Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 09:57 AM EDT

PDB ID	:	5UDD
Title	:	Crystal Structure of RSV F B9320 Bound to MEDI8897
Authors	:	McLellan, J.S.
Deposited on	:	2016-12-26
Resolution	:	4.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

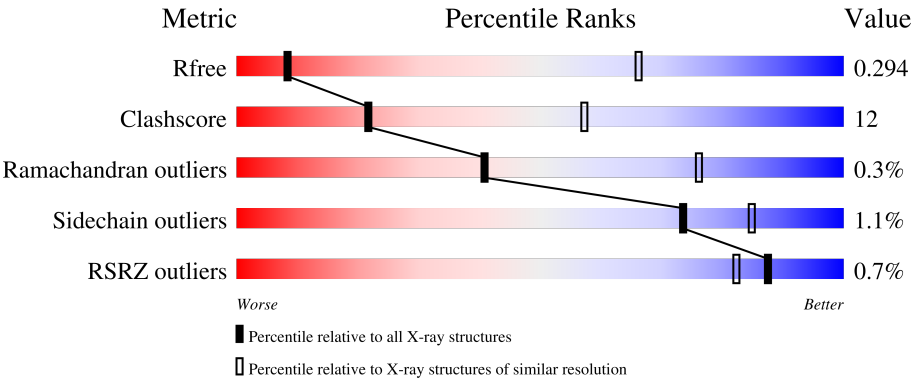
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	568	57% 23% 21%
1	B	568	55% 24% · 20%
1	C	568	55% 23% · 21%
1	D	568	57% 23% 20%
1	E	568	55% 23% · 21%

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Mol	Chain	Length	Quality of chain
1	F	568	52% 27% 20%
1	G	568	54% 26% 20%
1	H	568	56% 23% 21%
1	I	568	54% 25% 21%
2	J	228	72% 26%
2	K	228	% 75% 21%
2	L	228	73% 23%
2	M	228	76% 21%
2	N	228	81% 16%
2	O	228	4% 71% 24% 5%
3	P	214	79% 20%
3	Q	214	5% 77% 21%
3	R	214	77% 21%
3	S	214	74% 24%
3	T	214	79% 19%
3	U	214	9% 83% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	D	601	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 51201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3489	2201	578	688	22			
1	B	452	Total	C	N	O	S	0	0	0
			3511	2216	581	692	22			
1	C	450	Total	C	N	O	S	0	0	0
			3497	2208	578	689	22			
1	D	455	Total	C	N	O	S	0	0	0
			3532	2229	585	696	22			
1	E	451	Total	C	N	O	S	0	0	0
			3506	2213	580	691	22			
1	F	452	Total	C	N	O	S	0	0	0
			3515	2218	582	693	22			
1	G	453	Total	C	N	O	S	0	0	0
			3518	2221	582	693	22			
1	H	451	Total	C	N	O	S	0	0	0
			3502	2211	579	690	22			
1	I	448	Total	C	N	O	S	0	0	0
			3483	2199	576	686	22			

There are 531 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	CYS	SER	engineered mutation	UNP Q6V2E7
A	190	PHE	SER	engineered mutation	UNP Q6V2E7
A	207	LEU	VAL	engineered mutation	UNP Q6V2E7
A	290	CYS	SER	engineered mutation	UNP Q6V2E7
A	514	SER	-	expression tag	UNP Q6V2E7
A	515	ALA	-	expression tag	UNP Q6V2E7
A	516	ILE	-	expression tag	UNP Q6V2E7
A	517	GLY	-	expression tag	UNP Q6V2E7
A	518	GLY	-	expression tag	UNP Q6V2E7
A	519	TYR	-	expression tag	UNP Q6V2E7
A	520	ILE	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	521	PRO	-	expression tag	UNP Q6V2E7
A	522	GLU	-	expression tag	UNP Q6V2E7
A	523	ALA	-	expression tag	UNP Q6V2E7
A	524	PRO	-	expression tag	UNP Q6V2E7
A	525	ARG	-	expression tag	UNP Q6V2E7
A	526	ASP	-	expression tag	UNP Q6V2E7
A	527	GLY	-	expression tag	UNP Q6V2E7
A	528	GLN	-	expression tag	UNP Q6V2E7
A	529	ALA	-	expression tag	UNP Q6V2E7
A	530	TYR	-	expression tag	UNP Q6V2E7
A	531	VAL	-	expression tag	UNP Q6V2E7
A	532	ARG	-	expression tag	UNP Q6V2E7
A	533	LYS	-	expression tag	UNP Q6V2E7
A	534	ASP	-	expression tag	UNP Q6V2E7
A	535	GLY	-	expression tag	UNP Q6V2E7
A	536	GLU	-	expression tag	UNP Q6V2E7
A	537	TRP	-	expression tag	UNP Q6V2E7
A	538	VAL	-	expression tag	UNP Q6V2E7
A	539	LEU	-	expression tag	UNP Q6V2E7
A	540	LEU	-	expression tag	UNP Q6V2E7
A	541	SER	-	expression tag	UNP Q6V2E7
A	542	THR	-	expression tag	UNP Q6V2E7
A	543	PHE	-	expression tag	UNP Q6V2E7
A	544	LEU	-	expression tag	UNP Q6V2E7
A	545	GLY	-	expression tag	UNP Q6V2E7
A	546	GLY	-	expression tag	UNP Q6V2E7
A	547	LEU	-	expression tag	UNP Q6V2E7
A	548	VAL	-	expression tag	UNP Q6V2E7
A	549	PRO	-	expression tag	UNP Q6V2E7
A	550	ARG	-	expression tag	UNP Q6V2E7
A	551	GLY	-	expression tag	UNP Q6V2E7
A	552	SER	-	expression tag	UNP Q6V2E7
A	553	HIS	-	expression tag	UNP Q6V2E7
A	554	HIS	-	expression tag	UNP Q6V2E7
A	555	HIS	-	expression tag	UNP Q6V2E7
A	556	HIS	-	expression tag	UNP Q6V2E7
A	557	HIS	-	expression tag	UNP Q6V2E7
A	558	HIS	-	expression tag	UNP Q6V2E7
A	559	SER	-	expression tag	UNP Q6V2E7
A	560	ALA	-	expression tag	UNP Q6V2E7
A	561	TRP	-	expression tag	UNP Q6V2E7
A	562	SER	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	563	HIS	-	expression tag	UNP Q6V2E7
A	564	PRO	-	expression tag	UNP Q6V2E7
A	565	GLN	-	expression tag	UNP Q6V2E7
A	566	PHE	-	expression tag	UNP Q6V2E7
A	567	GLU	-	expression tag	UNP Q6V2E7
A	568	LYS	-	expression tag	UNP Q6V2E7
B	155	CYS	SER	engineered mutation	UNP Q6V2E7
B	190	PHE	SER	engineered mutation	UNP Q6V2E7
B	207	LEU	VAL	engineered mutation	UNP Q6V2E7
B	290	CYS	SER	engineered mutation	UNP Q6V2E7
B	514	SER	-	expression tag	UNP Q6V2E7
B	515	ALA	-	expression tag	UNP Q6V2E7
B	516	ILE	-	expression tag	UNP Q6V2E7
B	517	GLY	-	expression tag	UNP Q6V2E7
B	518	GLY	-	expression tag	UNP Q6V2E7
B	519	TYR	-	expression tag	UNP Q6V2E7
B	520	ILE	-	expression tag	UNP Q6V2E7
B	521	PRO	-	expression tag	UNP Q6V2E7
B	522	GLU	-	expression tag	UNP Q6V2E7
B	523	ALA	-	expression tag	UNP Q6V2E7
B	524	PRO	-	expression tag	UNP Q6V2E7
B	525	ARG	-	expression tag	UNP Q6V2E7
B	526	ASP	-	expression tag	UNP Q6V2E7
B	527	GLY	-	expression tag	UNP Q6V2E7
B	528	GLN	-	expression tag	UNP Q6V2E7
B	529	ALA	-	expression tag	UNP Q6V2E7
B	530	TYR	-	expression tag	UNP Q6V2E7
B	531	VAL	-	expression tag	UNP Q6V2E7
B	532	ARG	-	expression tag	UNP Q6V2E7
B	533	LYS	-	expression tag	UNP Q6V2E7
B	534	ASP	-	expression tag	UNP Q6V2E7
B	535	GLY	-	expression tag	UNP Q6V2E7
B	536	GLU	-	expression tag	UNP Q6V2E7
B	537	TRP	-	expression tag	UNP Q6V2E7
B	538	VAL	-	expression tag	UNP Q6V2E7
B	539	LEU	-	expression tag	UNP Q6V2E7
B	540	LEU	-	expression tag	UNP Q6V2E7
B	541	SER	-	expression tag	UNP Q6V2E7
B	542	THR	-	expression tag	UNP Q6V2E7
B	543	PHE	-	expression tag	UNP Q6V2E7
B	544	LEU	-	expression tag	UNP Q6V2E7
B	545	GLY	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLY	-	expression tag	UNP Q6V2E7
B	547	LEU	-	expression tag	UNP Q6V2E7
B	548	VAL	-	expression tag	UNP Q6V2E7
B	549	PRO	-	expression tag	UNP Q6V2E7
B	550	ARG	-	expression tag	UNP Q6V2E7
B	551	GLY	-	expression tag	UNP Q6V2E7
B	552	SER	-	expression tag	UNP Q6V2E7
B	553	HIS	-	expression tag	UNP Q6V2E7
B	554	HIS	-	expression tag	UNP Q6V2E7
B	555	HIS	-	expression tag	UNP Q6V2E7
B	556	HIS	-	expression tag	UNP Q6V2E7
B	557	HIS	-	expression tag	UNP Q6V2E7
B	558	HIS	-	expression tag	UNP Q6V2E7
B	559	SER	-	expression tag	UNP Q6V2E7
B	560	ALA	-	expression tag	UNP Q6V2E7
B	561	TRP	-	expression tag	UNP Q6V2E7
B	562	SER	-	expression tag	UNP Q6V2E7
B	563	HIS	-	expression tag	UNP Q6V2E7
B	564	PRO	-	expression tag	UNP Q6V2E7
B	565	GLN	-	expression tag	UNP Q6V2E7
B	566	PHE	-	expression tag	UNP Q6V2E7
B	567	GLU	-	expression tag	UNP Q6V2E7
B	568	LYS	-	expression tag	UNP Q6V2E7
C	155	CYS	SER	engineered mutation	UNP Q6V2E7
C	190	PHE	SER	engineered mutation	UNP Q6V2E7
C	207	LEU	VAL	engineered mutation	UNP Q6V2E7
C	290	CYS	SER	engineered mutation	UNP Q6V2E7
C	514	SER	-	expression tag	UNP Q6V2E7
C	515	ALA	-	expression tag	UNP Q6V2E7
C	516	ILE	-	expression tag	UNP Q6V2E7
C	517	GLY	-	expression tag	UNP Q6V2E7
C	518	GLY	-	expression tag	UNP Q6V2E7
C	519	TYR	-	expression tag	UNP Q6V2E7
C	520	ILE	-	expression tag	UNP Q6V2E7
C	521	PRO	-	expression tag	UNP Q6V2E7
C	522	GLU	-	expression tag	UNP Q6V2E7
C	523	ALA	-	expression tag	UNP Q6V2E7
C	524	PRO	-	expression tag	UNP Q6V2E7
C	525	ARG	-	expression tag	UNP Q6V2E7
C	526	ASP	-	expression tag	UNP Q6V2E7
C	527	GLY	-	expression tag	UNP Q6V2E7
C	528	GLN	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	529	ALA	-	expression tag	UNP Q6V2E7
C	530	TYR	-	expression tag	UNP Q6V2E7
C	531	VAL	-	expression tag	UNP Q6V2E7
C	532	ARG	-	expression tag	UNP Q6V2E7
C	533	LYS	-	expression tag	UNP Q6V2E7
C	534	ASP	-	expression tag	UNP Q6V2E7
C	535	GLY	-	expression tag	UNP Q6V2E7
C	536	GLU	-	expression tag	UNP Q6V2E7
C	537	TRP	-	expression tag	UNP Q6V2E7
C	538	VAL	-	expression tag	UNP Q6V2E7
C	539	LEU	-	expression tag	UNP Q6V2E7
C	540	LEU	-	expression tag	UNP Q6V2E7
C	541	SER	-	expression tag	UNP Q6V2E7
C	542	THR	-	expression tag	UNP Q6V2E7
C	543	PHE	-	expression tag	UNP Q6V2E7
C	544	LEU	-	expression tag	UNP Q6V2E7
C	545	GLY	-	expression tag	UNP Q6V2E7
C	546	GLY	-	expression tag	UNP Q6V2E7
C	547	LEU	-	expression tag	UNP Q6V2E7
C	548	VAL	-	expression tag	UNP Q6V2E7
C	549	PRO	-	expression tag	UNP Q6V2E7
C	550	ARG	-	expression tag	UNP Q6V2E7
C	551	GLY	-	expression tag	UNP Q6V2E7
C	552	SER	-	expression tag	UNP Q6V2E7
C	553	HIS	-	expression tag	UNP Q6V2E7
C	554	HIS	-	expression tag	UNP Q6V2E7
C	555	HIS	-	expression tag	UNP Q6V2E7
C	556	HIS	-	expression tag	UNP Q6V2E7
C	557	HIS	-	expression tag	UNP Q6V2E7
C	558	HIS	-	expression tag	UNP Q6V2E7
C	559	SER	-	expression tag	UNP Q6V2E7
C	560	ALA	-	expression tag	UNP Q6V2E7
C	561	TRP	-	expression tag	UNP Q6V2E7
C	562	SER	-	expression tag	UNP Q6V2E7
C	563	HIS	-	expression tag	UNP Q6V2E7
C	564	PRO	-	expression tag	UNP Q6V2E7
C	565	GLN	-	expression tag	UNP Q6V2E7
C	566	PHE	-	expression tag	UNP Q6V2E7
C	567	GLU	-	expression tag	UNP Q6V2E7
C	568	LYS	-	expression tag	UNP Q6V2E7
D	155	CYS	SER	engineered mutation	UNP Q6V2E7
D	190	PHE	SER	engineered mutation	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	207	LEU	VAL	engineered mutation	UNP Q6V2E7
D	290	CYS	SER	engineered mutation	UNP Q6V2E7
D	514	SER	-	expression tag	UNP Q6V2E7
D	515	ALA	-	expression tag	UNP Q6V2E7
D	516	ILE	-	expression tag	UNP Q6V2E7
D	517	GLY	-	expression tag	UNP Q6V2E7
D	518	GLY	-	expression tag	UNP Q6V2E7
D	519	TYR	-	expression tag	UNP Q6V2E7
D	520	ILE	-	expression tag	UNP Q6V2E7
D	521	PRO	-	expression tag	UNP Q6V2E7
D	522	GLU	-	expression tag	UNP Q6V2E7
D	523	ALA	-	expression tag	UNP Q6V2E7
D	524	PRO	-	expression tag	UNP Q6V2E7
D	525	ARG	-	expression tag	UNP Q6V2E7
D	526	ASP	-	expression tag	UNP Q6V2E7
D	527	GLY	-	expression tag	UNP Q6V2E7
D	528	GLN	-	expression tag	UNP Q6V2E7
D	529	ALA	-	expression tag	UNP Q6V2E7
D	530	TYR	-	expression tag	UNP Q6V2E7
D	531	VAL	-	expression tag	UNP Q6V2E7
D	532	ARG	-	expression tag	UNP Q6V2E7
D	533	LYS	-	expression tag	UNP Q6V2E7
D	534	ASP	-	expression tag	UNP Q6V2E7
D	535	GLY	-	expression tag	UNP Q6V2E7
D	536	GLU	-	expression tag	UNP Q6V2E7
D	537	TRP	-	expression tag	UNP Q6V2E7
D	538	VAL	-	expression tag	UNP Q6V2E7
D	539	LEU	-	expression tag	UNP Q6V2E7
D	540	LEU	-	expression tag	UNP Q6V2E7
D	541	SER	-	expression tag	UNP Q6V2E7
D	542	THR	-	expression tag	UNP Q6V2E7
D	543	PHE	-	expression tag	UNP Q6V2E7
D	544	LEU	-	expression tag	UNP Q6V2E7
D	545	GLY	-	expression tag	UNP Q6V2E7
D	546	GLY	-	expression tag	UNP Q6V2E7
D	547	LEU	-	expression tag	UNP Q6V2E7
D	548	VAL	-	expression tag	UNP Q6V2E7
D	549	PRO	-	expression tag	UNP Q6V2E7
D	550	ARG	-	expression tag	UNP Q6V2E7
D	551	GLY	-	expression tag	UNP Q6V2E7
D	552	SER	-	expression tag	UNP Q6V2E7
D	553	HIS	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	554	HIS	-	expression tag	UNP Q6V2E7
D	555	HIS	-	expression tag	UNP Q6V2E7
D	556	HIS	-	expression tag	UNP Q6V2E7
D	557	HIS	-	expression tag	UNP Q6V2E7
D	558	HIS	-	expression tag	UNP Q6V2E7
D	559	SER	-	expression tag	UNP Q6V2E7
D	560	ALA	-	expression tag	UNP Q6V2E7
D	561	TRP	-	expression tag	UNP Q6V2E7
D	562	SER	-	expression tag	UNP Q6V2E7
D	563	HIS	-	expression tag	UNP Q6V2E7
D	564	PRO	-	expression tag	UNP Q6V2E7
D	565	GLN	-	expression tag	UNP Q6V2E7
D	566	PHE	-	expression tag	UNP Q6V2E7
D	567	GLU	-	expression tag	UNP Q6V2E7
D	568	LYS	-	expression tag	UNP Q6V2E7
E	155	CYS	SER	engineered mutation	UNP Q6V2E7
E	190	PHE	SER	engineered mutation	UNP Q6V2E7
E	207	LEU	VAL	engineered mutation	UNP Q6V2E7
E	290	CYS	SER	engineered mutation	UNP Q6V2E7
E	514	SER	-	expression tag	UNP Q6V2E7
E	515	ALA	-	expression tag	UNP Q6V2E7
E	516	ILE	-	expression tag	UNP Q6V2E7
E	517	GLY	-	expression tag	UNP Q6V2E7
E	518	GLY	-	expression tag	UNP Q6V2E7
E	519	TYR	-	expression tag	UNP Q6V2E7
E	520	ILE	-	expression tag	UNP Q6V2E7
E	521	PRO	-	expression tag	UNP Q6V2E7
E	522	GLU	-	expression tag	UNP Q6V2E7
E	523	ALA	-	expression tag	UNP Q6V2E7
E	524	PRO	-	expression tag	UNP Q6V2E7
E	525	ARG	-	expression tag	UNP Q6V2E7
E	526	ASP	-	expression tag	UNP Q6V2E7
E	527	GLY	-	expression tag	UNP Q6V2E7
E	528	GLN	-	expression tag	UNP Q6V2E7
E	529	ALA	-	expression tag	UNP Q6V2E7
E	530	TYR	-	expression tag	UNP Q6V2E7
E	531	VAL	-	expression tag	UNP Q6V2E7
E	532	ARG	-	expression tag	UNP Q6V2E7
E	533	LYS	-	expression tag	UNP Q6V2E7
E	534	ASP	-	expression tag	UNP Q6V2E7
E	535	GLY	-	expression tag	UNP Q6V2E7
E	536	GLU	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	537	TRP	-	expression tag	UNP Q6V2E7
E	538	VAL	-	expression tag	UNP Q6V2E7
E	539	LEU	-	expression tag	UNP Q6V2E7
E	540	LEU	-	expression tag	UNP Q6V2E7
E	541	SER	-	expression tag	UNP Q6V2E7
E	542	THR	-	expression tag	UNP Q6V2E7
E	543	PHE	-	expression tag	UNP Q6V2E7
E	544	LEU	-	expression tag	UNP Q6V2E7
E	545	GLY	-	expression tag	UNP Q6V2E7
E	546	GLY	-	expression tag	UNP Q6V2E7
E	547	LEU	-	expression tag	UNP Q6V2E7
E	548	VAL	-	expression tag	UNP Q6V2E7
E	549	PRO	-	expression tag	UNP Q6V2E7
E	550	ARG	-	expression tag	UNP Q6V2E7
E	551	GLY	-	expression tag	UNP Q6V2E7
E	552	SER	-	expression tag	UNP Q6V2E7
E	553	HIS	-	expression tag	UNP Q6V2E7
E	554	HIS	-	expression tag	UNP Q6V2E7
E	555	HIS	-	expression tag	UNP Q6V2E7
E	556	HIS	-	expression tag	UNP Q6V2E7
E	557	HIS	-	expression tag	UNP Q6V2E7
E	558	HIS	-	expression tag	UNP Q6V2E7
E	559	SER	-	expression tag	UNP Q6V2E7
E	560	ALA	-	expression tag	UNP Q6V2E7
E	561	TRP	-	expression tag	UNP Q6V2E7
E	562	SER	-	expression tag	UNP Q6V2E7
E	563	HIS	-	expression tag	UNP Q6V2E7
E	564	PRO	-	expression tag	UNP Q6V2E7
E	565	GLN	-	expression tag	UNP Q6V2E7
E	566	PHE	-	expression tag	UNP Q6V2E7
E	567	GLU	-	expression tag	UNP Q6V2E7
E	568	LYS	-	expression tag	UNP Q6V2E7
F	155	CYS	SER	engineered mutation	UNP Q6V2E7
F	190	PHE	SER	engineered mutation	UNP Q6V2E7
F	207	LEU	VAL	engineered mutation	UNP Q6V2E7
F	290	CYS	SER	engineered mutation	UNP Q6V2E7
F	514	SER	-	expression tag	UNP Q6V2E7
F	515	ALA	-	expression tag	UNP Q6V2E7
F	516	ILE	-	expression tag	UNP Q6V2E7
F	517	GLY	-	expression tag	UNP Q6V2E7
F	518	GLY	-	expression tag	UNP Q6V2E7
F	519	TYR	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	520	ILE	-	expression tag	UNP Q6V2E7
F	521	PRO	-	expression tag	UNP Q6V2E7
F	522	GLU	-	expression tag	UNP Q6V2E7
F	523	ALA	-	expression tag	UNP Q6V2E7
F	524	PRO	-	expression tag	UNP Q6V2E7
F	525	ARG	-	expression tag	UNP Q6V2E7
F	526	ASP	-	expression tag	UNP Q6V2E7
F	527	GLY	-	expression tag	UNP Q6V2E7
F	528	GLN	-	expression tag	UNP Q6V2E7
F	529	ALA	-	expression tag	UNP Q6V2E7
F	530	TYR	-	expression tag	UNP Q6V2E7
F	531	VAL	-	expression tag	UNP Q6V2E7
F	532	ARG	-	expression tag	UNP Q6V2E7
F	533	LYS	-	expression tag	UNP Q6V2E7
F	534	ASP	-	expression tag	UNP Q6V2E7
F	535	GLY	-	expression tag	UNP Q6V2E7
F	536	GLU	-	expression tag	UNP Q6V2E7
F	537	TRP	-	expression tag	UNP Q6V2E7
F	538	VAL	-	expression tag	UNP Q6V2E7
F	539	LEU	-	expression tag	UNP Q6V2E7
F	540	LEU	-	expression tag	UNP Q6V2E7
F	541	SER	-	expression tag	UNP Q6V2E7
F	542	THR	-	expression tag	UNP Q6V2E7
F	543	PHE	-	expression tag	UNP Q6V2E7
F	544	LEU	-	expression tag	UNP Q6V2E7
F	545	GLY	-	expression tag	UNP Q6V2E7
F	546	GLY	-	expression tag	UNP Q6V2E7
F	547	LEU	-	expression tag	UNP Q6V2E7
F	548	VAL	-	expression tag	UNP Q6V2E7
F	549	PRO	-	expression tag	UNP Q6V2E7
F	550	ARG	-	expression tag	UNP Q6V2E7
F	551	GLY	-	expression tag	UNP Q6V2E7
F	552	SER	-	expression tag	UNP Q6V2E7
F	553	HIS	-	expression tag	UNP Q6V2E7
F	554	HIS	-	expression tag	UNP Q6V2E7
F	555	HIS	-	expression tag	UNP Q6V2E7
F	556	HIS	-	expression tag	UNP Q6V2E7
F	557	HIS	-	expression tag	UNP Q6V2E7
F	558	HIS	-	expression tag	UNP Q6V2E7
F	559	SER	-	expression tag	UNP Q6V2E7
F	560	ALA	-	expression tag	UNP Q6V2E7
F	561	TRP	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	562	SER	-	expression tag	UNP Q6V2E7
F	563	HIS	-	expression tag	UNP Q6V2E7
F	564	PRO	-	expression tag	UNP Q6V2E7
F	565	GLN	-	expression tag	UNP Q6V2E7
F	566	PHE	-	expression tag	UNP Q6V2E7
F	567	GLU	-	expression tag	UNP Q6V2E7
F	568	LYS	-	expression tag	UNP Q6V2E7
G	155	CYS	SER	engineered mutation	UNP Q6V2E7
G	190	PHE	SER	engineered mutation	UNP Q6V2E7
G	207	LEU	VAL	engineered mutation	UNP Q6V2E7
G	290	CYS	SER	engineered mutation	UNP Q6V2E7
G	514	SER	-	expression tag	UNP Q6V2E7
G	515	ALA	-	expression tag	UNP Q6V2E7
G	516	ILE	-	expression tag	UNP Q6V2E7
G	517	GLY	-	expression tag	UNP Q6V2E7
G	518	GLY	-	expression tag	UNP Q6V2E7
G	519	TYR	-	expression tag	UNP Q6V2E7
G	520	ILE	-	expression tag	UNP Q6V2E7
G	521	PRO	-	expression tag	UNP Q6V2E7
G	522	GLU	-	expression tag	UNP Q6V2E7
G	523	ALA	-	expression tag	UNP Q6V2E7
G	524	PRO	-	expression tag	UNP Q6V2E7
G	525	ARG	-	expression tag	UNP Q6V2E7
G	526	ASP	-	expression tag	UNP Q6V2E7
G	527	GLY	-	expression tag	UNP Q6V2E7
G	528	GLN	-	expression tag	UNP Q6V2E7
G	529	ALA	-	expression tag	UNP Q6V2E7
G	530	TYR	-	expression tag	UNP Q6V2E7
G	531	VAL	-	expression tag	UNP Q6V2E7
G	532	ARG	-	expression tag	UNP Q6V2E7
G	533	LYS	-	expression tag	UNP Q6V2E7
G	534	ASP	-	expression tag	UNP Q6V2E7
G	535	GLY	-	expression tag	UNP Q6V2E7
G	536	GLU	-	expression tag	UNP Q6V2E7
G	537	TRP	-	expression tag	UNP Q6V2E7
G	538	VAL	-	expression tag	UNP Q6V2E7
G	539	LEU	-	expression tag	UNP Q6V2E7
G	540	LEU	-	expression tag	UNP Q6V2E7
G	541	SER	-	expression tag	UNP Q6V2E7
G	542	THR	-	expression tag	UNP Q6V2E7
G	543	PHE	-	expression tag	UNP Q6V2E7
G	544	LEU	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	545	GLY	-	expression tag	UNP Q6V2E7
G	546	GLY	-	expression tag	UNP Q6V2E7
G	547	LEU	-	expression tag	UNP Q6V2E7
G	548	VAL	-	expression tag	UNP Q6V2E7
G	549	PRO	-	expression tag	UNP Q6V2E7
G	550	ARG	-	expression tag	UNP Q6V2E7
G	551	GLY	-	expression tag	UNP Q6V2E7
G	552	SER	-	expression tag	UNP Q6V2E7
G	553	HIS	-	expression tag	UNP Q6V2E7
G	554	HIS	-	expression tag	UNP Q6V2E7
G	555	HIS	-	expression tag	UNP Q6V2E7
G	556	HIS	-	expression tag	UNP Q6V2E7
G	557	HIS	-	expression tag	UNP Q6V2E7
G	558	HIS	-	expression tag	UNP Q6V2E7
G	559	SER	-	expression tag	UNP Q6V2E7
G	560	ALA	-	expression tag	UNP Q6V2E7
G	561	TRP	-	expression tag	UNP Q6V2E7
G	562	SER	-	expression tag	UNP Q6V2E7
G	563	HIS	-	expression tag	UNP Q6V2E7
G	564	PRO	-	expression tag	UNP Q6V2E7
G	565	GLN	-	expression tag	UNP Q6V2E7
G	566	PHE	-	expression tag	UNP Q6V2E7
G	567	GLU	-	expression tag	UNP Q6V2E7
G	568	LYS	-	expression tag	UNP Q6V2E7
H	155	CYS	SER	engineered mutation	UNP Q6V2E7
H	190	PHE	SER	engineered mutation	UNP Q6V2E7
H	207	LEU	VAL	engineered mutation	UNP Q6V2E7
H	290	CYS	SER	engineered mutation	UNP Q6V2E7
H	514	SER	-	expression tag	UNP Q6V2E7
H	515	ALA	-	expression tag	UNP Q6V2E7
H	516	ILE	-	expression tag	UNP Q6V2E7
H	517	GLY	-	expression tag	UNP Q6V2E7
H	518	GLY	-	expression tag	UNP Q6V2E7
H	519	TYR	-	expression tag	UNP Q6V2E7
H	520	ILE	-	expression tag	UNP Q6V2E7
H	521	PRO	-	expression tag	UNP Q6V2E7
H	522	GLU	-	expression tag	UNP Q6V2E7
H	523	ALA	-	expression tag	UNP Q6V2E7
H	524	PRO	-	expression tag	UNP Q6V2E7
H	525	ARG	-	expression tag	UNP Q6V2E7
H	526	ASP	-	expression tag	UNP Q6V2E7
H	527	GLY	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	528	GLN	-	expression tag	UNP Q6V2E7
H	529	ALA	-	expression tag	UNP Q6V2E7
H	530	TYR	-	expression tag	UNP Q6V2E7
H	531	VAL	-	expression tag	UNP Q6V2E7
H	532	ARG	-	expression tag	UNP Q6V2E7
H	533	LYS	-	expression tag	UNP Q6V2E7
H	534	ASP	-	expression tag	UNP Q6V2E7
H	535	GLY	-	expression tag	UNP Q6V2E7
H	536	GLU	-	expression tag	UNP Q6V2E7
H	537	TRP	-	expression tag	UNP Q6V2E7
H	538	VAL	-	expression tag	UNP Q6V2E7
H	539	LEU	-	expression tag	UNP Q6V2E7
H	540	LEU	-	expression tag	UNP Q6V2E7
H	541	SER	-	expression tag	UNP Q6V2E7
H	542	THR	-	expression tag	UNP Q6V2E7
H	543	PHE	-	expression tag	UNP Q6V2E7
H	544	LEU	-	expression tag	UNP Q6V2E7
H	545	GLY	-	expression tag	UNP Q6V2E7
H	546	GLY	-	expression tag	UNP Q6V2E7
H	547	LEU	-	expression tag	UNP Q6V2E7
H	548	VAL	-	expression tag	UNP Q6V2E7
H	549	PRO	-	expression tag	UNP Q6V2E7
H	550	ARG	-	expression tag	UNP Q6V2E7
H	551	GLY	-	expression tag	UNP Q6V2E7
H	552	SER	-	expression tag	UNP Q6V2E7
H	553	HIS	-	expression tag	UNP Q6V2E7
H	554	HIS	-	expression tag	UNP Q6V2E7
H	555	HIS	-	expression tag	UNP Q6V2E7
H	556	HIS	-	expression tag	UNP Q6V2E7
H	557	HIS	-	expression tag	UNP Q6V2E7
H	558	HIS	-	expression tag	UNP Q6V2E7
H	559	SER	-	expression tag	UNP Q6V2E7
H	560	ALA	-	expression tag	UNP Q6V2E7
H	561	TRP	-	expression tag	UNP Q6V2E7
H	562	SER	-	expression tag	UNP Q6V2E7
H	563	HIS	-	expression tag	UNP Q6V2E7
H	564	PRO	-	expression tag	UNP Q6V2E7
H	565	GLN	-	expression tag	UNP Q6V2E7
H	566	PHE	-	expression tag	UNP Q6V2E7
H	567	GLU	-	expression tag	UNP Q6V2E7
H	568	LYS	-	expression tag	UNP Q6V2E7
I	155	CYS	SER	engineered mutation	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	190	PHE	SER	engineered mutation	UNP Q6V2E7
I	207	LEU	VAL	engineered mutation	UNP Q6V2E7
I	290	CYS	SER	engineered mutation	UNP Q6V2E7
I	514	SER	-	expression tag	UNP Q6V2E7
I	515	ALA	-	expression tag	UNP Q6V2E7
I	516	ILE	-	expression tag	UNP Q6V2E7
I	517	GLY	-	expression tag	UNP Q6V2E7
I	518	GLY	-	expression tag	UNP Q6V2E7
I	519	TYR	-	expression tag	UNP Q6V2E7
I	520	ILE	-	expression tag	UNP Q6V2E7
I	521	PRO	-	expression tag	UNP Q6V2E7
I	522	GLU	-	expression tag	UNP Q6V2E7
I	523	ALA	-	expression tag	UNP Q6V2E7
I	524	PRO	-	expression tag	UNP Q6V2E7
I	525	ARG	-	expression tag	UNP Q6V2E7
I	526	ASP	-	expression tag	UNP Q6V2E7
I	527	GLY	-	expression tag	UNP Q6V2E7
I	528	GLN	-	expression tag	UNP Q6V2E7
I	529	ALA	-	expression tag	UNP Q6V2E7
I	530	TYR	-	expression tag	UNP Q6V2E7
I	531	VAL	-	expression tag	UNP Q6V2E7
I	532	ARG	-	expression tag	UNP Q6V2E7
I	533	LYS	-	expression tag	UNP Q6V2E7
I	534	ASP	-	expression tag	UNP Q6V2E7
I	535	GLY	-	expression tag	UNP Q6V2E7
I	536	GLU	-	expression tag	UNP Q6V2E7
I	537	TRP	-	expression tag	UNP Q6V2E7
I	538	VAL	-	expression tag	UNP Q6V2E7
I	539	LEU	-	expression tag	UNP Q6V2E7
I	540	LEU	-	expression tag	UNP Q6V2E7
I	541	SER	-	expression tag	UNP Q6V2E7
I	542	THR	-	expression tag	UNP Q6V2E7
I	543	PHE	-	expression tag	UNP Q6V2E7
I	544	LEU	-	expression tag	UNP Q6V2E7
I	545	GLY	-	expression tag	UNP Q6V2E7
I	546	GLY	-	expression tag	UNP Q6V2E7
I	547	LEU	-	expression tag	UNP Q6V2E7
I	548	VAL	-	expression tag	UNP Q6V2E7
I	549	PRO	-	expression tag	UNP Q6V2E7
I	550	ARG	-	expression tag	UNP Q6V2E7
I	551	GLY	-	expression tag	UNP Q6V2E7
I	552	SER	-	expression tag	UNP Q6V2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	553	HIS	-	expression tag	UNP Q6V2E7
I	554	HIS	-	expression tag	UNP Q6V2E7
I	555	HIS	-	expression tag	UNP Q6V2E7
I	556	HIS	-	expression tag	UNP Q6V2E7
I	557	HIS	-	expression tag	UNP Q6V2E7
I	558	HIS	-	expression tag	UNP Q6V2E7
I	559	SER	-	expression tag	UNP Q6V2E7
I	560	ALA	-	expression tag	UNP Q6V2E7
I	561	TRP	-	expression tag	UNP Q6V2E7
I	562	SER	-	expression tag	UNP Q6V2E7
I	563	HIS	-	expression tag	UNP Q6V2E7
I	564	PRO	-	expression tag	UNP Q6V2E7
I	565	GLN	-	expression tag	UNP Q6V2E7
I	566	PHE	-	expression tag	UNP Q6V2E7
I	567	GLU	-	expression tag	UNP Q6V2E7
I	568	LYS	-	expression tag	UNP Q6V2E7

- Molecule 2 is a protein called MEDI8897 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	224	Total	C	N	O	S	0	0	0
			1668	1054	273	333	8			
2	K	220	Total	C	N	O	S	0	0	0
			1643	1040	268	327	8			
2	L	221	Total	C	N	O	S	0	0	0
			1649	1043	269	329	8			
2	M	221	Total	C	N	O	S	0	0	0
			1649	1043	269	329	8			
2	N	221	Total	C	N	O	S	0	0	0
			1649	1043	269	329	8			
2	O	216	Total	C	N	O	S	0	0	0
			1622	1029	264	321	8			

- Molecule 3 is a protein called MEDI8897 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	212	Total	C	N	O	S	0	0	0
			1623	1016	270	332	5			
3	Q	211	Total	C	N	O	S	0	0	0
			1619	1014	269	331	5			
3	R	211	Total	C	N	O	S	0	0	0
			1619	1014	269	331	5			

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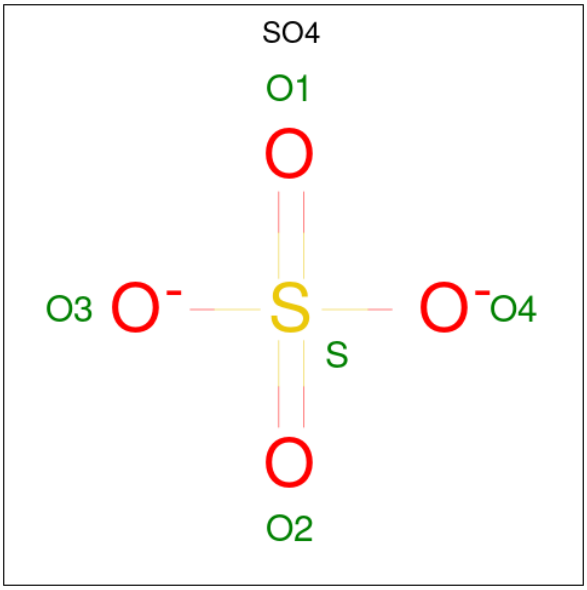
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	211	Total	C	N	O	S	0	0	0
			1619	1014	269	331	5			
3	T	211	Total	C	N	O	S	0	0	0
			1619	1014	269	331	5			
3	U	208	Total	C	N	O	S	0	0	0
			1594	999	263	327	5			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	O	S		0	0
			5	4	1			
4	B	1	Total	O	S		0	0
			5	4	1			
4	B	1	Total	O	S		0	0
			5	4	1			
4	B	1	Total	O	S		0	0
			5	4	1			
4	B	1	Total	O	S		0	0
			5	4	1			
4	C	1	Total	O	S		0	0
			5	4	1			
4	C	1	Total	O	S		0	0
			5	4	1			
4	D	1	Total	O	S		0	0
			5	4	1			

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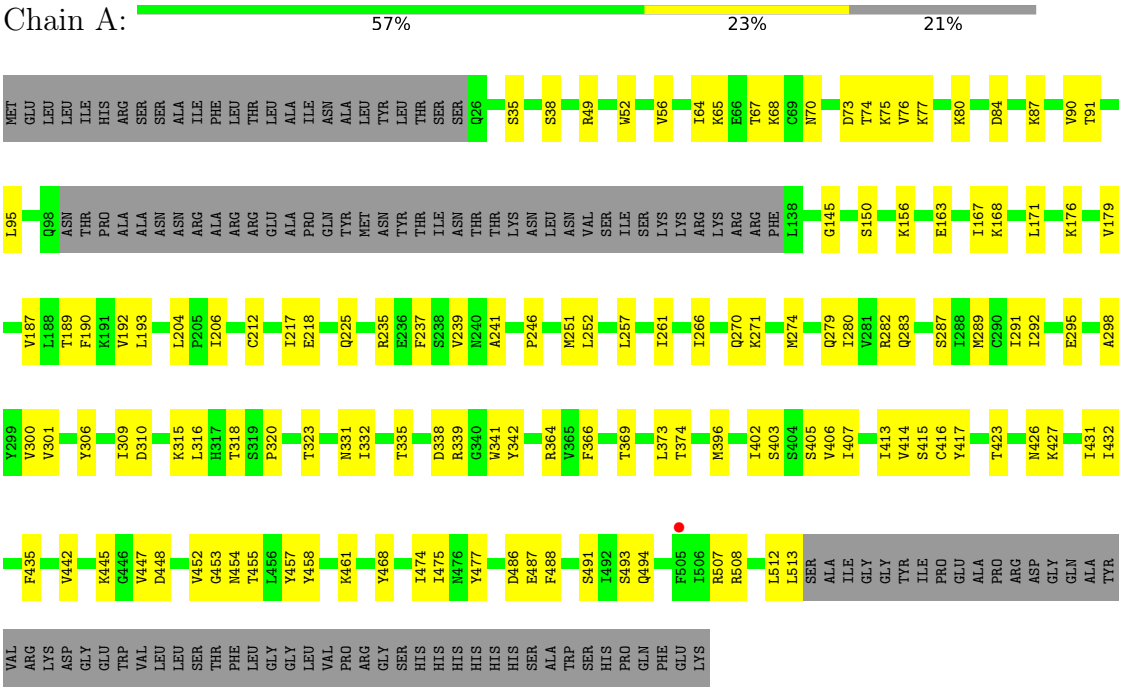
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

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

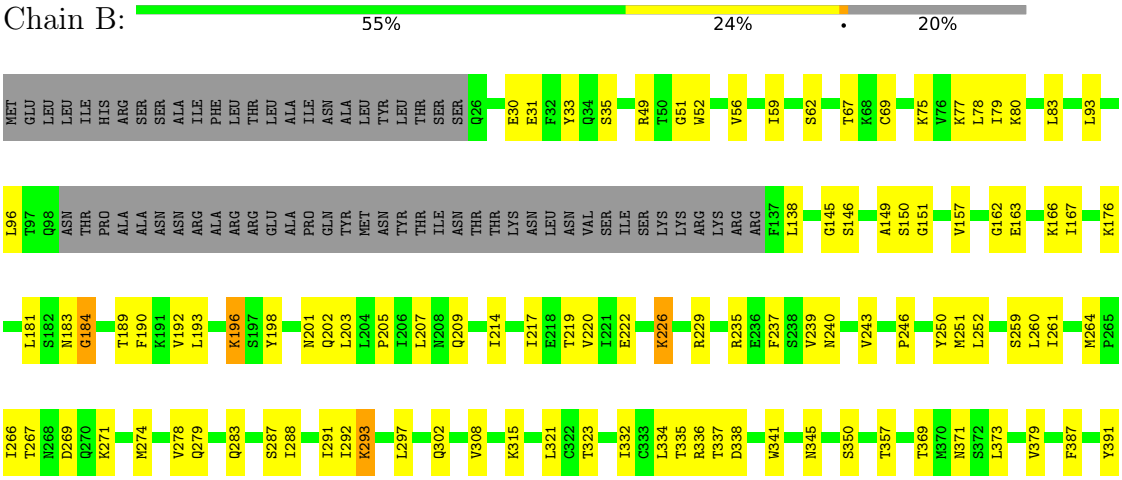
• Molecule 1: Fusion glycoprotein F0

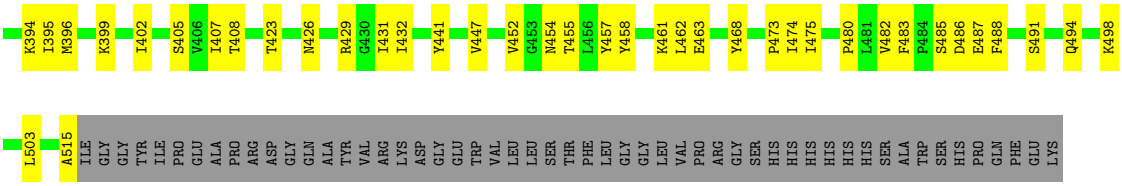
Chain A:



• Molecule 1: Fusion glycoprotein F0

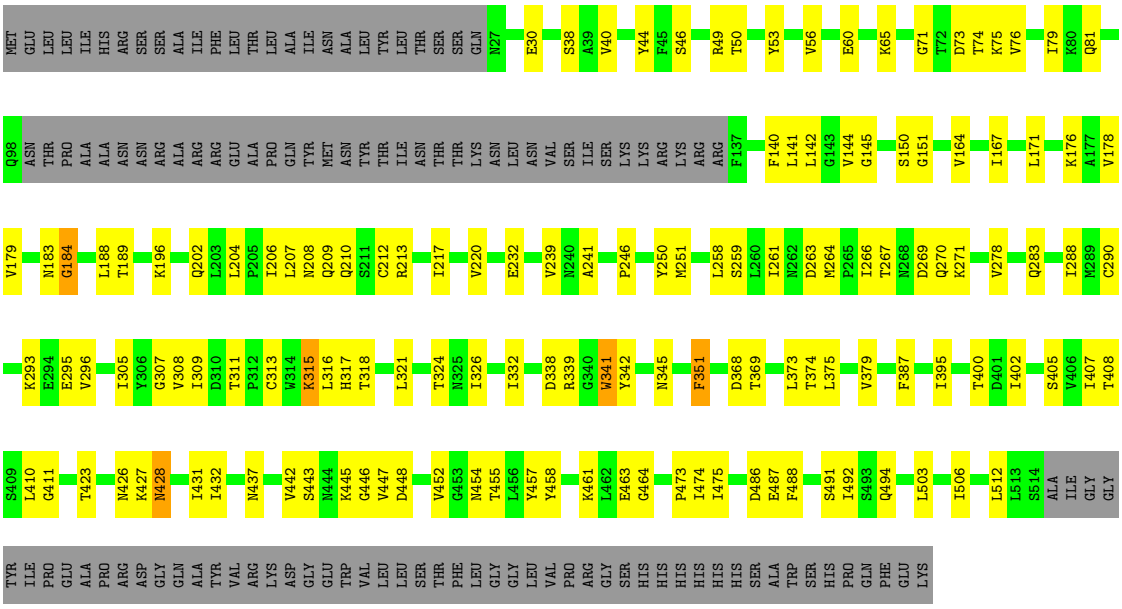
Chain B:





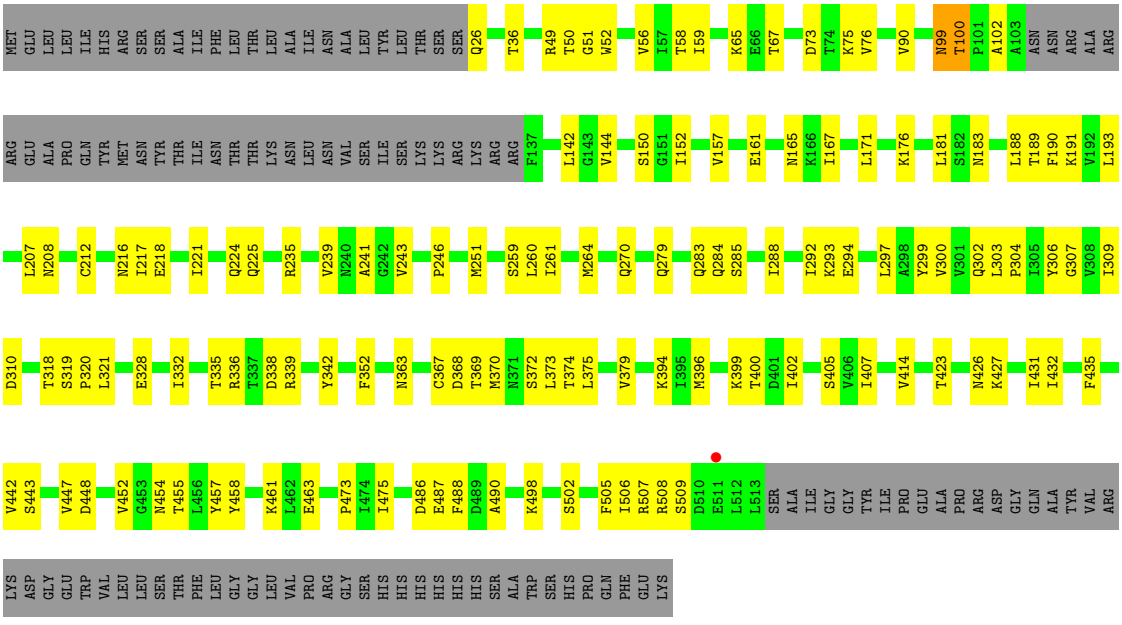
• Molecule 1: Fusion glycoprotein F0

Chain C:



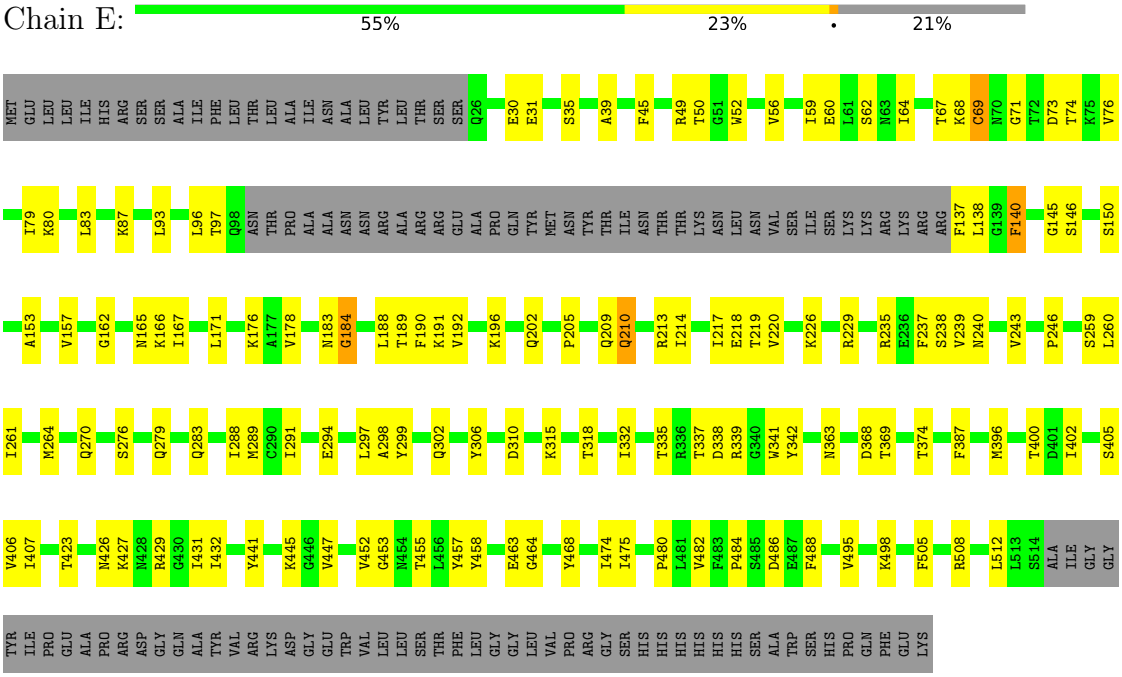
• Molecule 1: Fusion glycoprotein F0

Chain D:



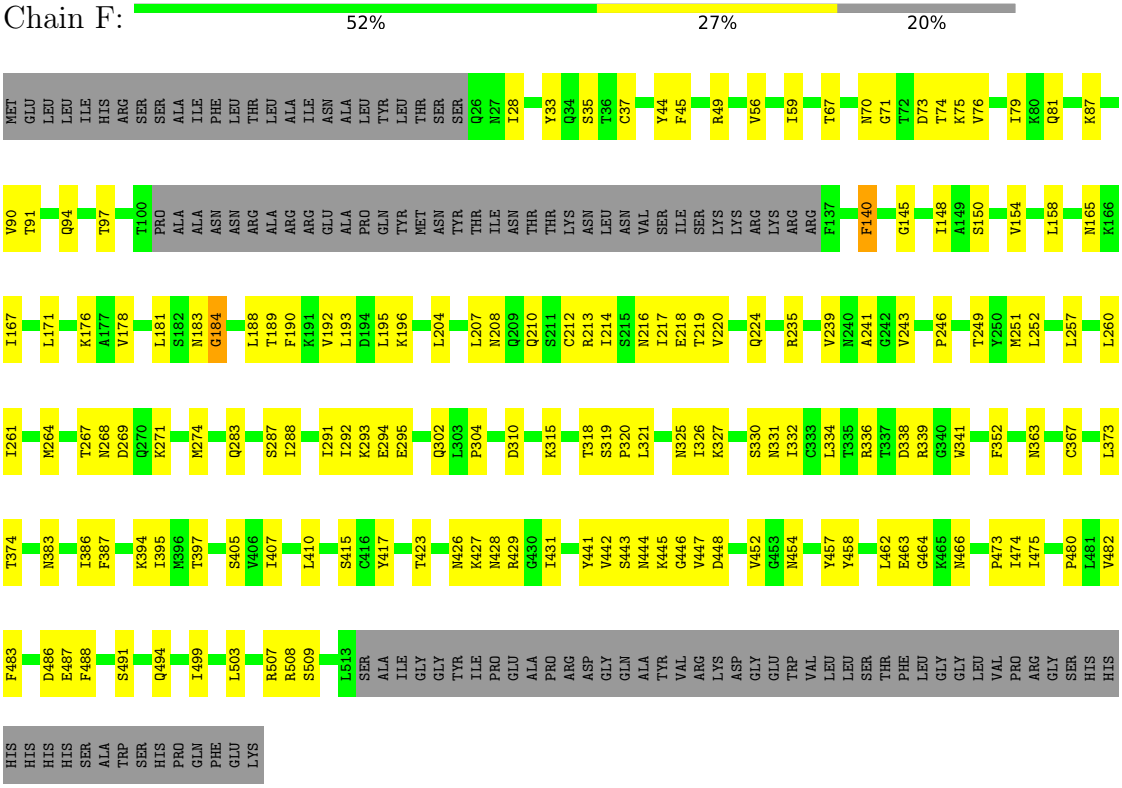
• Molecule 1: Fusion glycoprotein F0

Chain E:



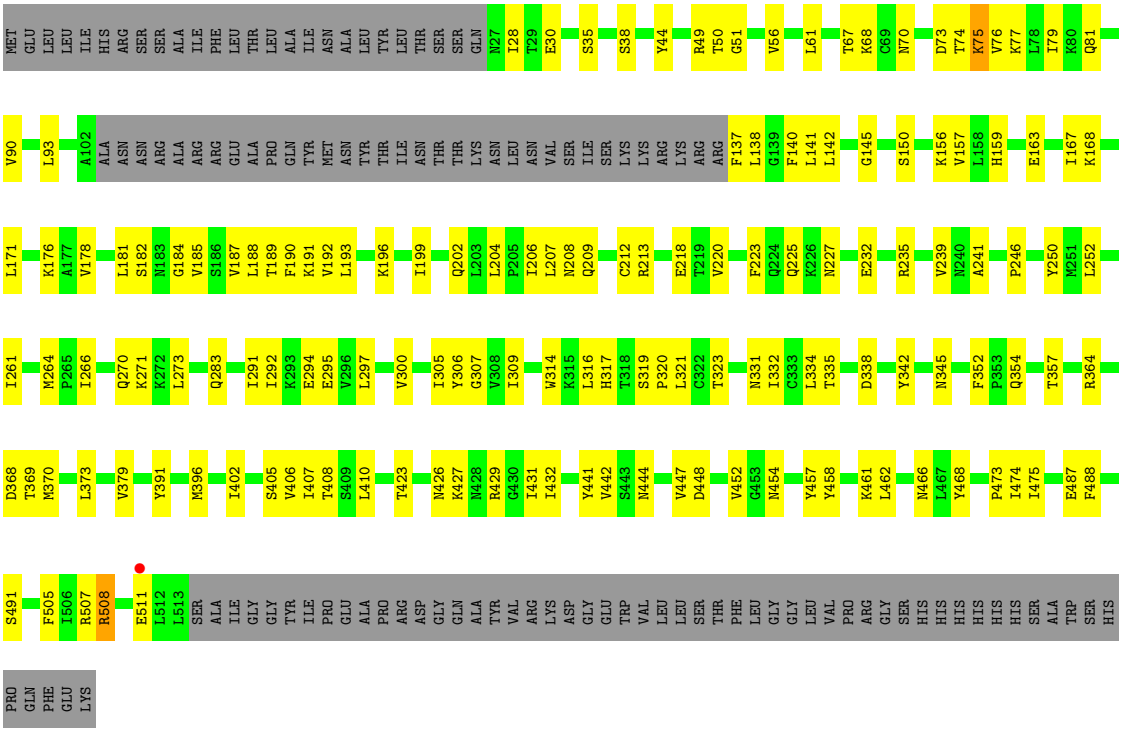
• Molecule 1: Fusion glycoprotein F0

Chain F:



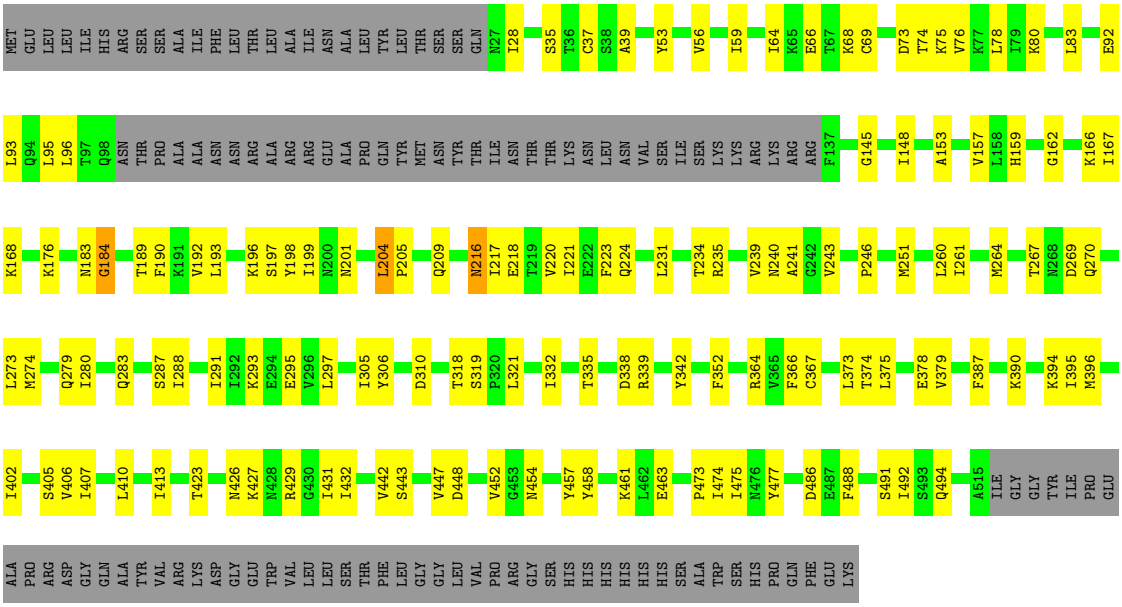
• Molecule 1: Fusion glycoprotein F0

Chain G:



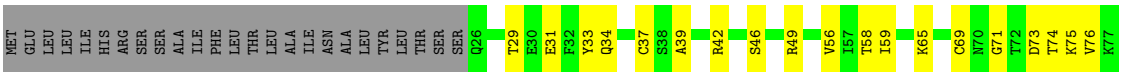
• Molecule 1: Fusion glycoprotein F0

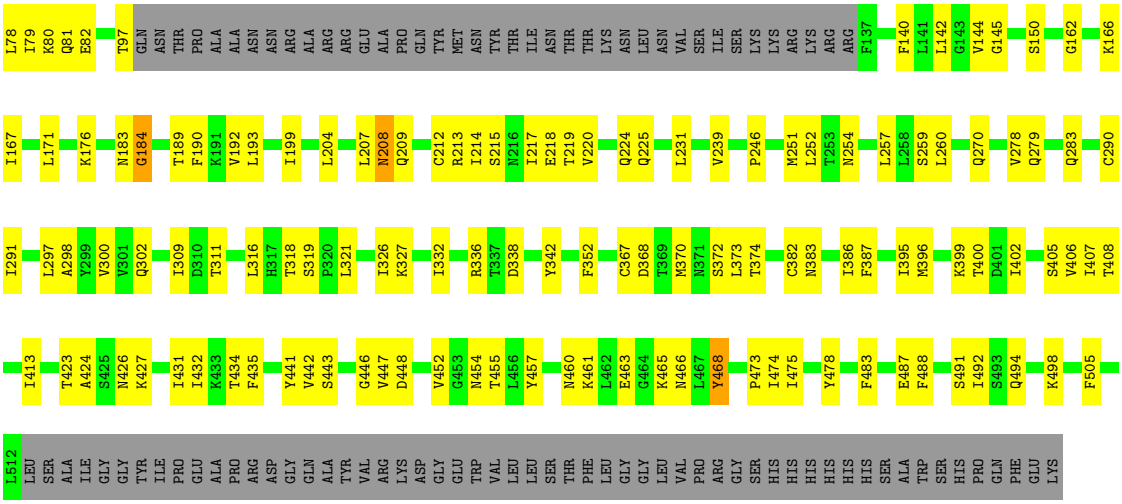
Chain H:



• Molecule 1: Fusion glycoprotein F0

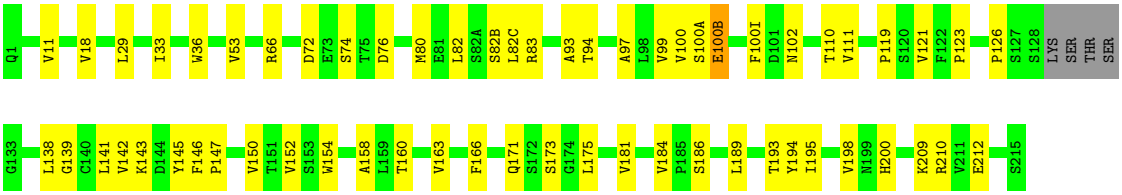
Chain I:





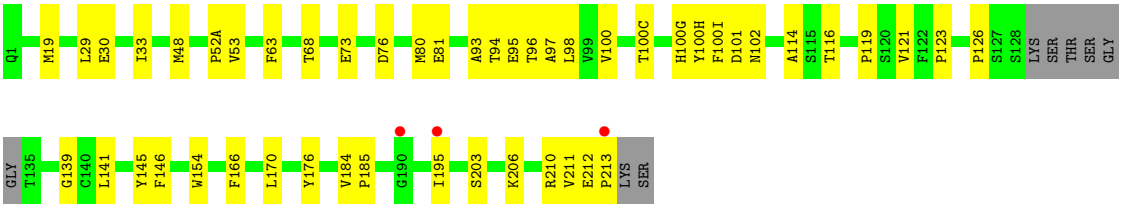
• Molecule 2: MEDI8897 Fab Heavy Chain

Chain J:



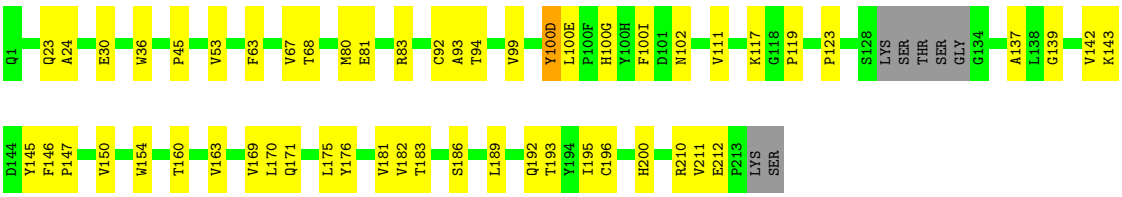
• Molecule 2: MEDI8897 Fab Heavy Chain

Chain K:



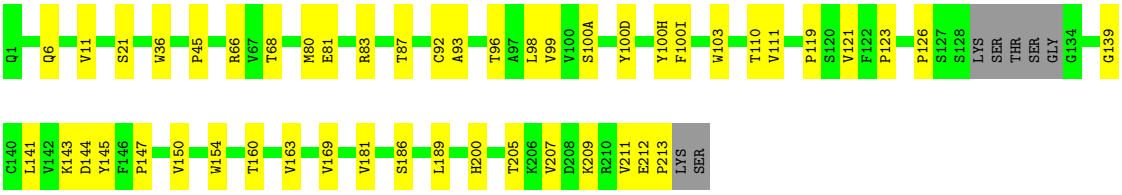
• Molecule 2: MEDI8897 Fab Heavy Chain

Chain L:

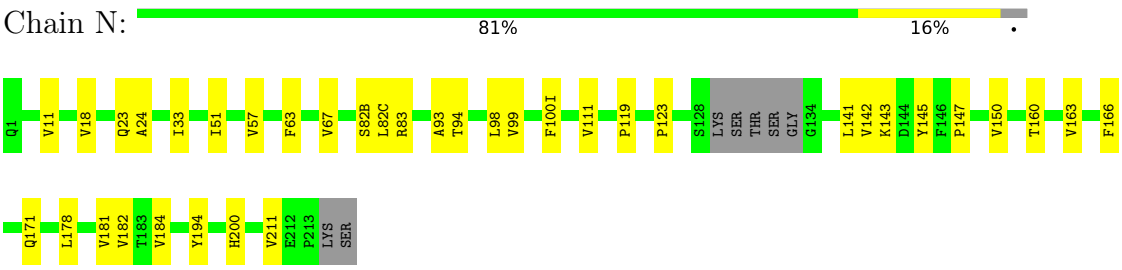


• Molecule 2: MEDI8897 Fab Heavy Chain

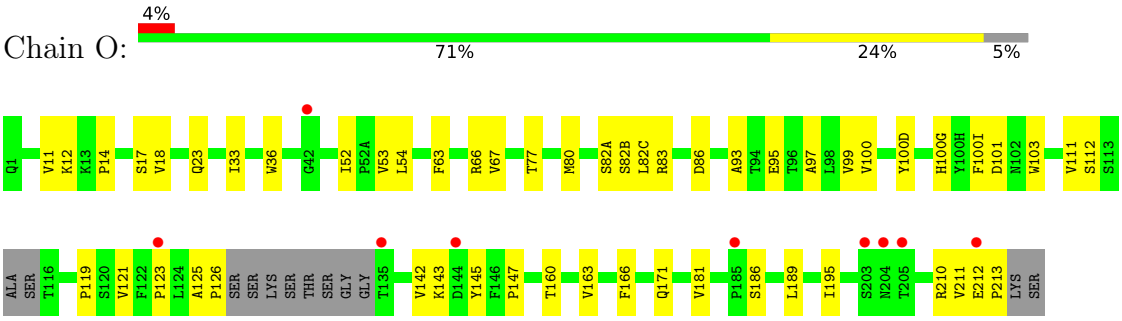
Chain M:



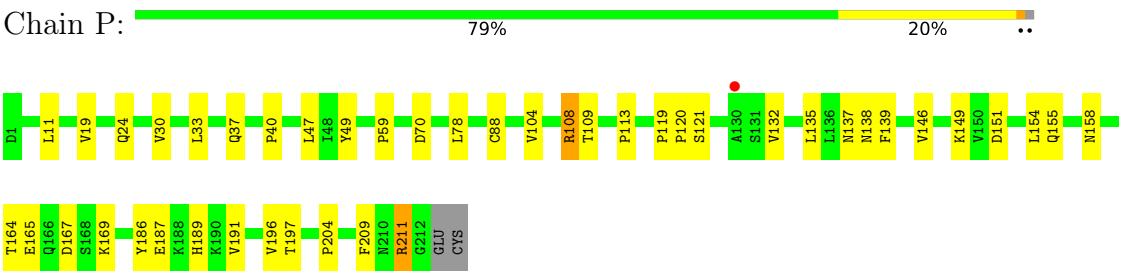
• Molecule 2: MEDI8897 Fab Heavy Chain



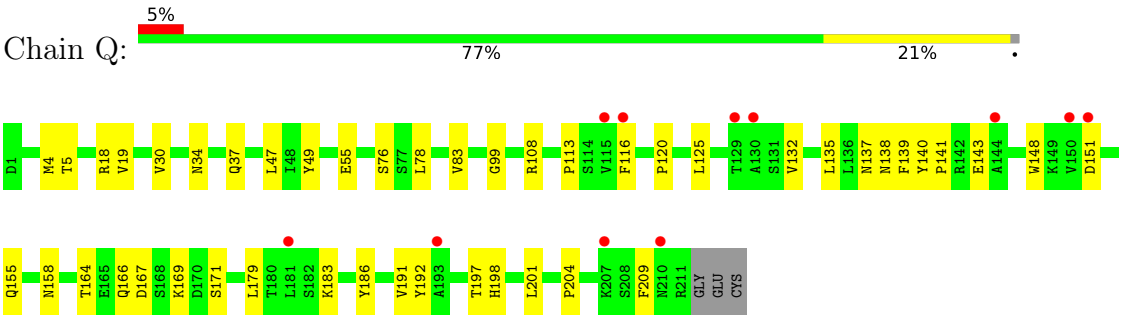
• Molecule 2: MEDI8897 Fab Heavy Chain



• Molecule 3: MEDI8897 Fab Light Chain

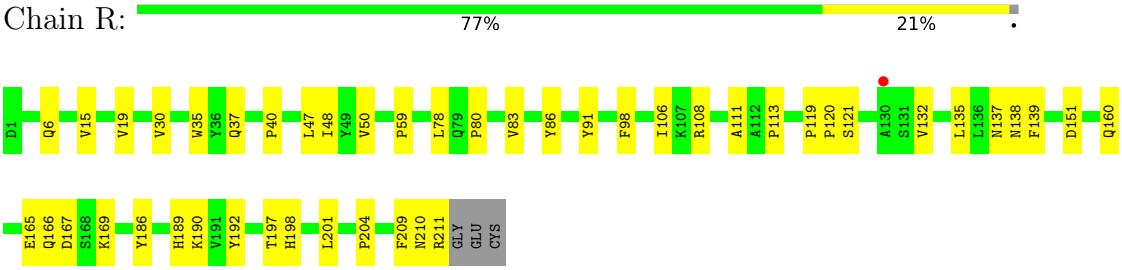


• Molecule 3: MEDI8897 Fab Light Chain



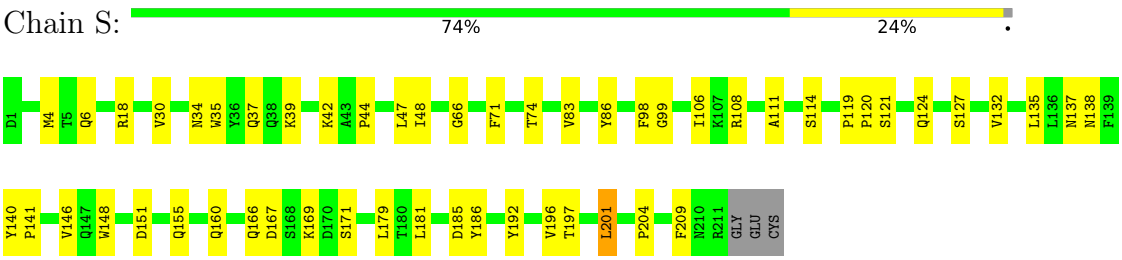
• Molecule 3: MEDI8897 Fab Light Chain

Chain R:



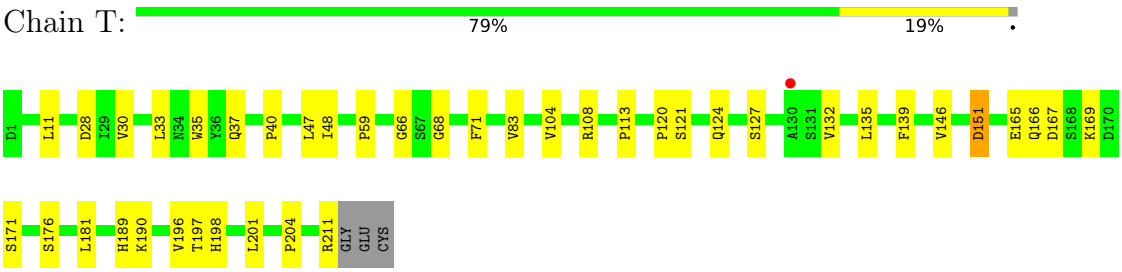
• Molecule 3: MEDI8897 Fab Light Chain

Chain S:



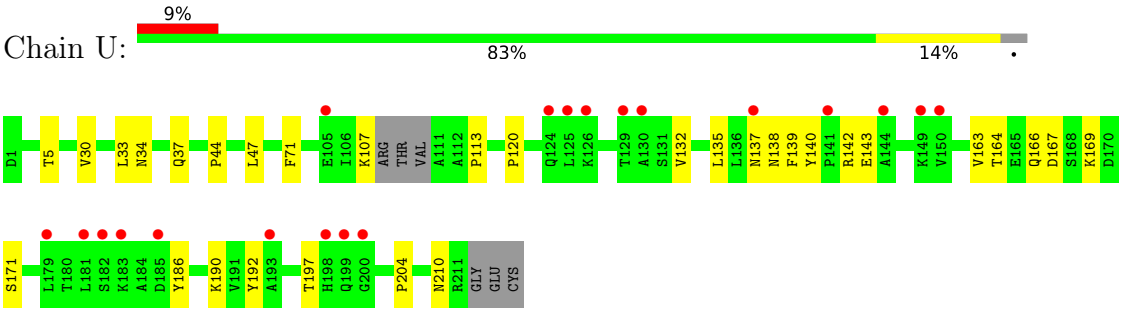
• Molecule 3: MEDI8897 Fab Light Chain

Chain T:



• Molecule 3: MEDI8897 Fab Light Chain

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	229.02Å 229.02Å 343.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.31 – 4.30 46.31 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.31-4.30) 100.0 (46.31-4.30)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 4.28Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.236 , 0.294 0.238 , 0.294	Depositor DCC
R_{free} test set	3466 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	82.9	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 65.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	51201	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.32	0/3538	0.53	0/4794
1	B	0.32	0/3561	0.52	0/4825
1	C	1.33	7/3547 (0.2%)	0.57	2/4806 (0.0%)
1	D	0.33	0/3583	0.53	2/4857 (0.0%)
1	E	0.32	0/3556	0.53	0/4818
1	F	0.31	0/3565	0.54	0/4831
1	G	0.32	0/3569	0.54	0/4838
1	H	0.32	0/3552	0.54	2/4813 (0.0%)
1	I	0.31	0/3533	0.54	1/4787 (0.0%)
2	J	0.29	0/1708	0.52	0/2334
2	K	0.29	0/1683	0.53	0/2302
2	L	0.29	0/1689	0.52	0/2310
2	M	0.29	0/1689	0.52	0/2310
2	N	0.30	0/1689	0.52	0/2310
2	O	0.28	0/1661	0.51	0/2271
3	P	0.29	0/1656	0.50	0/2252
3	Q	0.27	0/1652	0.50	0/2247
3	R	0.28	0/1652	0.49	0/2247
3	S	0.28	0/1652	0.51	1/2247 (0.0%)
3	T	0.29	0/1652	0.50	0/2247
3	U	0.30	0/1626	0.50	0/2210
All	All	0.46	7/52013 (0.0%)	0.53	8/70656 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	LYS	CE-NZ	58.12	2.94	1.49
1	C	341	TRP	CE3-CZ3	32.74	1.94	1.38
1	C	341	TRP	CZ3-CH2	22.46	1.75	1.40
1	C	341	TRP	CE2-CZ2	19.38	1.72	1.39
1	C	341	TRP	CD2-CE2	17.15	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	341	TRP	CZ2-CH2	11.78	1.59	1.37
1	C	341	TRP	CD2-CE3	11.55	1.57	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	315	LYS	CD-CE-NZ	9.90	134.48	111.70
3	S	201	LEU	CA-CB-CG	6.03	129.16	115.30
1	C	290	CYS	CA-CB-SG	5.88	124.59	114.00
1	H	310	ASP	C-N-CA	-5.53	107.88	121.70
1	H	204	LEU	CA-CB-CG	5.29	127.45	115.30
1	D	99	ASN	C-N-CA	5.26	134.86	121.70
1	D	310	ASP	C-N-CA	-5.13	108.86	121.70
1	I	290	CYS	CA-CB-SG	5.03	123.06	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3489	0	3527	108	0
1	B	3511	0	3546	116	0
1	C	3497	0	3533	143	0
1	D	3532	0	3566	106	0
1	E	3506	0	3541	106	0
1	F	3515	0	3549	128	0
1	G	3518	0	3553	120	0
1	H	3502	0	3538	105	0
1	I	3483	0	3517	118	0
2	J	1668	0	1630	38	1
2	K	1643	0	1602	31	1
2	L	1649	0	1609	39	0
2	M	1649	0	1609	31	0
2	N	1649	0	1609	24	0
2	O	1622	0	1585	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1623	0	1582	26	0
3	Q	1619	0	1579	30	1
3	R	1619	0	1579	27	0
3	S	1619	0	1579	31	0
3	T	1619	0	1579	22	0
3	U	1594	0	1549	18	1
4	A	5	0	0	1	0
4	B	20	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
4	H	10	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
4	L	5	0	0	0	0
All	All	51201	0	50961	1213	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:TRP:CH2	1:C:341:TRP:CZ3	1.76	1.66
1:C:341:TRP:CZ3	1:C:341:TRP:CE3	1.94	1.51
1:C:315:LYS:NZ	1:C:341:TRP:CE2	1.98	1.31
1:C:315:LYS:NZ	1:C:341:TRP:CD2	2.01	1.27
1:C:315:LYS:NZ	1:C:341:TRP:CE3	2.01	1.27
1:C:315:LYS:NZ	1:C:341:TRP:CZ3	2.02	1.27
1:C:315:LYS:NZ	1:C:341:TRP:CZ2	2.08	1.21
1:C:315:LYS:NZ	1:C:341:TRP:CH2	2.09	1.20
1:E:69:CYS:SG	1:E:80:LYS:NZ	2.28	1.07
1:A:448:ASP:OD1	1:A:461:LYS:NZ	1.93	1.01
1:C:315:LYS:CE	1:C:341:TRP:CE2	2.46	0.98
1:C:315:LYS:CE	1:C:341:TRP:CZ3	2.48	0.96
1:H:407:ILE:HD11	1:H:457:TYR:HB3	1.47	0.95
1:C:315:LYS:CE	1:C:341:TRP:CE3	2.49	0.95
1:C:315:LYS:CE	1:C:341:TRP:CD2	2.51	0.94
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.50	0.93
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:ILE:HD11	1:G:457:TYR:HB3	1.51	0.92
1:B:201:ASN:HB2	1:F:429:ARG:HH21	1.34	0.92
1:C:315:LYS:CE	1:C:341:TRP:CZ2	2.52	0.92
1:A:291:ILE:HD12	1:A:291:ILE:O	1.70	0.91
1:A:374:THR:HG21	1:B:454:ASN:H	1.32	0.91
1:C:315:LYS:CE	1:C:341:TRP:CH2	2.53	0.91
1:G:168:LYS:NZ	1:G:295:GLU:OE2	2.03	0.90
1:I:246:PRO:HB3	1:I:283:GLN:HA	1.53	0.90
1:D:407:ILE:HD11	1:D:457:TYR:HB3	1.54	0.89
1:B:176:LYS:NZ	1:B:259:SER:OG	2.04	0.89
1:F:214:ILE:HD11	1:F:219:THR:HB	1.54	0.88
1:D:448:ASP:OD1	1:D:461:LYS:NZ	2.08	0.86
1:E:432:ILE:HD11	1:E:447:VAL:HG22	1.57	0.86
1:H:246:PRO:HB3	1:H:283:GLN:HA	1.56	0.85
1:B:205:PRO:HB3	1:F:446:GLY:HA3	1.58	0.85
3:Q:158:ASN:HD22	3:Q:179:LEU:CD1	1.88	0.85
1:E:246:PRO:HB3	1:E:283:GLN:HA	1.58	0.85
1:F:246:PRO:HB3	1:F:283:GLN:HA	1.58	0.85
1:G:332:ILE:HG22	1:G:475:ILE:HD11	1.57	0.85
1:H:374:THR:HG21	1:I:454:ASN:H	1.42	0.85
1:I:332:ILE:HG22	1:I:475:ILE:HD11	1.58	0.85
1:A:407:ILE:HD11	1:A:457:TYR:HB3	1.58	0.84
1:G:225:GLN:OE1	1:I:81:GLN:NE2	2.10	0.84
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.58	0.84
1:I:176:LYS:NZ	1:I:259:SER:OG	2.10	0.83
1:H:426:ASN:HB3	1:H:429:ARG:HB2	1.61	0.83
1:H:332:ILE:HG22	1:H:475:ILE:HD11	1.58	0.83
1:B:214:ILE:HD11	1:B:219:THR:HB	1.59	0.82
1:E:205:PRO:HB3	1:I:446:GLY:HA3	1.61	0.81
1:H:168:LYS:NZ	1:H:295:GLU:HB2	1.95	0.81
1:E:407:ILE:HD11	1:E:457:TYR:HB3	1.62	0.81
1:H:273:LEU:HD13	1:H:364:ARG:NH1	1.96	0.81
1:F:67:THR:HA	2:M:99:VAL:HG22	1.63	0.80
1:C:332:ILE:HG22	1:C:475:ILE:HD11	1.62	0.80
1:G:157:VAL:HG11	1:G:181:LEU:HB3	1.63	0.80
1:I:150:SER:OG	1:I:302:GLN:NE2	2.14	0.80
2:O:125:ALA:HB1	2:O:213:PRO:HA	1.63	0.80
1:G:218:GLU:OE1	1:I:75:LYS:NZ	2.14	0.80
1:A:291:ILE:HD11	1:A:298:ALA:HB3	1.63	0.80
1:F:73:ASP:OD2	1:F:213:ARG:NH2	2.16	0.79
2:O:11:VAL:HB	2:O:147:PRO:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TYR:HB2	1:C:305:ILE:HD11	1.65	0.79
1:A:270:GLN:HG2	1:A:309:ILE:HD12	1.63	0.78
1:A:225:GLN:OE1	1:C:81:GLN:NE2	2.16	0.78
1:B:407:ILE:HD11	1:B:457:TYR:HB3	1.65	0.78
3:P:120:PRO:HD3	3:P:132:VAL:HG22	1.65	0.78
3:Q:120:PRO:HD3	3:Q:132:VAL:HG22	1.67	0.77
1:D:246:PRO:HB3	1:D:283:GLN:HA	1.66	0.77
3:Q:158:ASN:ND2	3:Q:179:LEU:CD1	2.47	0.77
1:E:374:THR:HG21	1:F:454:ASN:H	1.50	0.77
1:G:454:ASN:H	1:I:374:THR:HG21	1.50	0.77
1:C:407:ILE:HD11	1:C:457:TYR:HB3	1.67	0.76
1:C:446:GLY:HA3	1:H:205:PRO:HB3	1.67	0.76
2:O:12:LYS:HE3	2:O:17:SER:O	1.86	0.76
1:F:79:ILE:HD12	1:F:207:LEU:HD11	1.67	0.76
1:B:332:ILE:HG22	1:B:475:ILE:HD11	1.66	0.76
1:B:426:ASN:HB3	1:B:429:ARG:HB2	1.67	0.76
1:E:176:LYS:NZ	1:E:259:SER:OG	2.18	0.75
1:F:76:VAL:HG13	1:F:212:CYS:HB3	1.66	0.75
1:A:453:GLY:HA3	1:C:374:THR:HG21	1.67	0.75
2:O:119:PRO:HB3	2:O:145:TYR:HB3	1.67	0.75
1:A:332:ILE:HG22	1:A:475:ILE:HD11	1.67	0.75
1:A:488:PHE:HB3	1:B:488:PHE:CZ	2.22	0.75
1:E:332:ILE:HG22	1:E:475:ILE:HD11	1.67	0.74
1:D:270:GLN:NE2	1:D:306:TYR:O	2.19	0.74
1:C:315:LYS:HE2	1:C:341:TRP:CZ3	2.19	0.74
1:E:426:ASN:HB3	1:E:429:ARG:HB2	1.70	0.74
1:F:423:THR:HG21	1:F:431:ILE:HG12	1.67	0.74
1:B:426:ASN:HD22	1:B:429:ARG:HD2	1.53	0.74
1:A:402:ILE:HG21	1:C:373:LEU:HD13	1.69	0.73
1:G:75:LYS:HE3	1:G:213:ARG:HH21	1.52	0.73
2:N:119:PRO:HB3	2:N:145:TYR:HB3	1.69	0.73
1:G:79:ILE:HD13	1:G:207:LEU:HD11	1.71	0.73
2:J:123:PRO:O	3:P:121:SER:OG	2.07	0.73
1:D:407:ILE:HD12	1:F:145:GLY:HA2	1.69	0.73
1:E:261:ILE:HA	1:E:264:MET:HE2	1.71	0.73
1:C:315:LYS:HE3	1:C:341:TRP:CZ2	2.23	0.73
1:C:315:LYS:HG2	1:C:317:HIS:HE1	1.53	0.72
1:D:454:ASN:H	1:F:374:THR:HG21	1.53	0.72
1:E:171:LEU:O	1:E:191:LYS:NZ	2.19	0.72
1:I:336:ARG:NH1	1:I:382:CYS:O	2.22	0.72
1:E:498:LYS:NZ	1:F:486:ASP:HB2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:123:PRO:HB3	2:O:211:VAL:HG12	1.72	0.72
1:H:167:ILE:HD12	1:H:189:THR:HG21	1.72	0.72
2:L:143:LYS:NZ	2:L:171:GLN:OE1	2.22	0.72
1:G:270:GLN:HG2	1:G:309:ILE:HD12	1.72	0.72
1:B:69:CYS:HB2	1:B:80:LYS:HE3	1.72	0.72
2:K:68:THR:HB	2:K:81:GLU:HB3	1.72	0.72
1:A:323:THR:OG1	1:A:331:ASN:OD1	2.08	0.71
1:B:56:VAL:HB	1:B:189:THR:HG22	1.72	0.71
1:D:332:ILE:HG22	1:D:475:ILE:HD11	1.71	0.71
1:C:326:ILE:HD12	3:T:59:PRO:HA	1.72	0.71
1:G:321:LEU:HD11	1:G:473:PRO:HB3	1.72	0.71
2:O:143:LYS:NZ	2:O:171:GLN:OE1	2.24	0.71
1:F:165:ASN:ND2	1:F:294:GLU:OE2	2.23	0.71
1:G:488:PHE:HB2	1:H:488:PHE:CZ	2.25	0.71
1:D:56:VAL:HB	1:D:189:THR:HG22	1.72	0.71
1:I:427:LYS:HG2	1:I:448:ASP:OD2	1.90	0.71
3:T:120:PRO:HD3	3:T:132:VAL:HG22	1.73	0.71
1:I:396:MET:HG3	1:I:488:PHE:HA	1.73	0.70
1:F:325:ASN:ND2	1:F:331:ASN:OD1	2.25	0.70
1:B:31:GLU:OE1	1:B:33:TYR:OH	2.08	0.70
1:G:323:THR:OG1	1:G:331:ASN:OD1	2.07	0.70
1:A:318:THR:O	1:A:339:ARG:NH2	2.25	0.70
2:N:82(B):SER:O	2:N:83:ARG:NH2	2.24	0.70
1:F:407:ILE:HD11	1:F:457:TYR:HB3	1.73	0.70
2:O:23:GLN:OE1	2:O:77:THR:OG1	2.08	0.69
1:A:407:ILE:HD12	1:C:145:GLY:HA2	1.74	0.69
3:U:113:PRO:HB3	3:U:139:PHE:HB3	1.73	0.69
3:U:186:TYR:O	3:U:192:TYR:OH	2.10	0.69
1:I:75:LYS:HB3	1:I:214:ILE:HG22	1.74	0.69
2:N:181:VAL:HG11	3:T:135:LEU:HD22	1.75	0.69
1:B:59:ILE:HB	1:B:297:LEU:HD21	1.75	0.69
1:B:167:ILE:HD12	1:B:189:THR:HG21	1.74	0.69
1:B:183:ASN:OD1	1:B:184:GLY:N	2.25	0.68
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.74	0.68
3:S:197:THR:HG22	3:S:204:PRO:HB3	1.75	0.68
2:L:142:VAL:HG11	2:L:150:VAL:HG11	1.75	0.68
3:U:120:PRO:HD3	3:U:132:VAL:HG22	1.74	0.68
1:B:145:GLY:HA2	1:C:407:ILE:HD12	1.74	0.68
2:K:33:ILE:HB	2:K:95:GLU:HB3	1.76	0.68
1:E:79:ILE:HG23	1:E:220:VAL:HG23	1.76	0.68
1:A:270:GLN:NE2	1:A:306:TYR:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:82(B):SER:O	2:J:83:ARG:NH2	2.27	0.67
1:E:30:GLU:OE1	1:E:441:TYR:OH	2.09	0.67
1:G:196:LYS:NZ	1:G:295:GLU:OE1	2.25	0.67
3:T:151:ASP:OD1	3:T:189:HIS:ND1	2.26	0.67
1:H:92:GLU:HG2	1:I:254:ASN:HD22	1.59	0.67
1:H:64:ILE:HD11	1:H:199:ILE:HG21	1.76	0.67
1:D:56:VAL:HG22	1:D:300:VAL:HG22	1.77	0.67
1:B:405:SER:HB2	1:B:452:VAL:HG21	1.77	0.67
3:Q:83:VAL:HG11	3:Q:166:GLN:HB3	1.77	0.67
3:S:120:PRO:HD3	3:S:132:VAL:HG22	1.77	0.67
3:S:181:LEU:HD22	3:S:185:ASP:OD2	1.95	0.67
1:G:206:ILE:O	1:G:209:GLN:NE2	2.24	0.67
2:M:93:ALA:HB1	2:M:100(I):PHE:HB3	1.76	0.67
1:C:315:LYS:HG2	1:C:317:HIS:CE1	2.31	0.66
1:I:79:ILE:HD13	1:I:207:LEU:HD11	1.75	0.66
3:R:113:PRO:HB3	3:R:139:PHE:HB3	1.77	0.66
1:I:491:SER:HB2	1:I:494:GLN:HG3	1.78	0.66
1:H:291:ILE:HD11	1:H:293:LYS:HB2	1.77	0.66
1:D:73:ASP:OD1	1:I:434:THR:OG1	2.09	0.66
1:E:405:SER:HB3	1:E:457:TYR:CE2	2.30	0.66
2:L:181:VAL:HG11	3:R:135:LEU:HD22	1.77	0.66
1:E:405:SER:HB3	1:E:457:TYR:HE2	1.60	0.66
1:H:64:ILE:HG12	1:H:83:LEU:HD21	1.76	0.66
2:J:143:LYS:NZ	2:J:171:GLN:OE1	2.27	0.66
2:K:139:GLY:HA2	2:K:154:TRP:HH2	1.60	0.66
1:G:241:ALA:HA	1:H:279:GLN:HG2	1.77	0.66
2:J:83:ARG:O	2:J:111:VAL:HG11	1.96	0.66
1:H:168:LYS:HZ1	1:H:295:GLU:HB2	1.60	0.66
1:I:29:THR:HG23	1:I:42:ARG:HB2	1.77	0.66
1:F:150:SER:OG	1:F:302:GLN:OE1	2.13	0.65
1:F:261:ILE:HA	1:F:264:MET:HE2	1.77	0.65
2:J:195:ILE:HD12	2:J:210:ARG:HG2	1.78	0.65
1:B:229:ARG:NE	1:B:250:TYR:O	2.28	0.65
2:L:68:THR:HB	2:L:81:GLU:HB3	1.79	0.65
1:D:90:VAL:HG13	1:D:292:ILE:HD11	1.77	0.65
1:C:423:THR:HG21	1:C:431:ILE:HG13	1.78	0.65
1:D:335:THR:HB	1:D:396:MET:HG2	1.77	0.65
1:G:246:PRO:HB3	1:G:283:GLN:HA	1.79	0.65
3:S:146:VAL:HG22	3:S:196:VAL:HG22	1.79	0.65
1:B:291:ILE:HD11	1:B:293:LYS:HB3	1.79	0.65
1:F:148:ILE:HA	1:F:302:GLN:HE22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:ILE:HG23	1:F:475:ILE:HD11	1.79	0.65
1:G:423:THR:HG21	1:G:431:ILE:HG12	1.79	0.65
1:H:261:ILE:HA	1:H:264:MET:HE2	1.78	0.65
1:F:73:ASP:HB3	1:F:76:VAL:HG23	1.79	0.65
1:F:196:LYS:NZ	1:F:295:GLU:HG3	2.12	0.65
2:K:126:PRO:HG2	2:K:213:PRO:HG3	1.79	0.65
2:L:123:PRO:HB3	2:L:211:VAL:HG12	1.77	0.65
1:D:270:GLN:HG2	1:D:309:ILE:HD12	1.79	0.65
1:G:458:TYR:CD2	1:I:150:SER:HB3	2.32	0.65
1:B:350:SER:OG	1:C:454:ASN:ND2	2.30	0.64
1:G:488:PHE:CZ	1:I:488:PHE:HB2	2.32	0.64
1:G:442:VAL:HG11	1:G:447:VAL:HG21	1.79	0.64
1:B:488:PHE:HB2	1:C:488:PHE:CZ	2.32	0.64
1:F:243:VAL:HG22	1:F:288:ILE:HG23	1.79	0.64
1:H:168:LYS:HZ2	1:H:295:GLU:HB2	1.62	0.64
2:J:181:VAL:HG11	3:P:135:LEU:HD22	1.79	0.64
2:L:119:PRO:HB3	2:L:145:TYR:HB3	1.79	0.64
2:K:30:GLU:HB2	2:K:73:GLU:OE2	1.98	0.64
2:K:30:GLU:HG3	2:K:53:VAL:HG22	1.80	0.64
1:H:145:GLY:HA2	1:I:407:ILE:HD12	1.80	0.64
3:P:151:ASP:HA	3:P:191:VAL:HG13	1.79	0.64
3:Q:148:TRP:HB2	3:Q:155:GLN:HB2	1.79	0.64
2:N:143:LYS:NZ	2:N:171:GLN:OE1	2.30	0.64
1:D:452:VAL:O	1:D:455:THR:OG1	2.16	0.63
2:O:53:VAL:HG13	2:O:54:LEU:HD22	1.80	0.63
1:H:423:THR:HG21	1:H:431:ILE:HG12	1.80	0.63
1:G:159:HIS:NE2	1:G:291:ILE:HD13	2.14	0.63
1:G:292:ILE:HD12	1:G:297:LEU:HD12	1.80	0.63
2:K:93:ALA:HB1	2:K:100(I):PHE:HB3	1.81	0.63
1:D:402:ILE:HG21	1:F:373:LEU:HD13	1.81	0.63
1:G:261:ILE:HA	1:G:264:MET:HE2	1.81	0.62
3:P:167:ASP:OD1	3:P:169:LYS:HG2	1.99	0.62
2:K:123:PRO:HB3	2:K:211:VAL:HG12	1.82	0.62
1:C:318:THR:O	1:C:339:ARG:NH2	2.33	0.62
2:J:123:PRO:HD3	2:J:209:LYS:HE2	1.82	0.62
3:Q:197:THR:HG22	3:Q:204:PRO:HB3	1.81	0.62
1:A:373:LEU:HD13	1:B:402:ILE:HG21	1.81	0.62
1:D:423:THR:HG21	1:D:431:ILE:HG12	1.82	0.62
1:H:261:ILE:HD13	1:H:264:MET:HE1	1.82	0.62
3:Q:158:ASN:ND2	3:Q:179:LEU:HD13	2.14	0.62
1:B:209:GLN:NE2	1:F:441:TYR:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:494:GLN:NE2	1:I:399:LYS:HB3	2.14	0.62
1:H:405:SER:HB2	1:H:452:VAL:HG21	1.81	0.62
1:G:73:ASP:HB3	1:G:76:VAL:HG23	1.82	0.62
1:B:150:SER:HB3	1:C:458:TYR:CD2	2.35	0.62
1:C:56:VAL:HB	1:C:189:THR:HG22	1.81	0.62
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.82	0.62
1:G:488:PHE:HZ	1:I:488:PHE:HB2	1.64	0.61
3:R:35:TRP:HB2	3:R:48:ILE:HB	1.81	0.61
1:C:183:ASN:OD1	1:C:184:GLY:N	2.33	0.61
1:E:488:PHE:HB3	1:F:488:PHE:CZ	2.34	0.61
1:C:315:LYS:HE3	1:C:341:TRP:CH2	2.34	0.61
1:F:183:ASN:OD1	1:F:184:GLY:N	2.33	0.61
1:C:60:GLU:HG2	1:C:296:VAL:HG22	1.82	0.61
1:A:56:VAL:HB	1:A:189:THR:HG22	1.82	0.61
1:E:214:ILE:HD11	1:E:219:THR:HB	1.82	0.61
3:Q:137:ASN:OD1	3:Q:138:ASN:ND2	2.34	0.61
1:C:267:THR:HG22	1:C:269:ASP:H	1.66	0.61
1:B:432:ILE:HD11	1:B:447:VAL:HG22	1.83	0.61
1:D:374:THR:HG21	1:E:453:GLY:HA3	1.81	0.61
1:G:402:ILE:HG21	1:I:373:LEU:HD13	1.82	0.61
3:S:186:TYR:O	3:S:192:TYR:OH	2.18	0.61
1:I:33:TYR:HE2	1:I:383:ASN:HB3	1.65	0.60
1:D:49:ARG:NH1	1:D:51:GLY:O	2.34	0.60
3:U:37:GLN:HB2	3:U:47:LEU:HD11	1.82	0.60
1:H:335:THR:HB	1:H:396:MET:HG2	1.84	0.60
1:B:201:ASN:HB2	1:F:429:ARG:NH2	2.13	0.60
3:R:40:PRO:HB3	3:R:165:GLU:HG3	1.82	0.60
3:T:190:LYS:HD2	3:T:211:ARG:HB3	1.83	0.60
1:D:157:VAL:HG11	1:D:181:LEU:HB3	1.83	0.60
1:G:407:ILE:HD12	1:I:145:GLY:HA2	1.84	0.60
2:N:11:VAL:HB	2:N:147:PRO:HG3	1.84	0.60
1:B:394:LYS:HZ2	1:C:402:ILE:HD11	1.66	0.59
1:C:232:GLU:HG2	1:C:250:TYR:CD2	2.36	0.59
1:G:505:PHE:HE2	1:I:505:PHE:HB3	1.66	0.59
1:F:196:LYS:HZ3	1:F:295:GLU:HG3	1.67	0.59
3:R:120:PRO:HD3	3:R:132:VAL:HG22	1.83	0.59
1:B:261:ILE:HA	1:B:264:MET:HE2	1.84	0.59
1:E:289:MET:HG2	1:E:299:TYR:HB3	1.85	0.59
1:B:498:LYS:NZ	1:C:486:ASP:HB3	2.17	0.59
1:G:56:VAL:HB	1:G:189:THR:HG22	1.85	0.59
3:T:37:GLN:HB2	3:T:47:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:LEU:HD13	1:G:364:ARG:NH1	2.17	0.59
2:M:11:VAL:HB	2:M:147:PRO:HG3	1.85	0.59
3:P:108:ARG:NH1	3:P:109:THR:O	2.31	0.59
1:A:279:GLN:HG2	1:C:241:ALA:HA	1.84	0.59
1:A:452:VAL:O	1:A:455:THR:OG1	2.20	0.59
1:I:183:ASN:OD1	1:I:184:GLY:N	2.36	0.58
2:O:93:ALA:HB1	2:O:100(I):PHE:HB3	1.84	0.58
1:B:491:SER:HB2	1:B:494:GLN:HG3	1.84	0.58
1:D:167:ILE:HD12	1:D:189:THR:HG21	1.85	0.58
1:B:308:VAL:HG21	1:B:345:ASN:ND2	2.18	0.58
1:H:183:ASN:OD1	1:H:184:GLY:N	2.34	0.58
1:I:326:ILE:HG21	3:R:59:PRO:HA	1.85	0.58
1:G:167:ILE:HD12	1:G:189:THR:HG21	1.83	0.58
2:N:93:ALA:HB1	2:N:100(I):PHE:HB3	1.84	0.58
1:H:273:LEU:HD13	1:H:364:ARG:HH11	1.69	0.58
2:K:119:PRO:HB3	2:K:145:TYR:HB3	1.84	0.58
2:N:160:THR:O	2:N:163:VAL:HG22	2.03	0.58
1:B:176:LYS:HG2	1:B:190:PHE:CE1	2.38	0.58
1:C:79:ILE:HD12	1:C:207:LEU:HD11	1.85	0.58
1:E:423:THR:HG23	1:E:431:ILE:HG23	1.84	0.58
1:F:208:ASN:ND2	2:M:96:THR:O	2.35	0.58
1:G:505:PHE:CE2	1:I:505:PHE:HB3	2.38	0.58
3:T:66:GLY:HA3	3:T:71:PHE:HA	1.85	0.58
1:G:335:THR:HB	1:G:396:MET:HG2	1.86	0.58
1:G:426:ASN:HB3	1:G:429:ARG:HB2	1.85	0.58
3:U:137:ASN:OD1	3:U:138:ASN:ND2	2.36	0.58
2:M:36:TRP:CE2	2:M:80:MET:HB2	2.39	0.58
1:B:150:SER:OG	1:B:302:GLN:NE2	2.37	0.57
1:G:73:ASP:OD1	1:G:74:THR:N	2.37	0.57
1:F:429:ARG:HG3	1:F:429:ARG:NH1	2.19	0.57
3:Q:186:TYR:O	3:Q:192:TYR:OH	2.22	0.57
1:B:463:GLU:OE1	1:B:463:GLU:N	2.31	0.57
1:F:56:VAL:HB	1:F:189:THR:HG22	1.85	0.57
3:R:167:ASP:OD1	3:R:169:LYS:HG2	2.05	0.57
1:C:317:HIS:HD2	1:C:408:THR:HG22	1.69	0.57
1:A:67:THR:HA	2:J:99:VAL:HG13	1.86	0.57
1:C:463:GLU:OE1	1:C:463:GLU:N	2.26	0.57
1:D:165:ASN:ND2	1:D:294:GLU:OE2	2.32	0.57
1:A:423:THR:HG21	1:A:431:ILE:HG12	1.85	0.57
1:C:405:SER:HB3	1:C:457:TYR:CE2	2.40	0.57
1:D:157:VAL:HG21	1:D:183:ASN:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:407:ILE:HD11	1:I:457:TYR:HB3	1.86	0.57
3:S:6:GLN:NE2	3:S:86:TYR:O	2.34	0.57
1:A:427:LYS:HG2	1:A:448:ASP:OD2	2.05	0.57
1:B:192:VAL:HG11	1:B:229:ARG:HH22	1.69	0.57
1:C:40:VAL:HA	1:C:315:LYS:O	2.04	0.57
1:E:423:THR:HG21	1:E:431:ILE:HG12	1.86	0.57
1:I:336:ARG:NH2	1:I:383:ASN:OD1	2.37	0.57
2:M:66:ARG:CZ	2:M:83:ARG:HH12	2.18	0.57
1:B:190:PHE:HE2	1:B:260:LEU:HB2	1.69	0.57
1:A:335:THR:HB	1:A:396:MET:HG2	1.86	0.56
1:D:150:SER:OG	1:D:302:GLN:NE2	2.38	0.56
1:G:93:LEU:HD13	1:G:297:LEU:HD11	1.88	0.56
2:J:93:ALA:HB1	2:J:100(I):PHE:HB3	1.86	0.56
2:L:93:ALA:HB1	2:L:100(I):PHE:HB3	1.86	0.56
3:S:167:ASP:OD1	3:S:169:LYS:HG2	2.05	0.56
1:A:494:GLN:NE2	1:B:399:LYS:HB2	2.21	0.56
1:E:67:THR:OG1	1:E:80:LYS:HE3	2.03	0.56
1:G:56:VAL:HG22	1:G:300:VAL:HG22	1.86	0.56
1:H:176:LYS:HG2	1:H:190:PHE:CE1	2.39	0.56
1:I:49:ARG:HE	1:I:368:ASP:CG	2.08	0.56
1:I:214:ILE:HD11	1:I:219:THR:HB	1.86	0.56
1:I:405:SER:HB3	1:I:457:TYR:CE2	2.41	0.56
2:O:18:VAL:HB	2:O:82(C):LEU:HD11	1.86	0.56
3:P:137:ASN:OD1	3:P:138:ASN:ND2	2.38	0.56
3:U:190:LYS:NZ	3:U:210:ASN:HB3	2.20	0.56
1:E:318:THR:O	1:E:339:ARG:NH2	2.38	0.56
1:F:291:ILE:HD11	1:F:293:LYS:HG3	1.86	0.56
1:G:432:ILE:HD11	1:G:447:VAL:HG22	1.86	0.56
1:D:26:GLN:N	1:D:363:ASN:HD21	2.03	0.56
1:F:81:GLN:O	1:F:81:GLN:NE2	2.39	0.56
1:H:198:TYR:HE2	1:H:223:PHE:HD1	1.54	0.56
1:G:75:LYS:CE	1:G:213:ARG:HH21	2.19	0.56
3:P:146:VAL:HG22	3:P:196:VAL:HG22	1.88	0.56
1:B:394:LYS:NZ	1:C:400:THR:HG23	2.21	0.56
1:D:487:GLU:OE2	1:D:498:LYS:HD3	2.06	0.56
2:N:123:PRO:O	3:T:121:SER:OG	2.22	0.56
1:B:399:LYS:HG3	1:B:485:SER:HB2	1.88	0.55
1:C:405:SER:HB3	1:C:457:TYR:HE2	1.71	0.55
1:F:154:VAL:O	1:F:158:LEU:HD12	2.06	0.55
1:F:210:GLN:HB3	1:F:213:ARG:HG2	1.86	0.55
1:G:38:SER:HB2	1:G:316:LEU:HD11	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:123:PRO:O	3:S:121:SER:OG	2.24	0.55
1:A:68:LYS:H	2:J:99:VAL:HG22	1.71	0.55
1:D:442:VAL:HG11	1:D:447:VAL:HG21	1.88	0.55
1:H:59:ILE:HB	1:H:297:LEU:HD21	1.88	0.55
1:I:336:ARG:HH12	1:I:382:CYS:HB3	1.70	0.55
1:C:208:ASN:ND2	2:K:96:THR:O	2.38	0.55
1:D:284:GLN:OE1	1:D:306:TYR:OH	2.18	0.55
1:H:73:ASP:OD1	1:H:74:THR:N	2.40	0.55
2:J:150:VAL:HG22	2:J:200:HIS:HB2	1.87	0.55
3:P:37:GLN:HB2	3:P:47:LEU:HD11	1.87	0.55
1:B:369:THR:O	1:C:455:THR:HG22	2.05	0.55
1:F:429:ARG:HG3	1:F:429:ARG:HH11	1.71	0.55
2:L:169:VAL:HG21	3:R:160:GLN:HB3	1.89	0.55
1:A:512:LEU:HD11	1:B:515:ALA:HB3	1.89	0.55
1:G:163:GLU:OE2	1:G:182:SER:N	2.37	0.55
1:D:321:LEU:HD11	1:D:473:PRO:HB3	1.89	0.55
3:T:35:TRP:HB2	3:T:48:ILE:HB	1.89	0.55
1:A:405:SER:HB3	1:A:457:TYR:CE2	2.42	0.55
1:C:73:ASP:OD1	1:C:74:THR:N	2.40	0.55
1:G:373:LEU:HD13	1:H:402:ILE:HD13	1.89	0.55
1:I:39:ALA:HB2	1:I:413:ILE:HD11	1.88	0.55
1:C:428:ASN:O	1:C:428:ASN:ND2	2.24	0.55
3:S:114:SER:HB2	3:S:137:ASN:HB3	1.89	0.55
3:T:197:THR:HG22	3:T:204:PRO:HB3	1.88	0.55
1:E:93:LEU:O	1:E:97:THR:HG23	2.06	0.54
1:E:387:PHE:HE2	1:E:474:ILE:HD12	1.73	0.54
1:H:162:GLY:O	1:H:166:LYS:HG3	2.07	0.54
3:T:108:ARG:HD2	3:T:171:SER:HB2	1.89	0.54
1:A:320:PRO:HG3	1:C:141:LEU:HD11	1.89	0.54
1:C:452:VAL:O	1:C:455:THR:OG1	2.25	0.54
2:N:51:ILE:HG13	2:N:57:VAL:HG22	1.90	0.54
1:D:463:GLU:OE1	1:D:463:GLU:N	2.33	0.54
3:Q:19:VAL:HG21	3:Q:78:LEU:HD22	1.88	0.54
1:B:49:ARG:O	1:B:369:THR:HG23	2.08	0.54
1:B:394:LYS:HZ1	1:C:400:THR:HG23	1.72	0.54
1:H:92:GLU:HG2	1:I:254:ASN:ND2	2.22	0.54
2:L:30:GLU:HG3	2:L:53:VAL:HG22	1.89	0.54
3:P:187:GLU:HA	3:P:211:ARG:HH22	1.72	0.54
3:S:39:LYS:HB2	3:S:42:LYS:HD2	1.89	0.54
2:J:142:VAL:HG11	2:J:150:VAL:HG11	1.89	0.54
2:N:83:ARG:O	2:N:111:VAL:HG11	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:108:ARG:HH12	3:R:111:ALA:HB2	1.71	0.54
1:I:408:THR:O	1:I:460:ASN:ND2	2.40	0.54
1:A:150:SER:HB3	1:B:458:TYR:CD2	2.42	0.54
1:B:387:PHE:HE2	1:B:474:ILE:HD12	1.72	0.54
1:D:400:THR:OG1	1:F:394:LYS:NZ	2.40	0.54
1:I:46:SER:HG	1:I:311:THR:H	1.54	0.54
2:L:160:THR:O	2:L:163:VAL:HG22	2.07	0.54
2:N:23:GLN:NE2	2:N:24:ALA:O	2.39	0.54
3:R:151:ASP:OD1	3:R:189:HIS:ND1	2.40	0.54
3:S:148:TRP:HB2	3:S:155:GLN:HB2	1.89	0.54
1:I:162:GLY:O	1:I:166:LYS:HG3	2.07	0.54
1:A:90:VAL:HG13	1:A:292:ILE:HD11	1.89	0.53
1:F:321:LEU:HD11	1:F:473:PRO:HB3	1.89	0.53
2:K:139:GLY:HA2	2:K:154:TRP:CH2	2.43	0.53
3:R:190:LYS:HD2	3:R:211:ARG:HB3	1.89	0.53
1:A:291:ILE:O	1:A:291:ILE:CD1	2.51	0.53
1:C:442:VAL:HG11	1:C:447:VAL:HG21	1.90	0.53
1:D:458:TYR:CD2	1:F:150:SER:HB3	2.43	0.53
2:L:83:ARG:O	2:L:111:VAL:HG11	2.07	0.53
3:S:83:VAL:HG11	3:S:166:GLN:HB3	1.90	0.53
1:A:145:GLY:HA2	1:B:407:ILE:HD12	1.91	0.53
1:I:336:ARG:HH12	1:I:382:CYS:C	2.10	0.53
3:Q:167:ASP:OD1	3:Q:169:LYS:HG2	2.08	0.53
1:F:326:ILE:HD12	3:P:59:PRO:HA	1.90	0.53
1:G:232:GLU:HG2	1:G:250:TYR:CD2	2.44	0.53
1:I:69:CYS:HB2	1:I:80:LYS:HE3	1.89	0.53
2:J:146:PHE:HB2	2:J:175:LEU:HD22	1.89	0.53
3:P:186:TYR:O	3:P:211:ARG:NH2	2.41	0.53
1:D:218:GLU:OE1	1:F:75:LYS:HE3	2.08	0.53
1:E:498:LYS:HZ3	1:F:486:ASP:HB2	1.73	0.53
1:F:76:VAL:HG22	1:F:212:CYS:O	2.08	0.53
3:R:37:GLN:HB2	3:R:47:LEU:HD11	1.90	0.53
1:G:49:ARG:O	1:G:369:THR:HG23	2.09	0.53
1:G:56:VAL:HG23	1:G:187:VAL:HG21	1.88	0.53
1:C:176:LYS:NZ	1:C:259:SER:OG	2.33	0.53
1:E:183:ASN:OD1	1:E:184:GLY:N	2.42	0.53
1:E:445:LYS:HZ1	1:E:464:GLY:H	1.55	0.53
1:H:378:GLU:HG2	1:H:390:LYS:HD2	1.91	0.53
3:R:119:PRO:HB3	3:R:209:PHE:CE1	2.44	0.53
1:D:370:MET:HG3	1:E:457:TYR:HE1	1.73	0.53
3:P:19:VAL:HG21	3:P:78:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:LYS:HG2	1:C:448:ASP:OD2	2.09	0.53
1:E:209:GLN:NE2	1:I:442:VAL:HG13	2.23	0.53
1:F:73:ASP:OD1	1:F:74:THR:N	2.42	0.53
1:G:232:GLU:HG2	1:G:250:TYR:CG	2.44	0.53
1:A:455:THR:HG22	1:C:369:THR:O	2.08	0.52
1:D:73:ASP:HB3	1:D:76:VAL:HG23	1.91	0.52
1:F:176:LYS:HG2	1:F:190:PHE:CE1	2.44	0.52
1:D:279:GLN:HG2	1:F:241:ALA:HA	1.90	0.52
1:E:192:VAL:HG11	1:E:229:ARG:NH1	2.23	0.52
1:H:321:LEU:HD11	1:H:473:PRO:HB3	1.91	0.52
2:M:126:PRO:HG2	2:M:213:PRO:HG3	1.92	0.52
1:A:56:VAL:O	1:A:189:THR:HA	2.10	0.52
1:G:28:ILE:HG13	1:G:410:LEU:HD11	1.91	0.52
1:I:204:LEU:HD12	2:O:99:VAL:O	2.09	0.52
1:C:76:VAL:HG22	1:C:212:CYS:HB2	1.91	0.52
2:M:68:THR:HB	2:M:81:GLU:HB3	1.92	0.52
1:E:140:PHE:HD1	1:E:140:PHE:H	1.56	0.52
3:R:83:VAL:HG11	3:R:166:GLN:HB3	1.92	0.52
1:D:486:ASP:OD2	1:F:487:GLU:HA	2.09	0.52
1:E:338:ASP:HB2	1:E:342:TYR:OH	2.10	0.52
1:C:38:SER:HB2	1:C:316:LEU:HD11	1.92	0.52
1:F:445:LYS:HZ1	1:F:464:GLY:H	1.58	0.52
1:I:56:VAL:HG22	1:I:300:VAL:HG22	1.92	0.52
2:O:82(B):SER:O	2:O:83:ARG:NH2	2.42	0.52
3:T:167:ASP:OD1	3:T:169:LYS:HG2	2.09	0.52
1:A:454:ASN:H	1:C:374:THR:HG21	1.75	0.52
1:B:162:GLY:O	1:B:166:LYS:HG3	2.10	0.52
1:C:49:ARG:HE	1:C:368:ASP:CG	2.12	0.52
1:C:308:VAL:HG21	1:C:345:ASN:ND2	2.24	0.52
1:E:243:VAL:HG22	1:E:288:ILE:HG23	1.92	0.52
1:G:141:LEU:HD13	1:H:402:ILE:HD12	1.92	0.52
1:H:66:GLU:HB3	1:H:68:LYS:HE2	1.92	0.52
1:C:405:SER:HB2	1:C:452:VAL:HG21	1.92	0.52
1:F:268:ASN:HA	1:F:271:LYS:HB2	1.92	0.52
1:H:35:SER:O	1:H:474:ILE:HG12	2.10	0.52
1:C:151:GLY:HA3	1:C:288:ILE:HD12	1.92	0.51
1:G:270:GLN:NE2	1:G:306:TYR:O	2.43	0.51
1:E:59:ILE:HB	1:E:297:LEU:CD2	2.41	0.51
1:E:167:ILE:HD12	1:E:189:THR:HG21	1.92	0.51
1:F:415:SER:HB3	1:F:417:TYR:CE2	2.45	0.51
1:F:444:ASN:ND2	1:F:462:LEU:O	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:387:PHE:CE2	1:I:474:ILE:HD12	2.45	0.51
2:M:139:GLY:HA2	2:M:154:TRP:HH2	1.76	0.51
3:R:80:PRO:HA	3:R:106:ILE:HG13	1.93	0.51
1:E:188:LEU:HD23	1:E:260:LEU:HD12	1.92	0.51
1:G:405:SER:HB3	1:G:457:TYR:CE2	2.46	0.51
3:P:197:THR:HG22	3:P:204:PRO:HB3	1.92	0.51
3:U:190:LYS:HZ3	3:U:210:ASN:HB3	1.75	0.51
3:S:106:ILE:H	3:S:166:GLN:HE22	1.58	0.51
1:B:75:LYS:HE3	1:B:217:ILE:HG13	1.92	0.51
1:B:357:THR:HG21	1:B:371:ASN:HB2	1.92	0.51
1:C:178:VAL:HG12	1:C:188:LEU:HD12	1.92	0.51
1:E:217:ILE:HD13	1:F:218:GLU:HG2	1.92	0.51
1:C:445:LYS:NZ	1:C:464:GLY:H	2.09	0.51
1:D:405:SER:HB3	1:D:457:TYR:CE2	2.46	0.51
1:H:217:ILE:O	1:H:220:VAL:HG12	2.11	0.51
2:L:45:PRO:HG2	3:R:98:PHE:CD2	2.46	0.51
1:B:79:ILE:HD11	1:B:203:LEU:HD11	1.92	0.51
1:E:59:ILE:HB	1:E:297:LEU:HD21	1.91	0.51
1:F:167:ILE:HD11	1:F:181:LEU:HD21	1.93	0.51
1:H:423:THR:HG23	1:H:431:ILE:HG23	1.92	0.51
1:E:445:LYS:HZ3	1:E:463:GLU:HA	1.75	0.51
1:G:49:ARG:HE	1:G:368:ASP:CG	2.13	0.51
1:I:176:LYS:HG2	1:I:190:PHE:CE1	2.46	0.51
3:P:155:GLN:HB3	3:P:158:ASN:HD21	1.76	0.51
1:B:30:GLU:OE1	1:B:441:TYR:OH	2.28	0.51
1:B:67:THR:HG21	1:B:83:LEU:HD13	1.93	0.51
1:F:499:ILE:O	1:F:503:LEU:N	2.39	0.51
1:D:405:SER:HB2	1:D:452:VAL:HG21	1.93	0.50
1:F:267:THR:HG22	1:F:269:ASP:H	1.76	0.50
1:H:491:SER:HB2	1:H:494:GLN:HG3	1.93	0.50
2:K:94:THR:OG1	2:K:102:ASN:HB3	2.11	0.50
1:B:423:THR:HG23	1:B:431:ILE:HG23	1.92	0.50
1:G:448:ASP:OD1	1:G:461:LYS:NZ	2.33	0.50
2:K:121:VAL:HA	2:K:141:LEU:O	2.11	0.50
1:A:35:SER:O	1:A:474:ILE:HG12	2.12	0.50
1:G:68:LYS:H	2:N:99:VAL:HG22	1.77	0.50
1:I:463:GLU:OE1	1:I:463:GLU:N	2.31	0.50
2:L:117:LYS:HD3	2:L:175:LEU:HD11	1.94	0.50
2:O:126:PRO:HG2	2:O:213:PRO:HG3	1.92	0.50
2:O:181:VAL:HG11	3:U:135:LEU:HD22	1.94	0.50
1:D:241:ALA:HA	1:E:279:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:SER:HB3	1:F:457:TYR:CE2	2.47	0.50
1:G:178:VAL:HG12	1:G:188:LEU:HD12	1.92	0.50
2:K:100(H):TYR:HB3	3:Q:34:ASN:ND2	2.26	0.50
3:R:186:TYR:O	3:R:192:TYR:OH	2.27	0.50
1:A:266:ILE:HG13	1:A:271:LYS:HG3	1.94	0.50
1:B:62:SER:HB3	1:B:196:LYS:HG2	1.94	0.50
1:B:209:GLN:HG3	1:F:442:VAL:HG13	1.92	0.50
1:B:423:THR:HG21	1:B:431:ILE:HG12	1.94	0.50
1:D:270:GLN:HE22	1:D:307:GLY:HA2	1.77	0.50
1:H:375:LEU:HB3	1:H:379:VAL:HG21	1.94	0.50
1:I:73:ASP:OD1	1:I:74:THR:N	2.45	0.50
1:I:321:LEU:HD11	1:I:473:PRO:HB3	1.94	0.50
2:J:160:THR:O	2:J:163:VAL:HG22	2.11	0.50
2:L:154:TRP:CZ3	2:L:196:CYS:HB3	2.47	0.50
3:Q:125:LEU:HD22	3:Q:183:LYS:HG3	1.94	0.50
1:A:310:ASP:OD1	1:A:364:ARG:NH1	2.45	0.50
1:D:217:ILE:HG21	1:F:217:ILE:HG21	1.93	0.50
1:E:96:LEU:HD11	1:E:238:SER:HA	1.94	0.50
1:F:37:CYS:SG	1:F:319:SER:HB3	2.52	0.50
2:O:97:ALA:HB1	2:O:100:VAL:HG11	1.93	0.50
3:R:15:VAL:HG22	3:R:106:ILE:HD12	1.94	0.50
1:D:49:ARG:HE	1:D:368:ASP:CG	2.15	0.50
1:E:73:ASP:H	1:E:76:VAL:HG22	1.77	0.50
1:I:150:SER:HG	1:I:302:GLN:NE2	2.10	0.50
3:Q:151:ASP:HA	3:Q:191:VAL:HG13	1.92	0.50
1:F:321:LEU:HD21	1:F:473:PRO:HB3	1.94	0.50
1:F:397:THR:HB	1:F:483:PHE:HE2	1.75	0.50
1:F:491:SER:HB2	1:F:494:GLN:HG3	1.93	0.50
3:S:108:ARG:HD2	3:S:171:SER:HB2	1.94	0.50
1:A:338:ASP:HB2	1:A:342:TYR:OH	2.12	0.50
1:D:58:THR:O	1:D:191:LYS:HA	2.12	0.50
1:D:59:ILE:HB	1:D:297:LEU:HD21	1.94	0.50
1:G:334:LEU:HB2	1:G:475:ILE:HD13	1.94	0.50
3:R:19:VAL:HG21	3:R:78:LEU:HD22	1.92	0.50
1:C:308:VAL:HG21	1:C:345:ASN:HD21	1.77	0.49
1:D:414:VAL:HG21	1:D:435:PHE:CE2	2.47	0.49
1:F:190:PHE:HE2	1:F:260:LEU:HB2	1.76	0.49
1:I:386:ILE:HG21	1:I:474:ILE:HG13	1.94	0.49
2:L:137:ALA:HB2	2:L:183:THR:HG22	1.93	0.49
3:Q:158:ASN:HD22	3:Q:179:LEU:HD12	1.76	0.49
3:T:146:VAL:HG22	3:T:196:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ARG:NH2	1:A:508:ARG:HE	2.11	0.49
1:D:235:ARG:O	1:D:239:VAL:HG23	2.11	0.49
1:A:487:GLU:HA	1:B:486:ASP:OD2	2.11	0.49
1:E:315:LYS:HD2	1:E:341:TRP:CZ2	2.47	0.49
1:F:428:ASN:HB2	1:F:429:ARG:NH2	2.27	0.49
1:H:190:PHE:HE2	1:H:260:LEU:HB2	1.77	0.49
3:Q:116:PHE:HD2	3:Q:135:LEU:HD23	1.78	0.49
3:U:142:ARG:NH2	3:U:163:VAL:HG11	2.27	0.49
1:A:241:ALA:HA	1:B:279:GLN:CG	2.43	0.49
1:A:374:THR:HG21	1:B:454:ASN:N	2.13	0.49
1:E:190:PHE:HE2	1:E:260:LEU:HD13	1.75	0.49
1:H:56:VAL:HB	1:H:189:THR:HG22	1.94	0.49
1:I:56:VAL:HB	1:I:189:THR:HG22	1.94	0.49
2:O:66:ARG:NH2	2:O:86:ASP:OD1	2.37	0.49
1:H:477:TYR:HE1	2:L:195:ILE:HD13	1.78	0.49
1:A:49:ARG:NH1	1:A:52:TRP:CE2	2.81	0.49
1:B:315:LYS:HD2	1:B:341:TRP:CZ2	2.48	0.49
1:I:270:GLN:HG2	1:I:309:ILE:HD12	1.94	0.49
1:H:28:ILE:HG13	1:H:410:LEU:HD11	1.94	0.49
2:L:139:GLY:HA2	2:L:154:TRP:CH2	2.46	0.49
1:B:59:ILE:HB	1:B:297:LEU:CD2	2.43	0.49
1:I:424:ALA:HB2	1:I:435:PHE:CZ	2.47	0.49
1:A:405:SER:HB3	1:A:457:TYR:HE2	1.78	0.48
2:L:100(E):LEU:HB2	2:L:100(G):HIS:CE1	2.48	0.48
2:N:142:VAL:HG11	2:N:150:VAL:HG11	1.95	0.48
3:T:124:GLN:O	3:T:127:SER:OG	2.26	0.48
1:A:406:VAL:HB	1:A:413:ILE:HB	1.95	0.48
1:B:373:LEU:HD13	1:C:402:ILE:HD13	1.95	0.48
1:D:150:SER:HB3	1:E:458:TYR:CD2	2.48	0.48
1:G:185:VAL:HG13	1:H:427:LYS:NZ	2.27	0.48
1:H:64:ILE:HG21	1:H:83:LEU:HD11	1.95	0.48
1:I:31:GLU:OE1	1:I:33:TYR:OH	2.21	0.48
1:I:395:ILE:HD13	1:I:492:ILE:HD13	1.96	0.48
2:M:87:THR:OG1	2:M:111:VAL:HG12	2.13	0.48
2:M:139:GLY:HA2	2:M:154:TRP:CH2	2.48	0.48
1:B:93:LEU:HD23	1:B:96:LEU:HD12	1.95	0.48
1:G:373:LEU:HD13	1:H:402:ILE:HG21	1.95	0.48
1:H:270:GLN:NE2	1:H:306:TYR:O	2.38	0.48
3:Q:18:ARG:HG3	3:Q:76:SER:HA	1.94	0.48
1:A:56:VAL:HG23	1:A:187:VAL:HG21	1.94	0.48
1:A:95:LEU:HD22	1:B:278:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:SER:O	1:F:474:ILE:HG12	2.13	0.48
1:F:410:LEU:HB3	1:F:466:ASN:HD21	1.78	0.48
1:G:75:LYS:NZ	1:H:218:GLU:OE1	2.47	0.48
1:G:145:GLY:HA2	1:H:407:ILE:HD12	1.95	0.48
1:H:190:PHE:CE2	1:H:260:LEU:HB2	2.49	0.48
1:I:487:GLU:OE1	1:I:498:LYS:NZ	2.31	0.48
1:A:206:ILE:HD13	3:P:49:TYR:CE2	2.49	0.48
1:F:79:ILE:HD12	1:F:207:LEU:CD1	2.40	0.48
1:F:178:VAL:HG12	1:F:188:LEU:HD12	1.95	0.48
1:H:75:LYS:HE3	1:I:218:GLU:OE1	2.13	0.48
1:I:59:ILE:HB	1:I:297:LEU:HD21	1.95	0.48
2:L:94:THR:OG1	2:L:102:ASN:HB3	2.13	0.48
1:B:394:LYS:NZ	1:C:402:ILE:HD11	2.29	0.48
1:F:252:LEU:HD23	1:F:257:LEU:HD13	1.96	0.48
1:G:457:TYR:CE1	1:I:370:MET:HG3	2.49	0.48
1:I:423:THR:HG21	1:I:431:ILE:HG12	1.96	0.48
3:R:6:GLN:NE2	3:R:86:TYR:O	2.44	0.48
3:U:167:ASP:OD1	3:U:169:LYS:HG2	2.13	0.48
1:A:38:SER:HB2	1:A:316:LEU:HD11	1.96	0.48
1:C:491:SER:HB2	1:C:494:GLN:HG3	1.95	0.48
1:D:142:LEU:HA	1:D:373:LEU:HD21	1.95	0.48
1:E:71:GLY:O	1:E:76:VAL:HG21	2.13	0.48
1:G:171:LEU:O	1:G:191:LYS:NZ	2.35	0.48
2:K:100(G):HIS:HB2	2:K:100(H):TYR:HD1	1.79	0.48
2:M:123:PRO:HB3	2:M:211:VAL:HG12	1.95	0.48
1:E:498:LYS:HZ1	1:F:486:ASP:HB2	1.78	0.48
1:H:477:TYR:HA	2:L:192:GLN:HE22	1.79	0.48
2:O:186:SER:HA	2:O:189:LEU:HD13	1.95	0.48
3:S:37:GLN:HB2	3:S:47:LEU:HD11	1.96	0.48
1:A:405:SER:HB2	1:A:452:VAL:HG21	1.95	0.48
1:E:237:PHE:CE1	1:E:289:MET:HB2	2.49	0.48
1:G:441:TYR:OH	1:G:466:ASN:ND2	2.47	0.48
2:J:36:TRP:CE2	2:J:80:MET:HB2	2.49	0.48
2:L:36:TRP:CE2	2:L:80:MET:HB2	2.49	0.48
3:S:181:LEU:CD2	3:S:185:ASP:OD2	2.61	0.48
1:C:270:GLN:HG2	1:C:309:ILE:HD11	1.95	0.48
1:E:49:ARG:HE	1:E:368:ASP:CG	2.17	0.48
1:F:28:ILE:O	1:F:410:LEU:HD11	2.14	0.48
1:G:138:LEU:HA	1:G:140:PHE:CE1	2.49	0.48
1:G:405:SER:HB2	1:G:452:VAL:HG21	1.94	0.48
1:I:405:SER:HB3	1:I:457:TYR:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:24:GLN:HG2	3:P:70:ASP:OD1	2.14	0.48
3:R:137:ASN:OD1	3:R:138:ASN:ND2	2.46	0.48
1:G:35:SER:O	1:G:474:ILE:HG12	2.14	0.47
1:G:202:GLN:O	1:G:206:ILE:HG13	2.14	0.47
1:H:148:ILE:HB	1:H:288:ILE:HD11	1.96	0.47
1:A:176:LYS:HG2	1:A:190:PHE:CZ	2.49	0.47
1:B:336:ARG:HB3	1:B:338:ASP:OD1	2.15	0.47
1:D:36:THR:HB	1:D:336:ARG:HD2	1.95	0.47
1:D:352:PHE:CE2	1:D:367:CYS:HB3	2.49	0.47
1:D:487:GLU:CD	1:D:498:LYS:HZ3	2.17	0.47
1:G:444:ASN:ND2	1:G:462:LEU:O	2.35	0.47
1:B:261:ILE:HD12	1:B:274:MET:HB3	1.97	0.47
1:F:325:ASN:ND2	1:F:330:SER:O	2.47	0.47
1:G:61:LEU:HD13	1:G:90:VAL:HG22	1.96	0.47
2:K:96:THR:HG22	2:K:98:LEU:HD12	1.96	0.47
2:L:150:VAL:HG22	2:L:200:HIS:HB2	1.96	0.47
3:T:40:PRO:HB3	3:T:165:GLU:HG3	1.95	0.47
1:A:279:GLN:CG	1:C:241:ALA:HA	2.44	0.47
1:C:30:GLU:HB2	1:C:410:LEU:HD12	1.96	0.47
1:A:252:LEU:O	1:A:282:ARG:NH2	2.37	0.47
1:D:207:LEU:HD21	1:D:212:CYS:SG	2.54	0.47
1:G:273:LEU:HD13	1:G:364:ARG:HH11	1.77	0.47
1:A:76:VAL:HG22	1:A:212:CYS:O	2.15	0.47
1:A:291:ILE:HD12	1:A:291:ILE:C	2.34	0.47
1:A:458:TYR:CD2	1:C:150:SER:HB3	2.49	0.47
1:B:345:ASN:ND2	1:C:454:ASN:OD1	2.47	0.47
1:D:241:ALA:HA	1:E:279:GLN:CG	2.44	0.47
1:I:352:PHE:CE2	1:I:367:CYS:HB3	2.49	0.47
1:A:423:THR:CG2	1:A:431:ILE:HG12	2.45	0.47
1:A:426:ASN:HB2	1:A:432:ILE:HD11	1.96	0.47
1:B:292:ILE:HA	1:B:297:LEU:HA	1.96	0.47
1:C:142:LEU:HD23	1:C:373:LEU:HG	1.95	0.47
1:D:221:ILE:O	1:D:224:GLN:HG2	2.15	0.47
1:F:217:ILE:O	1:F:220:VAL:HG12	2.15	0.47
1:G:370:MET:HG3	1:H:457:TYR:CE1	2.50	0.47
1:H:76:VAL:HG12	1:H:80:LYS:HD3	1.96	0.47
1:H:216:ASN:ND2	1:H:218:GLU:OE2	2.48	0.47
2:N:184:VAL:HG21	2:N:194:TYR:CZ	2.49	0.47
2:O:33:ILE:HD11	2:O:100(D):TYR:HD2	1.79	0.47
1:A:246:PRO:HG2	1:C:239:VAL:HG12	1.96	0.47
1:B:240:ASN:HB3	1:B:243:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ILE:HD11	1:D:447:VAL:HG22	1.96	0.47
1:H:78:LEU:HB3	1:H:220:VAL:HG21	1.95	0.47
1:D:375:LEU:HD13	1:D:379:VAL:HG21	1.97	0.47
1:E:153:ALA:O	1:E:157:VAL:HG23	2.14	0.47
1:H:74:THR:O	1:H:78:LEU:HD23	2.13	0.47
2:K:184:VAL:HG22	2:K:185:PRO:HD2	1.96	0.47
1:E:202:GLN:HG3	1:I:432:ILE:HG22	1.96	0.47
1:F:407:ILE:HD13	1:F:458:TYR:O	2.14	0.47
1:G:150:SER:HB3	1:H:458:TYR:CD2	2.50	0.47
1:H:221:ILE:O	1:H:224:GLN:HG2	2.15	0.47
1:I:336:ARG:NH1	1:I:382:CYS:HB3	2.29	0.47
2:L:186:SER:HA	2:L:189:LEU:HD13	1.96	0.47
3:Q:37:GLN:HB2	3:Q:47:LEU:HD11	1.96	0.47
1:A:486:ASP:OD2	1:C:487:GLU:HA	2.15	0.46
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.97	0.46
1:C:75:LYS:HE3	1:C:75:LYS:HB2	1.70	0.46
1:C:338:ASP:HB2	1:C:342:TYR:OH	2.15	0.46
1:A:80:LYS:HE3	1:A:84:ASP:OD2	2.15	0.46
1:C:204:LEU:HD23	1:C:204:LEU:HA	1.71	0.46
1:D:373:LEU:HD13	1:E:402:ILE:HD13	1.97	0.46
1:H:448:ASP:OD1	1:H:461:LYS:NZ	2.37	0.46
3:T:113:PRO:HB3	3:T:139:PHE:HB3	1.96	0.46
1:A:68:LYS:N	2:J:99:VAL:HG22	2.30	0.46
1:A:513:LEU:HD11	1:C:512:LEU:HD11	1.97	0.46
1:C:208:ASN:ND2	2:K:97:ALA:HA	2.30	0.46
1:E:35:SER:O	1:E:474:ILE:HG12	2.14	0.46
1:H:338:ASP:HB2	1:H:342:TYR:OH	2.15	0.46
1:I:387:PHE:CZ	1:I:474:ILE:HG23	2.50	0.46
2:M:103:TRP:CE3	3:S:44:PRO:HD2	2.51	0.46
2:O:33:ILE:HB	2:O:95:GLU:HB3	1.97	0.46
1:A:56:VAL:HG22	1:A:300:VAL:HG22	1.98	0.46
1:A:218:GLU:HG2	1:C:75:LYS:CG	2.45	0.46
1:B:75:LYS:HD3	1:B:214:ILE:O	2.15	0.46
1:C:426:ASN:HB2	1:C:432:ILE:HD13	1.98	0.46
3:Q:155:GLN:HB3	3:Q:158:ASN:OD1	2.15	0.46
1:B:35:SER:O	1:B:474:ILE:HG12	2.15	0.46
1:B:78:LEU:HD23	1:B:220:VAL:HG11	1.96	0.46
1:F:427:LYS:HG2	1:F:448:ASP:OD2	2.16	0.46
1:F:507:ARG:HH22	1:F:508:ARG:HH21	1.62	0.46
1:H:53:TYR:HB2	1:H:305:ILE:HD11	1.96	0.46
1:A:237:PHE:HZ	1:A:287:SER:HG	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:PHE:CE2	1:C:474:ILE:HD12	2.50	0.46
1:C:461:LYS:HA	1:C:461:LYS:HD2	1.67	0.46
1:D:502:SER:O	1:D:506:ILE:HD13	2.16	0.46
2:M:160:THR:O	2:M:163:VAL:HG22	2.15	0.46
2:O:160:THR:O	2:O:163:VAL:HG22	2.16	0.46
1:A:171:LEU:HD21	1:A:189:THR:OG1	2.15	0.46
1:F:70:ASN:OD1	1:F:71:GLY:N	2.49	0.46
1:I:217:ILE:O	1:I:220:VAL:HG12	2.16	0.46
2:J:121:VAL:HA	2:J:141:LEU:O	2.15	0.46
2:O:11:VAL:HB	2:O:147:PRO:CG	2.42	0.46
3:U:197:THR:HG22	3:U:204:PRO:HB3	1.97	0.46
1:A:167:ILE:HD12	1:A:179:VAL:HG21	1.97	0.46
1:C:341:TRP:CZ3	1:C:341:TRP:CZ2	2.89	0.46
1:E:145:GLY:HA2	1:F:407:ILE:HD12	1.97	0.46
2:J:53:VAL:HG11	2:J:100:VAL:HG21	1.96	0.46
1:B:252:LEU:HD12	1:B:252:LEU:HA	1.82	0.46
1:D:394:LYS:HE2	1:E:400:THR:HG23	1.96	0.46
1:G:137:PHE:HE1	1:I:140:PHE:HB2	1.80	0.46
1:H:69:CYS:O	1:H:80:LYS:NZ	2.28	0.46
1:H:280:ILE:HG21	1:H:366:PHE:CG	2.51	0.46
1:C:188:LEU:HD21	1:C:263:ASP:HB3	1.98	0.46
1:E:178:VAL:HG12	1:E:188:LEU:HD12	1.98	0.46
1:E:261:ILE:HD13	1:E:264:MET:HE1	1.98	0.46
1:G:142:LEU:HA	1:G:373:LEU:HD21	1.98	0.46
1:H:224:GLN:OE1	1:I:225:GLN:NE2	2.49	0.46
2:J:18:VAL:HB	2:J:82(C):LEU:HD11	1.98	0.46
2:K:170:LEU:HD13	2:K:176:TYR:CE1	2.50	0.46
3:P:11:LEU:HD11	3:P:104:VAL:HG13	1.98	0.46
1:A:261:ILE:HD12	1:A:274:MET:HB3	1.98	0.45
1:A:454:ASN:HD22	1:C:345:ASN:CG	2.20	0.45
1:D:370:MET:HG3	1:E:457:TYR:CE1	2.51	0.45
1:G:345:ASN:O	1:H:454:ASN:ND2	2.49	0.45
1:H:235:ARG:O	1:H:239:VAL:HG23	2.16	0.45
1:I:97:THR:HG21	1:I:291:ILE:HA	1.97	0.45
1:I:167:ILE:HD12	1:I:189:THR:HG21	1.99	0.45
3:Q:108:ARG:HD2	3:Q:171:SER:HB2	1.97	0.45
1:A:73:ASP:OD1	1:A:74:THR:N	2.49	0.45
1:E:387:PHE:HZ	1:E:474:ILE:HG23	1.81	0.45
1:G:241:ALA:HA	1:H:279:GLN:CG	2.43	0.45
1:H:261:ILE:HD12	1:H:274:MET:HB3	1.97	0.45
2:J:184:VAL:HG21	2:J:194:TYR:OH	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:166:PHE:CE1	3:T:176:SER:HB3	2.52	0.45
3:T:33:LEU:HD22	3:T:71:PHE:CG	2.51	0.45
1:F:334:LEU:HD11	1:F:395:ILE:HB	1.97	0.45
1:H:243:VAL:HA	1:H:287:SER:O	2.15	0.45
1:I:142:LEU:HD23	1:I:373:LEU:HG	1.98	0.45
1:I:214:ILE:HD11	1:I:219:THR:CB	2.46	0.45
3:S:4:MET:HB2	3:S:99:GLY:HA2	1.99	0.45
1:A:77:LYS:HD2	1:A:77:LYS:HA	1.59	0.45
1:B:192:VAL:HG11	1:B:229:ARG:NH2	2.31	0.45
1:D:52:TRP:CE3	1:D:302:GLN:HG2	2.51	0.45
1:E:235:ARG:HG3	1:F:249:THR:OG1	2.17	0.45
1:F:140:PHE:HD1	1:F:140:PHE:H	1.64	0.45
1:F:320:PRO:O	1:F:417:TYR:OH	2.32	0.45
1:F:405:SER:HB3	1:F:457:TYR:CD2	2.51	0.45
1:F:445:LYS:HZ3	1:F:463:GLU:HA	1.80	0.45
1:I:220:VAL:O	1:I:224:GLN:HB2	2.17	0.45
1:I:452:VAL:O	1:I:455:THR:OG1	2.33	0.45
2:L:211:VAL:O	2:L:212:GLU:HG3	2.15	0.45
2:M:36:TRP:CZ3	2:M:92:CYS:HB2	2.52	0.45
1:A:87:LYS:O	1:A:91:THR:OG1	2.28	0.45
1:D:405:SER:HB3	1:D:457:TYR:CD2	2.52	0.45
1:D:414:VAL:HG21	1:D:435:PHE:HE2	1.80	0.45
1:F:426:ASN:OD1	1:F:427:LYS:N	2.50	0.45
1:G:181:LEU:HD12	1:G:185:VAL:HG23	1.99	0.45
1:G:223:PHE:O	1:G:227:ASN:N	2.44	0.45
1:H:204:LEU:N	1:H:205:PRO:HD2	2.32	0.45
1:H:231:LEU:HA	1:H:234:THR:HG22	1.98	0.45
2:N:18:VAL:HB	2:N:82(C):LEU:HD11	1.99	0.45
2:O:63:PHE:HB3	2:O:67:VAL:HG21	1.97	0.45
3:T:28:ASP:OD1	3:T:68:GLY:HA2	2.16	0.45
3:T:83:VAL:HG11	3:T:166:GLN:HB3	1.97	0.45
1:A:442:VAL:HG11	1:A:447:VAL:HG21	1.99	0.45
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.79	0.45
1:C:315:LYS:HE2	1:C:341:TRP:CE3	2.49	0.45
1:E:62:SER:HB3	1:E:196:LYS:HA	1.99	0.45
1:F:87:LYS:O	1:F:91:THR:OG1	2.28	0.45
1:G:199:ILE:HG23	1:G:204:LEU:HD23	1.99	0.45
2:J:29:LEU:HG	2:J:76:ASP:HA	1.98	0.45
2:L:163:VAL:HG12	2:L:182:VAL:HB	1.98	0.45
3:S:18:ARG:NH2	3:S:74:THR:HG21	2.32	0.45
1:A:192:VAL:HG23	1:A:193:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:HIS:CD2	1:C:408:THR:HA	2.52	0.45
1:D:328:GLU:OE1	1:D:328:GLU:N	2.29	0.45
1:E:56:VAL:HB	1:E:189:THR:HG22	1.99	0.45
1:H:39:ALA:HB2	1:H:413:ILE:HD11	1.99	0.45
1:I:338:ASP:HB2	1:I:342:TYR:OH	2.16	0.45
2:M:186:SER:HA	2:M:189:LEU:HD13	1.97	0.45
1:D:176:LYS:HG2	1:D:190:PHE:CZ	2.52	0.45
1:D:261:ILE:HA	1:D:264:MET:HE2	1.99	0.45
1:G:338:ASP:HB2	1:G:342:TYR:OH	2.16	0.45
1:H:241:ALA:H	1:I:279:GLN:NE2	2.15	0.45
1:I:386:ILE:HG12	1:I:492:ILE:HG13	1.99	0.45
1:I:461:LYS:HD2	1:I:461:LYS:HA	1.68	0.45
2:J:72:ASP:OD1	2:J:74:SER:OG	2.25	0.45
1:A:257:LEU:O	1:A:261:ILE:HG12	2.16	0.45
1:B:266:ILE:HG13	1:B:271:LYS:HG3	1.98	0.45
1:F:336:ARG:HB3	1:F:338:ASP:OD1	2.16	0.45
3:S:35:TRP:HB2	3:S:48:ILE:HB	1.99	0.45
3:U:166:GLN:NE2	3:U:171:SER:HB3	2.32	0.45
1:B:498:LYS:HZ3	1:C:486:ASP:HB3	1.80	0.45
1:C:202:GLN:O	1:C:206:ILE:HG13	2.16	0.45
1:D:260:LEU:HD22	1:D:303:LEU:HD12	1.99	0.45
1:E:73:ASP:OD1	1:E:74:THR:N	2.50	0.45
1:E:338:ASP:OD1	1:E:338:ASP:N	2.50	0.45
1:H:93:LEU:HD23	1:H:96:LEU:HD12	1.99	0.45
1:I:76:VAL:HG22	1:I:212:CYS:O	2.16	0.45
1:I:318:THR:O	1:I:406:VAL:HG21	2.16	0.45
2:M:181:VAL:HG11	3:S:135:LEU:HD22	1.99	0.45
1:A:176:LYS:NZ	1:A:190:PHE:CE2	2.84	0.44
1:C:209:GLN:HE22	2:K:101:ASP:HB2	1.82	0.44
1:F:90:VAL:HG13	1:F:292:ILE:HD11	1.99	0.44
1:F:171:LEU:HD21	1:F:189:THR:HB	1.99	0.44
1:F:235:ARG:O	1:F:239:VAL:HG23	2.17	0.44
1:H:198:TYR:CE2	1:H:223:PHE:HD1	2.35	0.44
1:H:432:ILE:HD11	1:H:447:VAL:HG22	1.99	0.44
1:B:52:TRP:CE3	1:B:302:GLN:HG2	2.52	0.44
1:B:146:SER:HB2	1:B:149:ALA:HB2	1.98	0.44
1:B:226:LYS:HD3	1:B:226:LYS:HA	1.65	0.44
1:D:99:ASN:O	1:D:100:THR:HG22	2.17	0.44
1:D:270:GLN:NE2	1:D:307:GLY:HA2	2.31	0.44
1:D:509:SER:HA	1:E:512:LEU:HD21	1.99	0.44
1:G:507:ARG:HH12	1:G:508:ARG:HH21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:GLN:HG2	3:Q:49:TYR:CZ	2.53	0.44
1:D:56:VAL:O	1:D:189:THR:HA	2.17	0.44
1:E:31:GLU:O	1:E:39:ALA:HA	2.18	0.44
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.88	0.44
1:G:56:VAL:O	1:G:189:THR:HA	2.17	0.44
1:I:190:PHE:HE2	1:I:260:LEU:HB2	1.83	0.44
2:O:166:PHE:CD2	3:U:164:THR:HG23	2.52	0.44
1:A:315:LYS:HD2	1:A:341:TRP:CZ2	2.51	0.44
1:A:415:SER:HB3	1:A:417:TYR:CE2	2.52	0.44
1:B:267:THR:HG22	1:B:269:ASP:H	1.83	0.44
1:E:484:PRO:HG2	1:E:495:VAL:HG13	1.99	0.44
1:E:508:ARG:HD3	1:F:509:SER:OG	2.18	0.44
1:F:33:TYR:CE2	1:F:383:ASN:HB3	2.52	0.44
1:F:195:LEU:HD23	1:F:195:LEU:HA	1.81	0.44
1:G:235:ARG:O	1:G:239:VAL:HG23	2.17	0.44
1:G:507:ARG:HH22	1:G:508:ARG:NH2	2.16	0.44
1:H:318:THR:O	1:H:339:ARG:NH2	2.50	0.44
3:U:143:GLU:OE1	3:U:143:GLU:N	2.49	0.44
1:B:202:GLN:HB2	1:F:429:ARG:HD2	1.98	0.44
1:B:235:ARG:O	1:B:239:VAL:HG23	2.18	0.44
1:B:308:VAL:HG21	1:B:345:ASN:HD21	1.83	0.44
1:C:318:THR:OG1	1:C:339:ARG:NH2	2.50	0.44
1:D:171:LEU:HD21	1:D:189:THR:OG1	2.17	0.44
1:D:243:VAL:HG22	1:D:288:ILE:HG22	1.99	0.44
1:E:64:ILE:HG21	1:E:83:LEU:HD11	1.99	0.44
1:E:217:ILE:O	1:E:220:VAL:HG12	2.18	0.44
1:G:50:THR:HG22	1:G:307:GLY:H	1.82	0.44
1:I:33:TYR:CE2	1:I:383:ASN:HB3	2.50	0.44
2:J:166:PHE:CD2	3:P:164:THR:HG23	2.52	0.44
2:L:170:LEU:HD13	2:L:176:TYR:CE1	2.53	0.44
3:P:108:ARG:HD3	3:P:109:THR:O	2.17	0.44
1:A:235:ARG:O	1:A:239:VAL:HG23	2.17	0.44
1:A:241:ALA:HA	1:B:279:GLN:HG2	1.99	0.44
1:B:235:ARG:HD3	1:C:250:TYR:CE2	2.53	0.44
1:C:75:LYS:O	1:C:79:ILE:HG12	2.18	0.44
1:D:414:VAL:HG11	1:D:435:PHE:HD2	1.83	0.44
1:E:270:GLN:NE2	1:E:306:TYR:O	2.51	0.44
1:E:387:PHE:CE2	2:J:158:ALA:HB2	2.52	0.44
1:F:405:SER:HB2	1:F:452:VAL:HG21	2.00	0.44
1:G:406:VAL:HG13	1:I:144:VAL:HG22	2.00	0.44
2:N:123:PRO:HB3	2:N:211:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:14:PRO:HD3	2:O:112:SER:C	2.37	0.44
2:O:123:PRO:CB	2:O:211:VAL:HG12	2.46	0.44
1:E:209:GLN:HE22	1:I:442:VAL:HG13	1.82	0.44
1:E:335:THR:HB	1:E:396:MET:HG2	1.98	0.44
1:F:97:THR:HG21	1:F:292:ILE:HG22	1.99	0.44
1:G:487:GLU:HA	1:H:486:ASP:OD2	2.18	0.44
1:H:159:HIS:CE1	1:H:291:ILE:HD13	2.52	0.44
1:E:50:THR:HG22	1:E:369:THR:HG21	1.99	0.44
1:E:291:ILE:HG22	1:E:298:ALA:O	2.18	0.44
1:F:386:ILE:HG21	1:F:474:ILE:HG13	2.00	0.44
2:J:66:ARG:NH1	2:J:82:LEU:HD11	2.33	0.44
2:O:33:ILE:HD11	2:O:100(D):TYR:CD2	2.52	0.44
3:Q:143:GLU:OE1	3:Q:143:GLU:N	2.49	0.44
1:C:261:ILE:HA	1:C:264:MET:HE2	1.99	0.44
1:G:317:HIS:CD2	1:G:408:THR:HA	2.52	0.44
1:I:432:ILE:HD11	1:I:447:VAL:HG22	1.99	0.44
1:I:491:SER:H	1:I:494:GLN:HB2	1.83	0.44
2:L:195:ILE:HD12	2:L:195:ILE:N	2.33	0.44
1:G:402:ILE:HD13	1:I:373:LEU:HD13	1.99	0.43
1:H:95:LEU:HD13	1:I:278:VAL:HG21	2.00	0.43
1:I:316:LEU:HD21	1:I:336:ARG:HH21	1.83	0.43
2:O:100(G):HIS:O	3:U:34:ASN:ND2	2.51	0.43
3:S:66:GLY:HA3	3:S:71:PHE:HA	1.99	0.43
3:S:124:GLN:O	3:S:127:SER:OG	2.31	0.43
3:U:33:LEU:HD22	3:U:71:PHE:CG	2.52	0.43
1:A:246:PRO:HG2	1:C:239:VAL:CG1	2.48	0.43
1:E:210:GLN:OE1	1:E:213:ARG:HB3	2.19	0.43
1:G:156:LYS:HE2	1:G:156:LYS:HB2	1.60	0.43
1:H:352:PHE:CE2	1:H:367:CYS:HB3	2.53	0.43
1:I:65:LYS:HA	1:I:65:LYS:HD3	1.81	0.43
1:I:209:GLN:NE2	2:O:101:ASP:OD2	2.39	0.43
2:K:29:LEU:HG	2:K:76:ASP:HA	2.00	0.43
2:K:114:ALA:HB3	2:K:146:PHE:CE2	2.53	0.43
2:M:169:VAL:HG21	3:S:160:GLN:HB3	2.00	0.43
1:A:414:VAL:HG21	1:A:435:PHE:CE2	2.53	0.43
1:C:164:VAL:HG21	1:C:293:LYS:HD3	1.99	0.43
1:F:315:LYS:HD2	1:F:341:TRP:CE2	2.53	0.43
1:G:30:GLU:OE1	1:G:441:TYR:OH	2.16	0.43
1:G:379:VAL:HG22	1:G:391:TYR:CZ	2.54	0.43
1:B:237:PHE:HZ	1:B:287:SER:HG	1.66	0.43
1:C:266:ILE:HG13	1:C:271:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:ALA:HB2	1:E:486:ASP:OD2	2.18	0.43
1:G:51:GLY:C	1:G:305:ILE:HG12	2.38	0.43
1:I:59:ILE:HG12	1:I:192:VAL:HG23	2.01	0.43
1:I:426:ASN:ND2	1:I:446:GLY:O	2.50	0.43
2:K:166:PHE:HA	3:Q:164:THR:HG22	1.99	0.43
2:L:100(D):TYR:HD1	2:L:100(E):LEU:H	1.66	0.43
2:O:33:ILE:HG12	2:O:52:ILE:HG23	2.01	0.43
3:P:119:PRO:HB3	3:P:209:PHE:CE1	2.53	0.43
1:C:44:TYR:CD2	1:C:341:TRP:HZ3	2.36	0.43
1:C:315:LYS:CD	1:C:341:TRP:CD2	3.01	0.43
1:C:446:GLY:HA3	1:H:205:PRO:CB	2.45	0.43
1:D:293:LYS:HG2	1:D:294:GLU:N	2.33	0.43
1:G:76:VAL:HG22	1:G:212:CYS:O	2.18	0.43
2:J:193:THR:HG22	2:J:195:ILE:HD11	1.99	0.43
2:L:123:PRO:O	3:R:121:SER:OG	2.36	0.43
3:P:33:LEU:HD11	3:P:88:CYS:HB2	2.01	0.43
3:S:137:ASN:OD1	3:S:138:ASN:ND2	2.44	0.43
1:G:79:ILE:HG22	1:G:220:VAL:HG23	2.00	0.43
1:G:442:VAL:CG1	1:G:447:VAL:HG21	2.48	0.43
2:N:150:VAL:HG22	2:N:200:HIS:HB2	2.01	0.43
3:P:40:PRO:CB	3:P:165:GLU:HG3	2.48	0.43
3:P:151:ASP:OD1	3:P:189:HIS:ND1	2.52	0.43
3:R:190:LYS:NZ	3:R:210:ASN:HB3	2.34	0.43
1:B:335:THR:HB	1:B:396:MET:HG2	2.00	0.43
1:C:207:LEU:HA	1:C:207:LEU:HD12	1.75	0.43
1:D:458:TYR:CE2	1:F:150:SER:HB3	2.54	0.43
1:H:394:LYS:HZ1	1:I:400:THR:CG2	2.31	0.43
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.84	0.43
1:A:403:SER:OG	1:A:416:CYS:HA	2.18	0.43
1:D:144:VAL:CG2	1:E:406:VAL:HG13	2.48	0.43
1:F:94:GLN:HG3	1:F:292:ILE:HD13	1.99	0.43
1:G:314:TRP:NE1	1:G:342:TYR:HB2	2.33	0.43
1:H:488:PHE:HB2	1:I:488:PHE:CZ	2.54	0.43
2:O:66:ARG:HH12	2:O:86:ASP:CG	2.21	0.43
1:B:379:VAL:HG22	1:B:391:TYR:CZ	2.53	0.43
1:C:73:ASP:OD2	1:C:213:ARG:NH2	2.52	0.43
1:C:210:GLN:O	1:C:213:ARG:HG3	2.19	0.43
1:D:319:SER:OG	1:D:320:PRO:HD2	2.19	0.43
1:E:426:ASN:OD1	1:E:427:LYS:N	2.51	0.43
1:F:243:VAL:HA	1:F:287:SER:O	2.18	0.43
1:H:153:ALA:O	1:H:157:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:ILE:HD13	1:H:492:ILE:HD13	2.01	0.43
2:K:195:ILE:HD12	2:K:210:ARG:HG2	2.01	0.43
2:L:170:LEU:HD13	2:L:176:TYR:CZ	2.53	0.43
2:M:11:VAL:HA	2:M:110:THR:O	2.19	0.43
3:S:119:PRO:HB3	3:S:209:PHE:CE1	2.54	0.43
1:A:369:THR:HG23	1:B:455:THR:HG23	2.00	0.43
1:D:369:THR:O	1:E:455:THR:HG22	2.19	0.43
1:E:137:PHE:HD2	1:E:337:THR:HA	1.84	0.43
3:P:113:PRO:HB3	3:P:139:PHE:HB3	2.00	0.43
1:A:217:ILE:HD12	1:A:217:ILE:HA	1.87	0.42
1:A:235:ARG:HD2	1:B:250:TYR:CE2	2.54	0.42
1:B:198:TYR:OH	1:B:222:GLU:OE2	2.30	0.42
1:C:315:LYS:HE2	1:C:315:LYS:HB2	1.14	0.42
1:F:49:ARG:HG3	1:F:304:PRO:CB	2.49	0.42
1:F:59:ILE:HG12	1:F:192:VAL:HG23	2.00	0.42
1:F:395:ILE:HG12	1:F:491:SER:HA	2.00	0.42
1:G:427:LYS:HG2	1:G:448:ASP:OD2	2.19	0.42
1:H:193:LEU:HD23	1:H:193:LEU:HA	1.89	0.42
1:I:78:LEU:HD12	1:I:78:LEU:HA	1.86	0.42
1:I:441:TYR:OH	1:I:466:ASN:ND2	2.45	0.42
2:J:33:ILE:HG13	2:J:97:ALA:HB2	2.01	0.42
2:M:209:LYS:HD2	2:M:209:LYS:HA	1.66	0.42
3:R:50:VAL:HG22	3:R:91:TYR:OH	2.18	0.42
1:E:45:PHE:HB3	1:E:310:ASP:HA	2.00	0.42
1:E:138:LEU:HD12	1:E:140:PHE:HE1	1.84	0.42
1:F:207:LEU:HD12	1:F:207:LEU:HA	1.66	0.42
1:G:77:LYS:O	1:G:81:GLN:HG2	2.19	0.42
2:L:63:PHE:HB3	2:L:67:VAL:HG21	2.01	0.42
3:S:179:LEU:HG	3:S:181:LEU:HD11	2.01	0.42
1:A:76:VAL:O	1:A:80:LYS:HB3	2.20	0.42
1:B:49:ARG:NH1	1:B:51:GLY:O	2.51	0.42
1:B:157:VAL:HG11	1:B:181:LEU:HB3	2.01	0.42
1:C:313:CYS:HA	1:C:342:TYR:O	2.20	0.42
1:C:491:SER:H	1:C:494:GLN:HB2	1.83	0.42
1:D:67:THR:HG22	2:L:99:VAL:HG13	2.01	0.42
1:D:285:SER:OG	1:D:304:PRO:HD3	2.18	0.42
1:G:61:LEU:O	1:G:295:GLU:HB2	2.19	0.42
1:G:252:LEU:HD12	1:G:252:LEU:HA	1.84	0.42
1:G:354:GLN:O	1:G:357:THR:OG1	2.37	0.42
2:L:193:THR:CG2	2:L:210:ARG:HD3	2.49	0.42
2:M:121:VAL:HA	2:M:141:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LYS:HZ1	1:C:486:ASP:HB3	1.82	0.42
1:C:71:GLY:O	1:C:76:VAL:HG11	2.19	0.42
1:D:193:LEU:HD23	1:D:193:LEU:HA	1.69	0.42
1:D:508:ARG:HG2	1:D:508:ARG:HH11	1.84	0.42
1:F:261:ILE:HD12	1:F:274:MET:HB3	2.01	0.42
1:I:171:LEU:HD21	1:I:189:THR:HB	2.02	0.42
2:L:36:TRP:CH2	2:L:92:CYS:HB2	2.54	0.42
1:B:157:VAL:HG21	1:B:183:ASN:ND2	2.34	0.42
1:D:338:ASP:HB2	1:D:342:TYR:OH	2.18	0.42
1:E:240:ASN:HB3	1:E:243:VAL:O	2.19	0.42
1:G:294:GLU:O	1:G:295:GLU:HG2	2.19	0.42
1:G:426:ASN:OD1	1:G:427:LYS:N	2.52	0.42
1:H:240:ASN:HB3	1:H:243:VAL:O	2.20	0.42
2:N:63:PHE:HB3	2:N:67:VAL:HG21	2.02	0.42
1:A:65:LYS:HG3	2:J:100(B):GLU:OE1	2.20	0.42
1:E:192:VAL:CG1	1:E:229:ARG:NH1	2.82	0.42
1:G:246:PRO:HG2	1:I:239:VAL:HG12	2.01	0.42
1:I:34:GLN:HB2	1:I:468:TYR:HE1	1.84	0.42
2:J:126:PRO:HD3	2:J:138:LEU:HB3	1.99	0.42
3:Q:113:PRO:HB3	3:Q:139:PHE:HB3	2.01	0.42
1:A:252:LEU:HD22	1:A:301:VAL:HG11	2.02	0.42
1:B:487:GLU:OE2	1:B:498:LYS:HD3	2.20	0.42
1:C:423:THR:CG2	1:C:431:ILE:HG13	2.46	0.42
1:D:59:ILE:HB	1:D:297:LEU:CD2	2.49	0.42
1:D:279:GLN:CG	1:F:241:ALA:HA	2.49	0.42
1:D:426:ASN:OD1	1:D:427:LYS:N	2.52	0.42
1:E:332:ILE:HD13	1:E:332:ILE:HA	1.93	0.42
1:F:318:THR:O	1:F:339:ARG:NH2	2.53	0.42
1:F:327:LYS:HB3	1:F:327:LYS:HE2	1.78	0.42
1:H:192:VAL:HG23	1:H:193:LEU:H	1.84	0.42
1:H:267:THR:HG22	1:H:269:ASP:H	1.85	0.42
2:K:166:PHE:CD2	3:Q:164:THR:HG23	2.55	0.42
2:M:205:THR:HG22	2:M:207:VAL:HG23	2.02	0.42
2:N:33:ILE:O	2:N:94:THR:HA	2.19	0.42
2:O:83:ARG:O	2:O:111:VAL:HG11	2.19	0.42
1:A:68:LYS:HD2	1:A:68:LYS:HA	1.82	0.42
1:E:150:SER:HB3	1:F:458:TYR:CD2	2.54	0.42
1:E:239:VAL:HG12	1:F:246:PRO:HG2	2.00	0.42
1:H:387:PHE:HZ	1:H:474:ILE:HG23	1.85	0.42
1:I:82:GLU:OE2	1:I:224:GLN:HG3	2.19	0.42
1:I:193:LEU:HD23	1:I:193:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:186:SER:HA	2:J:189:LEU:HD13	2.00	0.42
1:A:280:ILE:HG21	1:A:366:PHE:CG	2.55	0.42
1:A:406:VAL:HG13	1:C:144:VAL:CG2	2.50	0.42
1:B:30:GLU:OE2	1:B:408:THR:HB	2.20	0.42
1:D:225:GLN:HE21	1:F:224:GLN:NE2	2.17	0.42
1:E:60:GLU:OE1	1:E:196:LYS:HD3	2.20	0.42
1:E:79:ILE:CG2	1:E:220:VAL:HG23	2.48	0.42
1:F:44:TYR:HA	1:F:363:ASN:OD1	2.19	0.42
3:R:198:HIS:H	3:R:201:LEU:HD11	1.84	0.42
1:A:445:LYS:NZ	4:A:601:SO4:O1	2.46	0.42
1:C:46:SER:HG	1:C:311:THR:H	1.67	0.42
1:C:196:LYS:NZ	2:K:100(C):THR:OG1	2.53	0.42
1:D:176:LYS:HE2	1:D:190:PHE:CE2	2.55	0.42
1:I:405:SER:HB2	1:I:452:VAL:HG21	2.02	0.42
1:D:352:PHE:CD1	1:D:352:PHE:N	2.88	0.41
1:D:505:PHE:CG	1:E:505:PHE:HE1	2.38	0.41
1:G:204:LEU:HD13	1:G:204:LEU:HA	1.90	0.41
2:M:100(H):TYR:HB3	3:S:34:ASN:ND2	2.35	0.41
1:D:318:THR:O	1:D:339:ARG:NH2	2.53	0.41
1:E:192:VAL:HG11	1:E:229:ARG:CZ	2.50	0.41
1:I:37:CYS:SG	1:I:319:SER:HB3	2.60	0.41
2:K:48:MET:HG2	2:K:63:PHE:CE2	2.56	0.41
2:L:146:PHE:CD1	2:L:147:PRO:HA	2.55	0.41
2:M:45:PRO:HG2	3:S:98:PHE:CD2	2.54	0.41
2:O:36:TRP:CE2	2:O:80:MET:HB2	2.55	0.41
3:S:108:ARG:HH12	3:S:111:ALA:HB2	1.85	0.41
1:A:75:LYS:H	1:A:75:LYS:HG2	1.71	0.41
1:B:151:GLY:HA3	1:B:288:ILE:HD12	2.02	0.41
1:C:375:LEU:HB3	1:C:379:VAL:HG21	2.02	0.41
1:G:423:THR:HG23	1:G:431:ILE:HG23	2.01	0.41
2:J:11:VAL:HA	2:J:110:THR:O	2.20	0.41
2:M:98:LEU:HD23	2:M:98:LEU:HA	1.84	0.41
3:R:197:THR:HG22	3:R:204:PRO:HB3	2.02	0.41
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.88	0.41
1:F:397:THR:HB	1:F:483:PHE:CE2	2.55	0.41
1:G:319:SER:OG	1:G:320:PRO:HD2	2.20	0.41
2:J:94:THR:OG1	2:J:102:ASN:HB3	2.20	0.41
2:J:139:GLY:HA2	2:J:154:TRP:HH2	1.85	0.41
2:K:19:MET:HA	2:K:80:MET:O	2.21	0.41
2:O:33:ILE:HG23	2:O:52:ILE:HG12	2.02	0.41
1:A:237:PHE:CE2	1:A:289:MET:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ILE:HD13	1:C:179:VAL:HG11	2.02	0.41
1:C:171:LEU:HD21	1:C:189:THR:HB	2.03	0.41
1:C:217:ILE:O	1:C:220:VAL:HG12	2.21	0.41
1:C:258:LEU:HD11	1:C:278:VAL:HG11	2.02	0.41
1:D:50:THR:HG22	1:D:307:GLY:H	1.85	0.41
1:G:192:VAL:HG23	1:G:193:LEU:H	1.86	0.41
1:G:314:TRP:CE2	1:G:342:TYR:HB2	2.56	0.41
2:O:121:VAL:HG22	2:O:142:VAL:HG22	2.01	0.41
3:P:149:LYS:HG2	3:P:154:LEU:HG	2.02	0.41
3:S:140:TYR:CG	3:S:141:PRO:HA	2.54	0.41
3:U:107:LYS:HA	3:U:140:TYR:OH	2.20	0.41
1:C:151:GLY:HA3	1:C:288:ILE:CD1	2.50	0.41
1:C:171:LEU:HD21	1:C:189:THR:CB	2.50	0.41
1:C:321:LEU:HD11	1:C:473:PRO:HB3	2.02	0.41
1:C:503:LEU:HA	1:C:506:ILE:HB	2.01	0.41
1:D:407:ILE:HD13	1:D:458:TYR:O	2.20	0.41
1:E:146:SER:H	1:F:407:ILE:HD12	1.85	0.41
1:F:204:LEU:HD23	1:F:204:LEU:HA	1.77	0.41
1:I:204:LEU:O	1:I:208:ASN:HB2	2.20	0.41
1:I:231:LEU:HD23	1:I:231:LEU:HA	1.86	0.41
1:I:252:LEU:HD23	1:I:257:LEU:HD13	2.01	0.41
2:K:116:THR:HG22	2:K:203:SER:HB3	2.01	0.41
2:L:23:GLN:NE2	2:L:24:ALA:O	2.52	0.41
3:Q:140:TYR:CG	3:Q:141:PRO:HA	2.55	0.41
1:A:163:GLU:OE1	1:A:163:GLU:HA	2.20	0.41
1:B:480:PRO:C	1:B:482:VAL:H	2.24	0.41
1:C:442:VAL:HA	1:H:209:GLN:HG3	2.03	0.41
1:D:142:LEU:HD23	1:D:373:LEU:HG	2.03	0.41
1:D:399:LYS:HB2	1:F:494:GLN:NE2	2.35	0.41
1:D:507:ARG:HH22	1:D:508:ARG:NH2	2.19	0.41
1:E:452:VAL:O	1:E:455:THR:OG1	2.37	0.41
1:G:167:ILE:HD11	1:G:181:LEU:HD21	2.02	0.41
1:G:193:LEU:HD23	1:G:193:LEU:HA	1.91	0.41
1:H:406:VAL:O	1:H:413:ILE:N	2.44	0.41
1:H:442:VAL:HG11	1:H:447:VAL:HG21	2.03	0.41
1:I:199:ILE:O	1:I:204:LEU:HD23	2.20	0.41
2:O:100(D):TYR:CZ	2:O:100(G):HIS:HE1	2.38	0.41
1:B:207:LEU:HD12	1:B:207:LEU:HA	1.89	0.41
1:C:317:HIS:HD2	1:C:408:THR:CG2	2.33	0.41
1:C:324:THR:HB	1:C:437:ASN:HB3	2.03	0.41
1:C:351:PHE:C	1:C:351:PHE:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:SER:CA	1:E:512:LEU:HD21	2.49	0.41
1:E:140:PHE:CD1	1:E:140:PHE:N	2.88	0.41
1:E:165:ASN:ND2	1:E:294:GLU:OE2	2.53	0.41
1:F:387:PHE:CZ	1:F:474:ILE:HG23	2.56	0.41
1:G:507:ARG:O	1:G:511:GLU:HB3	2.21	0.41
1:I:204:LEU:HD13	1:I:204:LEU:HA	1.83	0.41
2:N:184:VAL:HG21	2:N:194:TYR:OH	2.20	0.41
1:A:426:ASN:OD1	1:A:427:LYS:N	2.53	0.41
1:A:491:SER:HB2	1:A:494:GLN:HG3	2.03	0.41
1:B:334:LEU:HD11	1:B:395:ILE:HB	2.03	0.41
1:B:461:LYS:HA	1:B:461:LYS:HD2	1.61	0.41
1:C:50:THR:HG23	1:C:307:GLY:H	1.85	0.41
1:C:65:LYS:HB2	2:K:100:VAL:O	2.21	0.41
1:C:217:ILE:HD12	1:C:217:ILE:HA	1.78	0.41
1:C:332:ILE:HD13	1:C:332:ILE:HA	1.96	0.41
1:D:75:LYS:HG3	1:E:218:GLU:OE2	2.21	0.41
1:F:387:PHE:CE2	1:F:474:ILE:HD12	2.56	0.41
1:G:28:ILE:HD12	1:G:44:TYR:CE1	2.56	0.41
1:G:67:THR:HA	2:N:99:VAL:HG22	2.02	0.41
1:G:176:LYS:HG2	1:G:190:PHE:CZ	2.56	0.41
1:G:185:VAL:HG13	1:H:427:LYS:HZ2	1.84	0.41
1:G:266:ILE:HG13	1:G:271:LYS:HG3	2.03	0.41
1:H:197:SER:O	1:H:201:ASN:HB2	2.21	0.41
2:J:11:VAL:HB	2:J:147:PRO:HG3	2.03	0.41
2:J:139:GLY:HA2	2:J:154:TRP:CH2	2.56	0.41
2:J:152:VAL:HG23	2:J:198:VAL:HG22	2.02	0.41
2:L:63:PHE:HB3	2:L:67:VAL:CG2	2.51	0.41
2:M:6:GLN:HA	2:M:21:SER:O	2.21	0.41
2:M:150:VAL:HG22	2:M:200:HIS:HB2	2.03	0.41
2:N:163:VAL:HG12	2:N:182:VAL:HB	2.03	0.41
3:Q:198:HIS:H	3:Q:201:LEU:HD11	1.85	0.41
3:T:198:HIS:H	3:T:201:LEU:HD11	1.85	0.41
1:A:156:LYS:HE3	1:B:462:LEU:HD23	2.03	0.41
1:B:189:THR:O	1:B:190:PHE:HD1	2.04	0.41
1:C:395:ILE:HD13	1:C:492:ILE:HD13	2.03	0.41
1:D:352:PHE:CE2	1:D:372:SER:HB3	2.56	0.41
1:E:52:TRP:CE3	1:E:302:GLN:HG2	2.56	0.41
1:F:352:PHE:CE2	1:F:367:CYS:HB3	2.56	0.41
1:I:478:TYR:HB3	1:I:483:PHE:HD2	1.86	0.41
2:L:100(D):TYR:HE1	2:L:100(G):HIS:CD2	2.39	0.41
2:N:141:LEU:HD12	2:N:178:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:17:SER:HA	2:O:82(A):SER:HA	2.03	0.41
2:O:103:TRP:CE3	3:U:44:PRO:HD2	2.56	0.41
3:Q:192:TYR:HB2	3:Q:209:PHE:CZ	2.56	0.41
3:T:11:LEU:HD11	3:T:104:VAL:HG13	2.02	0.41
1:A:323:THR:HG23	1:A:475:ILE:HG13	2.03	0.40
1:B:332:ILE:HG23	1:B:483:PHE:CE2	2.56	0.40
1:E:49:ARG:O	1:E:369:THR:HG23	2.21	0.40
1:G:352:PHE:CD1	1:G:352:PHE:N	2.88	0.40
1:I:59:ILE:HB	1:I:297:LEU:CD2	2.51	0.40
2:K:30:GLU:HA	2:K:52(A):PRO:HB2	2.04	0.40
2:M:143:LYS:HG2	2:M:144:ASP:CG	2.42	0.40
3:R:192:TYR:HB2	3:R:209:PHE:CE2	2.57	0.40
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.82	0.40
1:B:201:ASN:HB3	1:F:426:ASN:HD21	1.86	0.40
1:B:503:LEU:HD23	1:B:503:LEU:HA	1.94	0.40
1:C:426:ASN:OD1	1:C:427:LYS:N	2.54	0.40
1:E:162:GLY:O	1:E:166:LYS:HG3	2.21	0.40
1:F:394:LYS:HE2	1:F:394:LYS:HB3	1.91	0.40
1:H:37:CYS:SG	1:H:319:SER:HB3	2.61	0.40
1:H:373:LEU:HD13	1:I:402:ILE:HD13	2.03	0.40
2:O:195:ILE:HD12	2:O:210:ARG:HG2	2.04	0.40
1:A:64:ILE:HA	2:J:100(A):SER:HA	2.03	0.40
1:A:474:ILE:HA	1:A:477:TYR:HD2	1.87	0.40
1:C:209:GLN:NE2	3:Q:55:GLU:OE2	2.54	0.40
1:C:408:THR:OG1	1:C:411:GLY:N	2.54	0.40
1:D:176:LYS:NZ	1:D:259:SER:OG	2.54	0.40
1:G:461:LYS:HD2	1:G:461:LYS:HA	1.77	0.40
2:L:100(E):LEU:HB2	2:L:100(G):HIS:HE1	1.86	0.40
2:M:100(A):SER:O	2:M:100(D):TYR:HB2	2.21	0.40
1:B:138:LEU:HD21	1:B:337:THR:OG1	2.21	0.40
1:B:157:VAL:HG12	1:B:163:GLU:HG2	2.03	0.40
1:B:323:THR:HG23	1:B:475:ILE:HG13	2.03	0.40
1:D:288:ILE:O	1:D:288:ILE:HG13	2.21	0.40
1:D:293:LYS:HG2	1:D:294:GLU:H	1.86	0.40
1:E:480:PRO:C	1:E:482:VAL:H	2.24	0.40
1:F:480:PRO:C	1:F:482:VAL:H	2.25	0.40
1:H:59:ILE:HB	1:H:297:LEU:CD2	2.50	0.40
1:H:405:SER:HB3	1:H:457:TYR:CE2	2.57	0.40
1:I:58:THR:HG22	1:I:298:ALA:HB2	2.03	0.40
1:I:270:GLN:HG2	1:I:309:ILE:CD1	2.51	0.40
3:Q:4:MET:HB2	3:Q:99:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:NZ	1:A:295:GLU:HB2	2.37	0.40
1:B:338:ASP:OD1	1:B:338:ASP:N	2.46	0.40
1:D:102:ALA:HA	1:D:152:ILE:HD13	2.04	0.40
1:F:45:PHE:HB3	1:F:310:ASP:HA	2.03	0.40
1:F:334:LEU:CB	1:F:475:ILE:HD13	2.52	0.40
1:F:442:VAL:HG11	1:F:447:VAL:HG21	2.03	0.40
1:I:352:PHE:CE2	1:I:372:SER:HB3	2.57	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
2:J:173:SER:O	2:K:206:LYS:NZ[5_555]	1.98	0.22
3:Q:5:THR:OG1	3:U:5:THR:OG1[4_555]	1.98	0.22

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/568 (78%)	420 (94%)	25 (6%)	0	100	100
1	B	448/568 (79%)	427 (95%)	20 (4%)	1 (0%)	47	81
1	C	446/568 (78%)	426 (96%)	18 (4%)	2 (0%)	34	72
1	D	451/568 (79%)	430 (95%)	20 (4%)	1 (0%)	47	81
1	E	447/568 (79%)	428 (96%)	18 (4%)	1 (0%)	47	81
1	F	448/568 (79%)	429 (96%)	18 (4%)	1 (0%)	47	81
1	G	449/568 (79%)	427 (95%)	21 (5%)	1 (0%)	47	81
1	H	447/568 (79%)	429 (96%)	17 (4%)	1 (0%)	47	81
1	I	444/568 (78%)	422 (95%)	19 (4%)	3 (1%)	22	62
2	J	220/228 (96%)	214 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	216/228 (95%)	209 (97%)	7 (3%)	0	100	100
2	L	217/228 (95%)	208 (96%)	9 (4%)	0	100	100
2	M	217/228 (95%)	211 (97%)	6 (3%)	0	100	100
2	N	217/228 (95%)	210 (97%)	7 (3%)	0	100	100
2	O	210/228 (92%)	204 (97%)	6 (3%)	0	100	100
3	P	210/214 (98%)	201 (96%)	8 (4%)	1 (0%)	29	68
3	Q	209/214 (98%)	199 (95%)	9 (4%)	1 (0%)	29	68
3	R	209/214 (98%)	200 (96%)	8 (4%)	1 (0%)	29	68
3	S	209/214 (98%)	199 (95%)	8 (4%)	2 (1%)	15	54
3	T	209/214 (98%)	201 (96%)	6 (3%)	2 (1%)	15	54
3	U	204/214 (95%)	195 (96%)	8 (4%)	1 (0%)	29	68
All	All	6572/7764 (85%)	6289 (96%)	264 (4%)	19 (0%)	41	76

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	30	VAL
3	Q	30	VAL
3	R	30	VAL
3	S	30	VAL
3	T	30	VAL
3	U	30	VAL
1	C	295	GLU
1	I	71	GLY
1	I	215	SER
3	S	151	ASP
3	T	151	ASP
1	B	184	GLY
1	C	184	GLY
1	E	184	GLY
1	H	184	GLY
1	I	184	GLY
1	D	100	THR
1	F	184	GLY
1	G	184	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	411/512 (80%)	407 (99%)	4 (1%)	76 86
1	B	413/512 (81%)	407 (98%)	6 (2%)	65 80
1	C	412/512 (80%)	407 (99%)	5 (1%)	71 84
1	D	415/512 (81%)	407 (98%)	8 (2%)	57 75
1	E	413/512 (81%)	404 (98%)	9 (2%)	52 71
1	F	414/512 (81%)	410 (99%)	4 (1%)	76 86
1	G	414/512 (81%)	408 (99%)	6 (1%)	67 81
1	H	412/512 (80%)	407 (99%)	5 (1%)	71 84
1	I	410/512 (80%)	403 (98%)	7 (2%)	60 78
2	J	189/193 (98%)	187 (99%)	2 (1%)	73 85
2	K	186/193 (96%)	185 (100%)	1 (0%)	88 93
2	L	187/193 (97%)	186 (100%)	1 (0%)	88 93
2	M	187/193 (97%)	186 (100%)	1 (0%)	88 93
2	N	187/193 (97%)	186 (100%)	1 (0%)	88 93
2	O	184/193 (95%)	183 (100%)	1 (0%)	88 93
3	P	186/188 (99%)	184 (99%)	2 (1%)	73 85
3	Q	186/188 (99%)	186 (100%)	0	100 100
3	R	186/188 (99%)	186 (100%)	0	100 100
3	S	186/188 (99%)	185 (100%)	1 (0%)	88 93
3	T	186/188 (99%)	185 (100%)	1 (0%)	88 93
3	U	183/188 (97%)	183 (100%)	0	100 100
All	All	5947/6894 (86%)	5882 (99%)	65 (1%)	73 85

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	251	MET
1	A	468	TYR
1	A	493	SER
1	B	77	LYS
1	B	196	LYS
1	B	226	LYS
1	B	251	MET
1	B	293	LYS
1	B	468	TYR
1	C	140	PHE
1	C	251	MET
1	C	351	PHE
1	C	428	ASN
1	C	443	SER
1	D	65	LYS
1	D	161	GLU
1	D	208	ASN
1	D	216	ASN
1	D	251	MET
1	D	299	TYR
1	D	443	SER
1	D	488	PHE
1	E	68	LYS
1	E	69	CYS
1	E	87	LYS
1	E	140	PHE
1	E	210	GLN
1	E	226	LYS
1	E	276	SER
1	E	363	ASN
1	E	468	TYR
1	F	140	PHE
1	F	216	ASN
1	F	251	MET
1	F	443	SER
1	G	70	ASN
1	G	75	LYS
1	G	208	ASN
1	G	468	TYR
1	G	491	SER
1	G	508	ARG
1	H	196	LYS

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Mol	Chain	Res	Type
1	H	216	ASN
1	H	251	MET
1	H	443	SER
1	H	463	GLU
1	I	208	ASN
1	I	213	ARG
1	I	251	MET
1	I	327	LYS
1	I	443	SER
1	I	465	LYS
1	I	468	TYR
2	J	100(B)	GLU
2	J	212	GLU
2	K	212	GLU
2	L	100(D)	TYR
2	M	212	GLU
2	N	98	LEU
2	O	212	GLU
3	P	108	ARG
3	P	211	ARG
3	S	201	LEU
3	T	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	B	209	GLN
1	B	345	ASN
1	C	317	HIS
1	C	345	ASN
1	C	454	ASN
1	D	454	ASN
1	F	224	GLN
1	F	325	ASN
1	F	345	ASN
1	G	225	GLN
1	G	325	ASN
1	I	81	GLN
1	I	302	GLN
3	Q	158	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	C	602	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	B	603	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	G	601	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	601	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	H	602	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	J	301	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	H	601	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.09	0
4	SO4	D	601	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	L	301	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	E	601	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	B	601	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	I	601	-	4,4,4	0.13	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	SO4	1	0

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, 95^{th} 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	449/568 (79%)	-0.41	1 (0%) 95 93	62, 85, 113, 126	0
1	B	452/568 (79%)	-0.46	0 100 100	61, 83, 112, 128	0
1	C	450/568 (79%)	-0.41	0 100 100	58, 91, 118, 139	0
1	D	455/568 (80%)	-0.35	1 (0%) 95 93	59, 84, 117, 135	0
1	E	451/568 (79%)	-0.47	0 100 100	62, 82, 115, 132	0
1	F	452/568 (79%)	-0.43	0 100 100	66, 88, 116, 140	0
1	G	453/568 (79%)	-0.42	1 (0%) 95 93	63, 82, 112, 123	0
1	H	451/568 (79%)	-0.46	0 100 100	66, 84, 112, 128	0
1	I	448/568 (78%)	-0.40	0 100 100	60, 88, 111, 128	0
2	J	224/228 (98%)	-0.19	0 100 100	83, 103, 126, 145	0
2	K	220/228 (96%)	0.04	3 (1%) 75 66	96, 167, 209, 241	0
2	L	221/228 (96%)	-0.19	0 100 100	90, 111, 137, 156	0
2	M	221/228 (96%)	-0.31	0 100 100	75, 97, 137, 160	0
2	N	221/228 (96%)	-0.27	0 100 100	75, 93, 116, 142	0
2	O	216/228 (94%)	0.15	9 (4%) 36 29	90, 168, 201, 232	0
3	P	212/214 (99%)	-0.10	1 (0%) 91 86	84, 114, 156, 175	0
3	Q	211/214 (98%)	0.36	11 (5%) 27 24	92, 137, 210, 225	0
3	R	211/214 (98%)	-0.10	1 (0%) 91 86	87, 122, 169, 186	0
3	S	211/214 (98%)	-0.02	0 100 100	79, 108, 142, 150	0
3	T	211/214 (98%)	-0.20	1 (0%) 91 86	77, 106, 141, 164	0
3	U	208/214 (97%)	0.49	20 (9%) 8 7	87, 167, 211, 226	0
All	All	6648/7764 (85%)	-0.27	49 (0%) 87 82	58, 94, 173, 241	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	193	ALA	4.2
3	Q	193	ALA	3.7
3	U	149	LYS	3.6
2	O	203	SER	3.3
2	O	204	ASN	3.2
3	U	126	LYS	3.1
3	U	150	VAL	3.1
3	P	130	ALA	3.0
3	Q	116	PHE	3.0
3	Q	144	ALA	2.9
2	O	123	PRO	2.9
3	U	130	ALA	2.9
1	D	511	GLU	2.8
3	U	129	THR	2.7
3	Q	130	ALA	2.7
2	O	185	PRO	2.6
2	K	190	GLY	2.5
2	O	135	THR	2.5
3	U	198	HIS	2.5
3	U	199	GLN	2.5
3	U	125	LEU	2.4
3	Q	150	VAL	2.4
3	Q	151	ASP	2.4
2	K	195	ILE	2.4
3	Q	129	THR	2.4
3	Q	181	LEU	2.4
3	U	124	GLN	2.3
2	O	144	ASP	2.3
3	U	200	GLY	2.3
3	Q	115	VAL	2.2
2	O	205	THR	2.2
3	U	183	LYS	2.2
1	G	511	GLU	2.2
2	O	212	GLU	2.2
3	U	181	LEU	2.2
3	U	182	SER	2.2
3	T	130	ALA	2.2
3	U	105	GLU	2.1
3	U	137	ASN	2.1
3	U	144	ALA	2.1
2	O	42	GLY	2.1
3	U	141	PRO	2.1
1	A	505	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
3	R	130	ALA	2.0
3	U	179	LEU	2.0
3	Q	210	ASN	2.0
3	U	185	ASP	2.0
2	K	213	PRO	2.0
3	Q	207	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	D	601	5/5	0.77	0.47	147,147,147,147	0
4	SO4	B	602	5/5	0.80	0.31	172,172,172,172	0
4	SO4	C	601	5/5	0.82	0.28	138,138,138,138	0
4	SO4	H	601	5/5	0.83	0.21	119,119,119,119	0
4	SO4	C	602	5/5	0.86	0.31	121,121,122,122	0
4	SO4	G	601	5/5	0.87	0.26	119,120,120,120	0
4	SO4	I	601	5/5	0.88	0.34	136,136,136,136	0
4	SO4	B	603	5/5	0.89	0.33	145,145,145,145	0
4	SO4	E	601	5/5	0.90	0.20	96,96,97,97	0
4	SO4	A	601	5/5	0.90	0.23	145,146,146,146	0
4	SO4	J	301	5/5	0.90	0.27	128,129,129,129	0
4	SO4	B	601	5/5	0.91	0.15	132,132,132,132	0
4	SO4	L	301	5/5	0.94	0.19	115,115,115,116	0
4	SO4	H	602	5/5	0.95	0.37	103,103,103,104	0
4	SO4	B	604	5/5	0.96	0.22	105,106,106,107	0

6.5 Other polymers (i)

There are no such residues in this entry.