:LEU:CD2	1:B:518:GLU:OE2	2.23	0.87
1:H:571:TYR:CZ	1:H:590:MET:SD	2.69	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:496:LYS:CB	1:F:655:TRP:NE1	2.39	0.86
1:C:219:PHE:C	1:C:220:ARG:CG	2.43	0.86
1:C:497:TYR:O	1:C:497:TYR:CD2	2.28	0.85
1:E:497:TYR:O	1:E:497:TYR:CD2	2.29	0.85
1:A:497:TYR:O	1:A:497:TYR:CD2	2.30	0.85
1:B:497:TYR:O	1:B:497:TYR:CD2	2.30	0.85
1:D:497:TYR:CD2	1:D:497:TYR:O	2.30	0.84
1:C:533:LEU:CD2	1:C:629:VAL:CG1	2.54	0.84
1:E:655:TRP:CE3	1:F:654:LEU:CD1	2.59	0.84
1:H:434:TRP:CD1	1:H:435:GLN:N	2.45	0.84
1:E:153:LEU:CD2	1:E:162:HIS:ND1	2.41	0.84
1:E:170:ALA:O	1:E:172:GLU:N	2.11	0.84
1:E:219:PHE:C	1:E:220:ARG:CG	2.45	0.84
1:F:118:LYS:CG	1:F:264:HIS:O	2.26	0.84
1:A:547:LEU:CD1	1:A:615:THR:CG2	2.54	0.83
1:E:217:THR:OG1	1:E:218:GLY:N	2.08	0.83
1:C:153:LEU:CD2	1:C:162:HIS:ND1	2.42	0.83
1:B:217:THR:OG1	1:B:218:GLY:N	2.04	0.83
1:C:655:TRP:CE3	1:D:654:LEU:CD1	2.61	0.83
1:B:219:PHE:C	1:B:220:ARG:CG	2.44	0.82
1:A:236:ARG:NH2	1:D:231:TRP:CE3	2.47	0.82
1:D:217:THR:OG1	1:D:218:GLY:N	2.12	0.82
1:G:170:ALA:O	1:G:172:GLU:N	2.11	0.82
1:F:219:PHE:C	1:F:220:ARG:CG	2.45	0.82
1:G:475:GLU:CG	1:G:636:MET:CE	2.57	0.82
1:H:153:LEU:CD2	1:H:162:HIS:ND1	2.43	0.82
1:H:434:TRP:CE3	1:H:568:ARG:CA	2.63	0.82
1:E:434:TRP:CD1	1:E:435:GLN:N	2.48	0.82
1:G:153:LEU:CD2	1:G:162:HIS:ND1	2.43	0.82
1:A:231:TRP:CE3	1:D:236:ARG:NH2	2.48	0.82
1:B:540:LEU:CD2	1:B:621:LYS:NZ	2.42	0.82
1:F:153:LEU:CD2	1:F:162:HIS:ND1	2.43	0.81
1:G:217:THR:OG1	1:G:218:GLY:N	2.12	0.81
1:B:153:LEU:CD2	1:B:162:HIS:ND1	2.43	0.81
1:H:217:THR:OG1	1:H:218:GLY:N	2.08	0.81
1:A:170:ALA:O	1:A:172:GLU:N	2.13	0.81
1:A:533:LEU:CD2	1:A:629:VAL:CG1	2.57	0.81
1:D:153:LEU:CD2	1:D:162:HIS:ND1	2.44	0.81
1:D:170:ALA:O	1:D:172:GLU:N	2.14	0.81
1:B:170:ALA:O	1:B:172:GLU:N	2.14	0.81
1:C:170:ALA:O	1:C:172:GLU:N	2.14	0.81
1:E:571:TYR:CZ	1:E:590:MET:SD	2.73	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:LEU:CD2	1:A:162:HIS:ND1	2.44	0.80
1:F:217:THR:OG1	1:F:218:GLY:N	2.09	0.80
1:H:434:TRP:CZ3	1:H:568:ARG:CA	2.64	0.80
1:H:170:ALA:O	1:H:172:GLU:N	2.14	0.80
1:B:26:PHE:CE2	1:B:181:GLU:CD	2.55	0.80
1:G:434:TRP:CD1	1:G:435:GLN:N	2.49	0.80
1:F:497:TYR:O	1:F:497:TYR:CD2	2.35	0.80
1:F:170:ALA:O	1:F:172:GLU:N	2.14	0.80
1:D:434:TRP:CD1	1:D:435:GLN:N	2.50	0.80
1:E:26:PHE:CE2	1:E:181:GLU:CD	2.56	0.79
1:D:187:GLN:CB	1:D:223:LEU:CD2	2.60	0.79
1:E:120:GLY:O	1:E:124:THR:N	2.16	0.79
1:C:655:TRP:NE1	1:D:496:LYS:CB	2.45	0.79
1:C:120:GLY:O	1:C:124:THR:N	2.14	0.79
1:H:219:PHE:C	1:H:220:ARG:CG	2.49	0.79
1:D:219:PHE:C	1:D:220:ARG:CG	2.46	0.78
1:D:120:GLY:O	1:D:124:THR:N	2.17	0.78
1:H:26:PHE:CE2	1:H:181:GLU:OE1	2.37	0.78
1:A:496:LYS:CB	1:B:655:TRP:NE1	2.47	0.78
1:A:217:THR:OG1	1:A:218:GLY:N	2.12	0.78
1:B:434:TRP:CD1	1:B:435:GLN:N	2.51	0.78
1:D:424:THR:OG1	1:D:425:HIS:ND1	2.17	0.78
1:B:571:TYR:CZ	1:B:590:MET:SD	2.77	0.78
1:B:476:CYS:CB	1:B:636:MET:SD	2.72	0.77
1:G:120:GLY:O	1:G:124:THR:N	2.17	0.77
1:H:118:LYS:CG	1:H:264:HIS:O	2.31	0.77
1:G:219:PHE:C	1:G:220:ARG:CG	2.51	0.77
1:H:134:ARG:CA	1:H:300:PHE:CZ	2.68	0.77
1:C:217:THR:OG1	1:C:218:GLY:N	2.15	0.77
1:D:660:ILE:CG2	1:D:661:ALA:N	2.48	0.77
1:A:118:LYS:CG	1:A:264:HIS:O	2.32	0.77
1:A:120:GLY:O	1:A:124:THR:N	2.18	0.77
1:C:424:THR:OG1	1:C:425:HIS:ND1	2.17	0.77
1:A:434:TRP:CD1	1:A:435:GLN:N	2.53	0.77
1:B:479:LEU:C	1:B:640:GLU:OE2	2.24	0.76
1:C:107:TYR:O	1:C:110:GLN:N	2.18	0.76
1:B:120:GLY:O	1:B:124:THR:N	2.18	0.76
1:C:434:TRP:CD1	1:C:435:GLN:N	2.54	0.76
1:A:219:PHE:C	1:A:220:ARG:CG	2.49	0.76
1:D:434:TRP:CE3	1:D:568:ARG:CA	2.68	0.76
1:B:434:TRP:CE3	1:B:568:ARG:CA	2.68	0.76
1:F:443:ASP:O	1:F:446:ARG:CB	2.34	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:485:PHE:CE2	1:D:485:PHE:CB	2.69	0.76
1:B:424:THR:OG1	1:B:425:HIS:ND1	2.18	0.76
1:F:434:TRP:CD1	1:F:435:GLN:N	2.54	0.76
1:H:424:THR:OG1	1:H:425:HIS:ND1	2.18	0.76
1:E:424:THR:OG1	1:E:425:HIS:ND1	2.19	0.76
1:A:316:ASN:O	1:A:388:PHE:O	2.04	0.76
1:E:661:ALA:O	1:F:661:ALA:O	2.04	0.76
1:A:424:THR:OG1	1:A:425:HIS:ND1	2.19	0.76
1:A:186:LEU:O	1:A:188:TYR:N	2.18	0.76
1:H:120:GLY:O	1:H:124:THR:N	2.19	0.75
1:C:26:PHE:CE2	1:C:181:GLU:CD	2.58	0.75
1:F:424:THR:OG1	1:F:425:HIS:ND1	2.19	0.75
1:A:517:MET:SD	1:A:650:ARG:CG	2.75	0.75
1:H:110:GLN:O	1:H:111:PHE:CB	2.34	0.75
1:A:434:TRP:CZ3	1:A:568:ARG:CA	2.68	0.75
1:D:107:TYR:O	1:D:110:GLN:N	2.20	0.75
1:F:107:TYR:O	1:F:110:GLN:N	2.20	0.75
1:G:434:TRP:CZ3	1:G:568:ARG:CA	2.70	0.75
1:G:424:THR:OG1	1:G:425:HIS:ND1	2.20	0.74
1:C:654:LEU:CD1	1:D:655:TRP:CE3	2.69	0.74
1:F:660:ILE:CG2	1:F:661:ALA:N	2.51	0.74
1:A:107:TYR:O	1:A:110:GLN:N	2.20	0.74
1:B:246:TYR:CD1	1:B:258:VAL:CB	2.70	0.74
1:B:118:LYS:CG	1:B:264:HIS:O	2.34	0.74
1:F:120:GLY:O	1:F:124:THR:N	2.20	0.74
1:F:110:GLN:O	1:F:111:PHE:CB	2.34	0.74
1:A:246:TYR:CD1	1:A:258:VAL:CB	2.70	0.74
1:E:660:ILE:CG2	1:E:661:ALA:N	2.50	0.74
1:C:179:CYS:CB	1:C:181:GLU:CG	2.66	0.74
1:E:319:SER:OG	1:E:403:LEU:CB	2.35	0.74
1:F:246:TYR:CD1	1:F:258:VAL:CB	2.71	0.74
1:G:246:TYR:CD1	1:G:258:VAL:CB	2.70	0.74
1:C:316:ASN:O	1:C:388:PHE:O	2.06	0.74
1:H:466:SER:O	1:H:541:GLN:NE2	2.21	0.74
1:D:186:LEU:O	1:D:188:TYR:N	2.20	0.74
1:G:316:ASN:O	1:G:388:PHE:O	2.06	0.74
1:E:107:TYR:O	1:E:110:GLN:N	2.21	0.74
1:D:26:PHE:CE2	1:D:181:GLU:CD	2.61	0.74
1:B:107:TYR:O	1:B:110:GLN:N	2.20	0.74
1:C:110:GLN:O	1:C:111:PHE:CB	2.33	0.74
1:H:246:TYR:CD1	1:H:258:VAL:CB	2.70	0.74
1:H:179:CYS:CB	1:H:181:GLU:CG	2.66	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:660:ILE:CG2	1:C:661:ALA:N	2.50	0.73
1:H:451:GLN:CD	1:H:611:GLN:NE2	2.41	0.73
1:D:246:TYR:CD1	1:D:258:VAL:CB	2.70	0.73
1:B:479:LEU:CB	1:B:640:GLU:OE2	2.36	0.73
1:E:654:LEU:CD1	1:F:655:TRP:CZ3	2.70	0.73
1:H:107:TYR:O	1:H:110:GLN:N	2.21	0.73
1:E:110:GLN:O	1:E:111:PHE:CB	2.36	0.73
1:F:186:LEU:O	1:F:188:TYR:N	2.22	0.73
1:C:246:TYR:CD1	1:C:258:VAL:CB	2.71	0.73
1:B:186:LEU:O	1:B:188:TYR:N	2.22	0.73
1:C:646:ARG:CG	1:C:647:GLN:NE2	2.51	0.73
1:E:246:TYR:CD1	1:E:258:VAL:CB	2.72	0.73
1:G:111:PHE:CZ	1:G:572:ARG:CG	2.70	0.73
1:B:475:GLU:O	1:B:478:GLN:N	2.22	0.73
1:D:179:CYS:CB	1:D:181:GLU:CG	2.67	0.73
1:E:316:ASN:O	1:E:388:PHE:O	2.06	0.73
1:E:651:GLN:NE2	1:F:492:ILE:CG2	2.52	0.73
1:H:254:LYS:O	1:H:255:PHE:CD2	2.42	0.73
1:H:186:LEU:O	1:H:188:TYR:N	2.22	0.73
1:D:118:LYS:CG	1:D:264:HIS:O	2.37	0.73
1:B:547:LEU:CD1	1:B:614:LYS:CB	2.67	0.73
1:E:254:LYS:C	1:E:255:PHE:CG	2.62	0.73
1:F:387:ILE:CD1	1:F:450:GLY:CA	2.67	0.72
1:G:179:CYS:CB	1:G:181:GLU:CG	2.67	0.72
1:F:517:MET:CE	1:F:647:GLN:OE1	2.37	0.72
1:G:186:LEU:O	1:G:188:TYR:N	2.22	0.72
1:A:660:ILE:CG2	1:A:661:ALA:N	2.51	0.72
1:E:134:ARG:CA	1:E:300:PHE:CZ	2.72	0.72
1:E:646:ARG:CG	1:E:647:GLN:NE2	2.52	0.72
1:F:179:CYS:CB	1:F:181:GLU:CG	2.67	0.72
1:G:107:TYR:O	1:G:110:GLN:N	2.22	0.72
1:B:660:ILE:CG2	1:B:661:ALA:N	2.52	0.72
1:E:186:LEU:O	1:E:188:TYR:N	2.21	0.72
1:A:434:TRP:CE3	1:A:568:ARG:CA	2.72	0.72
1:A:110:GLN:O	1:A:111:PHE:CB	2.36	0.72
1:B:110:GLN:O	1:B:111:PHE:CB	2.37	0.72
1:D:230:GLN:C	1:D:232:HIS:N	2.43	0.71
1:B:254:LYS:C	1:B:255:PHE:CG	2.64	0.71
1:A:179:CYS:CB	1:A:181:GLU:CG	2.67	0.71
1:A:433:ILE:CG2	1:A:571:TYR:OH	2.38	0.71
1:C:284:HIS:NE2	1:E:342:GLN:NE2	2.38	0.71
1:A:646:ARG:CG	1:A:647:GLN:NE2	2.53	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:254:LYS:O	1:E:255:PHE:CD2	2.43	0.71
1:A:230:GLN:C	1:A:232:HIS:N	2.43	0.71
1:C:230:GLN:C	1:C:232:HIS:N	2.44	0.71
1:H:434:TRP:CD1	1:H:434:TRP:C	2.64	0.71
1:E:179:CYS:CB	1:E:181:GLU:CG	2.68	0.71
1:H:254:LYS:C	1:H:255:PHE:CG	2.64	0.71
1:B:646:ARG:CG	1:B:647:GLN:NE2	2.54	0.71
1:D:110:GLN:O	1:D:111:PHE:CB	2.37	0.71
1:H:248:ASP:C	1:H:248:ASP:OD1	2.29	0.71
1:B:230:GLN:C	1:B:232:HIS:N	2.43	0.71
1:C:422:THR:CB	1:C:585:GLY:CA	2.69	0.71
1:D:646:ARG:CG	1:D:647:GLN:NE2	2.54	0.71
1:H:316:ASN:O	1:H:388:PHE:O	2.08	0.71
1:F:533:LEU:CD2	1:F:629:VAL:CG1	2.68	0.71
1:C:254:LYS:C	1:C:255:PHE:CG	2.62	0.71
1:E:230:GLN:C	1:E:232:HIS:N	2.44	0.71
1:G:230:GLN:C	1:G:232:HIS:N	2.44	0.71
1:B:179:CYS:CB	1:B:181:GLU:CG	2.69	0.70
1:F:646:ARG:CG	1:F:647:GLN:NE2	2.53	0.70
1:G:110:GLN:O	1:G:111:PHE:CB	2.37	0.70
1:B:647:GLN:CD	1:B:647:GLN:N	2.44	0.70
1:G:130:SER:O	1:G:300:PHE:CE1	2.44	0.70
1:E:26:PHE:CE2	1:E:181:GLU:OE1	2.43	0.70
1:E:473:THR:CG2	1:E:533:LEU:CD2	2.70	0.70
1:D:316:ASN:O	1:D:388:PHE:O	2.09	0.70
1:F:134:ARG:CA	1:F:300:PHE:CZ	2.75	0.70
1:G:434:TRP:CE3	1:G:568:ARG:CA	2.75	0.70
1:A:655:TRP:CZ3	1:B:654:LEU:CD1	2.75	0.70
1:F:226:TRP:CG	1:F:227:GLN:N	2.59	0.70
1:G:571:TYR:CZ	1:G:590:MET:SD	2.85	0.70
1:E:248:ASP:C	1:E:248:ASP:OD1	2.30	0.69
1:F:230:GLN:C	1:F:232:HIS:N	2.44	0.69
1:F:254:LYS:C	1:F:255:PHE:CG	2.65	0.69
1:G:434:TRP:CD1	1:G:434:TRP:C	2.65	0.69
1:C:433:ILE:CG2	1:C:571:TYR:OH	2.40	0.69
1:C:26:PHE:CE2	1:C:181:GLU:OE1	2.46	0.69
1:G:254:LYS:C	1:G:255:PHE:CG	2.66	0.69
1:C:186:LEU:O	1:C:188:TYR:N	2.24	0.69
1:B:434:TRP:C	1:B:434:TRP:CD1	2.65	0.69
1:C:248:ASP:C	1:C:248:ASP:OD1	2.30	0.69
1:E:187:GLN:CB	1:E:223:LEU:CD2	2.71	0.69
1:C:485:PHE:CD2	1:D:485:PHE:CD2	2.80	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:647:GLN:CD	1:D:647:GLN:N	2.46	0.69
1:A:254:LYS:C	1:A:255:PHE:CG	2.65	0.69
1:E:434:TRP:C	1:E:434:TRP:CD1	2.63	0.68
1:D:254:LYS:C	1:D:255:PHE:CG	2.66	0.68
1:D:319:SER:OG	1:D:403:LEU:CB	2.41	0.68
1:D:505:ILE:O	1:D:506:THR:O	2.10	0.68
1:C:134:ARG:CA	1:C:300:PHE:CZ	2.76	0.68
1:E:665:VAL:CG2	1:F:665:VAL:CG2	2.71	0.68
1:H:433:ILE:CG2	1:H:571:TYR:OH	2.42	0.68
1:F:316:ASN:O	1:F:388:PHE:O	2.12	0.68
1:F:434:TRP:CZ3	1:F:568:ARG:CA	2.77	0.68
1:B:505:ILE:O	1:B:506:THR:O	2.11	0.68
1:D:434:TRP:C	1:D:434:TRP:CD1	2.65	0.68
1:C:647:GLN:N	1:C:647:GLN:CD	2.43	0.68
1:F:434:TRP:C	1:F:434:TRP:CD1	2.67	0.68
1:A:434:TRP:C	1:A:434:TRP:CD1	2.67	0.67
1:F:254:LYS:O	1:F:255:PHE:CD2	2.47	0.67
1:A:318:VAL:O	1:A:320:GLY:N	2.27	0.67
1:E:647:GLN:CD	1:E:647:GLN:N	2.46	0.67
1:B:254:LYS:O	1:B:255:PHE:CD2	2.46	0.67
1:G:318:VAL:O	1:G:320:GLY:N	2.28	0.67
1:B:479:LEU:O	1:B:640:GLU:OE2	2.13	0.67
1:E:226:TRP:CG	1:E:227:GLN:N	2.62	0.67
1:F:248:ASP:C	1:F:248:ASP:OD1	2.33	0.67
1:A:248:ASP:OD1	1:A:248:ASP:C	2.33	0.67
1:B:248:ASP:C	1:B:248:ASP:OD1	2.32	0.67
1:C:434:TRP:C	1:C:434:TRP:CD1	2.66	0.67
1:F:505:ILE:O	1:F:506:THR:O	2.13	0.67
1:C:226:TRP:CG	1:C:227:GLN:N	2.62	0.67
1:A:505:ILE:O	1:A:506:THR:O	2.12	0.67
1:A:105:ARG:O	1:A:108:LEU:N	2.28	0.67
1:B:637:ARG:O	1:B:641:LYS:N	2.28	0.67
1:H:230:GLN:C	1:H:232:HIS:N	2.44	0.67
1:C:254:LYS:O	1:C:255:PHE:CD2	2.47	0.67
1:G:245:VAL:O	1:G:257:SER:O	2.13	0.67
1:G:105:ARG:O	1:G:108:LEU:N	2.28	0.67
1:E:540:LEU:CD1	1:E:622:ALA:CB	2.73	0.67
1:G:248:ASP:C	1:G:248:ASP:OD1	2.33	0.66
1:D:120:GLY:O	1:D:123:ARG:N	2.29	0.66
1:D:254:LYS:O	1:D:255:PHE:CD2	2.48	0.66
1:A:254:LYS:O	1:A:255:PHE:CD2	2.49	0.66
1:G:254:LYS:O	1:G:255:PHE:CD2	2.48	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:316:ASN:O	1:B:388:PHE:O	2.13	0.66
1:C:505:ILE:O	1:C:506:THR:O	2.12	0.66
1:D:262:PRO:CB	1:D:409:SER:OG	2.44	0.66
1:C:514:TRP:O	1:C:518:GLU:N	2.28	0.66
1:B:475:GLU:O	1:B:476:CYS:C	2.32	0.66
1:A:647:GLN:N	1:A:647:GLN:CD	2.47	0.66
1:B:514:TRP:O	1:B:518:GLU:N	2.29	0.66
1:C:193:LEU:O	1:C:196:GLN:OE1	2.13	0.66
1:B:475:GLU:C	1:B:477:GLU:N	2.48	0.66
1:D:226:TRP:CG	1:D:227:GLN:N	2.61	0.66
1:F:647:GLN:N	1:F:647:GLN:CD	2.47	0.65
1:B:245:VAL:O	1:B:257:SER:O	2.14	0.65
1:D:550:ASN:OD1	1:D:611:GLN:OE1	2.14	0.65
1:D:105:ARG:O	1:D:108:LEU:N	2.29	0.65
1:B:387:ILE:CD1	1:B:450:GLY:CA	2.74	0.65
1:B:476:CYS:CA	1:B:636:MET:SD	2.84	0.65
1:C:245:VAL:O	1:C:257:SER:O	2.14	0.65
1:B:434:TRP:CB	1:B:571:TYR:CD1	2.80	0.65
1:H:434:TRP:CB	1:H:571:TYR:CD1	2.80	0.65
1:C:571:TYR:CZ	1:C:590:MET:SD	2.90	0.65
1:F:318:VAL:O	1:F:320:GLY:N	2.30	0.65
1:C:105:ARG:O	1:C:108:LEU:N	2.30	0.65
1:B:134:ARG:CA	1:B:300:PHE:CZ	2.80	0.65
1:E:505:ILE:O	1:E:506:THR:O	2.14	0.65
1:D:514:TRP:O	1:D:518:GLU:N	2.30	0.65
1:D:536:LYS:O	1:D:625:LEU:CD1	2.45	0.65
1:H:226:TRP:CG	1:H:227:GLN:N	2.61	0.65
1:C:318:VAL:O	1:C:320:GLY:N	2.29	0.65
1:D:119:GLU:CB	1:D:121:PRO:CD	2.75	0.65
1:H:193:LEU:O	1:H:196:GLN:OE1	2.14	0.65
1:D:248:ASP:C	1:D:248:ASP:OD1	2.34	0.65
1:F:514:TRP:O	1:F:518:GLU:N	2.29	0.64
1:H:318:VAL:O	1:H:320:GLY:N	2.30	0.64
1:D:318:VAL:O	1:D:320:GLY:N	2.30	0.64
1:A:514:TRP:O	1:A:518:GLU:N	2.30	0.64
1:E:120:GLY:O	1:E:123:ARG:N	2.31	0.64
1:H:193:LEU:CD2	1:H:231:TRP:CD1	2.80	0.64
1:F:105:ARG:O	1:F:108:LEU:N	2.31	0.64
1:F:187:GLN:CB	1:F:223:LEU:CD2	2.76	0.64
1:D:105:ARG:O	1:D:107:TYR:N	2.31	0.64
1:B:262:PRO:CB	1:B:409:SER:OG	2.45	0.64
1:G:226:TRP:CG	1:G:227:GLN:N	2.63	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:105:ARG:O	1:H:108:LEU:N	2.31	0.64
1:A:70:HIS:CD2	1:A:71:PRO:O	2.51	0.64
1:A:193:LEU:O	1:A:196:GLN:OE1	2.16	0.64
1:F:444:CYS:C	1:F:446:ARG:N	2.50	0.64
1:F:570:LEU:CB	1:F:590:MET:CE	2.75	0.64
1:C:485:PHE:CE2	1:D:485:PHE:CG	2.85	0.64
1:C:206:TRP:C	1:C:206:TRP:CD1	2.71	0.64
1:F:637:ARG:O	1:F:641:LYS:N	2.31	0.64
1:E:245:VAL:O	1:E:257:SER:O	2.15	0.64
1:D:245:VAL:O	1:D:257:SER:O	2.16	0.64
1:F:387:ILE:CD1	1:F:450:GLY:N	2.60	0.64
1:C:119:GLU:CB	1:C:121:PRO:CD	2.76	0.64
1:F:143:HIS:CD2	1:F:145:ASP:O	2.51	0.64
1:H:245:VAL:O	1:H:257:SER:O	2.16	0.63
1:D:193:LEU:O	1:D:196:GLN:OE1	2.16	0.63
1:E:105:ARG:O	1:E:108:LEU:N	2.30	0.63
1:H:70:HIS:CD2	1:H:71:PRO:O	2.52	0.63
1:E:193:LEU:O	1:E:196:GLN:OE1	2.16	0.63
1:E:514:TRP:O	1:E:518:GLU:N	2.31	0.63
1:B:226:TRP:CG	1:B:227:GLN:N	2.62	0.63
1:D:70:HIS:CD2	1:D:71:PRO:O	2.51	0.63
1:G:70:HIS:CD2	1:G:71:PRO:O	2.51	0.63
1:A:105:ARG:O	1:A:107:TYR:N	2.31	0.63
1:B:70:HIS:CD2	1:B:71:PRO:O	2.52	0.63
1:F:352:GLU:OE1	1:F:619:LYS:NZ	2.32	0.63
1:H:569:ASP:O	1:H:573:ARG:N	2.32	0.63
1:G:120:GLY:O	1:G:123:ARG:N	2.32	0.63
1:A:105:ARG:O	1:A:106:LYS:C	2.36	0.63
1:C:587:SER:OG	1:C:588:ASN:N	2.31	0.63
1:E:318:VAL:O	1:E:320:GLY:N	2.31	0.63
1:D:143:HIS:CD2	1:D:145:ASP:O	2.51	0.63
1:C:527:GLU:O	1:C:529:GLU:N	2.30	0.63
1:B:120:GLY:O	1:B:123:ARG:N	2.32	0.63
1:C:70:HIS:CD2	1:C:71:PRO:O	2.52	0.63
1:H:434:TRP:CZ3	1:H:568:ARG:CG	2.82	0.63
1:C:434:TRP:CZ3	1:C:568:ARG:CA	2.82	0.62
1:D:569:ASP:O	1:D:573:ARG:N	2.33	0.62
1:B:105:ARG:O	1:B:106:LYS:C	2.38	0.62
1:E:517:MET:CE	1:E:647:GLN:OE1	2.47	0.62
1:E:70:HIS:CD2	1:E:71:PRO:O	2.52	0.62
1:D:104:LEU:N	1:D:151:ILE:O	2.33	0.62
1:E:143:HIS:CD2	1:E:145:ASP:O	2.52	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:ASN:N	1:A:150:ASN:OD1	2.32	0.62
1:F:70:HIS:CD2	1:F:71:PRO:O	2.52	0.62
1:G:150:ASN:OD1	1:G:150:ASN:N	2.32	0.62
1:F:569:ASP:O	1:F:573:ARG:N	2.33	0.62
1:D:105:ARG:O	1:D:106:LYS:C	2.38	0.62
1:B:318:VAL:O	1:B:320:GLY:N	2.32	0.62
1:G:569:ASP:O	1:G:573:ARG:N	2.33	0.62
1:C:105:ARG:O	1:C:106:LYS:C	2.38	0.62
1:B:104:LEU:N	1:B:151:ILE:O	2.33	0.62
1:C:143:HIS:CD2	1:C:145:ASP:O	2.53	0.62
1:E:206:TRP:CD1	1:E:206:TRP:C	2.73	0.62
1:B:527:GLU:C	1:B:529:GLU:N	2.53	0.62
1:C:105:ARG:O	1:C:107:TYR:N	2.32	0.62
1:F:434:TRP:CE3	1:F:568:ARG:CA	2.83	0.62
1:B:105:ARG:O	1:B:108:LEU:N	2.32	0.62
1:C:422:THR:CB	1:C:585:GLY:C	2.67	0.62
1:B:193:LEU:O	1:B:196:GLN:OE1	2.17	0.62
1:F:105:ARG:O	1:F:106:LYS:C	2.38	0.62
1:F:105:ARG:O	1:F:107:TYR:N	2.33	0.62
1:A:143:HIS:CD2	1:A:145:ASP:O	2.52	0.61
1:B:143:HIS:CD2	1:B:145:ASP:O	2.53	0.61
1:A:571:TYR:CZ	1:A:590:MET:SD	2.93	0.61
1:G:104:LEU:N	1:G:151:ILE:O	2.34	0.61
1:A:104:LEU:N	1:A:151:ILE:O	2.33	0.61
1:B:521:VAL:CG1	1:B:643:VAL:CG1	2.78	0.61
1:C:272:LYS:CG	1:C:273:LEU:N	2.62	0.61
1:D:150:ASN:OD1	1:D:150:ASN:N	2.33	0.61
1:B:187:GLN:CB	1:B:223:LEU:CD2	2.79	0.61
1:H:187:GLN:CB	1:H:223:LEU:CD2	2.78	0.61
1:E:105:ARG:O	1:E:107:TYR:N	2.33	0.61
1:E:150:ASN:OD1	1:E:150:ASN:N	2.34	0.61
1:G:193:LEU:O	1:G:196:GLN:OE1	2.18	0.61
1:B:26:PHE:CE2	1:B:181:GLU:OE1	2.53	0.61
1:A:570:LEU:CB	1:A:590:MET:CE	2.78	0.61
1:A:245:VAL:O	1:A:257:SER:O	2.18	0.61
1:F:104:LEU:N	1:F:151:ILE:O	2.33	0.61
1:C:120:GLY:O	1:C:123:ARG:N	2.33	0.61
1:A:120:GLY:O	1:A:123:ARG:N	2.33	0.61
1:G:316:ASN:O	1:G:317:MET:CB	2.49	0.61
1:E:105:ARG:O	1:E:106:LYS:C	2.38	0.61
1:E:462:ASN:ND2	1:E:540:LEU:CB	2.63	0.61
1:B:319:SER:O	1:B:321:ARG:N	2.34	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:422:THR:CB	1:E:585:GLY:C	2.69	0.61
1:A:187:GLN:CB	1:A:223:LEU:CD2	2.79	0.61
1:D:531:GLN:O	1:D:535:ASP:N	2.34	0.61
1:C:373:ASP:C	1:C:374:CYS:SG	2.79	0.61
1:C:319:SER:O	1:C:321:ARG:N	2.34	0.61
1:B:105:ARG:O	1:B:107:TYR:N	2.34	0.61
1:G:206:TRP:C	1:G:206:TRP:CD1	2.74	0.61
1:A:226:TRP:CG	1:A:227:GLN:N	2.65	0.60
1:A:434:TRP:CB	1:A:571:TYR:CD1	2.83	0.60
1:H:143:HIS:CD2	1:H:145:ASP:O	2.54	0.60
1:F:272:LYS:CG	1:F:273:LEU:N	2.63	0.60
1:E:119:GLU:CB	1:E:121:PRO:CD	2.80	0.60
1:G:319:SER:O	1:G:321:ARG:N	2.35	0.60
1:E:492:ILE:CG2	1:F:651:GLN:NE2	2.63	0.60
1:F:120:GLY:O	1:F:123:ARG:N	2.35	0.60
1:D:26:PHE:CE2	1:D:181:GLU:OE1	2.55	0.60
1:G:143:HIS:CD2	1:G:145:ASP:O	2.54	0.60
1:D:185:THR:CG2	1:D:187:GLN:CG	2.80	0.60
1:C:569:ASP:O	1:C:573:ARG:N	2.34	0.60
1:E:527:GLU:O	1:E:529:GLU:N	2.35	0.60
1:C:189:LEU:CG	1:C:190:ALA:N	2.64	0.60
1:F:193:LEU:O	1:F:196:GLN:OE1	2.18	0.60
1:F:119:GLU:CB	1:F:121:PRO:CD	2.80	0.60
1:F:527:GLU:O	1:F:529:GLU:N	2.35	0.60
1:F:245:VAL:O	1:F:257:SER:O	2.19	0.60
1:E:189:LEU:CG	1:E:190:ALA:N	2.64	0.60
1:H:104:LEU:N	1:H:151:ILE:O	2.34	0.60
1:B:189:LEU:CG	1:B:190:ALA:N	2.65	0.60
1:H:387:ILE:CD1	1:H:450:GLY:N	2.64	0.60
1:B:569:ASP:O	1:B:573:ARG:N	2.35	0.60
1:H:319:SER:O	1:H:321:ARG:N	2.35	0.60
1:C:263:ASN:ND2	1:C:265:LEU:N	2.49	0.60
1:E:587:SER:OG	1:E:588:ASN:N	2.34	0.60
1:D:387:ILE:CD1	1:D:450:GLY:N	2.65	0.60
1:F:587:SER:OG	1:F:588:ASN:N	2.34	0.60
1:A:569:ASP:O	1:A:573:ARG:N	2.35	0.60
1:C:150:ASN:N	1:C:150:ASN:OD1	2.31	0.60
1:G:105:ARG:O	1:G:107:TYR:N	2.35	0.60
1:D:319:SER:O	1:D:321:ARG:N	2.35	0.60
1:E:104:LEU:N	1:E:151:ILE:O	2.35	0.60
1:E:319:SER:O	1:E:321:ARG:N	2.35	0.60
1:H:206:TRP:C	1:H:206:TRP:CD1	2.74	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:185:THR:CG2	1:C:187:GLN:CG	2.80	0.59
1:E:185:THR:CG2	1:E:187:GLN:CG	2.80	0.59
1:F:473:THR:CG2	1:F:533:LEU:CD2	2.80	0.59
1:E:531:GLN:O	1:E:535:ASP:N	2.35	0.59
1:E:569:ASP:O	1:E:573:ARG:N	2.34	0.59
1:A:189:LEU:CG	1:A:190:ALA:N	2.64	0.59
1:H:531:GLN:O	1:H:535:ASP:N	2.35	0.59
1:C:632:VAL:C	1:C:633:MET:SD	2.81	0.59
1:F:185:THR:CG2	1:F:187:GLN:CG	2.81	0.59
1:A:134:ARG:CA	1:A:300:PHE:CZ	2.84	0.59
1:A:319:SER:O	1:A:321:ARG:N	2.34	0.59
1:F:206:TRP:CD1	1:F:206:TRP:C	2.76	0.59
1:F:220:ARG:NH1	1:F:223:LEU:CD2	2.65	0.59
1:F:497:TYR:CE2	1:F:511:LEU:CD2	2.86	0.59
1:C:485:PHE:CE1	1:D:485:PHE:CD1	2.90	0.59
1:C:316:ASN:O	1:C:317:MET:CB	2.50	0.59
1:D:632:VAL:C	1:D:633:MET:SD	2.81	0.59
1:A:422:THR:CB	1:A:585:GLY:CA	2.80	0.59
1:B:150:ASN:OD1	1:B:150:ASN:N	2.35	0.59
1:D:433:ILE:CB	1:D:571:TYR:OH	2.49	0.59
1:H:316:ASN:O	1:H:317:MET:CB	2.50	0.59
1:A:531:GLN:O	1:A:535:ASP:N	2.35	0.59
1:G:185:THR:CG2	1:G:187:GLN:CG	2.80	0.59
1:F:319:SER:OG	1:F:403:LEU:CB	2.50	0.59
1:E:422:THR:CB	1:E:585:GLY:CA	2.79	0.59
1:B:119:GLU:CB	1:B:121:PRO:CD	2.80	0.59
1:C:187:GLN:CB	1:C:223:LEU:CD2	2.81	0.59
1:E:116:GLY:N	1:E:217:THR:O	2.36	0.59
1:G:200:THR:O	1:G:201:VAL:C	2.41	0.59
1:D:433:ILE:CG2	1:D:571:TYR:OH	2.50	0.59
1:C:419:ARG:CA	1:C:587:SER:OG	2.51	0.59
1:F:531:GLN:O	1:F:535:ASP:N	2.36	0.59
1:H:587:SER:OG	1:H:588:ASN:N	2.35	0.59
1:D:434:TRP:CB	1:D:571:TYR:CD1	2.85	0.59
1:F:319:SER:O	1:F:321:ARG:N	2.35	0.59
1:C:473:THR:CG2	1:C:533:LEU:CD2	2.80	0.59
1:H:105:ARG:O	1:H:107:TYR:N	2.36	0.59
1:H:119:GLU:CB	1:H:121:PRO:CD	2.81	0.59
1:A:527:GLU:C	1:A:529:GLU:N	2.55	0.59
1:C:200:THR:O	1:C:201:VAL:C	2.41	0.59
1:A:478:GLN:CG	1:A:479:LEU:N	2.66	0.59
1:C:531:GLN:O	1:C:535:ASP:N	2.36	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:150:ASN:N	1:H:150:ASN:OD1	2.33	0.59
1:E:655:TRP:CZ3	1:F:654:LEU:CD1	2.85	0.58
1:C:434:TRP:CB	1:C:571:TYR:CD1	2.87	0.58
1:E:272:LYS:CG	1:E:273:LEU:N	2.63	0.58
1:H:120:GLY:O	1:H:123:ARG:N	2.36	0.58
1:D:189:LEU:CG	1:D:190:ALA:N	2.66	0.58
1:G:531:GLN:O	1:G:535:ASP:N	2.36	0.58
1:F:484:ASP:C	1:F:486:PHE:N	2.56	0.58
1:A:504:GLY:N	1:B:662:CYS:SG	2.77	0.58
1:D:316:ASN:O	1:D:317:MET:CB	2.51	0.58
1:A:206:TRP:C	1:A:206:TRP:CD1	2.76	0.58
1:D:272:LYS:CG	1:D:273:LEU:N	2.65	0.58
1:A:222:PHE:CD2	1:A:255:PHE:CD2	2.92	0.58
1:B:484:ASP:C	1:B:486:PHE:N	2.56	0.58
1:B:531:GLN:O	1:B:535:ASP:N	2.36	0.58
1:B:206:TRP:CD1	1:B:206:TRP:C	2.77	0.58
1:H:26:PHE:CZ	1:H:179:CYS:CB	2.87	0.58
1:G:220:ARG:NH1	1:G:223:LEU:CD2	2.67	0.58
1:C:116:GLY:N	1:C:217:THR:O	2.36	0.58
1:G:134:ARG:CA	1:G:300:PHE:CZ	2.86	0.58
1:E:263:ASN:ND2	1:E:265:LEU:N	2.51	0.58
1:F:189:LEU:CG	1:F:190:ALA:N	2.66	0.58
1:A:521:VAL:CA	1:A:524:CYS:SG	2.92	0.58
1:G:587:SER:OG	1:G:588:ASN:N	2.37	0.58
1:B:185:THR:CG2	1:B:187:GLN:CG	2.81	0.58
1:F:433:ILE:CG2	1:F:571:TYR:OH	2.52	0.58
1:B:478:GLN:CG	1:B:479:LEU:N	2.66	0.57
1:H:105:ARG:O	1:H:106:LYS:C	2.42	0.57
1:F:222:PHE:CD2	1:F:255:PHE:CD2	2.91	0.57
1:B:587:SER:OG	1:B:588:ASN:N	2.35	0.57
1:A:263:ASN:ND2	1:A:265:LEU:N	2.52	0.57
1:G:119:GLU:CB	1:G:121:PRO:CD	2.82	0.57
1:A:119:GLU:CB	1:A:121:PRO:CD	2.81	0.57
1:C:478:GLN:CG	1:C:479:LEU:N	2.67	0.57
1:A:484:ASP:C	1:A:486:PHE:N	2.56	0.57
1:D:213:PHE:O	1:D:216:ILE:N	2.37	0.57
1:D:587:SER:OG	1:D:588:ASN:N	2.36	0.57
1:C:661:ALA:O	1:D:661:ALA:O	2.21	0.57
1:C:434:TRP:CE3	1:C:568:ARG:CA	2.88	0.57
1:G:187:GLN:CB	1:G:223:LEU:CD2	2.81	0.57
1:A:316:ASN:O	1:A:317:MET:CB	2.51	0.57
1:A:651:GLN:NE2	1:B:492:ILE:CG2	2.67	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:484:ASP:C	1:C:486:PHE:N	2.56	0.57
1:G:105:ARG:O	1:G:106:LYS:C	2.40	0.57
1:E:632:VAL:C	1:E:633:MET:SD	2.83	0.57
1:H:272:LYS:CG	1:H:273:LEU:N	2.65	0.57
1:C:104:LEU:N	1:C:151:ILE:O	2.37	0.57
1:A:200:THR:O	1:A:201:VAL:C	2.43	0.57
1:F:478:GLN:CG	1:F:479:LEU:N	2.67	0.57
1:B:494:LEU:CD1	1:B:514:TRP:CE3	2.88	0.57
1:C:497:TYR:N	1:D:655:TRP:CZ2	2.73	0.57
1:H:185:THR:CG2	1:H:187:GLN:CG	2.83	0.57
1:C:433:ILE:CB	1:C:571:TYR:OH	2.53	0.57
1:B:387:ILE:CD1	1:B:450:GLY:N	2.68	0.57
1:D:478:GLN:CG	1:D:479:LEU:N	2.68	0.57
1:A:111:PHE:CZ	1:A:572:ARG:CG	2.88	0.57
1:A:373:ASP:C	1:A:374:CYS:SG	2.83	0.57
1:C:107:TYR:O	1:C:110:GLN:CB	2.53	0.56
1:B:222:PHE:CE2	1:B:225:ASN:CB	2.89	0.56
1:F:213:PHE:O	1:F:216:ILE:N	2.38	0.56
1:C:222:PHE:CD2	1:C:224:PRO:O	2.59	0.56
1:C:373:ASP:CG	1:C:374:CYS:SG	2.83	0.56
1:C:451:GLN:CD	1:C:611:GLN:NE2	2.59	0.56
1:A:587:SER:OG	1:A:588:ASN:N	2.38	0.56
1:A:666:ARG:NH1	1:B:502:GLU:CG	2.68	0.56
1:C:222:PHE:CD2	1:C:255:PHE:CD2	2.93	0.56
1:D:222:PHE:CD2	1:D:255:PHE:CD2	2.93	0.56
1:A:416:ASP:N	1:A:416:ASP:OD1	2.39	0.56
1:B:451:GLN:NE2	1:B:608:ILE:O	2.38	0.56
1:A:479:LEU:CB	1:A:640:GLU:OE2	2.54	0.56
1:D:441:LYS:CB	1:D:560:LEU:CD2	2.83	0.56
1:G:263:ASN:ND2	1:G:265:LEU:N	2.53	0.56
1:E:480:LYS:NZ	1:E:525:GLY:C	2.59	0.56
1:B:632:VAL:C	1:B:633:MET:SD	2.84	0.56
1:B:200:THR:O	1:B:201:VAL:C	2.43	0.56
1:D:200:THR:O	1:D:201:VAL:C	2.42	0.56
1:G:189:LEU:CG	1:G:190:ALA:N	2.68	0.56
1:B:222:PHE:CD2	1:B:224:PRO:O	2.59	0.56
1:D:484:ASP:C	1:D:486:PHE:N	2.58	0.56
1:A:272:LYS:CG	1:A:273:LEU:N	2.68	0.56
1:B:362:ASN:O	1:B:364:ALA:N	2.39	0.56
1:H:200:THR:O	1:H:201:VAL:C	2.44	0.56
1:A:433:ILE:CB	1:A:571:TYR:OH	2.53	0.56
1:G:222:PHE:CD2	1:G:255:PHE:CD2	2.94	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:222:PHE:CD2	1:D:224:PRO:O	2.59	0.56
1:B:320:GLY:O	1:B:321:ARG:C	2.45	0.56
1:C:350:GLU:OE2	1:C:391:ASP:O	2.23	0.56
1:E:502:GLU:CG	1:F:666:ARG:NH1	2.69	0.56
1:D:220:ARG:NH1	1:D:223:LEU:CD2	2.69	0.55
1:B:571:TYR:OH	1:B:590:MET:SD	2.64	0.55
1:G:434:TRP:CB	1:G:571:TYR:CD1	2.89	0.55
1:A:116:GLY:N	1:A:217:THR:O	2.39	0.55
1:C:485:PHE:CD2	1:D:485:PHE:CG	2.94	0.55
1:E:478:GLN:CG	1:E:479:LEU:N	2.69	0.55
1:G:272:LYS:CG	1:G:273:LEU:N	2.67	0.55
1:B:220:ARG:NH1	1:B:223:LEU:CD2	2.70	0.55
1:H:222:PHE:CD2	1:H:224:PRO:O	2.60	0.55
1:A:222:PHE:CE2	1:A:225:ASN:CB	2.89	0.55
1:D:320:GLY:O	1:D:321:ARG:C	2.45	0.55
1:E:576:GLU:OE2	1:F:573:ARG:NH2	2.40	0.55
1:H:416:ASP:OD1	1:H:416:ASP:N	2.39	0.55
1:B:263:ASN:ND2	1:B:265:LEU:N	2.54	0.55
1:D:263:ASN:ND2	1:D:265:LEU:N	2.54	0.55
1:E:222:PHE:CE2	1:E:225:ASN:CB	2.89	0.55
1:B:316:ASN:O	1:B:317:MET:CB	2.55	0.55
1:F:416:ASP:OD1	1:F:416:ASP:N	2.39	0.55
1:C:262:PRO:CB	1:C:409:SER:OG	2.55	0.55
1:C:362:ASN:O	1:C:364:ALA:N	2.40	0.55
1:D:206:TRP:C	1:D:206:TRP:CD1	2.78	0.55
1:D:422:THR:CB	1:D:585:GLY:C	2.74	0.55
1:A:632:VAL:C	1:A:633:MET:SD	2.85	0.55
1:E:200:THR:O	1:E:201:VAL:C	2.45	0.55
1:H:263:ASN:ND2	1:H:265:LEU:N	2.54	0.55
1:B:107:TYR:O	1:B:110:GLN:CB	2.55	0.55
1:H:189:LEU:CG	1:H:190:ALA:N	2.70	0.55
1:A:185:THR:CG2	1:A:187:GLN:CG	2.84	0.55
1:H:125:LEU:CA	1:H:162:HIS:NE2	2.70	0.55
1:E:107:TYR:O	1:E:110:GLN:CB	2.54	0.55
1:C:647:GLN:OE1	1:C:647:GLN:CA	2.55	0.55
1:B:660:ILE:O	1:B:662:CYS:N	2.40	0.55
1:D:222:PHE:CE2	1:D:225:ASN:CB	2.89	0.55
1:B:416:ASP:OD1	1:B:416:ASP:N	2.39	0.55
1:C:633:MET:N	1:C:633:MET:SD	2.80	0.55
1:C:478:GLN:OE1	1:D:481:ALA:CB	2.55	0.55
1:B:433:ILE:CG2	1:B:571:TYR:OH	2.55	0.55
1:C:660:ILE:O	1:C:662:CYS:N	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:316:ASN:O	1:F:317:MET:CB	2.55	0.55
1:F:320:GLY:O	1:F:321:ARG:C	2.44	0.55
1:C:666:ARG:CG	1:D:503:PHE:CE1	2.90	0.55
1:E:373:ASP:C	1:E:374:CYS:SG	2.85	0.55
1:E:416:ASP:OD1	1:E:416:ASP:N	2.40	0.55
1:D:362:ASN:O	1:D:364:ALA:N	2.40	0.55
1:G:125:LEU:CA	1:G:162:HIS:NE2	2.70	0.55
1:B:125:LEU:CA	1:B:162:HIS:NE2	2.70	0.55
1:H:222:PHE:CD2	1:H:255:PHE:CD2	2.94	0.55
1:C:416:ASP:N	1:C:416:ASP:OD1	2.39	0.55
1:D:527:GLU:O	1:D:529:GLU:N	2.40	0.55
1:H:564:GLU:OE2	1:H:568:ARG:NH2	2.41	0.54
1:E:497:TYR:CE2	1:E:511:LEU:CD2	2.90	0.54
1:G:222:PHE:CE2	1:G:225:ASN:CB	2.91	0.54
1:D:350:GLU:OE2	1:D:391:ASP:O	2.26	0.54
1:F:200:THR:O	1:F:201:VAL:C	2.44	0.54
1:G:632:VAL:C	1:G:633:MET:SD	2.86	0.54
1:D:475:GLU:CG	1:D:636:MET:CE	2.85	0.54
1:F:632:VAL:C	1:F:633:MET:SD	2.86	0.54
1:D:416:ASP:OD1	1:D:416:ASP:N	2.40	0.54
1:E:373:ASP:CG	1:E:374:CYS:SG	2.85	0.54
1:D:430:TRP:CB	1:D:571:TYR:CD2	2.90	0.54
1:E:222:PHE:CD2	1:E:224:PRO:O	2.61	0.54
1:G:362:ASN:O	1:G:364:ALA:N	2.40	0.54
1:F:107:TYR:O	1:F:110:GLN:CB	2.55	0.54
1:E:484:ASP:C	1:E:486:PHE:N	2.58	0.54
1:F:524:CYS:SG	1:F:643:VAL:CG1	2.96	0.54
1:H:362:ASN:O	1:H:364:ALA:N	2.41	0.54
1:F:150:ASN:OD1	1:F:150:ASN:N	2.39	0.54
1:B:501:MET:CA	1:B:505:ILE:CD1	2.85	0.54
1:G:416:ASP:N	1:G:416:ASP:OD1	2.41	0.54
1:H:571:TYR:CE2	1:H:590:MET:CG	2.91	0.54
1:A:26:PHE:CE2	1:A:181:GLU:CD	2.81	0.54
1:E:220:ARG:NH1	1:E:223:LEU:CD2	2.71	0.54
1:G:71:PRO:O	1:G:72:ASN:CB	2.55	0.54
1:D:422:THR:CB	1:D:585:GLY:CA	2.85	0.54
1:G:419:ARG:N	1:G:420:PRO:CD	2.71	0.54
1:F:263:ASN:ND2	1:F:265:LEU:N	2.56	0.54
1:C:71:PRO:O	1:C:72:ASN:CB	2.56	0.54
1:C:235:VAL:CG1	1:C:243:ILE:N	2.71	0.54
1:H:212:ALA:O	1:H:213:PHE:C	2.45	0.54
1:C:220:ARG:NH1	1:C:223:LEU:CD2	2.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:494:LEU:CD1	1:B:514:TRP:CB	2.85	0.54
1:E:316:ASN:O	1:E:317:MET:CB	2.55	0.54
1:H:222:PHE:CE2	1:H:225:ASN:CB	2.90	0.54
1:G:359:LEU:CA	1:G:460:ARG:NH1	2.71	0.54
1:H:472:MET:SD	1:H:633:MET:CB	2.96	0.54
1:B:475:GLU:O	1:B:477:GLU:N	2.41	0.53
1:H:220:ARG:NH1	1:H:223:LEU:CD2	2.70	0.53
1:E:350:GLU:OE2	1:E:391:ASP:O	2.26	0.53
1:A:213:PHE:O	1:A:216:ILE:N	2.42	0.53
1:D:107:TYR:O	1:D:110:GLN:CB	2.57	0.53
1:A:660:ILE:O	1:A:662:CYS:N	2.40	0.53
1:B:419:ARG:N	1:B:420:PRO:CD	2.72	0.53
1:F:362:ASN:O	1:F:364:ALA:N	2.41	0.53
1:A:580:ASP:CB	1:D:579:ARG:NH2	2.71	0.53
1:C:213:PHE:O	1:C:216:ILE:N	2.41	0.53
1:E:222:PHE:CD2	1:E:255:PHE:CD2	2.96	0.53
1:F:262:PRO:CB	1:F:409:SER:OG	2.57	0.53
1:B:272:LYS:CG	1:B:273:LEU:N	2.67	0.53
1:D:235:VAL:CG1	1:D:243:ILE:N	2.71	0.53
1:A:220:ARG:NH1	1:A:223:LEU:CD2	2.71	0.53
1:E:564:GLU:OE2	1:E:568:ARG:NH2	2.41	0.53
1:A:107:TYR:O	1:A:110:GLN:CB	2.57	0.53
1:B:222:PHE:CD2	1:B:255:PHE:CD2	2.96	0.53
1:D:434:TRP:CZ3	1:D:568:ARG:CB	2.91	0.53
1:E:125:LEU:CA	1:E:162:HIS:NE2	2.72	0.53
1:D:647:GLN:CA	1:D:647:GLN:OE1	2.57	0.53
1:B:500:GLN:CB	1:B:505:ILE:CG1	2.86	0.53
1:A:71:PRO:O	1:A:72:ASN:CB	2.57	0.53
1:B:442:GLU:O	1:B:446:ARG:NE	2.42	0.53
1:G:373:ASP:C	1:G:374:CYS:SG	2.87	0.53
1:B:656:ASN:OD1	1:B:656:ASN:C	2.46	0.53
1:F:125:LEU:CA	1:F:162:HIS:NE2	2.71	0.53
1:G:564:GLU:OE2	1:G:568:ARG:NH2	2.41	0.53
1:C:419:ARG:N	1:C:420:PRO:CD	2.72	0.53
1:D:588:ASN:CG	1:D:589:ASP:N	2.62	0.53
1:E:362:ASN:O	1:E:364:ALA:N	2.42	0.53
1:F:419:ARG:N	1:F:420:PRO:CD	2.72	0.53
1:D:125:LEU:CA	1:D:162:HIS:NE2	2.71	0.53
1:H:134:ARG:CB	1:H:300:PHE:CE1	2.91	0.53
1:F:317:MET:CE	1:F:609:TYR:CZ	2.92	0.53
1:F:426:LEU:O	1:F:430:TRP:N	2.41	0.53
1:E:387:ILE:CD1	1:E:450:GLY:N	2.71	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:373:ASP:C	1:B:374:CYS:SG	2.87	0.53
1:E:118:LYS:CB	1:E:264:HIS:O	2.57	0.53
1:E:433:ILE:CG2	1:E:571:TYR:OH	2.56	0.53
1:G:116:GLY:N	1:G:217:THR:O	2.42	0.53
1:C:109:ASN:O	1:C:111:PHE:N	2.42	0.53
1:F:444:CYS:O	1:F:446:ARG:N	2.41	0.53
1:H:107:TYR:O	1:H:110:GLN:CB	2.56	0.53
1:G:107:TYR:O	1:G:110:GLN:CB	2.56	0.53
1:B:71:PRO:O	1:B:72:ASN:CB	2.57	0.53
1:G:198:LYS:O	1:G:200:THR:N	2.42	0.53
1:E:633:MET:N	1:E:633:MET:SD	2.82	0.53
1:D:426:LEU:O	1:D:430:TRP:N	2.42	0.53
1:E:116:GLY:CA	1:E:217:THR:O	2.57	0.53
1:A:419:ARG:N	1:A:420:PRO:CD	2.72	0.53
1:A:362:ASN:O	1:A:364:ALA:N	2.42	0.53
1:A:373:ASP:CG	1:A:374:CYS:SG	2.88	0.53
1:C:462:ASN:ND2	1:C:540:LEU:CB	2.71	0.53
1:C:485:PHE:CZ	1:D:485:PHE:CB	2.91	0.52
1:E:320:GLY:O	1:E:321:ARG:C	2.47	0.52
1:H:419:ARG:N	1:H:420:PRO:CD	2.72	0.52
1:F:235:VAL:CG1	1:F:243:ILE:N	2.72	0.52
1:G:213:PHE:O	1:G:216:ILE:N	2.42	0.52
1:F:116:GLY:CA	1:F:217:THR:O	2.57	0.52
1:B:109:ASN:O	1:B:111:PHE:N	2.42	0.52
1:F:222:PHE:CE2	1:F:225:ASN:CB	2.92	0.52
1:G:70:HIS:NE2	1:G:131:SER:O	2.43	0.52
1:E:419:ARG:N	1:E:420:PRO:CD	2.73	0.52
1:B:213:PHE:O	1:B:216:ILE:N	2.42	0.52
1:D:660:ILE:O	1:D:662:CYS:N	2.42	0.52
1:D:633:MET:SD	1:D:633:MET:N	2.82	0.52
1:G:387:ILE:CD1	1:G:450:GLY:CA	2.87	0.52
1:G:320:GLY:O	1:G:321:ARG:C	2.47	0.52
1:F:647:GLN:CA	1:F:647:GLN:OE1	2.58	0.52
1:F:222:PHE:CD2	1:F:224:PRO:O	2.63	0.52
1:F:521:VAL:CA	1:F:524:CYS:SG	2.97	0.52
1:D:109:ASN:O	1:D:111:PHE:N	2.43	0.52
1:D:26:PHE:CZ	1:D:179:CYS:CB	2.93	0.52
1:B:647:GLN:CA	1:B:647:GLN:OE1	2.57	0.52
1:H:71:PRO:O	1:H:72:ASN:CB	2.57	0.52
1:C:521:VAL:CA	1:C:524:CYS:SG	2.97	0.52
1:A:213:PHE:C	1:A:213:PHE:CD2	2.83	0.52
1:A:222:PHE:CD2	1:A:224:PRO:O	2.63	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:632:VAL:C	1:H:633:MET:SD	2.88	0.52
1:B:235:VAL:CG1	1:B:243:ILE:N	2.73	0.52
1:F:656:ASN:OD1	1:F:656:ASN:C	2.48	0.52
1:C:484:ASP:O	1:C:487:ARG:N	2.43	0.52
1:F:434:TRP:CB	1:F:571:TYR:CD1	2.93	0.52
1:D:322:VAL:CG1	1:D:323:HIS:N	2.73	0.52
1:D:419:ARG:N	1:D:420:PRO:CD	2.72	0.52
1:G:475:GLU:OE2	1:G:637:ARG:CG	2.58	0.52
1:F:571:TYR:CZ	1:F:590:MET:SD	3.03	0.52
1:A:373:ASP:OD1	1:A:374:CYS:N	2.43	0.52
1:H:563:LEU:CD2	1:H:596:LEU:CB	2.87	0.52
1:H:248:ASP:O	1:H:248:ASP:OD1	2.28	0.52
1:E:213:PHE:O	1:E:216:ILE:N	2.43	0.52
1:D:476:CYS:CA	1:D:636:MET:SD	2.98	0.51
1:G:433:ILE:CG2	1:G:571:TYR:OH	2.57	0.51
1:E:662:CYS:SG	1:F:661:ALA:CB	2.97	0.51
1:F:484:ASP:O	1:F:487:ARG:N	2.43	0.51
1:A:536:LYS:CB	1:A:625:LEU:CD1	2.87	0.51
1:H:426:LEU:O	1:H:430:TRP:N	2.43	0.51
1:E:71:PRO:O	1:E:72:ASN:CB	2.58	0.51
1:C:373:ASP:OD1	1:C:374:CYS:N	2.42	0.51
1:G:341:GLN:O	1:G:345:GLY:N	2.43	0.51
1:B:547:LEU:O	1:B:550:ASN:ND2	2.44	0.51
1:C:426:LEU:O	1:C:430:TRP:N	2.43	0.51
1:G:426:LEU:O	1:G:430:TRP:N	2.43	0.51
1:B:350:GLU:OE2	1:B:391:ASP:O	2.29	0.51
1:E:571:TYR:OH	1:E:590:MET:SD	2.69	0.51
1:C:111:PHE:CZ	1:C:572:ARG:CG	2.93	0.51
1:A:320:GLY:O	1:A:321:ARG:C	2.48	0.51
1:C:26:PHE:CZ	1:C:179:CYS:CB	2.93	0.51
1:A:588:ASN:OD1	1:A:589:ASP:N	2.43	0.51
1:H:547:LEU:O	1:H:550:ASN:ND2	2.44	0.51
1:D:473:THR:CG2	1:D:533:LEU:CD2	2.88	0.51
1:A:120:GLY:C	1:A:122:ILE:N	2.63	0.51
1:C:320:GLY:O	1:C:321:ARG:C	2.48	0.51
1:F:213:PHE:CD2	1:F:213:PHE:C	2.84	0.51
1:B:444:CYS:C	1:B:446:ARG:N	2.63	0.51
1:F:373:ASP:CG	1:F:374:CYS:SG	2.89	0.51
1:H:451:GLN:OE1	1:H:611:GLN:NE2	2.44	0.51
1:E:533:LEU:CD2	1:E:629:VAL:CG1	2.88	0.51
1:D:120:GLY:C	1:D:122:ILE:N	2.63	0.51
1:F:564:GLU:OE2	1:F:568:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:643:VAL:O	1:C:644:VAL:CG2	2.59	0.51
1:H:235:VAL:CG1	1:H:243:ILE:N	2.73	0.51
1:A:350:GLU:OE2	1:A:391:ASP:O	2.28	0.51
1:A:647:GLN:CA	1:A:647:GLN:OE1	2.58	0.51
1:E:254:LYS:N	1:E:255:PHE:CE1	2.79	0.51
1:G:222:PHE:CD2	1:G:224:PRO:O	2.63	0.51
1:E:235:VAL:CG1	1:E:243:ILE:N	2.74	0.51
1:D:341:GLN:O	1:D:345:GLY:N	2.44	0.51
1:A:171:LYS:CG	1:A:171:LYS:O	2.59	0.51
1:E:647:GLN:OE1	1:E:647:GLN:CA	2.58	0.51
1:F:71:PRO:O	1:F:72:ASN:CB	2.58	0.51
1:D:588:ASN:OD1	1:D:589:ASP:N	2.44	0.51
1:G:633:MET:N	1:G:633:MET:SD	2.84	0.51
1:D:444:CYS:O	1:D:446:ARG:N	2.44	0.51
1:D:171:LYS:CG	1:D:171:LYS:O	2.59	0.51
1:C:656:ASN:OD1	1:C:656:ASN:C	2.48	0.51
1:C:116:GLY:CA	1:C:217:THR:O	2.59	0.51
1:A:122:ILE:O	1:A:126:LEU:N	2.44	0.51
1:A:109:ASN:O	1:A:111:PHE:N	2.44	0.51
1:G:26:PHE:CE2	1:G:181:GLU:CD	2.84	0.51
1:H:320:GLY:O	1:H:321:ARG:C	2.49	0.51
1:H:312:LEU:O	1:H:325:TYR:N	2.44	0.51
1:C:358:GLY:O	1:C:359:LEU:CB	2.60	0.51
1:B:660:ILE:C	1:B:662:CYS:N	2.65	0.50
1:H:588:ASN:CG	1:H:589:ASP:N	2.63	0.50
1:A:588:ASN:CG	1:A:589:ASP:N	2.63	0.50
1:E:387:ILE:CD1	1:E:449:GLN:CG	2.88	0.50
1:F:350:GLU:OE2	1:F:391:ASP:O	2.29	0.50
1:E:426:LEU:O	1:E:430:TRP:N	2.45	0.50
1:C:222:PHE:CE2	1:C:225:ASN:CB	2.93	0.50
1:B:588:ASN:CG	1:B:589:ASP:N	2.65	0.50
1:B:588:ASN:OD1	1:B:589:ASP:N	2.44	0.50
1:H:633:MET:SD	1:H:633:MET:N	2.84	0.50
1:E:358:GLY:O	1:E:359:LEU:CB	2.60	0.50
1:A:547:LEU:O	1:A:550:ASN:ND2	2.45	0.50
1:A:125:LEU:CA	1:A:162:HIS:NE2	2.74	0.50
1:E:494:LEU:CD2	1:E:518:GLU:OE2	2.59	0.50
1:B:521:VAL:CA	1:B:524:CYS:SG	3.00	0.50
1:H:213:PHE:O	1:H:216:ILE:N	2.45	0.50
1:D:438:ARG:CG	1:D:564:GLU:CG	2.90	0.50
1:C:564:GLU:OE2	1:C:568:ARG:NH2	2.43	0.50
1:E:661:ALA:CB	1:F:662:CYS:SG	2.99	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:322:VAL:CG1	1:F:323:HIS:N	2.75	0.50
1:D:656:ASN:OD1	1:D:656:ASN:C	2.49	0.50
1:F:120:GLY:C	1:F:122:ILE:N	2.65	0.50
1:H:254:LYS:N	1:H:255:PHE:CE1	2.80	0.50
1:F:248:ASP:OD1	1:F:248:ASP:O	2.30	0.50
1:G:443:ASP:O	1:G:446:ARG:CB	2.59	0.50
1:C:485:PHE:CD1	1:D:485:PHE:CD1	3.00	0.50
1:F:660:ILE:O	1:F:662:CYS:N	2.45	0.50
1:H:109:ASN:O	1:H:111:PHE:N	2.45	0.50
1:F:109:ASN:O	1:F:111:PHE:N	2.45	0.50
1:D:222:PHE:CE2	1:D:224:PRO:O	2.64	0.50
1:H:588:ASN:OD1	1:H:589:ASP:N	2.44	0.50
1:A:235:VAL:CG1	1:A:243:ILE:N	2.74	0.50
1:D:564:GLU:OE2	1:D:568:ARG:NH2	2.44	0.50
1:C:125:LEU:CA	1:C:162:HIS:NE2	2.74	0.50
1:E:484:ASP:O	1:E:487:ARG:N	2.44	0.50
1:F:26:PHE:CE2	1:F:181:GLU:CD	2.85	0.50
1:F:534:VAL:CG1	1:F:535:ASP:N	2.75	0.50
1:B:484:ASP:O	1:B:487:ARG:N	2.44	0.50
1:C:547:LEU:O	1:C:550:ASN:ND2	2.44	0.50
1:A:660:ILE:C	1:A:662:CYS:N	2.65	0.50
1:C:418:LYS:O	1:C:419:ARG:CB	2.60	0.50
1:F:373:ASP:C	1:F:374:CYS:SG	2.90	0.50
1:A:358:GLY:O	1:A:359:LEU:CB	2.59	0.50
1:A:484:ASP:O	1:A:487:ARG:N	2.45	0.50
1:H:319:SER:C	1:H:321:ARG:N	2.65	0.50
1:D:71:PRO:O	1:D:72:ASN:CB	2.59	0.50
1:B:643:VAL:O	1:B:644:VAL:CG2	2.60	0.50
1:E:534:VAL:CG1	1:E:535:ASP:N	2.75	0.50
1:G:235:VAL:CG1	1:G:243:ILE:N	2.75	0.50
1:A:341:GLN:O	1:A:345:GLY:N	2.45	0.50
1:G:547:LEU:O	1:G:550:ASN:ND2	2.44	0.50
1:D:358:GLY:O	1:D:359:LEU:CB	2.59	0.50
1:E:120:GLY:C	1:E:122:ILE:N	2.65	0.49
1:E:588:ASN:CG	1:E:589:ASP:N	2.66	0.49
1:A:534:VAL:CG1	1:A:535:ASP:N	2.74	0.49
1:G:534:VAL:CG1	1:G:535:ASP:N	2.75	0.49
1:F:341:GLN:O	1:F:345:GLY:N	2.45	0.49
1:C:322:VAL:CG1	1:C:323:HIS:N	2.75	0.49
1:B:116:GLY:N	1:B:217:THR:O	2.45	0.49
1:F:116:GLY:N	1:F:217:THR:O	2.44	0.49
1:H:120:GLY:C	1:H:122:ILE:N	2.66	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:423:TYR:O	1:E:425:HIS:N	2.45	0.49
1:E:109:ASN:O	1:E:111:PHE:N	2.45	0.49
1:D:534:VAL:CG1	1:D:535:ASP:N	2.74	0.49
1:G:109:ASN:O	1:G:111:PHE:N	2.45	0.49
1:G:588:ASN:OD1	1:G:589:ASP:N	2.45	0.49
1:G:443:ASP:O	1:G:446:ARG:N	2.45	0.49
1:E:547:LEU:O	1:E:550:ASN:ND2	2.45	0.49
1:G:434:TRP:CZ3	1:G:568:ARG:CG	2.95	0.49
1:G:319:SER:C	1:G:321:ARG:N	2.66	0.49
1:B:130:SER:O	1:B:300:PHE:CE1	2.66	0.49
1:B:373:ASP:OD1	1:B:374:CYS:N	2.45	0.49
1:G:322:VAL:CG1	1:G:323:HIS:N	2.75	0.49
1:H:113:ASN:O	1:H:116:GLY:N	2.45	0.49
1:G:116:GLY:CA	1:G:216:ILE:O	2.60	0.49
1:C:212:ALA:O	1:C:213:PHE:C	2.51	0.49
1:A:319:SER:C	1:A:321:ARG:N	2.65	0.49
1:C:319:SER:C	1:C:321:ARG:N	2.66	0.49
1:C:254:LYS:N	1:C:255:PHE:CE1	2.80	0.49
1:C:588:ASN:CG	1:C:589:ASP:N	2.66	0.49
1:G:588:ASN:CG	1:G:589:ASP:N	2.65	0.49
1:A:656:ASN:OD1	1:A:656:ASN:C	2.50	0.49
1:C:655:TRP:CD1	1:D:496:LYS:CB	2.95	0.49
1:B:433:ILE:CB	1:B:571:TYR:OH	2.61	0.49
1:C:118:LYS:CB	1:C:264:HIS:O	2.59	0.49
1:B:113:ASN:O	1:B:116:GLY:N	2.45	0.49
1:A:564:GLU:OE2	1:A:568:ARG:NH2	2.45	0.49
1:A:633:MET:SD	1:A:633:MET:N	2.85	0.49
1:D:521:VAL:CA	1:D:524:CYS:SG	3.01	0.49
1:E:550:ASN:OD1	1:E:611:GLN:OE1	2.30	0.49
1:H:122:ILE:O	1:H:126:LEU:N	2.46	0.49
1:C:660:ILE:C	1:C:662:CYS:N	2.65	0.49
1:H:423:TYR:O	1:H:425:HIS:N	2.45	0.49
1:E:486:PHE:CZ	1:E:517:MET:CE	2.95	0.49
1:G:198:LYS:C	1:G:200:THR:N	2.66	0.49
1:C:342:GLN:NE2	1:E:284:HIS:NE2	2.59	0.49
1:B:435:GLN:O	1:B:439:ALA:N	2.46	0.49
1:G:213:PHE:CD2	1:G:213:PHE:C	2.86	0.49
1:H:111:PHE:CZ	1:H:572:ARG:CG	2.96	0.49
1:A:262:PRO:CB	1:A:409:SER:OG	2.61	0.49
1:A:322:VAL:CG1	1:A:323:HIS:N	2.75	0.49
1:F:358:GLY:O	1:F:359:LEU:CB	2.60	0.49
1:E:113:ASN:O	1:E:116:GLY:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:423:TYR:O	1:C:425:HIS:N	2.45	0.49
1:E:660:ILE:O	1:E:662:CYS:N	2.45	0.49
1:H:402:SER:CA	1:H:609:TYR:CG	2.96	0.49
1:D:319:SER:C	1:D:321:ARG:N	2.66	0.49
1:D:418:LYS:O	1:D:419:ARG:CB	2.61	0.49
1:B:322:VAL:CG1	1:B:323:HIS:N	2.76	0.49
1:E:319:SER:C	1:E:321:ARG:N	2.67	0.49
1:C:534:VAL:CG1	1:C:535:ASP:N	2.75	0.49
1:B:341:GLN:O	1:B:345:GLY:N	2.45	0.49
1:G:171:LYS:CG	1:G:171:LYS:O	2.60	0.49
1:H:534:VAL:CG1	1:H:535:ASP:N	2.76	0.48
1:B:534:VAL:CG1	1:B:535:ASP:N	2.75	0.48
1:E:262:PRO:CB	1:E:409:SER:OG	2.60	0.48
1:E:234:LYS:O	1:E:235:VAL:O	2.31	0.48
1:H:350:GLU:OE2	1:H:391:ASP:O	2.30	0.48
1:E:656:ASN:OD1	1:E:656:ASN:C	2.50	0.48
1:G:120:GLY:C	1:G:122:ILE:N	2.66	0.48
1:B:120:GLY:C	1:B:122:ILE:N	2.64	0.48
1:B:319:SER:C	1:B:321:ARG:N	2.66	0.48
1:D:444:CYS:C	1:D:446:ARG:N	2.66	0.48
1:A:426:LEU:O	1:A:430:TRP:N	2.46	0.48
1:H:444:CYS:O	1:H:446:ARG:N	2.46	0.48
1:D:570:LEU:CB	1:D:590:MET:CE	2.91	0.48
1:F:122:ILE:O	1:F:126:LEU:N	2.47	0.48
1:F:319:SER:C	1:F:321:ARG:N	2.66	0.48
1:B:633:MET:N	1:B:633:MET:SD	2.86	0.48
1:E:373:ASP:OD1	1:E:374:CYS:N	2.46	0.48
1:F:418:LYS:O	1:F:419:ARG:CB	2.61	0.48
1:G:444:CYS:C	1:G:446:ARG:N	2.66	0.48
1:C:341:GLN:O	1:C:345:GLY:N	2.47	0.48
1:B:276:TRP:CE3	1:B:277:LEU:CD2	2.96	0.48
1:E:171:LYS:CG	1:E:171:LYS:O	2.61	0.48
1:H:171:LYS:O	1:H:171:LYS:CG	2.60	0.48
1:B:213:PHE:C	1:B:213:PHE:CD2	2.86	0.48
1:E:322:VAL:CG1	1:E:323:HIS:N	2.75	0.48
1:C:171:LYS:O	1:C:171:LYS:CG	2.62	0.48
1:B:426:LEU:O	1:B:430:TRP:N	2.45	0.48
1:C:122:ILE:O	1:C:126:LEU:N	2.46	0.48
1:D:423:TYR:O	1:D:425:HIS:N	2.46	0.48
1:D:660:ILE:C	1:D:662:CYS:N	2.67	0.48
1:C:485:PHE:CD1	1:D:485:PHE:CE1	3.02	0.48
1:B:540:LEU:CD2	1:B:621:LYS:CE	2.91	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:130:SER:O	1:E:300:PHE:CE1	2.65	0.48
1:C:248:ASP:O	1:C:248:ASP:OD1	2.30	0.48
1:B:248:ASP:OD1	1:B:248:ASP:O	2.31	0.48
1:E:588:ASN:OD1	1:E:589:ASP:N	2.47	0.48
1:B:418:LYS:O	1:B:419:ARG:CB	2.61	0.48
1:G:97:GLU:OE2	1:G:163:LYS:NZ	2.46	0.48
1:E:643:VAL:O	1:E:644:VAL:CG2	2.61	0.48
1:F:547:LEU:O	1:F:550:ASN:ND2	2.47	0.48
1:D:134:ARG:CA	1:D:300:PHE:CZ	2.97	0.48
1:G:118:LYS:CG	1:G:264:HIS:O	2.62	0.48
1:C:449:GLN:O	1:C:450:GLY:C	2.51	0.48
1:E:122:ILE:O	1:E:126:LEU:N	2.46	0.48
1:F:435:GLN:O	1:F:439:ALA:N	2.46	0.48
1:F:193:LEU:CD2	1:F:231:TRP:CD1	2.97	0.48
1:E:418:LYS:O	1:E:419:ARG:CB	2.62	0.48
1:B:373:ASP:CG	1:B:374:CYS:SG	2.92	0.48
1:A:418:LYS:O	1:A:419:ARG:CB	2.61	0.48
1:H:373:ASP:C	1:H:374:CYS:SG	2.92	0.48
1:C:497:TYR:CE2	1:C:511:LEU:CD2	2.97	0.48
1:D:547:LEU:O	1:D:550:ASN:ND2	2.46	0.48
1:F:588:ASN:CG	1:F:589:ASP:N	2.66	0.48
1:A:643:VAL:O	1:A:644:VAL:CG2	2.62	0.48
1:H:434:TRP:O	1:H:438:ARG:N	2.46	0.48
1:D:212:ALA:O	1:D:213:PHE:C	2.52	0.48
1:A:113:ASN:O	1:A:116:GLY:N	2.47	0.48
1:C:148:PRO:CD	1:C:188:TYR:CE2	2.97	0.48
1:H:418:LYS:O	1:H:419:ARG:CB	2.61	0.48
1:E:581:GLN:O	1:E:582:ARG:C	2.53	0.48
1:E:210:THR:O	1:E:211:LEU:C	2.52	0.48
1:A:286:ARG:CG	1:A:286:ARG:NH1	2.77	0.48
1:E:312:LEU:O	1:E:325:TYR:N	2.46	0.48
1:F:171:LYS:CG	1:F:171:LYS:O	2.60	0.48
1:B:171:LYS:O	1:B:171:LYS:CG	2.61	0.48
1:B:423:TYR:O	1:B:425:HIS:N	2.47	0.48
1:E:248:ASP:OD1	1:E:248:ASP:O	2.31	0.48
1:D:210:THR:O	1:D:211:LEU:C	2.52	0.48
1:D:113:ASN:O	1:D:116:GLY:N	2.47	0.47
1:H:130:SER:O	1:H:300:PHE:CE1	2.66	0.47
1:H:317:MET:O	1:H:609:TYR:OH	2.32	0.47
1:F:588:ASN:OD1	1:F:589:ASP:N	2.47	0.47
1:E:213:PHE:C	1:E:213:PHE:CD2	2.87	0.47
1:C:581:GLN:O	1:C:582:ARG:C	2.52	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:570:LEU:CB	1:H:590:MET:CE	2.92	0.47
1:H:571:TYR:OH	1:H:590:MET:SD	2.72	0.47
1:A:423:TYR:O	1:A:425:HIS:N	2.47	0.47
1:F:423:TYR:O	1:F:425:HIS:N	2.47	0.47
1:B:254:LYS:N	1:B:255:PHE:CE1	2.82	0.47
1:C:480:LYS:NZ	1:C:525:GLY:C	2.67	0.47
1:D:449:GLN:O	1:D:450:GLY:C	2.53	0.47
1:B:402:SER:O	1:B:403:LEU:CB	2.61	0.47
1:H:341:GLN:O	1:H:345:GLY:N	2.47	0.47
1:F:113:ASN:O	1:F:116:GLY:N	2.48	0.47
1:C:113:ASN:O	1:C:116:GLY:N	2.47	0.47
1:F:660:ILE:C	1:F:662:CYS:N	2.68	0.47
1:B:222:PHE:CE2	1:B:224:PRO:O	2.67	0.47
1:G:248:ASP:OD1	1:G:248:ASP:O	2.32	0.47
1:E:198:LYS:C	1:E:200:THR:N	2.68	0.47
1:F:643:VAL:O	1:F:644:VAL:CG2	2.62	0.47
1:G:409:SER:CB	1:G:412:ILE:CD1	2.92	0.47
1:G:418:LYS:O	1:G:419:ARG:CB	2.62	0.47
1:E:469:LYS:NZ	1:E:630:LYS:CE	2.77	0.47
1:D:451:GLN:NE2	1:D:608:ILE:O	2.47	0.47
1:F:135:TYR:O	1:F:139:ASN:ND2	2.47	0.47
1:G:390:PHE:N	1:G:390:PHE:CD1	2.83	0.47
1:B:286:ARG:NH1	1:B:286:ARG:CG	2.76	0.47
1:D:213:PHE:CD2	1:D:213:PHE:C	2.88	0.47
1:A:116:GLY:CA	1:A:217:THR:O	2.62	0.47
1:D:484:ASP:O	1:D:487:ARG:N	2.46	0.47
1:A:409:SER:CB	1:A:412:ILE:CD1	2.92	0.47
1:F:144:ARG:CD	1:F:169:TYR:O	2.62	0.47
1:B:581:GLN:O	1:B:582:ARG:C	2.52	0.47
1:E:134:ARG:CB	1:E:300:PHE:CE1	2.97	0.47
1:C:434:TRP:O	1:C:438:ARG:N	2.47	0.47
1:H:222:PHE:CE2	1:H:224:PRO:O	2.67	0.47
1:F:26:PHE:CE2	1:F:181:GLU:OE1	2.68	0.47
1:C:222:PHE:CE2	1:C:224:PRO:O	2.66	0.47
1:B:133:LEU:O	1:B:134:ARG:C	2.53	0.47
1:G:358:GLY:O	1:G:359:LEU:CB	2.61	0.47
1:H:373:ASP:CG	1:H:374:CYS:SG	2.93	0.47
1:C:402:SER:O	1:C:403:LEU:CB	2.62	0.47
1:C:312:LEU:O	1:C:325:TYR:N	2.47	0.47
1:G:473:THR:CG2	1:G:533:LEU:CD2	2.93	0.47
1:F:402:SER:O	1:F:403:LEU:CB	2.62	0.47
1:B:409:SER:CB	1:B:412:ILE:CD1	2.92	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:373:ASP:CG	1:D:374:CYS:SG	2.93	0.47
1:C:144:ARG:CD	1:C:169:TYR:O	2.63	0.47
1:C:459:LEU:CD1	1:C:548:GLN:OE1	2.62	0.47
1:B:434:TRP:CZ3	1:B:568:ARG:CB	2.97	0.47
1:B:122:ILE:O	1:B:126:LEU:N	2.47	0.47
1:F:444:CYS:O	1:F:447:LEU:N	2.47	0.47
1:C:494:LEU:CD2	1:C:518:GLU:OE2	2.63	0.47
1:D:248:ASP:O	1:D:248:ASP:OD1	2.33	0.47
1:G:276:TRP:CE3	1:G:277:LEU:CD2	2.98	0.47
1:F:633:MET:N	1:F:633:MET:SD	2.87	0.47
1:B:444:CYS:O	1:B:446:ARG:N	2.47	0.47
1:F:373:ASP:OD1	1:F:374:CYS:N	2.47	0.47
1:H:443:ASP:O	1:H:446:ARG:CB	2.62	0.47
1:F:165:ILE:O	1:F:167:LEU:N	2.48	0.47
1:E:341:GLN:O	1:E:345:GLY:N	2.48	0.47
1:G:402:SER:O	1:G:403:LEU:CB	2.63	0.47
1:H:433:ILE:CB	1:H:571:TYR:OH	2.63	0.47
1:H:402:SER:O	1:H:403:LEU:CB	2.62	0.47
1:G:359:LEU:N	1:G:460:ARG:NH1	2.62	0.47
1:B:212:ALA:O	1:B:213:PHE:C	2.53	0.47
1:D:373:ASP:OD1	1:D:374:CYS:N	2.48	0.47
1:B:358:GLY:O	1:B:359:LEU:CB	2.63	0.47
1:C:573:ARG:NH2	1:D:573:ARG:NH1	2.63	0.47
1:B:564:GLU:OE2	1:B:568:ARG:NH2	2.47	0.47
1:E:222:PHE:CE2	1:E:224:PRO:O	2.68	0.47
1:C:130:SER:O	1:C:300:PHE:CE1	2.68	0.47
1:H:449:GLN:NE2	1:H:453:THR:CG2	2.78	0.47
1:D:479:LEU:O	1:D:640:GLU:OE2	2.32	0.47
1:G:373:ASP:OD1	1:G:374:CYS:N	2.48	0.47
1:E:212:ALA:O	1:E:213:PHE:C	2.53	0.47
1:C:654:LEU:CD1	1:D:655:TRP:CZ3	2.98	0.47
1:G:434:TRP:O	1:G:438:ARG:N	2.48	0.47
1:G:122:ILE:O	1:G:126:LEU:N	2.47	0.47
1:C:213:PHE:CD2	1:C:213:PHE:C	2.88	0.47
1:G:423:TYR:O	1:G:425:HIS:N	2.48	0.47
1:H:276:TRP:CE3	1:H:277:LEU:CD2	2.98	0.47
1:G:449:GLN:NE2	1:G:453:THR:CG2	2.78	0.47
1:H:135:TYR:O	1:H:139:ASN:ND2	2.48	0.47
1:H:358:GLY:O	1:H:359:LEU:CB	2.62	0.47
1:F:210:THR:O	1:F:211:LEU:C	2.53	0.47
1:C:120:GLY:C	1:C:122:ILE:N	2.69	0.46
1:C:588:ASN:OD1	1:C:589:ASP:N	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:390:PHE:N	1:A:390:PHE:CD1	2.83	0.46
1:E:660:ILE:C	1:E:662:CYS:N	2.68	0.46
1:F:130:SER:O	1:F:300:PHE:CE1	2.68	0.46
1:F:134:ARG:CB	1:F:300:PHE:CE1	2.98	0.46
1:A:276:TRP:CE3	1:A:277:LEU:CD2	2.98	0.46
1:D:643:VAL:O	1:D:644:VAL:CG2	2.62	0.46
1:A:144:ARG:CD	1:A:169:TYR:O	2.63	0.46
1:B:312:LEU:O	1:B:325:TYR:N	2.48	0.46
1:B:144:ARG:CD	1:B:169:TYR:O	2.64	0.46
1:E:658:LEU:CD1	1:F:658:LEU:CA	2.93	0.46
1:A:634:ASN:OD1	1:A:637:ARG:NH1	2.49	0.46
1:E:521:VAL:CA	1:E:524:CYS:SG	3.03	0.46
1:G:581:GLN:O	1:G:582:ARG:C	2.53	0.46
1:D:390:PHE:CD1	1:D:390:PHE:N	2.84	0.46
1:G:571:TYR:CE2	1:G:590:MET:CG	2.98	0.46
1:H:409:SER:CB	1:H:412:ILE:CD1	2.93	0.46
1:H:234:LYS:O	1:H:235:VAL:O	2.33	0.46
1:A:502:GLU:CG	1:B:666:ARG:NH1	2.78	0.46
1:D:581:GLN:O	1:D:582:ARG:C	2.53	0.46
1:F:312:LEU:O	1:F:325:TYR:N	2.49	0.46
1:E:144:ARG:CD	1:E:169:TYR:O	2.63	0.46
1:B:390:PHE:CD1	1:B:390:PHE:N	2.83	0.46
1:F:390:PHE:N	1:F:390:PHE:CD1	2.83	0.46
1:B:475:GLU:CG	1:B:476:CYS:N	2.79	0.46
1:H:571:TYR:CE2	1:H:590:MET:SD	3.07	0.46
1:A:118:LYS:CG	1:A:118:LYS:O	2.63	0.46
1:A:118:LYS:CB	1:A:264:HIS:O	2.64	0.46
1:F:276:TRP:CE3	1:F:277:LEU:CD2	2.99	0.46
1:C:409:SER:CB	1:C:412:ILE:CD1	2.93	0.46
1:E:322:VAL:CG2	1:E:446:ARG:NH1	2.77	0.46
1:D:373:ASP:C	1:D:374:CYS:SG	2.93	0.46
1:B:165:ILE:O	1:B:167:LEU:N	2.48	0.46
1:H:118:LYS:CB	1:H:264:HIS:O	2.63	0.46
1:B:449:GLN:O	1:B:450:GLY:C	2.52	0.46
1:B:394:LYS:CG	1:B:401:ILE:N	2.78	0.46
1:F:449:GLN:NE2	1:F:453:THR:CG2	2.79	0.46
1:C:133:LEU:O	1:C:134:ARG:C	2.53	0.46
1:E:233:GLY:O	1:E:235:VAL:N	2.49	0.46
1:G:144:ARG:CD	1:G:169:TYR:O	2.64	0.46
1:G:135:TYR:O	1:G:139:ASN:ND2	2.48	0.46
1:C:276:TRP:CE3	1:C:277:LEU:CD2	2.98	0.46
1:E:265:LEU:CD2	1:E:269:LEU:CB	2.94	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:409:SER:CB	1:F:412:ILE:CD1	2.93	0.46
1:E:409:SER:CB	1:E:412:ILE:CD1	2.93	0.46
1:D:233:GLY:O	1:D:235:VAL:N	2.49	0.46
1:H:444:CYS:C	1:H:446:ARG:N	2.69	0.46
1:D:634:ASN:OD1	1:D:637:ARG:NH1	2.49	0.46
1:H:250:THR:C	1:H:251:GLY:O	2.54	0.46
1:F:581:GLN:O	1:F:582:ARG:C	2.53	0.46
1:A:581:GLN:O	1:A:582:ARG:C	2.54	0.46
1:H:390:PHE:N	1:H:390:PHE:CD1	2.83	0.46
1:H:581:GLN:O	1:H:582:ARG:C	2.53	0.46
1:H:434:TRP:CZ3	1:H:568:ARG:CB	2.99	0.46
1:G:105:ARG:CZ	1:G:149:GLU:OE2	2.64	0.46
1:B:634:ASN:OD1	1:B:637:ARG:NH1	2.49	0.46
1:B:269:LEU:C	1:B:271:GLY:N	2.68	0.46
1:E:434:TRP:CB	1:E:571:TYR:CD1	2.99	0.46
1:C:213:PHE:CE2	1:C:217:THR:OG1	2.69	0.46
1:E:105:ARG:CZ	1:E:149:GLU:OE2	2.64	0.46
1:D:317:MET:O	1:D:609:TYR:OH	2.34	0.46
1:D:402:SER:O	1:D:403:LEU:CB	2.64	0.46
1:D:480:LYS:NZ	1:D:640:GLU:OE1	2.49	0.46
1:C:638:GLU:O	1:C:642:ILE:N	2.49	0.46
1:B:598:ILE:O	1:B:602:GLU:N	2.49	0.46
1:B:434:TRP:O	1:B:438:ARG:N	2.49	0.46
1:G:212:ALA:O	1:G:213:PHE:C	2.54	0.46
1:E:412:ILE:O	1:E:416:ASP:OD1	2.34	0.46
1:G:373:ASP:CG	1:G:374:CYS:SG	2.94	0.46
1:B:651:GLN:O	1:B:652:GLN:C	2.55	0.46
1:G:634:ASN:OD1	1:G:637:ARG:NH1	2.49	0.45
1:H:133:LEU:O	1:H:134:ARG:C	2.54	0.45
1:A:316:ASN:N	1:A:321:ARG:O	2.49	0.45
1:C:316:ASN:N	1:C:321:ARG:O	2.49	0.45
1:E:527:GLU:O	1:E:530:VAL:N	2.49	0.45
1:D:441:LYS:CD	1:D:561:ASP:OD1	2.64	0.45
1:G:118:LYS:CG	1:G:118:LYS:O	2.64	0.45
1:D:135:TYR:O	1:D:139:ASN:ND2	2.49	0.45
1:H:634:ASN:OD1	1:H:637:ARG:NH1	2.49	0.45
1:F:598:ILE:O	1:F:602:GLU:N	2.48	0.45
1:C:634:ASN:OD1	1:C:637:ARG:NH1	2.49	0.45
1:F:148:PRO:CD	1:F:188:TYR:CE2	2.99	0.45
1:F:634:ASN:OD1	1:F:637:ARG:NH1	2.49	0.45
1:E:449:GLN:O	1:E:450:GLY:C	2.55	0.45
1:A:140:ARG:NH2	1:A:174:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:449:GLN:O	1:A:450:GLY:C	2.54	0.45
1:A:248:ASP:OD1	1:A:248:ASP:O	2.34	0.45
1:E:434:TRP:O	1:E:438:ARG:N	2.50	0.45
1:G:124:THR:O	1:G:127:SER:N	2.48	0.45
1:F:434:TRP:O	1:F:438:ARG:N	2.49	0.45
1:A:148:PRO:CD	1:A:188:TYR:CE2	3.00	0.45
1:B:118:LYS:CG	1:B:118:LYS:O	2.64	0.45
1:E:148:PRO:CD	1:E:188:TYR:CE2	2.99	0.45
1:A:222:PHE:CE2	1:A:224:PRO:O	2.70	0.45
1:D:409:SER:CB	1:D:412:ILE:CD1	2.94	0.45
1:C:272:LYS:O	1:C:273:LEU:C	2.55	0.45
1:F:412:ILE:O	1:F:416:ASP:OD1	2.34	0.45
1:B:443:ASP:O	1:B:446:ARG:CB	2.65	0.45
1:D:140:ARG:NH2	1:D:174:ASP:OD2	2.49	0.45
1:B:550:ASN:ND2	1:B:611:GLN:CG	2.80	0.45
1:D:208:PHE:O	1:D:212:ALA:N	2.49	0.45
1:A:212:ALA:O	1:A:213:PHE:C	2.55	0.45
1:A:133:LEU:O	1:A:134:ARG:C	2.54	0.45
1:G:133:LEU:O	1:G:134:ARG:C	2.54	0.45
1:D:276:TRP:CE3	1:D:277:LEU:CD2	3.00	0.45
1:D:479:LEU:C	1:D:640:GLU:OE2	2.55	0.45
1:H:373:ASP:OD1	1:H:374:CYS:N	2.49	0.45
1:G:350:GLU:OE2	1:G:391:ASP:O	2.33	0.45
1:B:140:ARG:NH2	1:B:174:ASP:OD2	2.50	0.45
1:G:312:LEU:O	1:G:325:TYR:N	2.50	0.45
1:B:114:CYS:O	1:B:115:CYS:CB	2.64	0.45
1:D:213:PHE:O	1:D:214:GLU:C	2.54	0.45
1:E:103:ASP:O	1:E:105:ARG:N	2.50	0.45
1:G:300:PHE:O	1:G:301:GLN:C	2.55	0.45
1:G:234:LYS:O	1:G:235:VAL:O	2.35	0.45
1:H:322:VAL:CG1	1:H:323:HIS:N	2.79	0.45
1:H:26:PHE:CE2	1:H:181:GLU:CG	2.99	0.45
1:D:122:ILE:O	1:D:126:LEU:N	2.49	0.45
1:A:130:SER:O	1:A:300:PHE:CE1	2.69	0.45
1:F:103:ASP:O	1:F:105:ARG:N	2.50	0.45
1:A:105:ARG:CZ	1:A:149:GLU:OE2	2.65	0.45
1:F:449:GLN:O	1:F:450:GLY:C	2.54	0.45
1:A:254:LYS:N	1:A:255:PHE:CE1	2.85	0.45
1:G:165:ILE:O	1:G:167:LEU:N	2.50	0.45
1:B:394:LYS:CE	1:B:401:ILE:CA	2.94	0.45
1:B:300:PHE:O	1:B:301:GLN:C	2.55	0.45
1:C:373:ASP:O	1:C:374:CYS:CB	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:206:TRP:CD1	1:G:207:SER:N	2.85	0.45
1:E:276:TRP:CE3	1:E:277:LEU:CD2	3.00	0.45
1:F:443:ASP:O	1:F:446:ARG:N	2.50	0.45
1:C:485:PHE:CZ	1:D:485:PHE:CG	3.04	0.45
1:H:105:ARG:CZ	1:H:149:GLU:OE2	2.65	0.45
1:F:222:PHE:CE2	1:F:224:PRO:O	2.70	0.45
1:C:114:CYS:O	1:C:115:CYS:CB	2.64	0.45
1:D:144:ARG:CD	1:D:169:TYR:O	2.64	0.45
1:E:249:LEU:CG	1:E:253:VAL:O	2.64	0.45
1:A:402:SER:O	1:A:403:LEU:CB	2.64	0.45
1:E:118:LYS:CB	1:E:264:HIS:C	2.85	0.45
1:E:124:THR:O	1:E:127:SER:N	2.50	0.45
1:E:127:SER:O	1:E:130:SER:OG	2.34	0.45
1:G:402:SER:CA	1:G:609:TYR:CG	2.99	0.45
1:A:312:LEU:O	1:A:325:TYR:N	2.51	0.45
1:E:634:ASN:OD1	1:E:637:ARG:NH1	2.49	0.45
1:A:598:ILE:O	1:A:602:GLU:N	2.50	0.45
1:A:455:MET:CE	1:A:455:MET:O	2.65	0.45
1:H:583:THR:O	1:H:584:PRO:C	2.56	0.45
1:D:435:GLN:O	1:D:439:ALA:N	2.50	0.44
1:B:438:ARG:CG	1:B:564:GLU:CG	2.95	0.44
1:A:517:MET:CE	1:A:647:GLN:OE1	2.65	0.44
1:A:434:TRP:CZ3	1:A:568:ARG:CG	3.00	0.44
1:B:111:PHE:CZ	1:B:572:ARG:CG	3.00	0.44
1:B:105:ARG:CZ	1:B:149:GLU:OE2	2.66	0.44
1:B:148:PRO:CD	1:B:188:TYR:CE2	3.01	0.44
1:C:206:TRP:CD1	1:C:207:SER:N	2.85	0.44
1:B:233:GLY:O	1:B:235:VAL:N	2.50	0.44
1:A:135:TYR:O	1:A:139:ASN:ND2	2.50	0.44
1:E:638:GLU:O	1:E:642:ILE:N	2.50	0.44
1:G:286:ARG:CG	1:G:286:ARG:NH1	2.79	0.44
1:G:113:ASN:O	1:G:116:GLY:N	2.51	0.44
1:G:222:PHE:CE2	1:G:224:PRO:O	2.70	0.44
1:E:527:GLU:C	1:E:529:GLU:N	2.69	0.44
1:H:387:ILE:CD1	1:H:449:GLN:CG	2.95	0.44
1:A:422:THR:CB	1:A:585:GLY:C	2.84	0.44
1:F:484:ASP:O	1:F:485:PHE:C	2.55	0.44
1:G:272:LYS:O	1:G:273:LEU:C	2.55	0.44
1:B:234:LYS:O	1:B:235:VAL:O	2.35	0.44
1:C:387:ILE:CD1	1:C:450:GLY:N	2.80	0.44
1:F:249:LEU:CG	1:F:253:VAL:O	2.64	0.44
1:B:135:TYR:O	1:B:139:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:165:ILE:O	1:H:167:LEU:N	2.49	0.44
1:G:136:LEU:O	1:G:141:ILE:N	2.50	0.44
1:A:435:GLN:O	1:A:439:ALA:N	2.50	0.44
1:E:316:ASN:N	1:E:321:ARG:O	2.50	0.44
1:D:148:PRO:CD	1:D:188:TYR:CE2	3.00	0.44
1:H:272:LYS:O	1:H:273:LEU:C	2.55	0.44
1:H:265:LEU:CD2	1:H:269:LEU:CB	2.94	0.44
1:C:234:LYS:O	1:C:235:VAL:O	2.35	0.44
1:H:213:PHE:CD2	1:H:213:PHE:C	2.90	0.44
1:B:208:PHE:O	1:B:212:ALA:N	2.51	0.44
1:B:249:LEU:CG	1:B:253:VAL:O	2.65	0.44
1:G:77:ARG:N	1:G:95:ALA:O	2.50	0.44
1:C:496:LYS:C	1:D:655:TRP:CZ2	2.91	0.44
1:C:484:ASP:O	1:C:485:PHE:C	2.55	0.44
1:D:105:ARG:CZ	1:D:149:GLU:OE2	2.66	0.44
1:C:422:THR:OG1	1:C:585:GLY:O	2.36	0.44
1:D:254:LYS:N	1:D:255:PHE:CE1	2.85	0.44
1:B:412:ILE:O	1:B:416:ASP:OD1	2.36	0.44
1:G:598:ILE:O	1:G:602:GLU:N	2.50	0.44
1:E:286:ARG:CG	1:E:286:ARG:NH1	2.80	0.44
1:H:144:ARG:CD	1:H:169:TYR:O	2.65	0.44
1:C:140:ARG:NH2	1:C:174:ASP:OD2	2.51	0.44
1:C:390:PHE:CD1	1:C:390:PHE:N	2.85	0.44
1:D:434:TRP:O	1:D:438:ARG:N	2.51	0.44
1:C:118:LYS:O	1:C:118:LYS:CG	2.65	0.44
1:B:26:PHE:CZ	1:B:179:CYS:CB	3.01	0.44
1:E:482:LYS:C	1:E:484:ASP:N	2.71	0.44
1:A:269:LEU:C	1:A:271:GLY:N	2.68	0.44
1:A:234:LYS:O	1:A:235:VAL:O	2.36	0.44
1:A:249:LEU:CG	1:A:253:VAL:O	2.65	0.44
1:F:140:ARG:NH2	1:F:174:ASP:OD2	2.50	0.44
1:B:538:MET:O	1:B:542:THR:OG1	2.35	0.44
1:E:165:ILE:O	1:E:167:LEU:N	2.50	0.44
1:B:571:TYR:CE2	1:B:590:MET:CG	3.00	0.44
1:C:124:THR:O	1:C:127:SER:N	2.50	0.44
1:G:435:GLN:O	1:G:439:ALA:N	2.50	0.44
1:G:254:LYS:N	1:G:255:PHE:CE1	2.86	0.44
1:B:124:THR:O	1:B:127:SER:N	2.51	0.44
1:E:449:GLN:NE2	1:E:453:THR:CG2	2.81	0.44
1:D:286:ARG:NH1	1:D:286:ARG:CG	2.78	0.44
1:E:300:PHE:O	1:E:301:GLN:C	2.55	0.44
1:A:210:THR:O	1:A:211:LEU:C	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:ASP:O	1:A:105:ARG:N	2.50	0.44
1:F:300:PHE:O	1:F:301:GLN:C	2.56	0.44
1:C:269:LEU:C	1:C:271:GLY:N	2.68	0.44
1:F:212:ALA:O	1:F:213:PHE:C	2.56	0.44
1:G:362:ASN:C	1:G:364:ALA:N	2.71	0.44
1:H:598:ILE:O	1:H:602:GLU:N	2.51	0.44
1:H:249:LEU:CG	1:H:253:VAL:O	2.66	0.44
1:D:312:LEU:O	1:D:325:TYR:N	2.50	0.44
1:D:538:MET:O	1:D:542:THR:OG1	2.36	0.44
1:G:103:ASP:O	1:G:105:ARG:N	2.51	0.44
1:C:284:HIS:NE2	1:E:342:GLN:CD	2.71	0.44
1:H:316:ASN:N	1:H:321:ARG:O	2.51	0.44
1:C:134:ARG:CB	1:C:300:PHE:CE1	3.00	0.44
1:D:547:LEU:CD1	1:D:615:THR:CG2	2.95	0.44
1:C:286:ARG:CG	1:C:286:ARG:NH1	2.79	0.44
1:E:435:GLN:O	1:E:439:ALA:N	2.51	0.43
1:C:105:ARG:CZ	1:C:149:GLU:OE2	2.65	0.43
1:C:570:LEU:CB	1:C:590:MET:CE	2.96	0.43
1:D:118:LYS:CG	1:D:118:LYS:O	2.65	0.43
1:D:362:ASN:C	1:D:364:ALA:N	2.71	0.43
1:H:362:ASN:C	1:H:364:ALA:N	2.71	0.43
1:H:233:GLY:O	1:H:235:VAL:N	2.52	0.43
1:D:133:LEU:O	1:D:134:ARG:C	2.56	0.43
1:C:333:LEU:O	1:C:336:LEU:N	2.51	0.43
1:C:422:THR:OG1	1:C:585:GLY:C	2.56	0.43
1:A:165:ILE:O	1:A:167:LEU:N	2.51	0.43
1:E:419:ARG:CA	1:E:587:SER:OG	2.66	0.43
1:H:212:ALA:O	1:H:215:CYS:N	2.51	0.43
1:G:449:GLN:O	1:G:450:GLY:C	2.56	0.43
1:A:233:GLY:O	1:A:235:VAL:N	2.51	0.43
1:D:57:ARG:NE	1:D:177:GLU:O	2.51	0.43
1:A:451:GLN:CD	1:A:611:GLN:NE2	2.71	0.43
1:F:269:LEU:C	1:F:271:GLY:N	2.71	0.43
1:F:286:ARG:NH1	1:F:286:ARG:CG	2.79	0.43
1:E:114:CYS:O	1:E:115:CYS:CB	2.66	0.43
1:C:338:SER:OG	1:C:339:TRP:N	2.52	0.43
1:H:538:MET:O	1:H:542:THR:OG1	2.37	0.43
1:D:502:GLU:OE1	1:D:502:GLU:N	2.51	0.43
1:H:286:ARG:NH1	1:H:286:ARG:CG	2.79	0.43
1:H:153:LEU:CD2	1:H:162:HIS:CG	3.01	0.43
1:E:402:SER:O	1:E:403:LEU:CB	2.66	0.43
1:D:412:ILE:O	1:D:416:ASP:OD1	2.36	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:362:ASN:C	1:B:364:ALA:N	2.71	0.43
1:B:250:THR:C	1:B:251:GLY:O	2.54	0.43
1:C:598:ILE:O	1:C:602:GLU:N	2.51	0.43
1:E:598:ILE:O	1:E:602:GLU:N	2.51	0.43
1:G:389:LEU:CD1	1:G:454:SER:OG	2.66	0.43
1:D:430:TRP:C	1:D:571:TYR:CD2	2.92	0.43
1:D:116:GLY:N	1:D:217:THR:O	2.50	0.43
1:E:133:LEU:O	1:E:134:ARG:C	2.56	0.43
1:C:435:GLN:O	1:C:439:ALA:N	2.51	0.43
1:B:501:MET:C	1:B:505:ILE:CD1	2.87	0.43
1:G:412:ILE:O	1:G:416:ASP:OD1	2.36	0.43
1:B:272:LYS:O	1:B:273:LEU:C	2.56	0.43
1:E:140:ARG:NH2	1:E:174:ASP:OD2	2.51	0.43
1:C:583:THR:O	1:C:584:PRO:C	2.57	0.43
1:G:249:LEU:CG	1:G:253:VAL:O	2.66	0.43
1:A:540:LEU:CD1	1:A:622:ALA:CB	2.97	0.43
1:F:114:CYS:O	1:F:115:CYS:CB	2.66	0.43
1:H:300:PHE:O	1:H:301:GLN:C	2.57	0.43
1:F:538:MET:O	1:F:542:THR:OG1	2.36	0.43
1:C:249:LEU:CG	1:C:253:VAL:O	2.66	0.43
1:E:490:ILE:O	1:E:490:ILE:CG2	2.67	0.43
1:D:193:LEU:CD2	1:D:231:TRP:CD1	3.01	0.43
1:A:213:PHE:CE2	1:A:217:THR:OG1	2.72	0.43
1:A:300:PHE:O	1:A:301:GLN:C	2.56	0.43
1:A:433:ILE:CB	1:A:571:TYR:CZ	3.02	0.43
1:E:269:LEU:C	1:E:271:GLY:N	2.70	0.43
1:A:412:ILE:O	1:A:416:ASP:OD1	2.37	0.43
1:A:502:GLU:N	1:A:502:GLU:OE1	2.51	0.43
1:C:153:LEU:CD2	1:C:162:HIS:CG	3.01	0.43
1:E:571:TYR:CE2	1:E:590:MET:CG	3.00	0.43
1:H:148:PRO:CD	1:H:188:TYR:CE2	3.01	0.43
1:C:254:LYS:O	1:C:255:PHE:CG	2.72	0.43
1:C:233:GLY:O	1:C:235:VAL:N	2.52	0.43
1:D:300:PHE:O	1:D:301:GLN:C	2.57	0.43
1:A:449:GLN:NE2	1:A:453:THR:CG2	2.82	0.43
1:C:165:ILE:O	1:C:167:LEU:N	2.51	0.43
1:C:651:GLN:O	1:C:652:GLN:C	2.57	0.43
1:E:571:TYR:CE2	1:E:590:MET:SD	3.11	0.43
1:C:662:CYS:SG	1:D:661:ALA:CB	3.07	0.43
1:B:118:LYS:CB	1:B:264:HIS:O	2.66	0.43
1:G:148:PRO:CD	1:G:188:TYR:CE2	3.01	0.43
1:E:206:TRP:CD1	1:E:207:SER:N	2.87	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:449:GLN:O	1:H:450:GLY:C	2.57	0.43
1:F:206:TRP:CD1	1:F:207:SER:N	2.87	0.43
1:F:77:ARG:N	1:F:95:ALA:O	2.52	0.43
1:D:219:PHE:CE1	1:D:428:ARG:NE	2.87	0.43
1:B:153:LEU:CD2	1:B:162:HIS:CG	3.02	0.43
1:C:430:TRP:CB	1:C:571:TYR:CD2	3.02	0.43
1:C:485:PHE:CG	1:D:485:PHE:CD2	3.06	0.43
1:E:254:LYS:O	1:E:255:PHE:CG	2.70	0.43
1:A:97:GLU:OE2	1:A:163:LYS:NZ	2.51	0.43
1:A:579:ARG:NH2	1:D:580:ASP:CB	2.82	0.43
1:G:538:MET:O	1:G:542:THR:OG1	2.36	0.43
1:A:638:GLU:O	1:A:642:ILE:N	2.52	0.43
1:E:390:PHE:CD1	1:E:390:PHE:N	2.87	0.43
1:C:348:GLU:OE2	1:C:348:GLU:N	2.52	0.43
1:D:212:ALA:O	1:D:215:CYS:N	2.52	0.43
1:F:153:LEU:CD2	1:F:162:HIS:CG	3.02	0.43
1:H:118:LYS:CG	1:H:118:LYS:O	2.67	0.43
1:B:449:GLN:NE2	1:B:453:THR:CG2	2.82	0.43
1:D:272:LYS:O	1:D:273:LEU:C	2.57	0.43
1:C:362:ASN:C	1:C:364:ALA:N	2.71	0.43
1:E:198:LYS:O	1:E:200:THR:N	2.51	0.43
1:A:362:ASN:C	1:A:364:ALA:N	2.72	0.43
1:G:430:TRP:O	1:G:431:GLY:C	2.57	0.43
1:G:140:ARG:NH2	1:G:174:ASP:OD2	2.51	0.43
1:C:665:VAL:CG2	1:D:665:VAL:CG2	2.96	0.43
1:E:296:ASN:CG	1:E:297:VAL:N	2.72	0.43
1:D:153:LEU:CD2	1:D:162:HIS:CG	3.02	0.42
1:E:26:PHE:CZ	1:E:179:CYS:CB	3.02	0.42
1:A:434:TRP:O	1:A:438:ARG:N	2.51	0.42
1:B:103:ASP:O	1:B:105:ARG:N	2.52	0.42
1:D:632:VAL:O	1:D:633:MET:SD	2.77	0.42
1:A:373:ASP:O	1:A:374:CYS:CB	2.67	0.42
1:D:265:LEU:CD2	1:D:269:LEU:CB	2.98	0.42
1:F:233:GLY:O	1:F:235:VAL:N	2.52	0.42
1:B:336:LEU:O	1:B:340:LEU:N	2.52	0.42
1:D:638:GLU:O	1:D:642:ILE:N	2.51	0.42
1:H:26:PHE:CE2	1:H:181:GLU:OE2	2.70	0.42
1:A:153:LEU:CD2	1:A:162:HIS:CG	3.03	0.42
1:D:103:ASP:O	1:D:105:ARG:N	2.52	0.42
1:F:105:ARG:CZ	1:F:149:GLU:OE2	2.67	0.42
1:H:206:TRP:CD1	1:H:207:SER:N	2.88	0.42
1:A:272:LYS:O	1:A:276:TRP:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:362:ASN:C	1:E:364:ALA:N	2.72	0.42
1:B:340:LEU:O	1:B:344:THR:OG1	2.37	0.42
1:F:451:GLN:CD	1:F:611:GLN:NE2	2.72	0.42
1:D:598:ILE:O	1:D:602:GLU:N	2.51	0.42
1:G:213:PHE:CE2	1:G:217:THR:OG1	2.73	0.42
1:H:190:ALA:O	1:H:191:PRO:C	2.58	0.42
1:B:210:THR:O	1:B:211:LEU:C	2.58	0.42
1:D:583:THR:O	1:D:584:PRO:C	2.57	0.42
1:H:338:SER:OG	1:H:339:TRP:N	2.52	0.42
1:C:135:TYR:O	1:C:139:ASN:ND2	2.52	0.42
1:C:410:VAL:O	1:C:411:SER:C	2.57	0.42
1:H:140:ARG:NH2	1:H:174:ASP:OD2	2.52	0.42
1:E:455:MET:O	1:E:455:MET:CE	2.68	0.42
1:D:570:LEU:CD2	1:D:590:MET:CE	2.98	0.42
1:F:118:LYS:CB	1:F:264:HIS:O	2.67	0.42
1:G:316:ASN:N	1:G:321:ARG:O	2.52	0.42
1:B:317:MET:O	1:B:609:TYR:OH	2.38	0.42
1:C:263:ASN:ND2	1:C:265:LEU:CB	2.82	0.42
1:B:198:LYS:C	1:B:200:THR:N	2.73	0.42
1:F:362:ASN:C	1:F:364:ALA:N	2.73	0.42
1:C:449:GLN:NE2	1:C:453:THR:CG2	2.82	0.42
1:B:410:VAL:O	1:B:411:SER:C	2.58	0.42
1:F:136:LEU:O	1:F:141:ILE:N	2.52	0.42
1:C:340:LEU:O	1:C:344:THR:OG1	2.37	0.42
1:G:583:THR:O	1:G:584:PRO:C	2.58	0.42
1:E:434:TRP:CZ3	1:E:568:ARG:CA	3.02	0.42
1:D:484:ASP:O	1:D:485:PHE:C	2.58	0.42
1:C:300:PHE:O	1:C:301:GLN:C	2.55	0.42
1:G:269:LEU:C	1:G:271:GLY:N	2.71	0.42
1:C:412:ILE:O	1:C:416:ASP:OD1	2.38	0.42
1:F:583:THR:O	1:F:584:PRO:C	2.58	0.42
1:E:135:TYR:O	1:E:139:ASN:ND2	2.52	0.42
1:B:638:GLU:O	1:B:642:ILE:N	2.53	0.42
1:E:340:LEU:O	1:E:344:THR:OG1	2.38	0.42
1:A:583:THR:O	1:A:584:PRO:C	2.58	0.42
1:D:571:TYR:CZ	1:D:590:MET:SD	3.12	0.42
1:C:118:LYS:NZ	1:C:123:ARG:NH2	2.68	0.42
1:C:486:PHE:CG	1:C:486:PHE:O	2.72	0.42
1:H:272:LYS:O	1:H:276:TRP:N	2.52	0.42
1:E:658:LEU:CA	1:F:658:LEU:CD1	2.98	0.42
1:D:637:ARG:O	1:D:641:LYS:N	2.53	0.42
1:E:333:LEU:O	1:E:336:LEU:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:210:THR:O	1:G:211:LEU:C	2.58	0.42
1:H:336:LEU:O	1:H:340:LEU:N	2.52	0.42
1:F:422:THR:CB	1:F:585:GLY:CA	2.98	0.42
1:C:502:GLU:OE1	1:C:502:GLU:N	2.53	0.42
1:F:118:LYS:CG	1:F:118:LYS:O	2.68	0.42
1:A:124:THR:O	1:A:127:SER:N	2.53	0.42
1:C:103:ASP:O	1:C:105:ARG:N	2.53	0.42
1:C:430:TRP:O	1:C:431:GLY:C	2.58	0.42
1:E:502:GLU:OE1	1:E:502:GLU:N	2.53	0.42
1:E:373:ASP:O	1:E:374:CYS:CB	2.67	0.42
1:F:521:VAL:CG2	1:F:643:VAL:CG1	2.97	0.42
1:H:77:ARG:N	1:H:95:ALA:O	2.53	0.42
1:B:260:PRO:O	1:B:261:THR:OG1	2.37	0.42
1:E:348:GLU:N	1:E:348:GLU:OE2	2.53	0.42
1:B:490:ILE:CG2	1:B:490:ILE:O	2.67	0.42
1:D:651:GLN:O	1:D:652:GLN:C	2.57	0.42
1:E:120:GLY:O	1:E:123:ARG:CA	2.68	0.42
1:C:213:PHE:O	1:C:214:GLU:C	2.58	0.42
1:C:646:ARG:C	1:C:647:GLN:OE1	2.57	0.42
1:C:480:LYS:CE	1:C:527:GLU:CB	2.98	0.42
1:C:190:ALA:O	1:C:191:PRO:C	2.58	0.42
1:H:273:LEU:O	1:H:276:TRP:N	2.53	0.42
1:F:430:TRP:O	1:F:431:GLY:C	2.58	0.42
1:B:77:ARG:N	1:B:95:ALA:O	2.53	0.42
1:B:441:LYS:CB	1:B:560:LEU:CD2	2.98	0.42
1:A:114:CYS:O	1:A:115:CYS:CB	2.68	0.42
1:B:455:MET:CE	1:B:455:MET:O	2.68	0.42
1:G:213:PHE:O	1:G:214:GLU:C	2.58	0.42
1:C:517:MET:CE	1:C:647:GLN:OE1	2.68	0.42
1:F:272:LYS:O	1:F:273:LEU:C	2.58	0.42
1:A:263:ASN:ND2	1:A:265:LEU:CB	2.83	0.42
1:A:651:GLN:O	1:A:652:GLN:C	2.57	0.42
1:H:412:ILE:O	1:H:416:ASP:OD1	2.38	0.42
1:H:419:ARG:CG	1:H:419:ARG:O	2.68	0.42
1:B:583:THR:O	1:B:584:PRO:C	2.58	0.42
1:H:136:LEU:O	1:H:141:ILE:N	2.53	0.42
1:E:549:ARG:O	1:E:550:ASN:CB	2.68	0.42
1:C:496:LYS:CB	1:D:655:TRP:CD1	2.97	0.42
1:A:484:ASP:O	1:A:485:PHE:C	2.57	0.42
1:A:209:GLY:O	1:A:213:PHE:N	2.53	0.42
1:H:127:SER:O	1:H:130:SER:OG	2.38	0.42
1:A:150:ASN:ND2	1:A:167:LEU:CD1	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:265:LEU:CD2	1:C:269:LEU:CB	2.98	0.42
1:A:265:LEU:CD2	1:A:269:LEU:CB	2.98	0.42
1:F:263:ASN:ND2	1:F:265:LEU:CB	2.83	0.42
1:H:340:LEU:O	1:H:344:THR:OG1	2.38	0.42
1:A:348:GLU:OE2	1:A:348:GLU:N	2.53	0.42
1:B:430:TRP:O	1:B:431:GLY:C	2.58	0.41
1:B:434:TRP:O	1:B:435:GLN:C	2.55	0.41
1:D:127:SER:O	1:D:130:SER:OG	2.37	0.41
1:A:434:TRP:CZ3	1:A:568:ARG:CB	3.03	0.41
1:C:109:ASN:O	1:C:110:GLN:C	2.58	0.41
1:C:484:ASP:OD1	1:C:487:ARG:NH1	2.53	0.41
1:F:133:LEU:O	1:F:134:ARG:C	2.57	0.41
1:B:193:LEU:CD2	1:B:231:TRP:CD1	3.03	0.41
1:C:273:LEU:O	1:C:276:TRP:N	2.53	0.41
1:E:190:ALA:O	1:E:191:PRO:C	2.58	0.41
1:A:198:LYS:C	1:A:200:THR:N	2.73	0.41
1:A:272:LYS:O	1:A:273:LEU:C	2.58	0.41
1:H:263:ASN:ND2	1:H:265:LEU:CB	2.83	0.41
1:A:77:ARG:N	1:A:95:ALA:O	2.53	0.41
1:D:77:ARG:N	1:D:95:ALA:O	2.53	0.41
1:D:249:LEU:CG	1:D:253:VAL:O	2.68	0.41
1:D:165:ILE:O	1:D:167:LEU:N	2.53	0.41
1:G:114:CYS:O	1:G:115:CYS:CB	2.68	0.41
1:A:476:CYS:CB	1:A:636:MET:SD	3.08	0.41
1:H:433:ILE:CB	1:H:571:TYR:CZ	3.03	0.41
1:A:210:THR:O	1:A:213:PHE:N	2.53	0.41
1:H:124:THR:O	1:H:127:SER:N	2.52	0.41
1:F:254:LYS:N	1:F:255:PHE:CE1	2.87	0.41
1:E:272:LYS:O	1:E:273:LEU:C	2.57	0.41
1:E:272:LYS:O	1:E:276:TRP:N	2.53	0.41
1:E:485:PHE:CD2	1:F:485:PHE:CD2	3.08	0.41
1:G:263:ASN:ND2	1:G:265:LEU:CB	2.83	0.41
1:G:340:LEU:O	1:G:344:THR:OG1	2.38	0.41
1:A:250:THR:C	1:A:251:GLY:O	2.58	0.41
1:E:583:THR:O	1:E:584:PRO:C	2.58	0.41
1:D:340:LEU:O	1:D:344:THR:OG1	2.38	0.41
1:E:103:ASP:O	1:E:106:LYS:N	2.53	0.41
1:F:503:PHE:O	1:F:505:ILE:CG1	2.68	0.41
1:A:410:VAL:O	1:A:411:SER:C	2.59	0.41
1:E:77:ARG:N	1:E:95:ALA:O	2.53	0.41
1:E:152:VAL:N	1:E:163:LYS:O	2.54	0.41
1:F:502:GLU:OE1	1:F:502:GLU:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:430:TRP:O	1:D:431:GLY:C	2.59	0.41
1:D:434:TRP:O	1:D:435:GLN:C	2.56	0.41
1:H:451:GLN:NE2	1:H:611:GLN:NE2	2.68	0.41
1:C:277:LEU:C	1:C:279:CYS:N	2.74	0.41
1:F:213:PHE:O	1:F:214:GLU:C	2.58	0.41
1:D:198:LYS:C	1:D:200:THR:N	2.74	0.41
1:D:263:ASN:ND2	1:D:265:LEU:CB	2.83	0.41
1:D:234:LYS:O	1:D:235:VAL:O	2.38	0.41
1:E:336:LEU:O	1:E:337:LYS:C	2.57	0.41
1:E:497:TYR:CD2	1:E:497:TYR:C	2.94	0.41
1:E:153:LEU:CD2	1:E:162:HIS:CG	3.02	0.41
1:G:570:LEU:CB	1:G:590:MET:CE	2.97	0.41
1:A:208:PHE:O	1:A:212:ALA:N	2.53	0.41
1:D:423:TYR:CE2	1:D:425:HIS:CB	3.03	0.41
1:H:423:TYR:CE1	1:H:425:HIS:O	2.74	0.41
1:G:265:LEU:CD2	1:G:269:LEU:CB	2.99	0.41
1:A:430:TRP:O	1:A:431:GLY:C	2.59	0.41
1:D:637:ARG:O	1:D:641:LYS:CB	2.68	0.41
1:B:606:ILE:O	1:B:607:LEU:C	2.58	0.41
1:C:136:LEU:O	1:C:141:ILE:N	2.53	0.41
1:F:488:SER:O	1:F:491:GLN:N	2.53	0.41
1:D:497:TYR:CE2	1:D:511:LEU:CD2	3.03	0.41
1:B:120:GLY:O	1:B:123:ARG:CA	2.69	0.41
1:A:198:LYS:O	1:A:200:THR:N	2.54	0.41
1:C:451:GLN:OE1	1:C:611:GLN:NE2	2.54	0.41
1:G:472:MET:CG	1:G:633:MET:CB	2.99	0.41
1:F:234:LYS:O	1:F:235:VAL:O	2.38	0.41
1:C:210:THR:O	1:C:211:LEU:C	2.59	0.41
1:F:638:GLU:O	1:F:642:ILE:N	2.53	0.41
1:A:488:SER:O	1:A:491:GLN:N	2.54	0.41
1:G:455:MET:CE	1:G:455:MET:O	2.68	0.41
1:C:208:PHE:O	1:C:212:ALA:N	2.54	0.41
1:C:527:GLU:C	1:C:529:GLU:N	2.73	0.41
1:F:272:LYS:O	1:F:276:TRP:N	2.54	0.41
1:D:449:GLN:NE2	1:D:453:THR:CG2	2.83	0.41
1:A:206:TRP:CD1	1:A:207:SER:N	2.88	0.41
1:C:538:MET:O	1:C:542:THR:OG1	2.39	0.41
1:D:497:TYR:C	1:D:497:TYR:CD2	2.93	0.41
1:G:153:LEU:CD2	1:G:162:HIS:CG	3.03	0.41
1:D:124:THR:O	1:D:127:SER:N	2.54	0.41
1:B:265:LEU:CD2	1:B:269:LEU:CB	2.99	0.41
1:A:285:GLN:O	1:A:285:GLN:CG	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:114:CYS:SG	1:C:114:CYS:O	2.79	0.41
1:D:336:LEU:O	1:D:340:LEU:N	2.54	0.41
1:E:538:MET:O	1:E:542:THR:OG1	2.38	0.41
1:D:114:CYS:O	1:D:115:CYS:CB	2.69	0.41
1:B:434:TRP:CZ3	1:B:568:ARG:CG	3.04	0.41
1:B:430:TRP:CB	1:B:571:TYR:CD2	3.03	0.41
1:E:118:LYS:CG	1:E:118:LYS:O	2.68	0.41
1:C:549:ARG:O	1:C:550:ASN:CB	2.69	0.41
1:D:213:PHE:CE2	1:D:217:THR:OG1	2.74	0.41
1:G:567:ALA:O	1:G:571:TYR:CD1	2.74	0.41
1:A:212:ALA:O	1:A:215:CYS:N	2.54	0.41
1:D:485:PHE:C	1:D:485:PHE:CD1	2.94	0.41
1:D:484:ASP:OD1	1:D:487:ARG:NH1	2.54	0.41
1:E:423:TYR:CE2	1:E:425:HIS:CB	3.04	0.41
1:A:423:TYR:CE2	1:A:425:HIS:CB	3.04	0.41
1:E:321:ARG:NE	1:E:443:ASP:OD1	2.54	0.41
1:D:118:LYS:CB	1:D:264:HIS:O	2.69	0.41
1:E:486:PHE:O	1:E:486:PHE:CG	2.73	0.41
1:E:273:LEU:O	1:E:276:TRP:N	2.54	0.41
1:D:272:LYS:O	1:D:276:TRP:N	2.54	0.41
1:G:273:LEU:O	1:G:276:TRP:N	2.54	0.41
1:B:656:ASN:OD1	1:B:656:ASN:O	2.39	0.41
1:A:282:MET:CB	1:A:286:ARG:CG	2.99	0.41
1:G:282:MET:CB	1:G:286:ARG:CG	2.98	0.41
1:H:169:TYR:N	1:H:169:TYR:CD2	2.89	0.41
1:C:77:ARG:N	1:C:95:ALA:O	2.54	0.41
1:A:340:LEU:O	1:A:344:THR:OG1	2.39	0.41
1:B:285:GLN:CG	1:B:285:GLN:O	2.69	0.41
1:A:336:LEU:O	1:A:337:LYS:C	2.59	0.41
1:A:136:LEU:O	1:A:141:ILE:N	2.54	0.41
1:C:488:SER:O	1:C:491:GLN:N	2.54	0.41
1:F:455:MET:CE	1:F:455:MET:O	2.69	0.41
1:D:434:TRP:CZ3	1:D:568:ARG:CG	3.04	0.41
1:B:497:TYR:CD2	1:B:497:TYR:C	2.93	0.41
1:G:434:TRP:CZ3	1:G:568:ARG:CB	3.04	0.41
1:A:127:SER:O	1:A:130:SER:OG	2.38	0.41
1:C:102:GLY:O	1:C:103:ASP:C	2.60	0.41
1:H:423:TYR:CE2	1:H:425:HIS:CB	3.04	0.41
1:E:651:GLN:O	1:E:652:GLN:C	2.59	0.41
1:A:222:PHE:CZ	1:A:225:ASN:CB	3.04	0.41
1:B:502:GLU:N	1:B:502:GLU:OE1	2.54	0.41
1:G:419:ARG:O	1:G:419:ARG:CG	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:373:ASP:O	1:B:374:CYS:CB	2.69	0.41
1:H:583:THR:O	1:H:585:GLY:N	2.54	0.41
1:C:336:LEU:O	1:C:337:LYS:C	2.60	0.41
1:F:282:MET:CB	1:F:286:ARG:CG	2.98	0.41
1:A:336:LEU:O	1:A:340:LEU:N	2.54	0.41
1:H:210:THR:O	1:H:211:LEU:C	2.60	0.41
1:E:488:SER:O	1:E:491:GLN:N	2.54	0.41
1:C:250:THR:C	1:C:251:GLY:O	2.58	0.41
1:E:250:THR:C	1:E:251:GLY:O	2.58	0.41
1:G:348:GLU:N	1:G:348:GLU:OE2	2.54	0.41
1:D:476:CYS:CB	1:D:636:MET:SD	3.09	0.40
1:A:497:TYR:C	1:A:497:TYR:CD2	2.94	0.40
1:G:438:ARG:NH1	1:G:568:ARG:NH2	2.69	0.40
1:G:571:TYR:OH	1:G:590:MET:SD	2.79	0.40
1:B:102:GLY:O	1:B:103:ASP:C	2.60	0.40
1:D:222:PHE:CZ	1:D:225:ASN:CB	3.04	0.40
1:G:272:LYS:O	1:G:276:TRP:N	2.54	0.40
1:D:206:TRP:CD1	1:D:207:SER:N	2.89	0.40
1:G:373:ASP:O	1:G:374:CYS:CB	2.68	0.40
1:D:169:TYR:N	1:D:169:TYR:CD2	2.89	0.40
1:F:336:LEU:O	1:F:340:LEU:N	2.54	0.40
1:F:296:ASN:CG	1:F:297:VAL:N	2.75	0.40
1:D:250:THR:C	1:D:251:GLY:O	2.59	0.40
1:D:567:ALA:O	1:D:571:TYR:CD1	2.74	0.40
1:G:212:ALA:O	1:G:215:CYS:N	2.55	0.40
1:A:213:PHE:O	1:A:214:GLU:C	2.59	0.40
1:F:423:TYR:CE2	1:F:425:HIS:CB	3.04	0.40
1:G:423:TYR:CE1	1:G:425:HIS:O	2.74	0.40
1:E:102:GLY:O	1:E:103:ASP:C	2.59	0.40
1:C:419:ARG:CG	1:C:419:ARG:O	2.69	0.40
1:F:651:GLN:O	1:F:652:GLN:C	2.59	0.40
1:A:190:ALA:O	1:A:191:PRO:C	2.60	0.40
1:G:190:ALA:O	1:G:191:PRO:C	2.59	0.40
1:A:285:GLN:NE2	1:A:286:ARG:NH1	2.70	0.40
1:D:580:ASP:O	1:D:580:ASP:CG	2.60	0.40
1:E:336:LEU:O	1:E:340:LEU:N	2.54	0.40
1:E:136:LEU:O	1:E:141:ILE:N	2.55	0.40
1:F:606:ILE:O	1:F:607:LEU:C	2.58	0.40
1:C:497:TYR:C	1:C:497:TYR:CD2	2.93	0.40
1:B:438:ARG:NH1	1:B:568:ARG:NH2	2.69	0.40
1:A:482:LYS:C	1:A:484:ASP:N	2.74	0.40
1:C:120:GLY:O	1:C:123:ARG:CA	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:423:TYR:CE2	1:C:425:HIS:CB	3.04	0.40
1:C:485:PHE:CB	1:D:485:PHE:CE2	3.05	0.40
1:D:109:ASN:O	1:D:110:GLN:C	2.60	0.40
1:F:124:THR:O	1:F:127:SER:N	2.53	0.40
1:G:105:ARG:NE	1:G:149:GLU:OE2	2.55	0.40
1:F:486:PHE:O	1:F:486:PHE:CG	2.75	0.40
1:H:208:PHE:O	1:H:212:ALA:N	2.54	0.40
1:G:336:LEU:O	1:G:340:LEU:N	2.54	0.40
1:E:536:LYS:CB	1:E:625:LEU:CD1	2.99	0.40
1:B:136:LEU:O	1:B:141:ILE:N	2.55	0.40
1:E:410:VAL:O	1:E:411:SER:C	2.59	0.40
1:B:485:PHE:C	1:B:485:PHE:CD1	2.95	0.40
1:D:434:TRP:NE1	1:D:435:GLN:OE1	2.55	0.40
1:G:208:PHE:O	1:G:212:ALA:N	2.54	0.40
1:C:485:PHE:CG	1:D:485:PHE:CE2	3.09	0.40
1:B:316:ASN:N	1:B:321:ARG:O	2.54	0.40
1:D:549:ARG:O	1:D:550:ASN:CB	2.70	0.40
1:F:480:LYS:NZ	1:F:527:GLU:CB	2.85	0.40
1:C:632:VAL:O	1:C:633:MET:SD	2.79	0.40
1:B:484:ASP:OD1	1:B:487:ARG:NH1	2.54	0.40
1:E:282:MET:CB	1:E:286:ARG:CG	2.99	0.40
1:D:282:MET:CB	1:D:286:ARG:CG	3.00	0.40
1:D:136:LEU:O	1:D:141:ILE:N	2.54	0.40
1:H:114:CYS:O	1:H:115:CYS:CB	2.70	0.40
1:F:490:ILE:CG2	1:F:490:ILE:O	2.68	0.40
1:B:124:THR:O	1:B:128:ASP:N	2.54	0.40
1:G:423:TYR:CE2	1:G:425:HIS:CB	3.05	0.40
1:D:70:HIS:NE2	1:D:131:SER:O	2.54	0.40
1:G:150:ASN:ND2	1:G:167:LEU:CD1	2.84	0.40
1:C:260:PRO:CB	1:C:273:LEU:CD1	3.00	0.40
1:E:419:ARG:O	1:E:419:ARG:CG	2.69	0.40
1:B:277:LEU:C	1:B:279:CYS:N	2.74	0.40
1:F:549:ARG:O	1:F:550:ASN:CB	2.70	0.40
1:F:114:CYS:SG	1:F:114:CYS:O	2.80	0.40
1:A:152:VAL:N	1:A:163:LYS:O	2.55	0.40
1:B:333:LEU:O	1:B:336:LEU:N	2.54	0.40
1:H:333:LEU:O	1:H:336:LEU:N	2.55	0.40
1:F:63:GLN:O	1:F:67:LYS:N	2.55	0.40
1:C:296:ASN:CG	1:C:297:VAL:N	2.75	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:501:MET:SD	1:E:364:ALA:O[1_565]	1.61	0.59
1:E:515:ARG:NH1	1:H:394:LYS:NZ[1_465]	1.76	0.44
1:B:617:VAL:CG2	1:C:519:GLN:OE1[1_465]	1.96	0.24
1:A:522:GLU:OE1	1:C:295:PRO:CB[1_565]	2.01	0.19
1:A:522:GLU:OE1	1:C:295:PRO:CG[1_565]	2.04	0.16
1:B:394:LYS:NZ	1:C:515:ARG:NH1[1_465]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	610/676 (90%)	360 (59%)	145 (24%)	105 (17%)	0	5
1	B	610/676 (90%)	362 (59%)	143 (23%)	105 (17%)	0	5
1	C	610/676 (90%)	359 (59%)	147 (24%)	104 (17%)	0	5
1	D	610/676 (90%)	363 (60%)	143 (23%)	104 (17%)	0	5
1	E	610/676 (90%)	361 (59%)	147 (24%)	102 (17%)	0	6
1	F	610/676 (90%)	362 (59%)	144 (24%)	104 (17%)	0	5
1	G	527/676 (78%)	310 (59%)	126 (24%)	91 (17%)	0	5
1	H	527/676 (78%)	313 (59%)	121 (23%)	93 (18%)	0	4
All	All	4714/5408 (87%)	2790 (59%)	1116 (24%)	808 (17%)	0	5

All (808) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	106	LYS
1	A	110	GLN
1	A	111	PHE
1	A	166	ASP
1	A	171	LYS
1	A	183	VAL
1	A	187	GLN
1	A	191	PRO

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Mol	Chain	Res	Type
1	A	195	GLU
1	A	202	THR
1	A	214	GLU
1	A	231	TRP
1	A	235	VAL
1	A	300	PHE
1	A	319	SER
1	A	330	ASN
1	A	350	GLU
1	A	359	LEU
1	A	372	ILE
1	A	403	LEU
1	A	419	ARG
1	A	420	PRO
1	A	424	THR
1	A	506	THR
1	A	528	ARG
1	A	582	ARG
1	A	584	PRO
1	A	588	ASN
1	B	101	GLY
1	B	106	LYS
1	B	110	GLN
1	B	111	PHE
1	B	166	ASP
1	B	171	LYS
1	B	183	VAL
1	B	187	GLN
1	B	191	PRO
1	B	195	GLU
1	B	201	VAL
1	B	202	THR
1	B	231	TRP
1	B	235	VAL
1	B	300	PHE
1	B	319	SER
1	B	330	ASN
1	B	350	GLU
1	B	359	LEU
1	B	363	SER
1	B	372	ILE
1	B	403	LEU

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Mol	Chain	Res	Type
1	B	419	ARG
1	B	420	PRO
1	B	424	THR
1	B	506	THR
1	B	528	ARG
1	B	582	ARG
1	B	584	PRO
1	B	661	ALA
1	C	101	GLY
1	C	106	LYS
1	C	110	GLN
1	C	111	PHE
1	C	166	ASP
1	C	171	LYS
1	C	183	VAL
1	C	187	GLN
1	C	191	PRO
1	C	195	GLU
1	C	201	VAL
1	C	202	THR
1	C	231	TRP
1	C	235	VAL
1	C	273	LEU
1	C	300	PHE
1	C	319	SER
1	C	330	ASN
1	C	350	GLU
1	C	359	LEU
1	C	363	SER
1	C	372	ILE
1	C	403	LEU
1	C	419	ARG
1	C	420	PRO
1	C	424	THR
1	C	506	THR
1	C	528	ARG
1	C	582	ARG
1	C	584	PRO
1	C	661	ALA
1	D	101	GLY
1	D	106	LYS
1	D	110	GLN

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Mol	Chain	Res	Type
1	D	111	PHE
1	D	166	ASP
1	D	171	LYS
1	D	183	VAL
1	D	187	GLN
1	D	191	PRO
1	D	195	GLU
1	D	201	VAL
1	D	202	THR
1	D	231	TRP
1	D	235	VAL
1	D	300	PHE
1	D	319	SER
1	D	330	ASN
1	D	350	GLU
1	D	359	LEU
1	D	363	SER
1	D	372	ILE
1	D	386	LEU
1	D	403	LEU
1	D	419	ARG
1	D	420	PRO
1	D	424	THR
1	D	506	THR
1	D	582	ARG
1	D	584	PRO
1	D	661	ALA
1	E	101	GLY
1	E	106	LYS
1	E	110	GLN
1	E	111	PHE
1	E	166	ASP
1	E	171	LYS
1	E	183	VAL
1	E	187	GLN
1	E	191	PRO
1	E	195	GLU
1	E	202	THR
1	E	231	TRP
1	E	235	VAL
1	E	273	LEU
1	E	300	PHE

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Mol	Chain	Res	Type
1	E	319	SER
1	E	330	ASN
1	E	350	GLU
1	E	359	LEU
1	E	372	ILE
1	E	403	LEU
1	E	419	ARG
1	E	420	PRO
1	E	424	THR
1	E	506	THR
1	E	582	ARG
1	E	584	PRO
1	E	661	ALA
1	F	101	GLY
1	F	106	LYS
1	F	110	GLN
1	F	111	PHE
1	F	166	ASP
1	F	171	LYS
1	F	183	VAL
1	F	187	GLN
1	F	191	PRO
1	F	195	GLU
1	F	201	VAL
1	F	202	THR
1	F	214	GLU
1	F	231	TRP
1	F	235	VAL
1	F	273	LEU
1	F	300	PHE
1	F	319	SER
1	F	330	ASN
1	F	350	GLU
1	F	359	LEU
1	F	372	ILE
1	F	403	LEU
1	F	419	ARG
1	F	420	PRO
1	F	424	THR
1	F	506	THR
1	F	582	ARG
1	F	584	PRO

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Mol	Chain	Res	Type
1	G	101	GLY
1	G	106	LYS
1	G	110	GLN
1	G	111	PHE
1	G	166	ASP
1	G	171	LYS
1	G	183	VAL
1	G	187	GLN
1	G	191	PRO
1	G	195	GLU
1	G	201	VAL
1	G	202	THR
1	G	231	TRP
1	G	235	VAL
1	G	273	LEU
1	G	300	PHE
1	G	319	SER
1	G	330	ASN
1	G	350	GLU
1	G	359	LEU
1	G	363	SER
1	G	372	ILE
1	G	403	LEU
1	G	419	ARG
1	G	420	PRO
1	G	424	THR
1	G	582	ARG
1	G	584	PRO
1	H	101	GLY
1	H	106	LYS
1	H	110	GLN
1	H	111	PHE
1	H	166	ASP
1	H	171	LYS
1	H	183	VAL
1	H	187	GLN
1	H	191	PRO
1	H	195	GLU
1	H	201	VAL
1	H	202	THR
1	H	231	TRP
1	H	235	VAL

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Mol	Chain	Res	Type
1	H	273	LEU
1	H	300	PHE
1	H	319	SER
1	H	330	ASN
1	H	350	GLU
1	H	359	LEU
1	H	372	ILE
1	H	403	LEU
1	H	419	ARG
1	H	420	PRO
1	H	424	THR
1	H	582	ARG
1	H	584	PRO
1	H	588	ASN
1	A	36	ASP
1	A	74	VAL
1	A	103	ASP
1	A	134	ARG
1	A	179	CYS
1	A	184	GLY
1	A	189	LEU
1	A	201	VAL
1	A	222	PHE
1	A	250	THR
1	A	251	GLY
1	A	273	LEU
1	A	298	GLY
1	A	308	SER
1	A	317	MET
1	A	363	SER
1	A	371	VAL
1	A	374	CYS
1	A	385	ASP
1	A	386	LEU
1	A	503	PHE
1	A	661	ALA
1	B	36	ASP
1	B	74	VAL
1	B	103	ASP
1	B	134	ARG
1	B	160	LEU
1	B	179	CYS

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Mol	Chain	Res	Type
1	B	184	GLY
1	B	189	LEU
1	B	214	GLU
1	B	222	PHE
1	B	250	THR
1	B	251	GLY
1	B	273	LEU
1	B	298	GLY
1	B	317	MET
1	B	320	GLY
1	B	321	ARG
1	B	371	VAL
1	B	374	CYS
1	B	385	ASP
1	B	386	LEU
1	B	476	CYS
1	B	588	ASN
1	C	36	ASP
1	C	74	VAL
1	C	85	LYS
1	C	134	ARG
1	C	160	LEU
1	C	179	CYS
1	C	184	GLY
1	C	214	GLU
1	C	222	PHE
1	C	230	GLN
1	C	250	THR
1	C	251	GLY
1	C	298	GLY
1	C	308	SER
1	C	317	MET
1	C	371	VAL
1	C	374	CYS
1	C	385	ASP
1	C	386	LEU
1	C	427	ARG
1	C	588	ASN
1	C	643	VAL
1	D	36	ASP
1	D	74	VAL
1	D	103	ASP

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Mol	Chain	Res	Type
1	D	134	ARG
1	D	160	LEU
1	D	179	CYS
1	D	184	GLY
1	D	189	LEU
1	D	213	PHE
1	D	214	GLU
1	D	222	PHE
1	D	250	THR
1	D	251	GLY
1	D	273	LEU
1	D	298	GLY
1	D	317	MET
1	D	320	GLY
1	D	321	ARG
1	D	371	VAL
1	D	374	CYS
1	D	385	ASP
1	D	528	ARG
1	D	588	ASN
1	D	643	VAL
1	E	36	ASP
1	E	74	VAL
1	E	103	ASP
1	E	134	ARG
1	E	160	LEU
1	E	179	CYS
1	E	184	GLY
1	E	189	LEU
1	E	201	VAL
1	E	214	GLU
1	E	222	PHE
1	E	250	THR
1	E	251	GLY
1	E	298	GLY
1	E	308	SER
1	E	317	MET
1	E	320	GLY
1	E	363	SER
1	E	371	VAL
1	E	374	CYS
1	E	385	ASP

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Mol	Chain	Res	Type
1	E	386	LEU
1	E	503	PHE
1	E	528	ARG
1	E	588	ASN
1	E	643	VAL
1	F	36	ASP
1	F	74	VAL
1	F	103	ASP
1	F	134	ARG
1	F	160	LEU
1	F	179	CYS
1	F	184	GLY
1	F	189	LEU
1	F	213	PHE
1	F	222	PHE
1	F	250	THR
1	F	251	GLY
1	F	298	GLY
1	F	308	SER
1	F	317	MET
1	F	320	GLY
1	F	363	SER
1	F	371	VAL
1	F	374	CYS
1	F	385	ASP
1	F	386	LEU
1	F	503	PHE
1	F	588	ASN
1	F	643	VAL
1	F	661	ALA
1	G	36	ASP
1	G	74	VAL
1	G	103	ASP
1	G	134	ARG
1	G	160	LEU
1	G	179	CYS
1	G	184	GLY
1	G	189	LEU
1	G	214	GLU
1	G	222	PHE
1	G	230	GLN
1	G	250	THR

Continued on next page...

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Mol	Chain	Res	Type
1	G	251	GLY
1	G	298	GLY
1	G	308	SER
1	G	317	MET
1	G	371	VAL
1	G	374	CYS
1	G	385	ASP
1	G	386	LEU
1	G	588	ASN
1	H	36	ASP
1	H	74	VAL
1	H	103	ASP
1	H	134	ARG
1	H	160	LEU
1	H	179	CYS
1	H	184	GLY
1	H	189	LEU
1	H	222	PHE
1	H	230	GLN
1	H	250	THR
1	H	251	GLY
1	H	298	GLY
1	H	308	SER
1	H	317	MET
1	H	363	SER
1	H	371	VAL
1	H	374	CYS
1	H	385	ASP
1	H	386	LEU
1	A	48	GLN
1	A	49	GLU
1	A	85	LYS
1	A	105	ARG
1	A	115	CYS
1	A	160	LEU
1	A	194	LEU
1	A	213	PHE
1	A	218	GLY
1	A	230	GLN
1	A	234	LYS
1	A	320	GLY
1	A	321	ARG

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Mol	Chain	Res	Type
1	A	333	LEU
1	A	348	GLU
1	A	364	ALA
1	A	409	SER
1	A	507	SER
1	A	508	GLU
1	A	530	VAL
1	A	550	ASN
1	A	583	THR
1	A	587	SER
1	A	597	ALA
1	A	643	VAL
1	B	48	GLN
1	B	49	GLU
1	B	85	LYS
1	B	105	ARG
1	B	115	CYS
1	B	194	LEU
1	B	213	PHE
1	B	218	GLY
1	B	230	GLN
1	B	234	LYS
1	B	308	SER
1	B	333	LEU
1	B	348	GLU
1	B	364	ALA
1	B	409	SER
1	B	427	ARG
1	B	450	GLY
1	B	489	SER
1	B	507	SER
1	B	508	GLU
1	B	530	VAL
1	B	550	ASN
1	B	583	THR
1	B	587	SER
1	B	597	ALA
1	B	643	VAL
1	C	48	GLN
1	C	49	GLU
1	C	103	ASP
1	C	105	ARG

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Mol	Chain	Res	Type
1	C	115	CYS
1	C	189	LEU
1	C	194	LEU
1	C	213	PHE
1	C	234	LYS
1	C	320	GLY
1	C	321	ARG
1	C	333	LEU
1	C	348	GLU
1	C	364	ALA
1	C	409	SER
1	C	450	GLY
1	C	483	LEU
1	C	489	SER
1	C	503	PHE
1	C	508	GLU
1	C	530	VAL
1	C	550	ASN
1	C	583	THR
1	C	587	SER
1	C	597	ALA
1	D	48	GLN
1	D	49	GLU
1	D	85	LYS
1	D	105	ARG
1	D	115	CYS
1	D	194	LEU
1	D	230	GLN
1	D	234	LYS
1	D	308	SER
1	D	333	LEU
1	D	348	GLU
1	D	364	ALA
1	D	409	SER
1	D	450	GLY
1	D	483	LEU
1	D	503	PHE
1	D	508	GLU
1	D	530	VAL
1	D	550	ASN
1	D	583	THR
1	D	587	SER

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Mol	Chain	Res	Type
1	D	597	ALA
1	E	48	GLN
1	E	49	GLU
1	E	85	LYS
1	E	115	CYS
1	E	194	LEU
1	E	213	PHE
1	E	230	GLN
1	E	234	LYS
1	E	321	ARG
1	E	333	LEU
1	E	348	GLU
1	E	364	ALA
1	E	409	SER
1	E	427	ARG
1	E	483	LEU
1	E	507	SER
1	E	508	GLU
1	E	530	VAL
1	E	550	ASN
1	E	583	THR
1	E	587	SER
1	F	49	GLU
1	F	85	LYS
1	F	105	ARG
1	F	115	CYS
1	F	194	LEU
1	F	218	GLY
1	F	230	GLN
1	F	234	LYS
1	F	321	ARG
1	F	333	LEU
1	F	348	GLU
1	F	364	ALA
1	F	409	SER
1	F	489	SER
1	F	507	SER
1	F	508	GLU
1	F	528	ARG
1	F	530	VAL
1	F	550	ASN
1	F	583	THR

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Mol	Chain	Res	Type
1	F	587	SER
1	G	48	GLN
1	G	49	GLU
1	G	85	LYS
1	G	194	LEU
1	G	213	PHE
1	G	218	GLY
1	G	234	LYS
1	G	320	GLY
1	G	321	ARG
1	G	333	LEU
1	G	348	GLU
1	G	409	SER
1	G	530	VAL
1	G	550	ASN
1	G	583	THR
1	G	587	SER
1	G	597	ALA
1	H	48	GLN
1	H	49	GLU
1	H	85	LYS
1	H	105	ARG
1	H	115	CYS
1	H	194	LEU
1	H	214	GLU
1	H	234	LYS
1	H	320	GLY
1	H	321	ARG
1	H	333	LEU
1	H	348	GLU
1	H	364	ALA
1	H	409	SER
1	H	427	ARG
1	H	450	GLY
1	H	530	VAL
1	H	550	ASN
1	H	583	THR
1	H	587	SER
1	H	597	ALA
1	A	121	PRO
1	A	144	ARG
1	A	199	TYR

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Mol	Chain	Res	Type
1	A	284	HIS
1	A	418	LYS
1	A	427	ARG
1	A	450	GLY
1	A	483	LEU
1	A	489	SER
1	A	549	ARG
1	A	629	VAL
1	B	121	PRO
1	B	144	ARG
1	B	199	TYR
1	B	284	HIS
1	B	309	LEU
1	B	418	LYS
1	B	503	PHE
1	B	549	ARG
1	B	629	VAL
1	C	78	GLU
1	C	121	PRO
1	C	144	ARG
1	C	218	GLY
1	C	284	HIS
1	C	418	LYS
1	C	507	SER
1	C	549	ARG
1	C	629	VAL
1	D	121	PRO
1	D	144	ARG
1	D	218	GLY
1	D	418	LYS
1	D	427	ARG
1	D	489	SER
1	D	507	SER
1	D	549	ARG
1	D	629	VAL
1	D	644	VAL
1	E	105	ARG
1	E	121	PRO
1	E	144	ARG
1	E	218	GLY
1	E	418	LYS
1	E	450	GLY

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Mol	Chain	Res	Type
1	E	489	SER
1	E	549	ARG
1	E	597	ALA
1	E	629	VAL
1	F	48	GLN
1	F	144	ARG
1	F	418	LYS
1	F	427	ARG
1	F	450	GLY
1	F	483	LEU
1	F	549	ARG
1	F	597	ALA
1	F	629	VAL
1	G	105	ARG
1	G	115	CYS
1	G	121	PRO
1	G	144	ARG
1	G	364	ALA
1	G	418	LYS
1	G	427	ARG
1	G	549	ARG
1	G	629	VAL
1	H	121	PRO
1	H	144	ARG
1	H	213	PHE
1	H	218	GLY
1	H	284	HIS
1	H	309	LEU
1	H	418	LYS
1	H	549	ARG
1	H	629	VAL
1	A	72	ASN
1	A	78	GLU
1	A	220	ARG
1	A	227	GLN
1	A	261	THR
1	A	309	LEU
1	A	445	ALA
1	A	644	VAL
1	B	72	ASN
1	B	78	GLU
1	B	220	ARG

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Mol	Chain	Res	Type
1	B	261	THR
1	B	388	PHE
1	B	483	LEU
1	B	644	VAL
1	C	72	ASN
1	C	220	ARG
1	C	261	THR
1	C	445	ALA
1	C	644	VAL
1	D	78	GLU
1	D	220	ARG
1	D	261	THR
1	D	284	HIS
1	D	309	LEU
1	D	388	PHE
1	D	445	ALA
1	E	35	GLN
1	E	78	GLU
1	E	220	ARG
1	E	261	THR
1	E	284	HIS
1	E	644	VAL
1	F	78	GLU
1	F	121	PRO
1	F	199	TYR
1	F	220	ARG
1	F	261	THR
1	F	284	HIS
1	F	388	PHE
1	F	431	GLY
1	F	445	ALA
1	F	644	VAL
1	G	72	ASN
1	G	78	GLU
1	G	193	LEU
1	G	220	ARG
1	G	227	GLN
1	G	261	THR
1	G	284	HIS
1	G	309	LEU
1	G	450	GLY
1	H	78	GLU

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Mol	Chain	Res	Type
1	H	220	ARG
1	H	261	THR
1	H	431	GLY
1	H	445	ALA
1	A	35	GLN
1	A	388	PHE
1	A	431	GLY
1	A	626	SER
1	A	665	VAL
1	B	227	GLN
1	B	431	GLY
1	B	577	ARG
1	B	626	SER
1	B	665	VAL
1	C	193	LEU
1	C	199	TYR
1	C	227	GLN
1	C	388	PHE
1	C	431	GLY
1	C	577	ARG
1	C	626	SER
1	C	665	VAL
1	D	199	TYR
1	D	227	GLN
1	D	626	SER
1	D	665	VAL
1	E	72	ASN
1	E	431	GLY
1	E	445	ALA
1	E	577	ARG
1	E	626	SER
1	E	665	VAL
1	F	72	ASN
1	F	227	GLN
1	F	626	SER
1	F	665	VAL
1	G	388	PHE
1	G	577	ARG
1	H	72	ASN
1	H	199	TYR
1	A	407	PRO
1	A	577	ARG

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Mol	Chain	Res	Type
1	D	407	PRO
1	D	431	GLY
1	F	577	ARG
1	G	407	PRO
1	G	431	GLY
1	G	626	SER
1	H	227	GLN
1	H	407	PRO
1	H	577	ARG
1	H	626	SER
1	B	165	ILE
1	B	407	PRO
1	C	407	PRO
1	D	165	ILE
1	D	577	ARG
1	E	227	GLN
1	E	407	PRO
1	F	165	ILE
1	F	407	PRO
1	A	165	ILE
1	B	387	ILE
1	C	165	ILE
1	E	165	ILE
1	F	387	ILE
1	G	165	ILE
1	H	165	ILE
1	B	260	PRO
1	D	260	PRO
1	D	295	PRO
1	D	387	ILE
1	E	295	PRO
1	E	387	ILE
1	F	260	PRO
1	F	295	PRO
1	G	260	PRO
1	H	260	PRO
1	H	295	PRO
1	A	260	PRO
1	A	295	PRO
1	B	295	PRO
1	C	260	PRO
1	C	295	PRO

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Mol	Chain	Res	Type
1	H	387	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	563/609 (92%)	520 (92%)	43 (8%)	19	66
1	B	563/609 (92%)	521 (92%)	42 (8%)	19	67
1	C	563/609 (92%)	520 (92%)	43 (8%)	19	66
1	D	563/609 (92%)	519 (92%)	44 (8%)	18	65
1	E	563/609 (92%)	520 (92%)	43 (8%)	19	66
1	F	563/609 (92%)	521 (92%)	42 (8%)	19	67
1	G	488/609 (80%)	456 (93%)	32 (7%)	24	73
1	H	488/609 (80%)	455 (93%)	33 (7%)	22	71
All	All	4354/4872 (89%)	4032 (93%)	322 (7%)	20	67

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	51	SER
1	A	114	CYS
1	A	123	ARG
1	A	134	ARG
1	A	145	ASP
1	A	150	ASN
1	A	210	THR
1	A	234	LYS
1	A	248	ASP
1	A	263	ASN
1	A	266	SER
1	A	278	GLN
1	A	301	GLN
1	A	313	SER
1	A	314	VAL

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Mol	Chain	Res	Type
1	A	330	ASN
1	A	357	SER
1	A	390	PHE
1	A	408	GLU
1	A	422	THR
1	A	424	THR
1	A	429	VAL
1	A	434	TRP
1	A	436	THR
1	A	444	CYS
1	A	448	LEU
1	A	453	THR
1	A	455	MET
1	A	479	LEU
1	A	490	ILE
1	A	494	LEU
1	A	497	TYR
1	A	505	ILE
1	A	517	MET
1	A	535	ASP
1	A	564	GLU
1	A	590	MET
1	A	610	ASP
1	A	616	VAL
1	A	654	LEU
1	A	659	LYS
1	A	662	CYS
1	B	16	GLU
1	B	51	SER
1	B	114	CYS
1	B	123	ARG
1	B	134	ARG
1	B	145	ASP
1	B	150	ASN
1	B	210	THR
1	B	234	LYS
1	B	248	ASP
1	B	263	ASN
1	B	266	SER
1	B	278	GLN
1	B	301	GLN
1	B	313	SER

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Mol	Chain	Res	Type
1	B	330	ASN
1	B	339	TRP
1	B	357	SER
1	B	390	PHE
1	B	408	GLU
1	B	422	THR
1	B	424	THR
1	B	429	VAL
1	B	434	TRP
1	B	436	THR
1	B	444	CYS
1	B	448	LEU
1	B	453	THR
1	B	455	MET
1	B	479	LEU
1	B	490	ILE
1	B	494	LEU
1	B	497	TYR
1	B	505	ILE
1	B	517	MET
1	B	535	ASP
1	B	564	GLU
1	B	590	MET
1	B	616	VAL
1	B	654	LEU
1	B	659	LYS
1	B	662	CYS
1	C	16	GLU
1	C	51	SER
1	C	114	CYS
1	C	123	ARG
1	C	134	ARG
1	C	145	ASP
1	C	150	ASN
1	C	210	THR
1	C	234	LYS
1	C	248	ASP
1	C	263	ASN
1	C	266	SER
1	C	278	GLN
1	C	301	GLN
1	C	313	SER

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Mol	Chain	Res	Type
1	C	314	VAL
1	C	330	ASN
1	C	357	SER
1	C	390	PHE
1	C	408	GLU
1	C	422	THR
1	C	424	THR
1	C	429	VAL
1	C	434	TRP
1	C	436	THR
1	C	444	CYS
1	C	448	LEU
1	C	453	THR
1	C	455	MET
1	C	479	LEU
1	C	490	ILE
1	C	497	TYR
1	C	505	ILE
1	C	517	MET
1	C	564	GLU
1	C	590	MET
1	C	602	GLU
1	C	606	ILE
1	C	610	ASP
1	C	616	VAL
1	C	654	LEU
1	C	659	LYS
1	C	662	CYS
1	D	16	GLU
1	D	51	SER
1	D	114	CYS
1	D	123	ARG
1	D	134	ARG
1	D	145	ASP
1	D	150	ASN
1	D	210	THR
1	D	219	PHE
1	D	234	LYS
1	D	248	ASP
1	D	263	ASN
1	D	266	SER
1	D	278	GLN

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Mol	Chain	Res	Type
1	D	301	GLN
1	D	313	SER
1	D	330	ASN
1	D	339	TRP
1	D	357	SER
1	D	390	PHE
1	D	408	GLU
1	D	422	THR
1	D	424	THR
1	D	429	VAL
1	D	434	TRP
1	D	436	THR
1	D	444	CYS
1	D	448	LEU
1	D	453	THR
1	D	455	MET
1	D	479	LEU
1	D	490	ILE
1	D	494	LEU
1	D	497	TYR
1	D	505	ILE
1	D	517	MET
1	D	564	GLU
1	D	590	MET
1	D	602	GLU
1	D	610	ASP
1	D	616	VAL
1	D	654	LEU
1	D	659	LYS
1	D	662	CYS
1	E	16	GLU
1	E	51	SER
1	E	114	CYS
1	E	123	ARG
1	E	134	ARG
1	E	145	ASP
1	E	150	ASN
1	E	210	THR
1	E	219	PHE
1	E	234	LYS
1	E	248	ASP
1	E	263	ASN

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Mol	Chain	Res	Type
1	E	266	SER
1	E	278	GLN
1	E	301	GLN
1	E	313	SER
1	E	314	VAL
1	E	330	ASN
1	E	357	SER
1	E	390	PHE
1	E	408	GLU
1	E	422	THR
1	E	424	THR
1	E	429	VAL
1	E	434	TRP
1	E	436	THR
1	E	444	CYS
1	E	448	LEU
1	E	453	THR
1	E	455	MET
1	E	479	LEU
1	E	490	ILE
1	E	497	TYR
1	E	505	ILE
1	E	517	MET
1	E	564	GLU
1	E	590	MET
1	E	606	ILE
1	E	610	ASP
1	E	616	VAL
1	E	654	LEU
1	E	659	LYS
1	E	662	CYS
1	F	16	GLU
1	F	51	SER
1	F	114	CYS
1	F	123	ARG
1	F	134	ARG
1	F	145	ASP
1	F	150	ASN
1	F	210	THR
1	F	219	PHE
1	F	234	LYS
1	F	248	ASP

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Mol	Chain	Res	Type
1	F	263	ASN
1	F	266	SER
1	F	278	GLN
1	F	301	GLN
1	F	313	SER
1	F	330	ASN
1	F	339	TRP
1	F	357	SER
1	F	390	PHE
1	F	408	GLU
1	F	422	THR
1	F	424	THR
1	F	429	VAL
1	F	434	TRP
1	F	444	CYS
1	F	448	LEU
1	F	453	THR
1	F	455	MET
1	F	479	LEU
1	F	490	ILE
1	F	497	TYR
1	F	505	ILE
1	F	517	MET
1	F	564	GLU
1	F	590	MET
1	F	602	GLU
1	F	610	ASP
1	F	616	VAL
1	F	654	LEU
1	F	659	LYS
1	F	662	CYS
1	G	16	GLU
1	G	51	SER
1	G	114	CYS
1	G	123	ARG
1	G	134	ARG
1	G	145	ASP
1	G	150	ASN
1	G	210	THR
1	G	234	LYS
1	G	248	ASP
1	G	263	ASN

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Mol	Chain	Res	Type
1	G	266	SER
1	G	278	GLN
1	G	301	GLN
1	G	313	SER
1	G	330	ASN
1	G	357	SER
1	G	390	PHE
1	G	408	GLU
1	G	422	THR
1	G	424	THR
1	G	429	VAL
1	G	434	TRP
1	G	444	CYS
1	G	448	LEU
1	G	453	THR
1	G	455	MET
1	G	564	GLU
1	G	590	MET
1	G	602	GLU
1	G	610	ASP
1	G	616	VAL
1	H	16	GLU
1	H	51	SER
1	H	114	CYS
1	H	123	ARG
1	H	134	ARG
1	H	145	ASP
1	H	150	ASN
1	H	210	THR
1	H	234	LYS
1	H	248	ASP
1	H	263	ASN
1	H	266	SER
1	H	278	GLN
1	H	301	GLN
1	H	313	SER
1	H	330	ASN
1	H	339	TRP
1	H	357	SER
1	H	390	PHE
1	H	408	GLU
1	H	422	THR

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Mol	Chain	Res	Type
1	H	424	THR
1	H	429	VAL
1	H	434	TRP
1	H	436	THR
1	H	444	CYS
1	H	448	LEU
1	H	453	THR
1	H	455	MET
1	H	535	ASP
1	H	564	GLU
1	H	590	MET
1	H	616	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	622/676 (92%)	0.24	22 (3%) 42 23	76, 189, 275, 337	0
1	B	622/676 (92%)	0.14	11 (1%) 65 39	71, 191, 274, 336	0
1	C	622/676 (92%)	0.22	6 (0%) 79 53	58, 188, 275, 327	0
1	D	622/676 (92%)	0.14	24 (3%) 37 21	85, 194, 278, 327	0
1	E	622/676 (92%)	0.21	12 (1%) 64 37	74, 190, 274, 330	0
1	F	622/676 (92%)	0.26	35 (5%) 24 13	93, 200, 283, 331	0
1	G	541/676 (80%)	0.36	34 (6%) 19 11	96, 214, 302, 387	0
1	H	541/676 (80%)	0.27	19 (3%) 42 23	79, 194, 293, 423	0
All	All	4814/5408 (89%)	0.23	163 (3%) 43 24	58, 195, 283, 423	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	537	MET	7.8
1	A	65	MET	7.0
1	A	93	LEU	6.9
1	F	155	PRO	6.4
1	G	571	TYR	6.3
1	D	65	MET	6.2
1	G	65	MET	5.6
1	G	236	ARG	5.5
1	F	510	LEU	5.2
1	F	157	PRO	5.1
1	F	65	MET	4.9
1	A	172	GLU	4.8
1	H	528	ARG	4.8
1	A	236	ARG	4.7
1	D	93	LEU	4.6
1	H	65	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	87	ALA	4.1
1	H	571	TYR	4.0
1	G	46	CYS	4.0
1	G	360	ALA	3.9
1	G	47	ARG	3.9
1	H	47	ARG	3.8
1	F	93	LEU	3.8
1	D	654	LEU	3.7
1	F	497	TYR	3.7
1	F	158	GLN	3.6
1	B	666	ARG	3.5
1	F	571	TYR	3.5
1	G	93	LEU	3.5
1	F	298	GLY	3.5
1	D	236	ARG	3.5
1	E	61	GLU	3.4
1	H	388	PHE	3.3
1	A	506	THR	3.3
1	E	199	TYR	3.3
1	A	86	LEU	3.3
1	A	143	HIS	3.3
1	G	327	VAL	3.3
1	F	88	PRO	3.3
1	H	533	LEU	3.1
1	B	353	LEU	3.1
1	F	87	ALA	3.1
1	H	159	ARG	3.1
1	F	61	GLU	3.1
1	F	73	VAL	3.1
1	G	389	LEU	3.1
1	A	88	PRO	3.1
1	A	87	ALA	3.0
1	H	61	GLU	3.0
1	A	141	ILE	3.0
1	E	17	MET	3.0
1	G	535	ASP	3.0
1	H	37	THR	2.9
1	D	625	LEU	2.9
1	H	541	GLN	2.9
1	G	353	LEU	2.9
1	E	47	ARG	2.9
1	A	367	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	354	LEU	2.9
1	E	160	LEU	2.8
1	F	156	GLY	2.8
1	C	88	PRO	2.8
1	G	390	PHE	2.8
1	F	591	VAL	2.8
1	F	40	GLN	2.8
1	G	62	ILE	2.8
1	D	164	ILE	2.8
1	A	175	GLN	2.8
1	G	548	GLN	2.7
1	B	310	LYS	2.7
1	D	94	LEU	2.7
1	G	528	ARG	2.7
1	D	117	LEU	2.7
1	B	143	HIS	2.7
1	F	590	MET	2.7
1	G	45	GLN	2.7
1	H	96	MET	2.6
1	H	544	SER	2.6
1	F	175	GLN	2.6
1	C	89	ASN	2.6
1	G	404	PRO	2.6
1	A	503	PHE	2.6
1	F	176	GLY	2.6
1	G	407	PRO	2.6
1	E	167	LEU	2.5
1	F	299	CYS	2.5
1	A	41	VAL	2.5
1	D	17	MET	2.5
1	G	469	LYS	2.5
1	A	176	GLY	2.5
1	D	85	LYS	2.5
1	A	170	ALA	2.4
1	G	168	GLY	2.4
1	G	406	HIS	2.4
1	D	166	ASP	2.4
1	F	394	LYS	2.4
1	G	531	GLN	2.4
1	F	41	VAL	2.4
1	C	93	LEU	2.4
1	A	171	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	401	ILE	2.4
1	F	236	ARG	2.4
1	E	571	TYR	2.4
1	F	172	GLU	2.4
1	E	384	GLY	2.4
1	H	153	LEU	2.4
1	B	327	VAL	2.4
1	G	393	ARG	2.4
1	D	437	ILE	2.4
1	G	437	ILE	2.4
1	D	21	LEU	2.4
1	G	549	ARG	2.4
1	H	88	PRO	2.3
1	D	60	LEU	2.3
1	E	198	LYS	2.3
1	G	370	TYR	2.3
1	G	61	GLU	2.3
1	F	54	ASN	2.3
1	E	244	VAL	2.3
1	G	63	GLN	2.3
1	D	62	ILE	2.3
1	D	141	ILE	2.3
1	B	571	TYR	2.3
1	H	38	GLY	2.3
1	C	244	VAL	2.3
1	G	166	ASP	2.3
1	D	510	LEU	2.2
1	F	74	VAL	2.2
1	B	146	LEU	2.2
1	B	68	LEU	2.2
1	B	394	LYS	2.2
1	H	39	GLU	2.2
1	H	461	TYR	2.2
1	D	215	CYS	2.2
1	G	388	PHE	2.2
1	C	96	MET	2.2
1	D	197	LYS	2.2
1	A	61	GLU	2.2
1	D	208	PHE	2.2
1	A	536	LYS	2.1
1	D	571	TYR	2.1
1	A	507	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	199	TYR	2.1
1	H	31	ARG	2.1
1	D	80	PRO	2.1
1	B	164	ILE	2.1
1	C	279	CYS	2.1
1	G	538	MET	2.1
1	F	32	TRP	2.1
1	F	549	ARG	2.1
1	A	327	VAL	2.1
1	E	175	GLN	2.1
1	G	592	ARG	2.1
1	D	388	PHE	2.1
1	F	653	GLU	2.0
1	F	164	ILE	2.0
1	G	603	LYS	2.0
1	F	205	TYR	2.0
1	F	286	ARG	2.0
1	F	654	LEU	2.0
1	E	393	ARG	2.0
1	A	548	GLN	2.0
1	F	593	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.