Full wwPDB EM Validation Report ⓘ

Jun 1, 2026 – 07:17 PM EDT

PDB ID	:	9YF4 / pdb_00009yf4
EMDB ID	:	EMD-72876
Title	:	N4 Full Virion C6 Tail
Authors	:	Bellis, N.F.; Cingolani, G.
Deposited on	:	2025-09-25
Resolution	:	3.28 Å(reported)

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

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

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

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

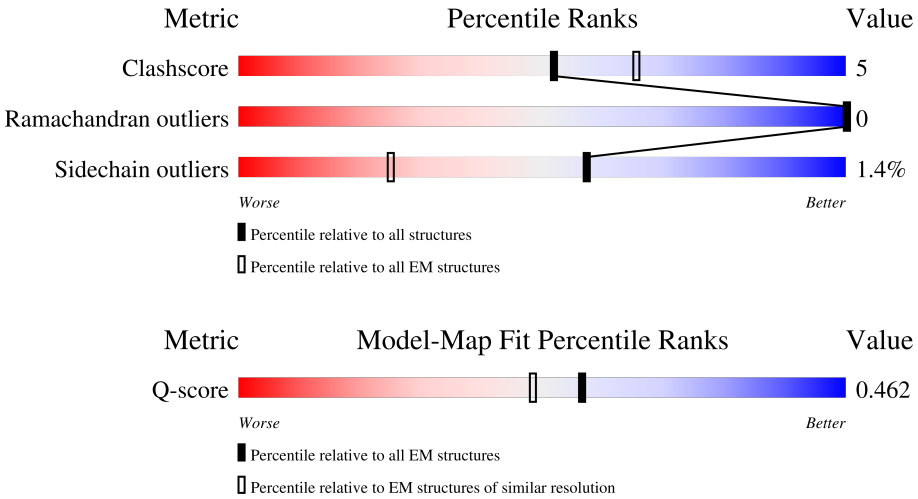
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14492 (2.78 - 3.78)

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

Mol	Chain	Length	Quality of chain
1	AA	236	92% 8%
1	AB	236	87% 12%
1	AC	236	92% 8%
1	AD	236	88% 11%

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Mol	Chain	Length	Quality of chain
1	AE	236	91% 8%
1	AF	236	88% 11%
1	AG	236	92% 7%
1	AH	236	87% 12%
1	AI	236	92% 8%
1	AJ	236	86% 13%
1	AK	236	92% 8%
1	AL	236	88% 11%
2	LA	1382	71% 15% 15%
2	LB	1382	70% 15% 15%
2	LC	1382	71% 15% 15%
2	LD	1382	70% 15% 15%
2	LE	1382	71% 15% 15%
2	LF	1382	70% 15% 15%
3	PA	763	73% 16% 12%
3	PB	763	72% 16% 12%
3	PC	763	72% 16% 12%
3	PD	763	73% 16% 12%
3	PE	763	72% 16% 12%
3	PF	763	73% 15% 12%
3	PG	763	72% 16% 12%
3	PH	763	72% 16% 12%
3	PI	763	72% 16% 12%
3	PJ	763	73% 15% 12%
3	PK	763	72% 16% 12%

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Mol	Chain	Length	Quality of chain
3	PL	763	74% 15% 12%
4	SA	417	83% 16%
4	SB	417	84% 16%
4	SC	417	83% 16%
4	SD	417	83% 17%
4	SE	417	83% 16%
4	SF	417	84% 15%
5	TA	299	89% 11%
5	TB	299	87% 12%
5	TC	299	89% 11%
5	TD	299	88% 11%
5	TE	299	88% 11%
5	TF	299	87% 13%
5	TG	299	89% 11%
5	TH	299	87% 13%
5	TI	299	88% 11%
5	TJ	299	88% 12%
5	TK	299	88% 11%
5	TL	299	87% 12%
6	XA	556	10% 87%
6	XB	556	11% 87%
6	XC	556	9% 87%
6	XD	556	11% 87%
6	XE	556	9% 87%
6	XF	556	11% 87%

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Mol	Chain	Length	Quality of chain
6	XG	556	10% 87%
6	XH	556	12% 87%
6	XI	556	10% 87%
6	XJ	556	11% 87%
6	XK	556	10% 87%
6	XL	556	11% 87%
6	YA	556	11% 88%
6	YB	556	10% 88%
6	YC	556	11% 88%
6	YD	556	10% 88%
6	YE	556	11% 88%
6	YF	556	10% 88%
6	YG	556	11% 88%
6	YH	556	10% 88%
6	YI	556	11% 88%
6	YJ	556	10% 88%
6	YK	556	11% 88%
6	YL	556	9% 88%
6	ZA	556	10% 89%
6	ZB	556	10% 89%
6	ZC	556	10% 89%
6	ZD	556	10% 89%
6	ZE	556	9% 89%
6	ZF	556	10% 89%
6	ZG	556	9% 89%

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Mol	Chain	Length	Quality of chain
6	ZH	556	10% 89%
6	ZI	556	9% 89%
6	ZJ	556	10% 89%
6	ZK	556	10% 89%
6	ZL	556	10% 89%
7	OA	150	9% 91%
7	OB	150	9% 91%
7	OC	150	9% 91%
7	OD	150	9% 91%
7	OE	150	9% 91%
7	OF	150	9% 91%
7	OG	150	9% 91%
7	OH	150	9% 91%
7	OI	150	9% 91%
7	OJ	150	9% 91%
7	OK	150	9% 91%
7	OL	150	8% 91%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 211500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AB	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AC	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AD	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AE	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AF	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AG	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AH	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AI	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AJ	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AK	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		
1	AL	236	Total	C	N	O	S	0	0
			1912	1201	327	375	9		

- Molecule 2 is a protein called Non-contractile tail sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	LA	1181	Total	C	N	O	S	0	0
			9341	5952	1572	1776	41		
2	LB	1181	Total	C	N	O	S	0	0
			9341	5952	1572	1776	41		
2	LC	1181	Total	C	N	O	S	0	0
			9341	5952	1572	1776	41		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	LD	1181	Total	C	N	O	S	0	0
			9341	5952	1572	1776	41		
2	LE	1181	Total	C	N	O	S	0	0
			9341	5952	1572	1776	41		
2	LF	1181	Total	C	N	O	S	0	0
			9341	5952	1572	1776	41		

- Molecule 3 is a protein called Probable portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	PA	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PB	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PC	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PD	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PE	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PF	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PG	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PH	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PI	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PJ	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PK	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		
3	PL	675	Total	C	N	O	S	0	0
			5357	3358	943	1033	23		

- Molecule 4 is a protein called Gp64.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SA	415	Total	C	N	O	S	0	0
			3383	2212	537	616	18		
4	SB	415	Total	C	N	O	S	0	0
			3383	2212	537	616	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	SC	415	Total	C	N	O	S	0	0
			3383	2212	537	616	18		
4	SD	415	Total	C	N	O	S	0	0
			3383	2212	537	616	18		
4	SE	415	Total	C	N	O	S	0	0
			3383	2212	537	616	18		
4	SF	415	Total	C	N	O	S	0	0
			3383	2212	537	616	18		

- Molecule 5 is a protein called Gp54.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	TA	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TB	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TC	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TD	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TE	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TF	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TG	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TH	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TI	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TJ	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TK	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		
5	TL	298	Total	C	N	O	S	0	0
			2263	1408	381	464	10		

- Molecule 6 is a protein called 60 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	XA	72	Total	C	N	O	S	0	0
			575	371	92	107	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	XB	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	YA	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	YB	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	ZA	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	ZB	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	XC	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	XD	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	YC	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	YD	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	ZC	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	ZD	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	XE	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	XF	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	YE	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	YF	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	ZE	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	ZF	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	XG	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	XH	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	YG	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	YH	68	Total	C	N	O	S	0	0
			543	355	89	96	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	ZG	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	ZH	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	XI	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	XJ	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	YI	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	YJ	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	ZI	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	ZJ	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	XK	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	XL	72	Total	C	N	O	S	0	0
			575	371	92	107	5		
6	YK	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	YL	68	Total	C	N	O	S	0	0
			543	355	89	96	3		
6	ZK	63	Total	C	N	O	S	0	0
			508	330	82	93	3		
6	ZL	63	Total	C	N	O	S	0	0
			508	330	82	93	3		

- Molecule 7 is a protein called 16.5 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	OA	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OB	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OC	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OD	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OE	14	Total	C	N	O	S	0	0
			105	66	16	22	1		

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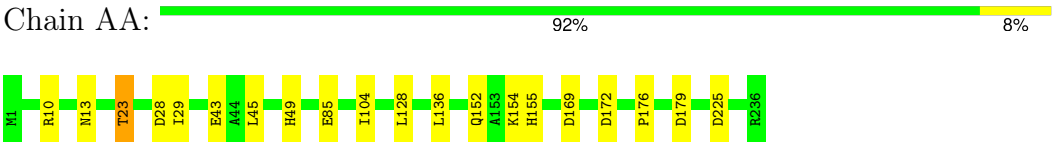
Mol	Chain	Residues	Atoms					AltConf	Trace
7	OF	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OG	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OH	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OI	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OJ	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OK	14	Total	C	N	O	S	0	0
			105	66	16	22	1		
7	OL	14	Total	C	N	O	S	0	0
			105	66	16	22	1		

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

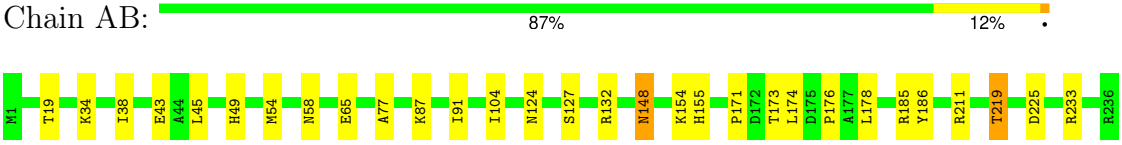
- Molecule 1: 30 kDa protein

Chain AA:



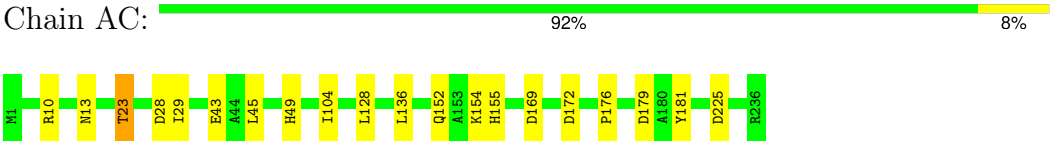
- Molecule 1: 30 kDa protein

Chain AB:



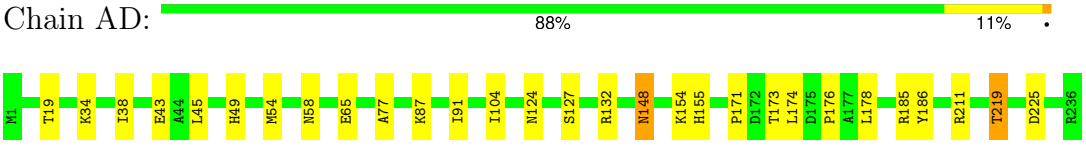
- Molecule 1: 30 kDa protein

Chain AC:



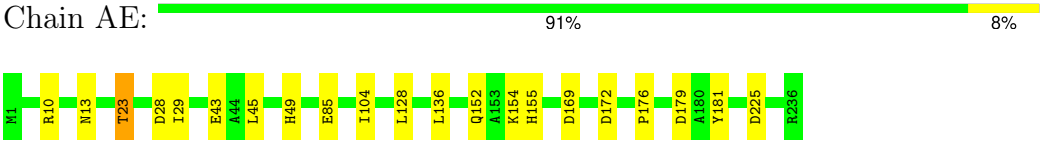
- Molecule 1: 30 kDa protein

Chain AD:



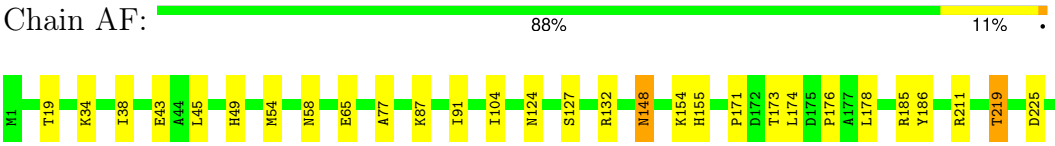
- Molecule 1: 30 kDa protein

Chain AE:



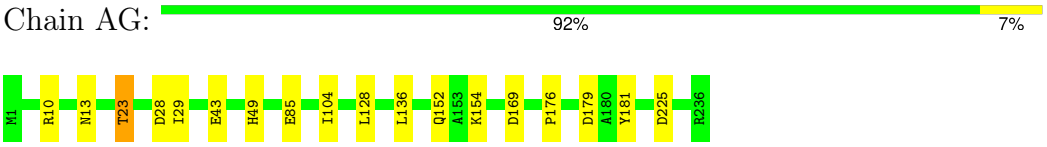
- Molecule 1: 30 kDa protein

Chain AF:



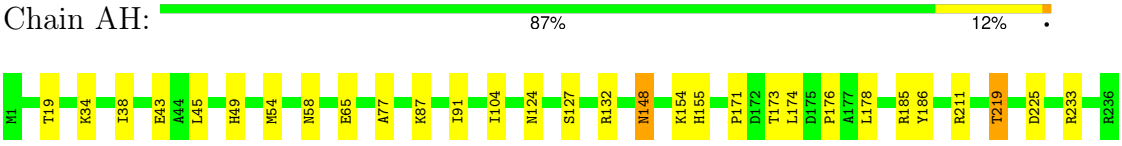
• Molecule 1: 30 kDa protein

Chain AG:



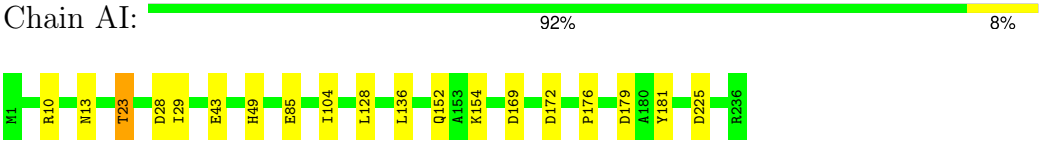
• Molecule 1: 30 kDa protein

Chain AH:



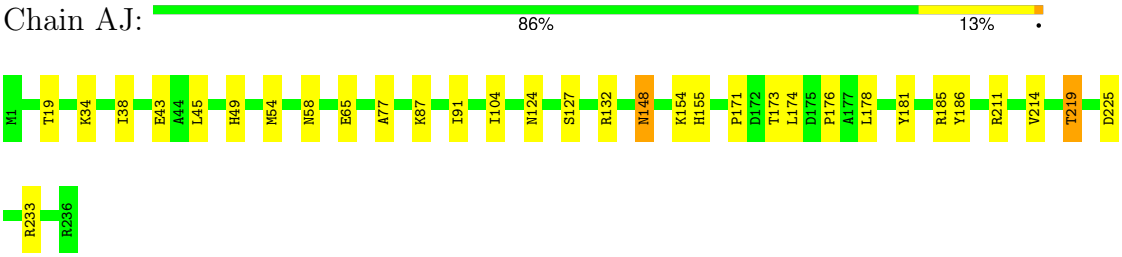
• Molecule 1: 30 kDa protein

Chain AI:



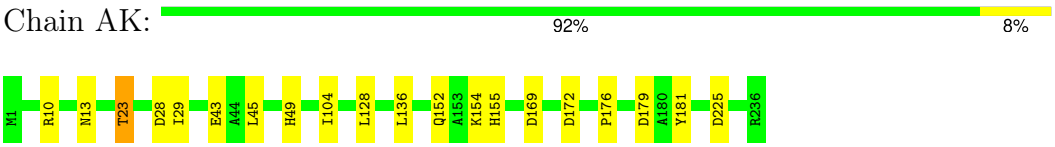
• Molecule 1: 30 kDa protein

Chain AJ:



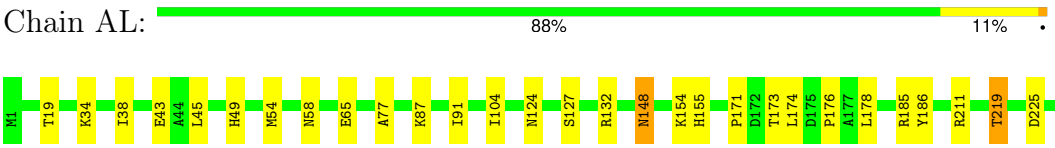
• Molecule 1: 30 kDa protein

Chain AK:



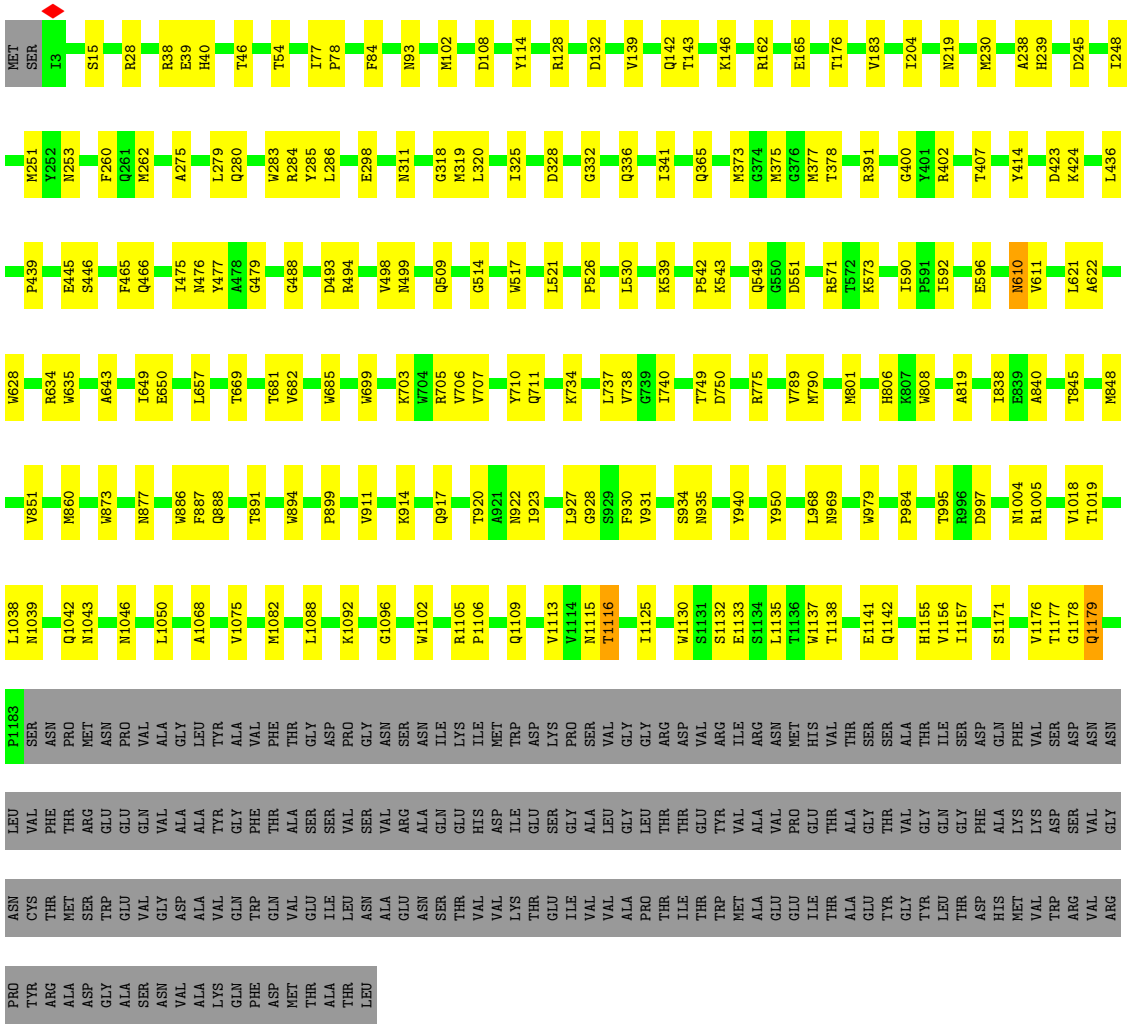
• Molecule 1: 30 kDa protein

Chain AL:



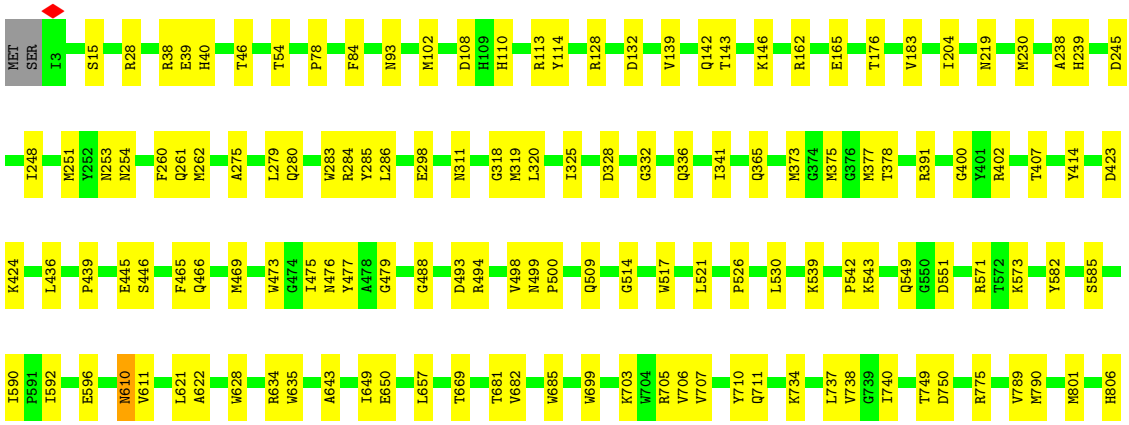
• Molecule 2: Non-contractile tail sheath

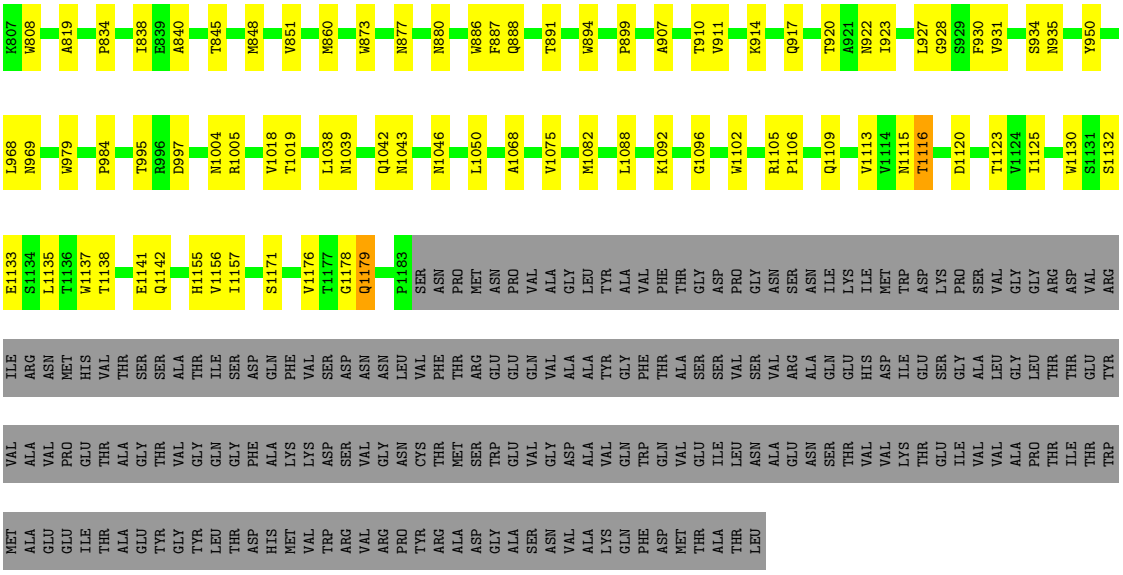
Chain LA:



• Molecule 2: Non-contractile tail sheath

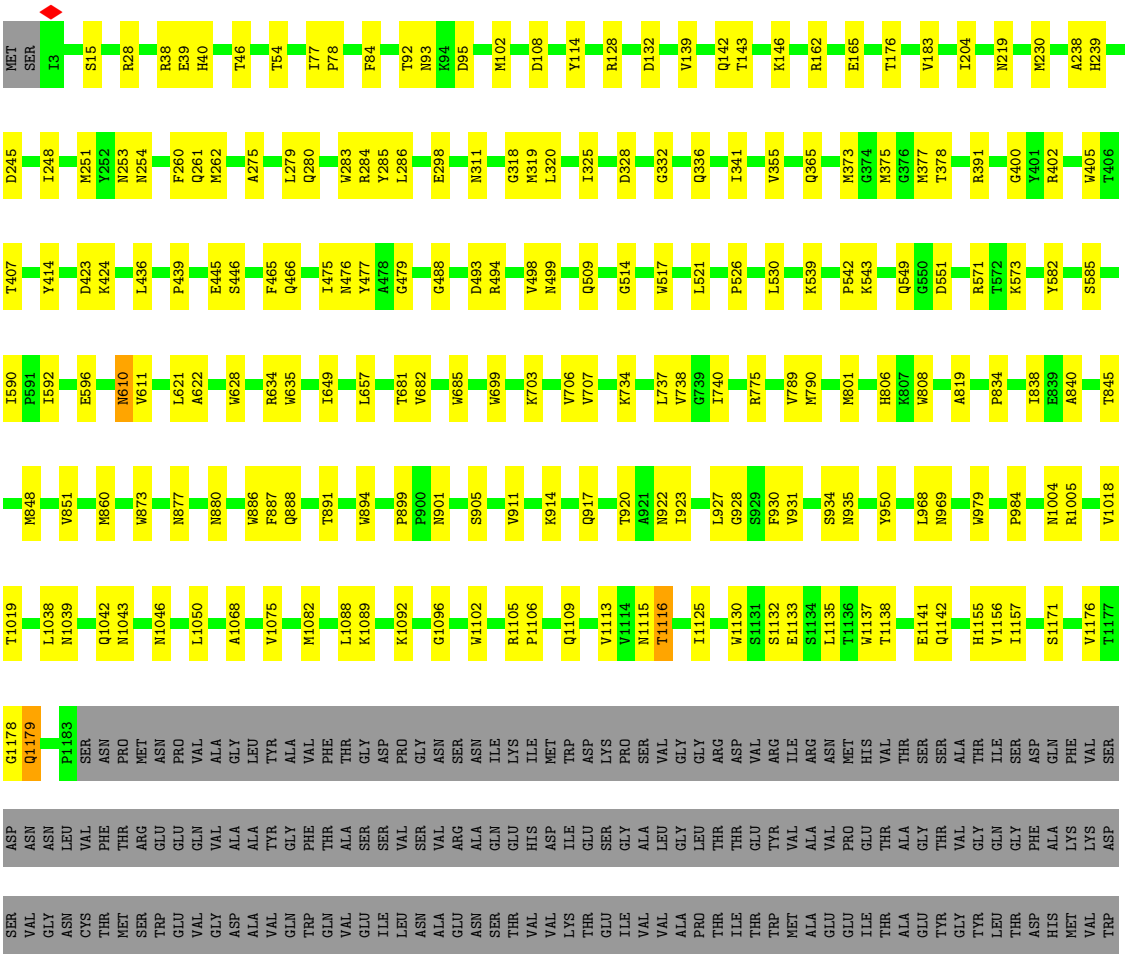
Chain LB:

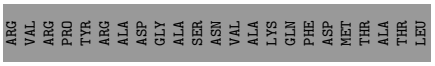




• Molecule 2: Non-contractile tail sheath

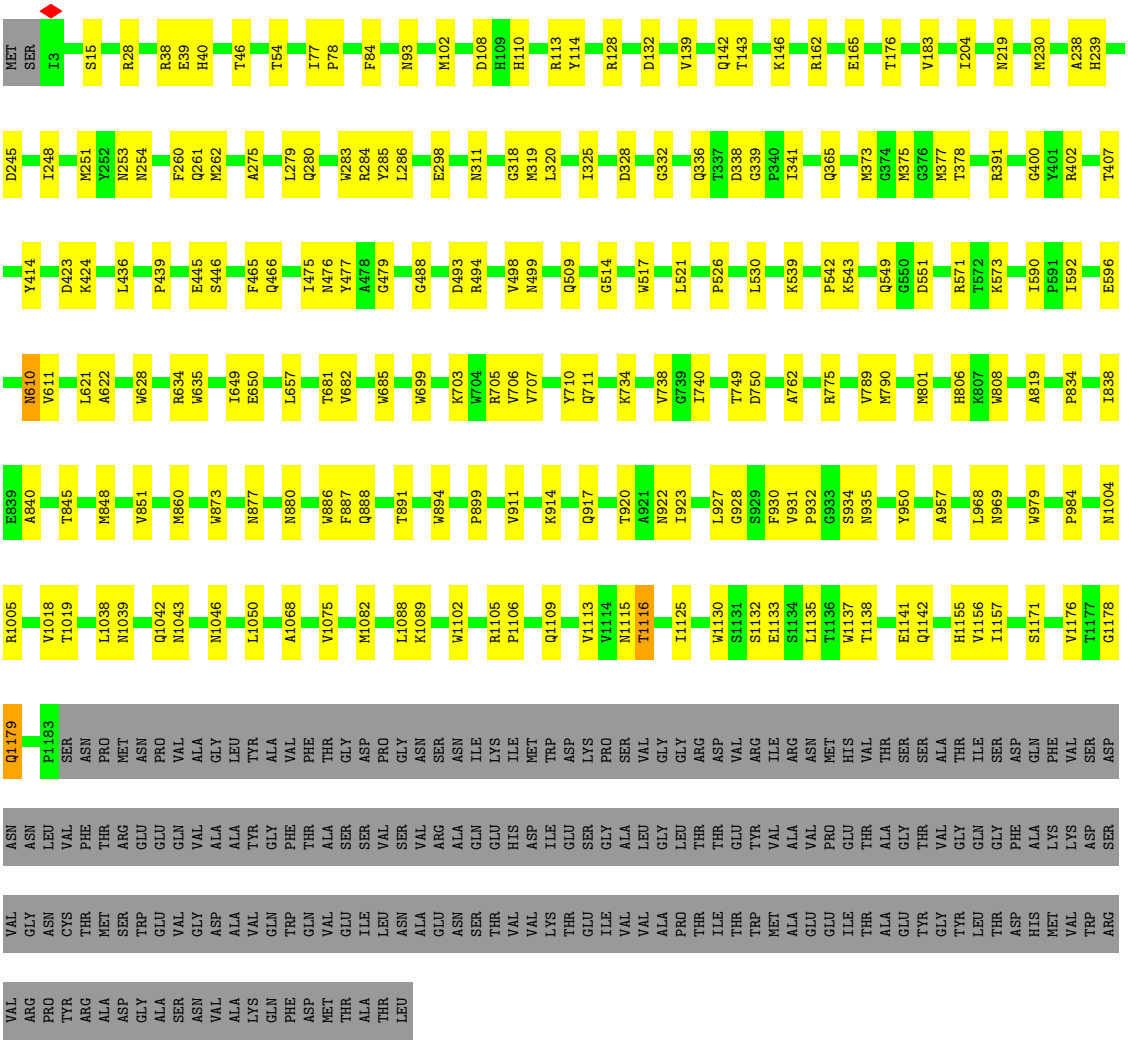
Chain LC:





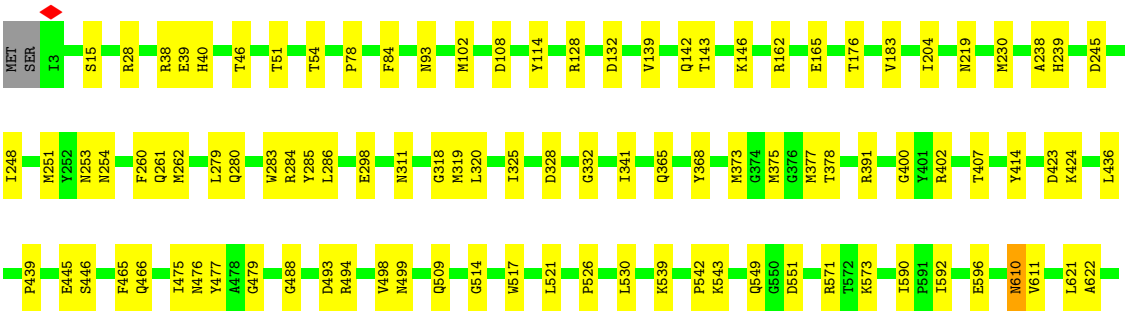
• Molecule 2: Non-contractile tail sheath

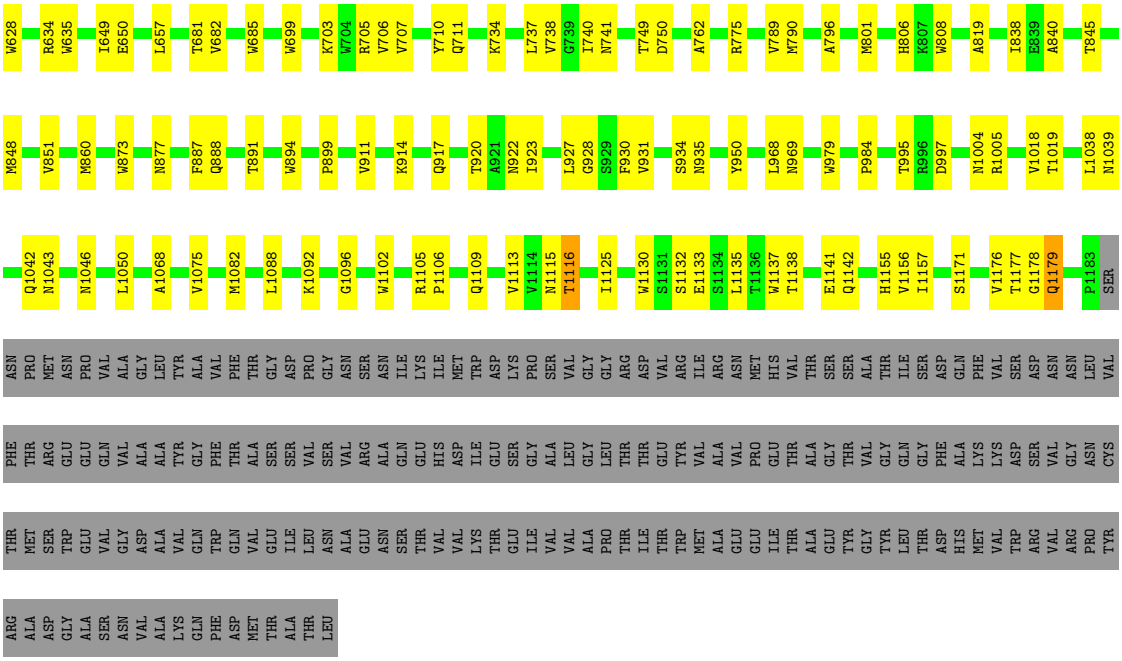
Chain LD:



• Molecule 2: Non-contractile tail sheath

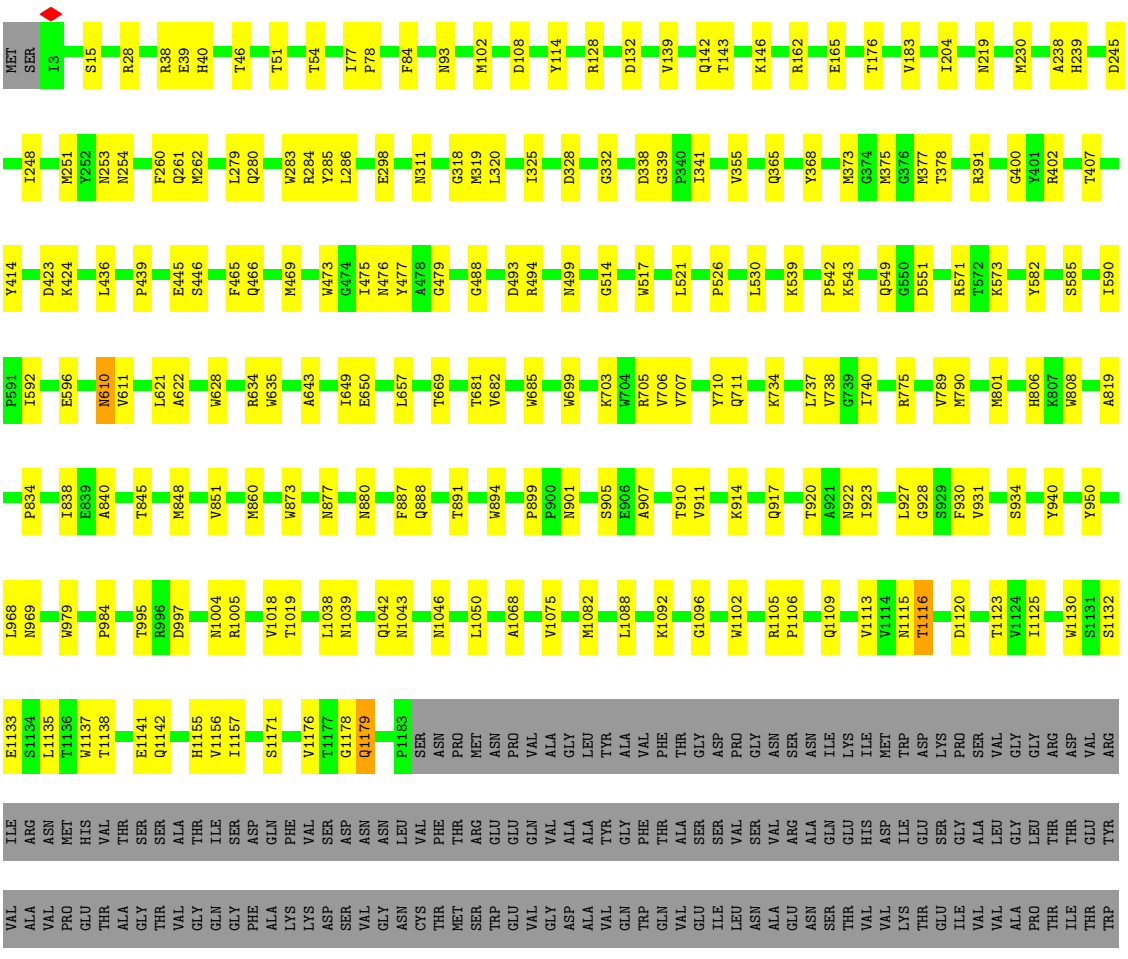
Chain LE:





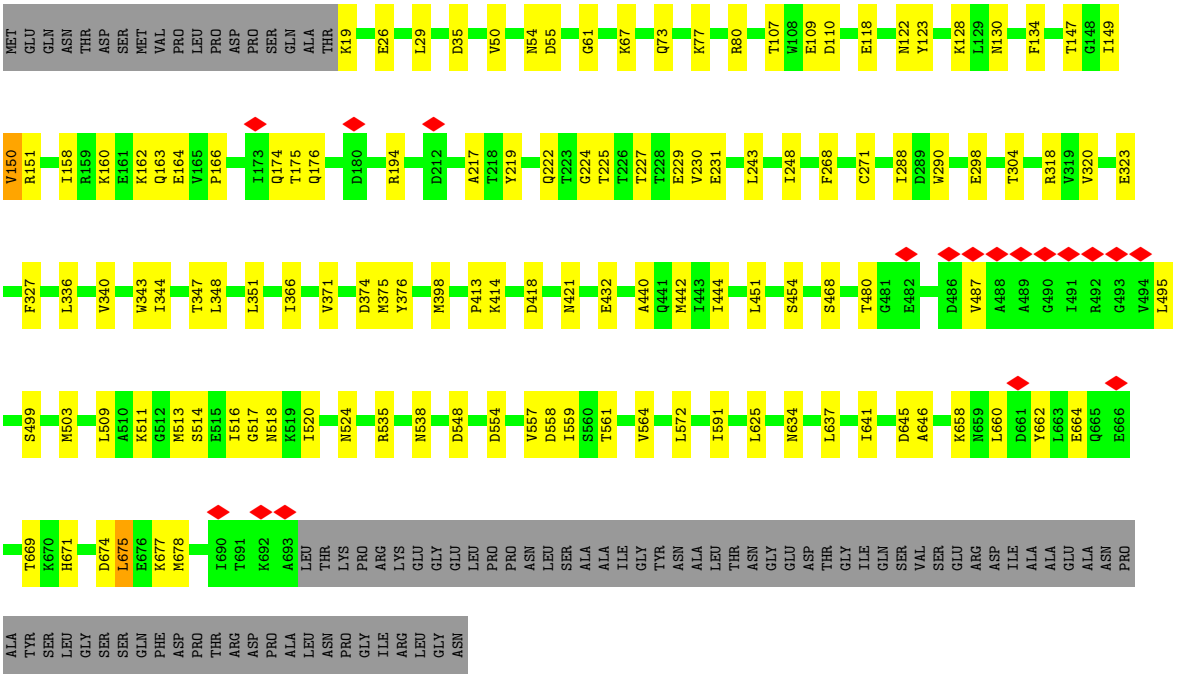
• Molecule 2: Non-contractile tail sheath

Chain LF:



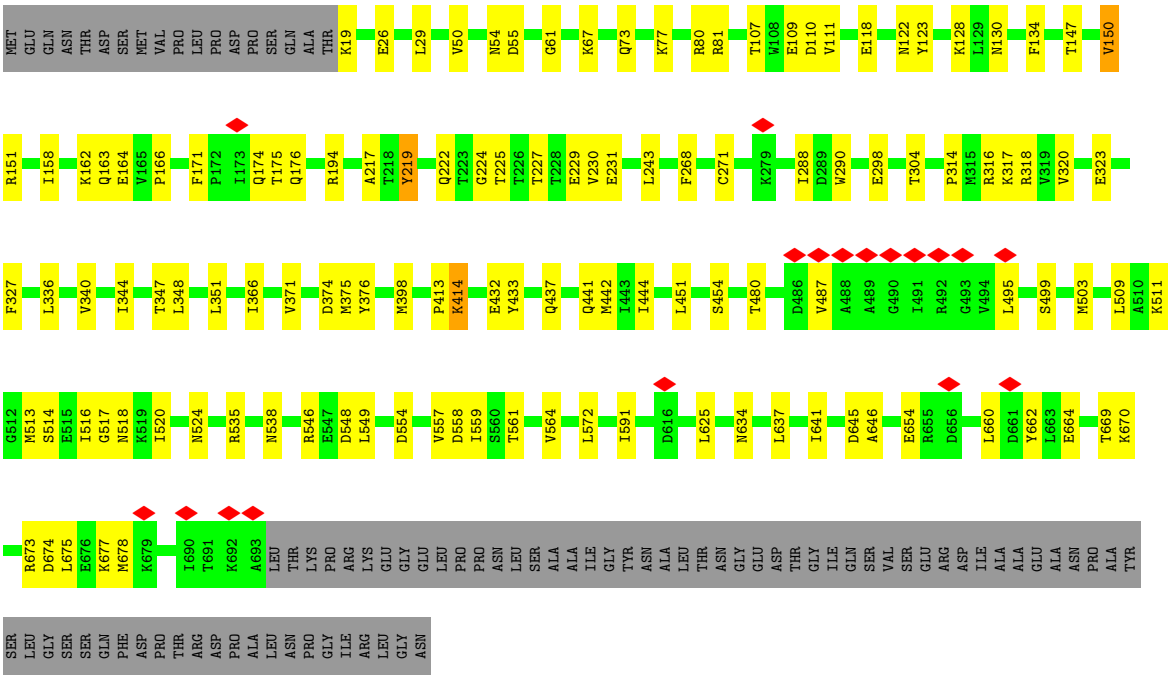
• Molecule 3: Probable portal protein

Chain PA:



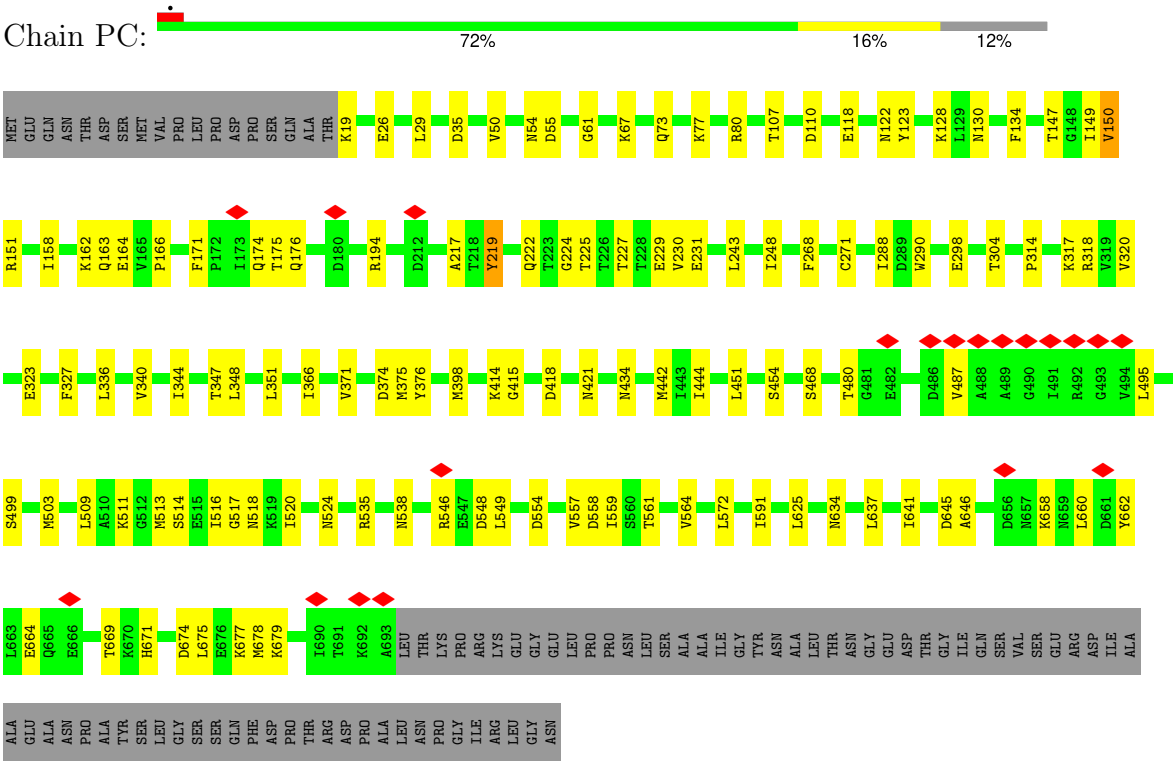
• Molecule 3: Probable portal protein

Chain PB:



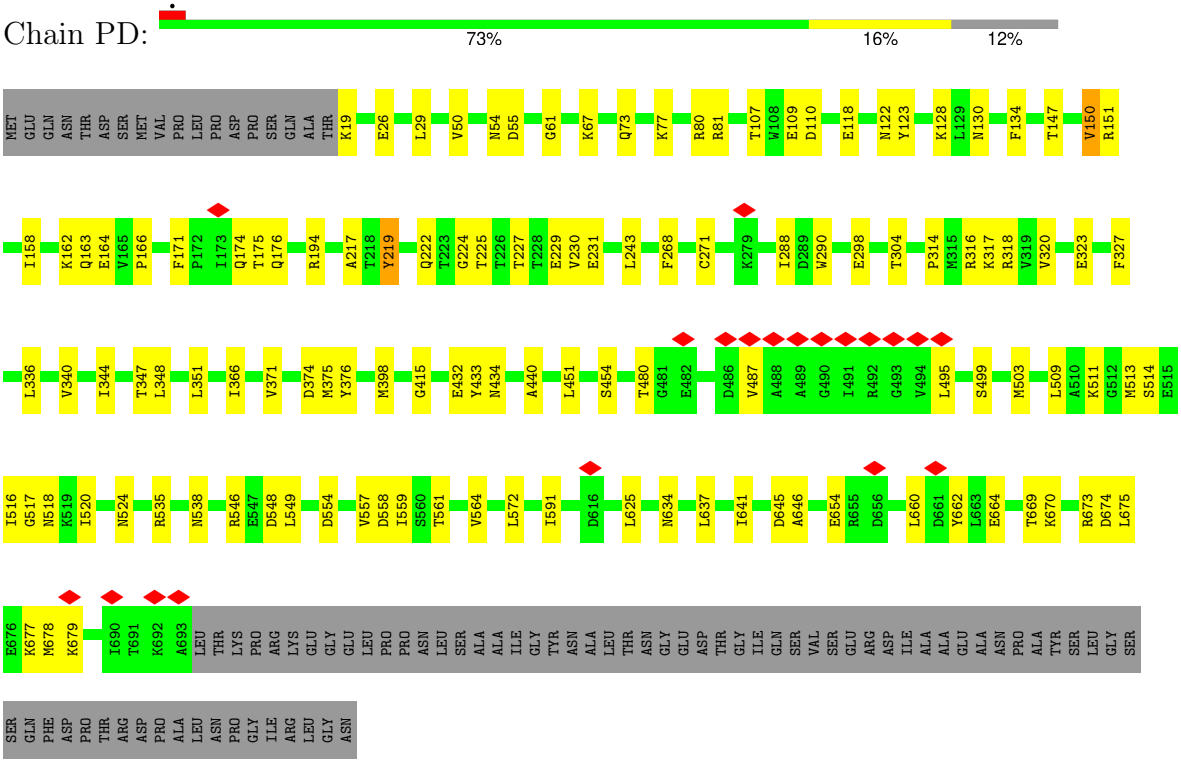
• Molecule 3: Probable portal protein

Chain PC:



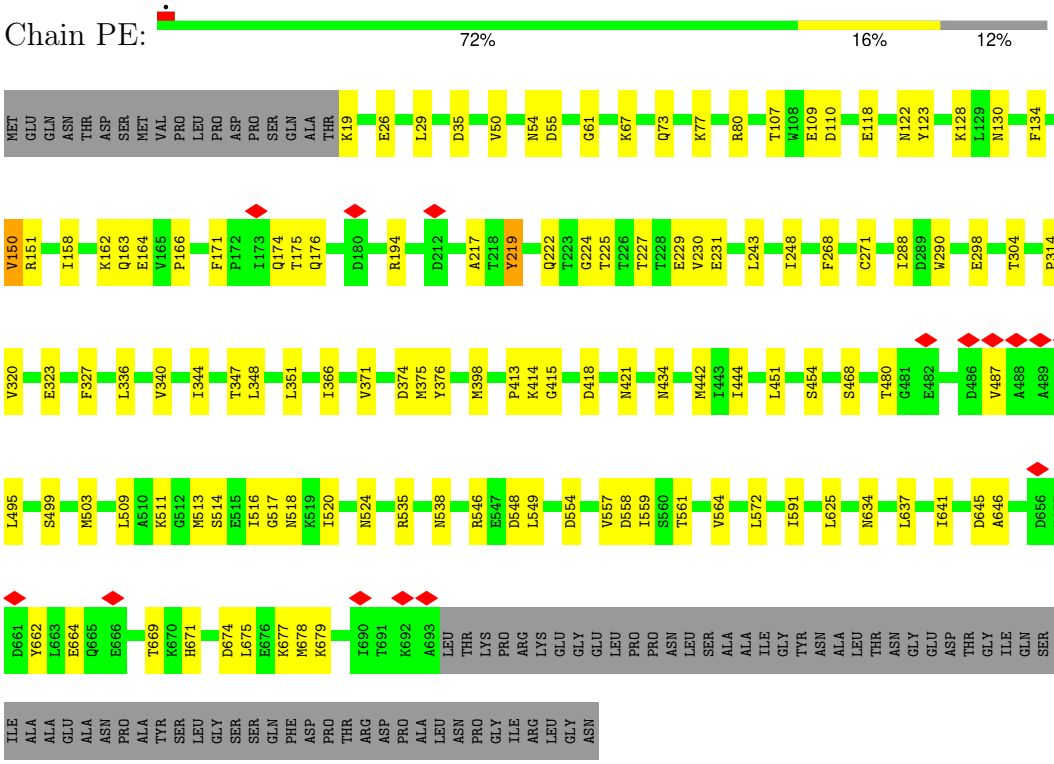
• Molecule 3: Probable portal protein

Chain PD:



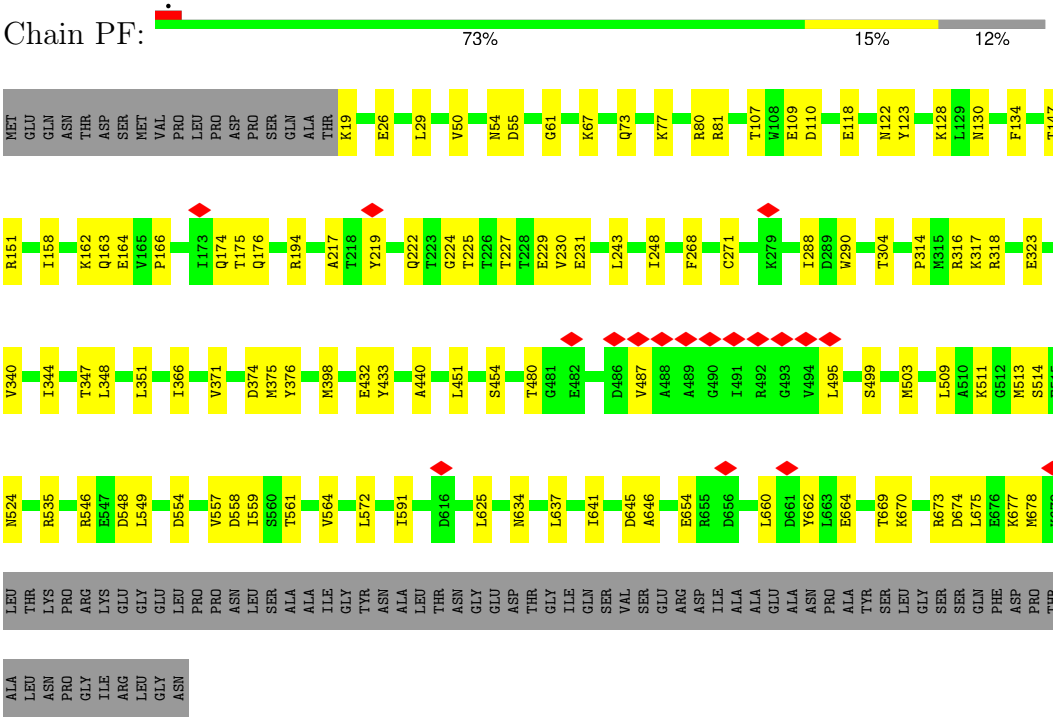
• Molecule 3: Probable portal protein

Chain PE:



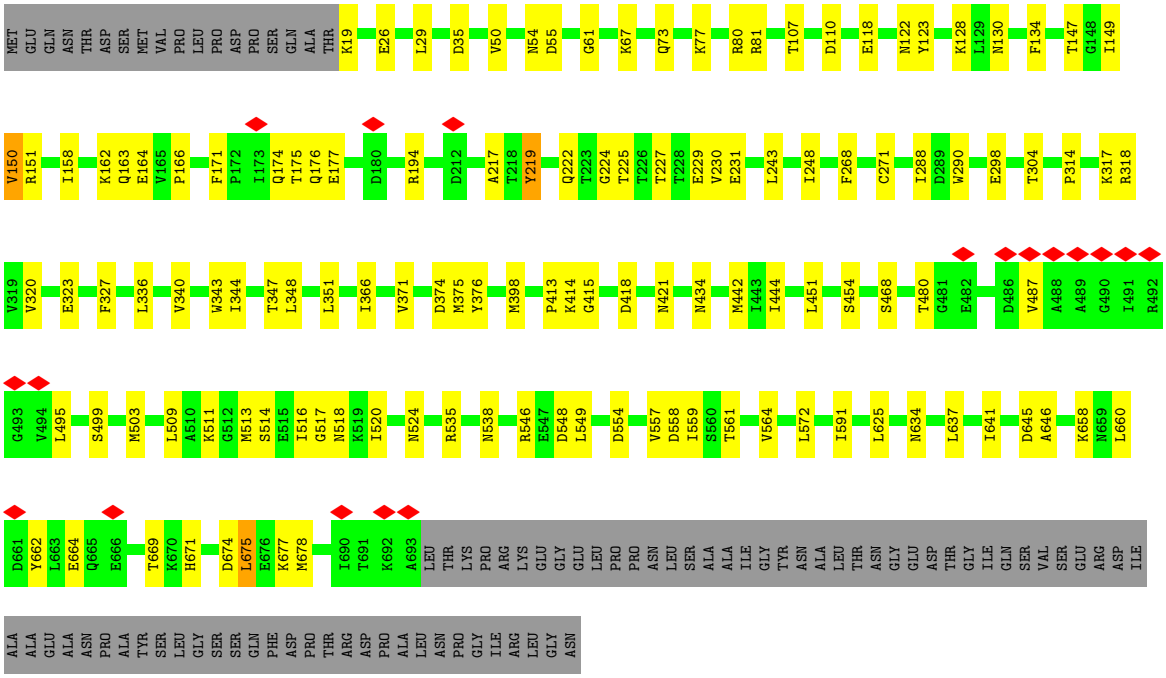
• Molecule 3: Probable portal protein

Chain PF:



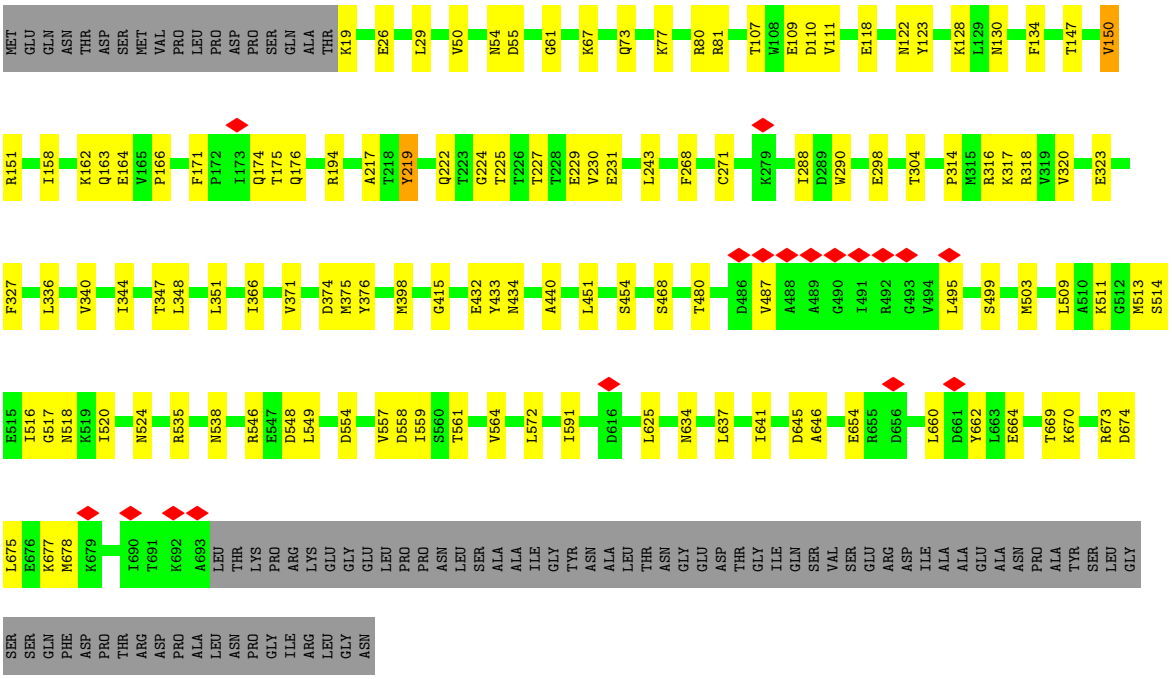
• Molecule 3: Probable portal protein

Chain PG:



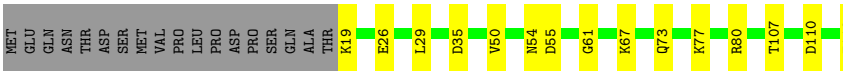
• Molecule 3: Probable portal protein

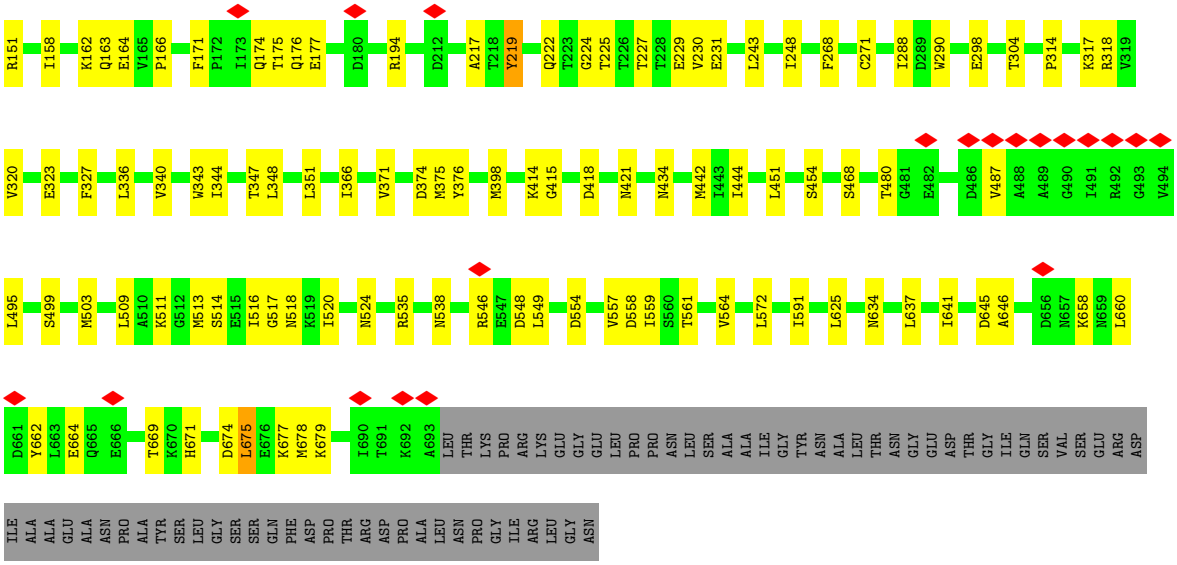
Chain PH:



• Molecule 3: Probable portal protein

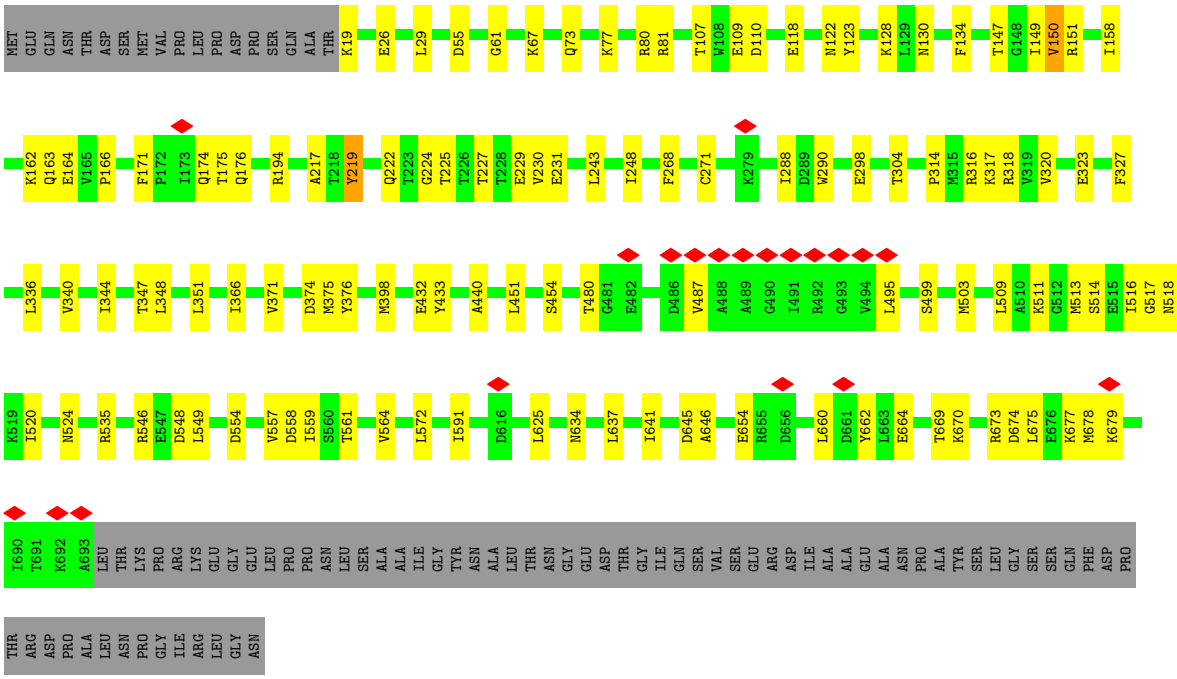
Chain PI:





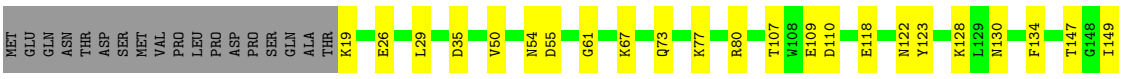
• Molecule 3: Probable portal protein

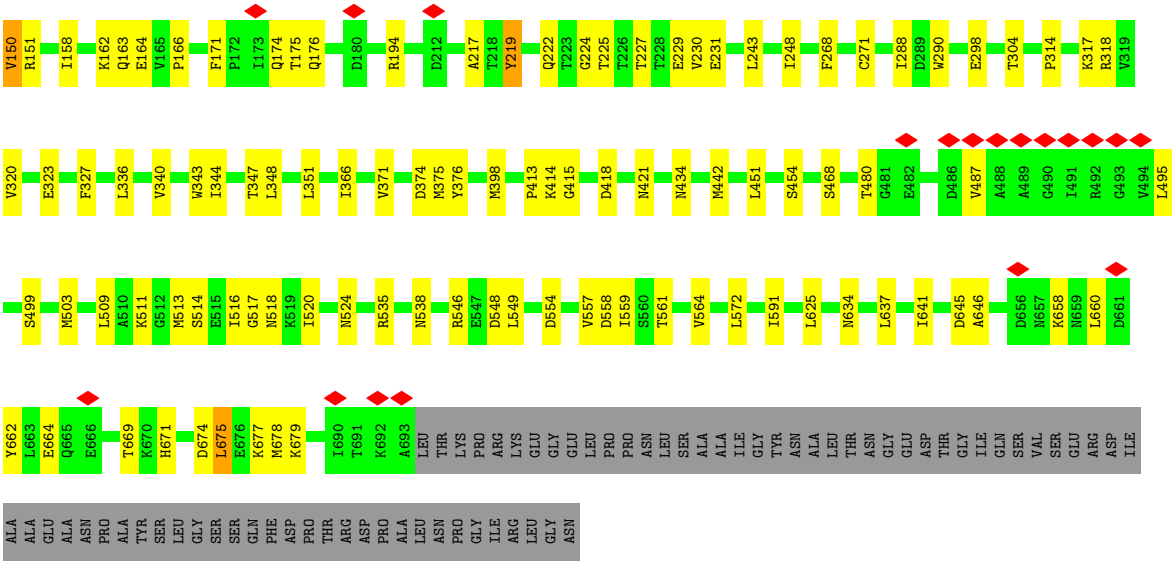
Chain PJ:



• Molecule 3: Probable portal protein

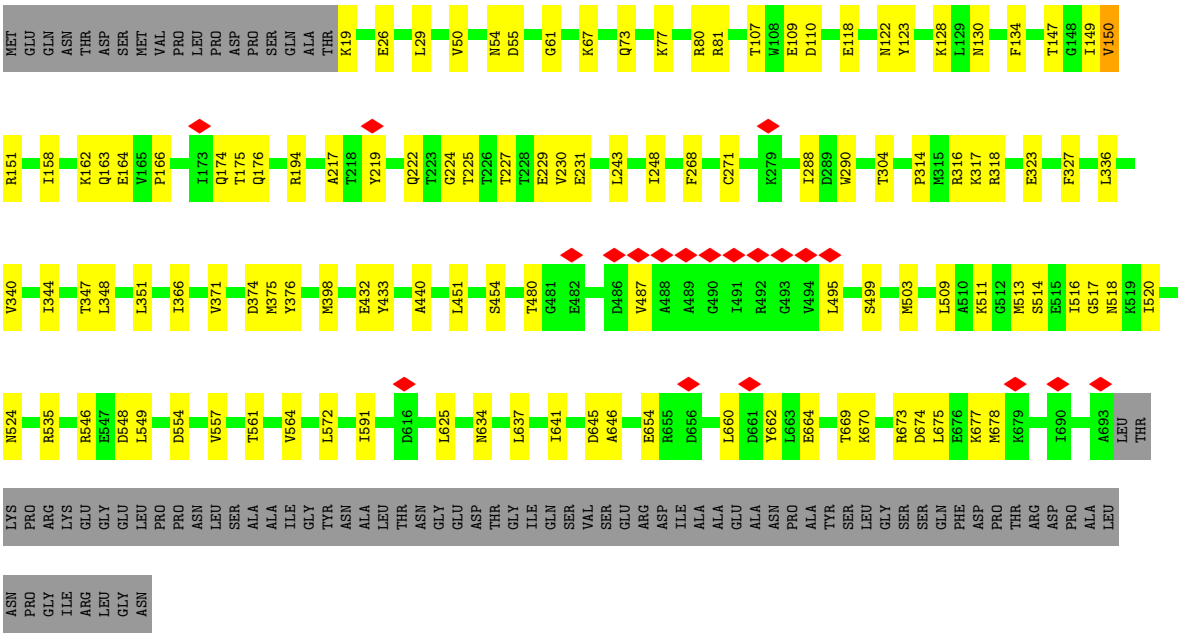
Chain PK:





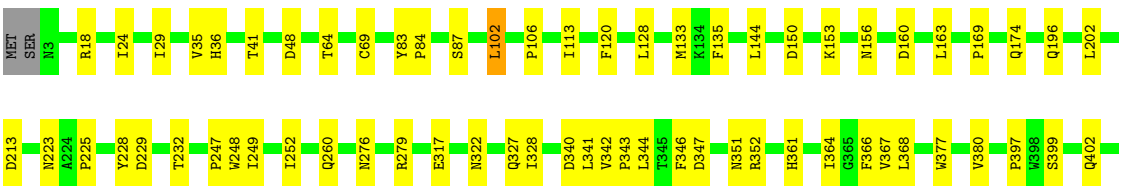
• Molecule 3: Probable portal protein

Chain PL:



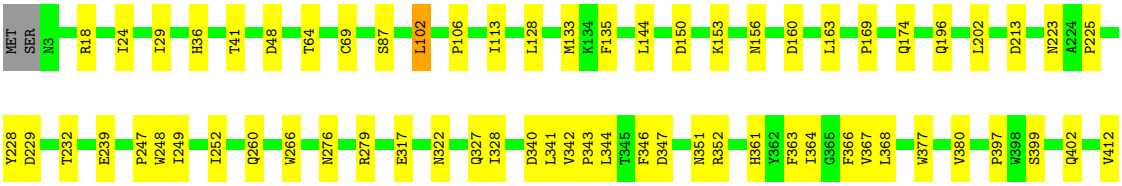
• Molecule 4: Gp64

Chain SA:



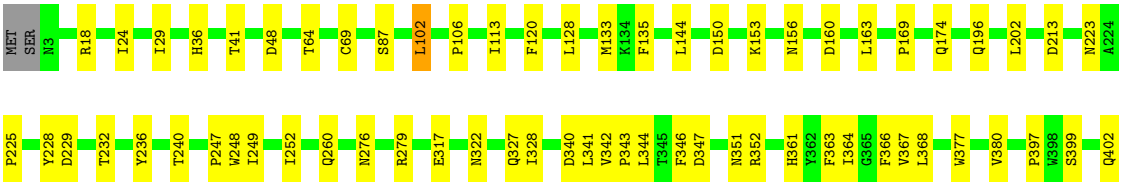
• Molecule 4: Gp64

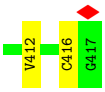
Chain SB:



• Molecule 4: Gp64

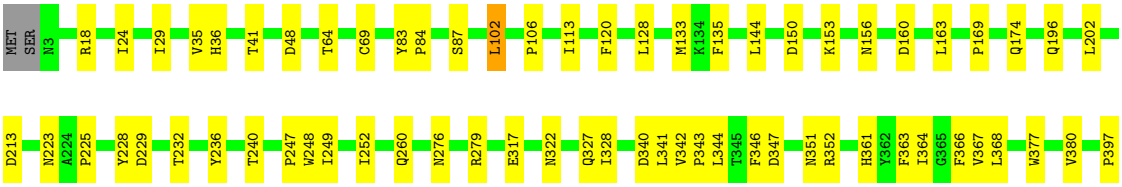
Chain SC:





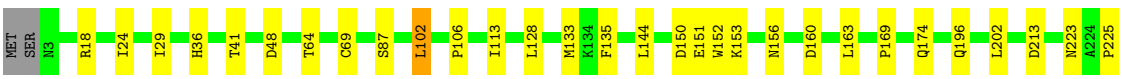
• Molecule 4: Gp64

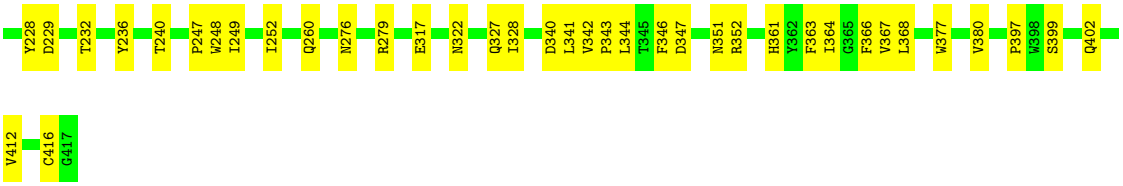
Chain SD:



• Molecule 4: Gp64

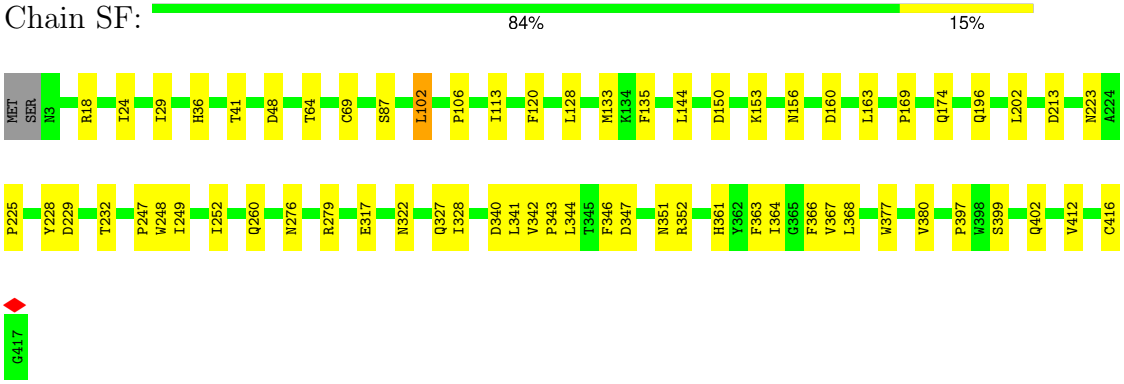
Chain SE:





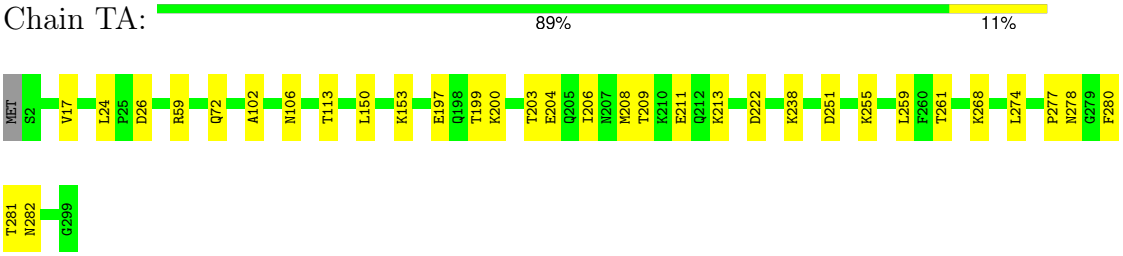
• Molecule 4: Gp64

Chain SF:



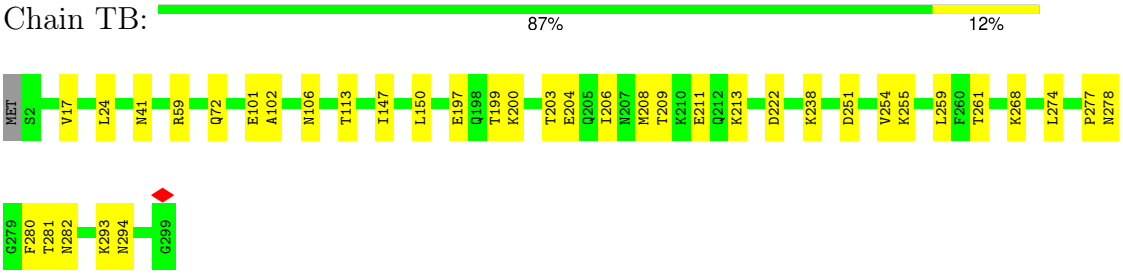
• Molecule 5: Gp54

Chain TA:



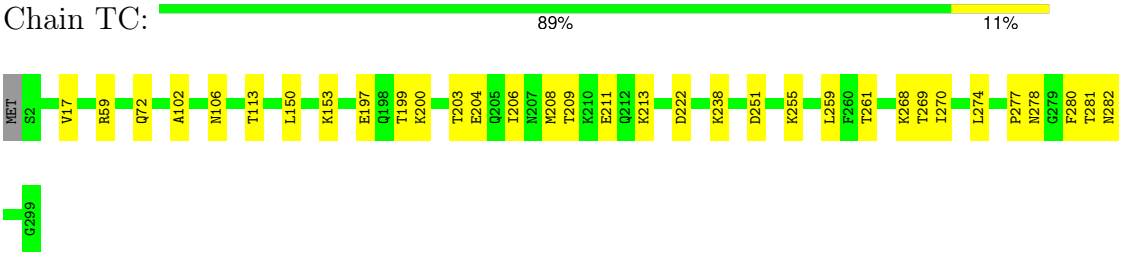
• Molecule 5: Gp54

Chain TB:



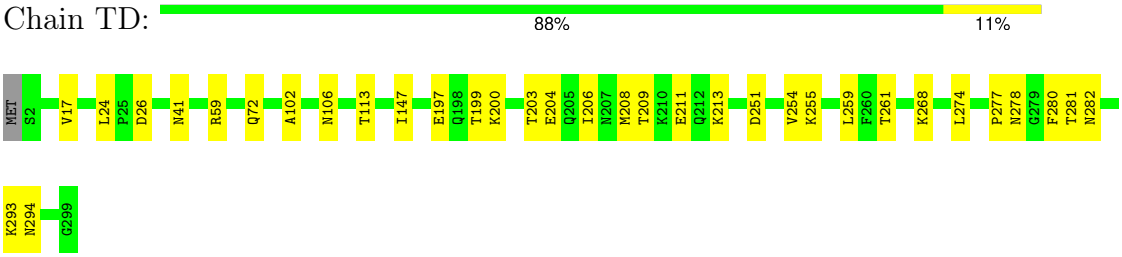
• Molecule 5: Gp54

Chain TC:



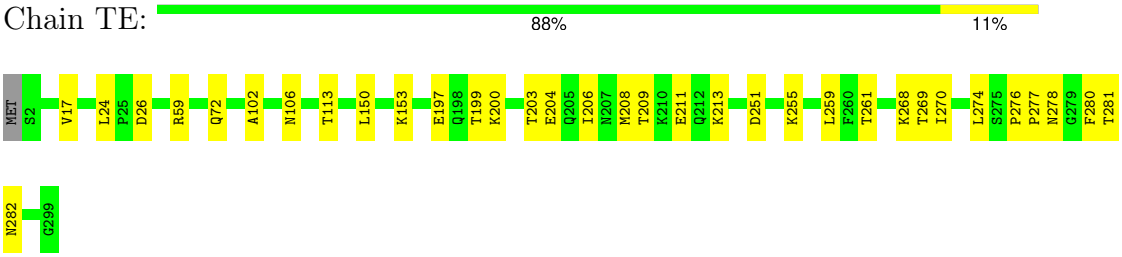
• Molecule 5: Gp54

Chain TD:



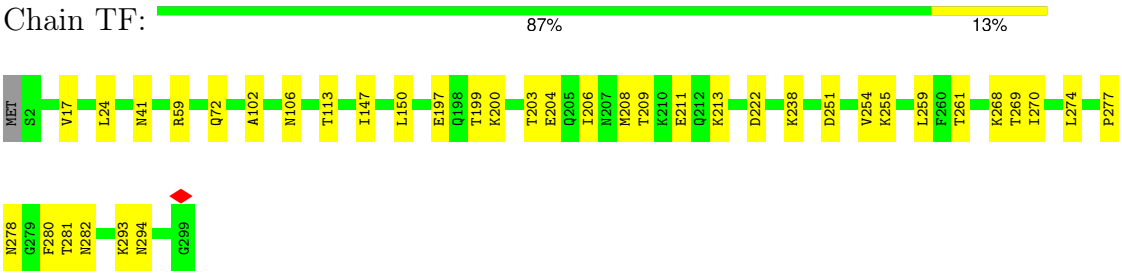
• Molecule 5: Gp54

Chain TE:



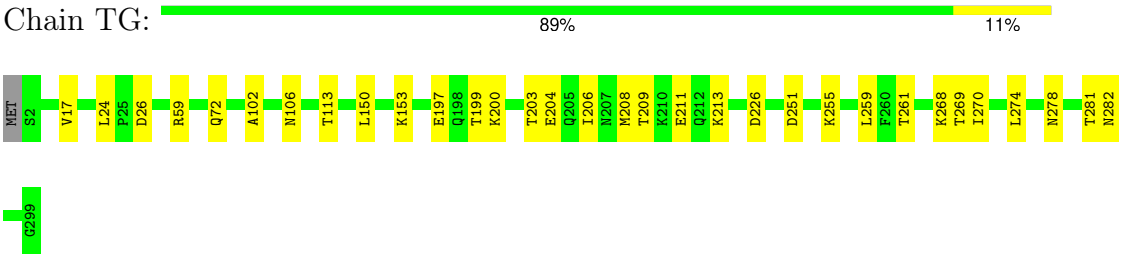
• Molecule 5: Gp54

Chain TF:



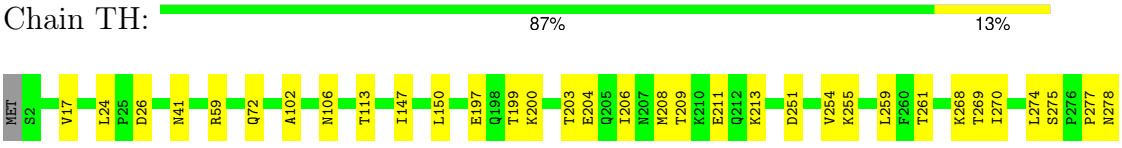
• Molecule 5: Gp54

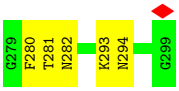
Chain TG:



• Molecule 5: Gp54

Chain TH:





• Molecule 5: Gp54

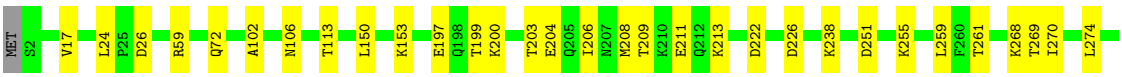
Chain TI:

• Molecule 5: Gp54

Chain TJ:

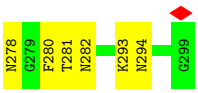
• Molecule 5: Gp54

Chain TK:



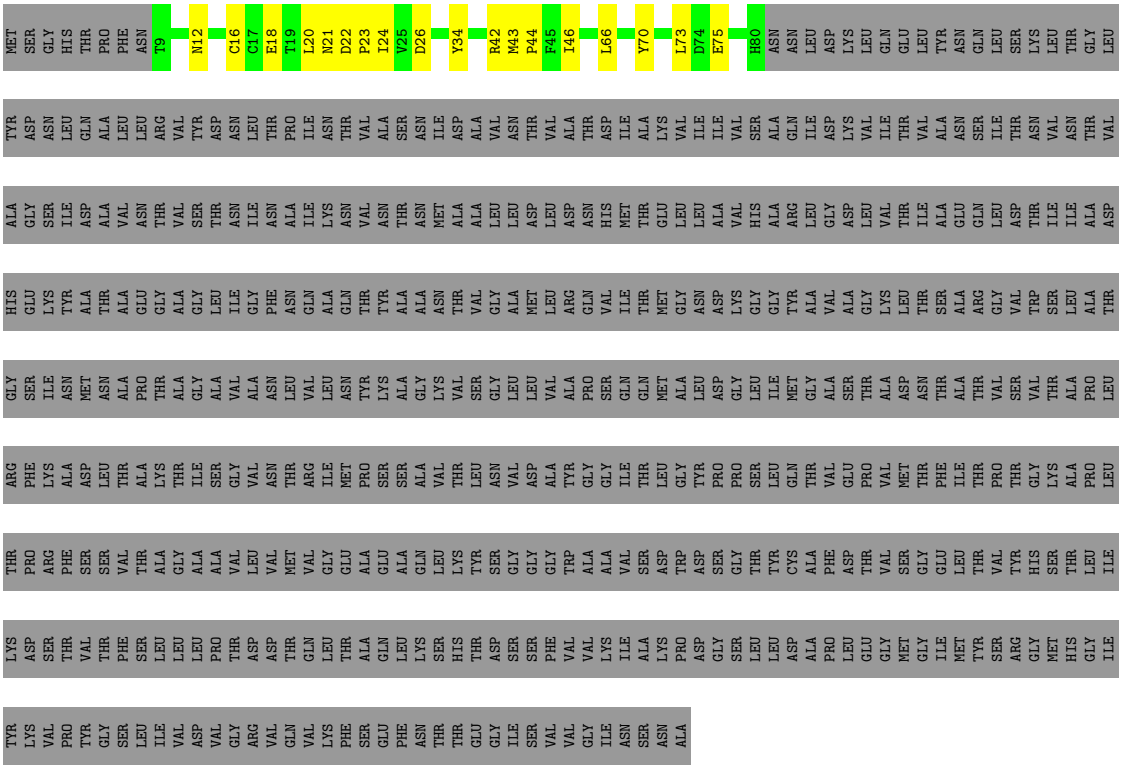
• Molecule 5: Gp54

Chain TL:



• Molecule 6: 60 kDa protein

Chain XA:

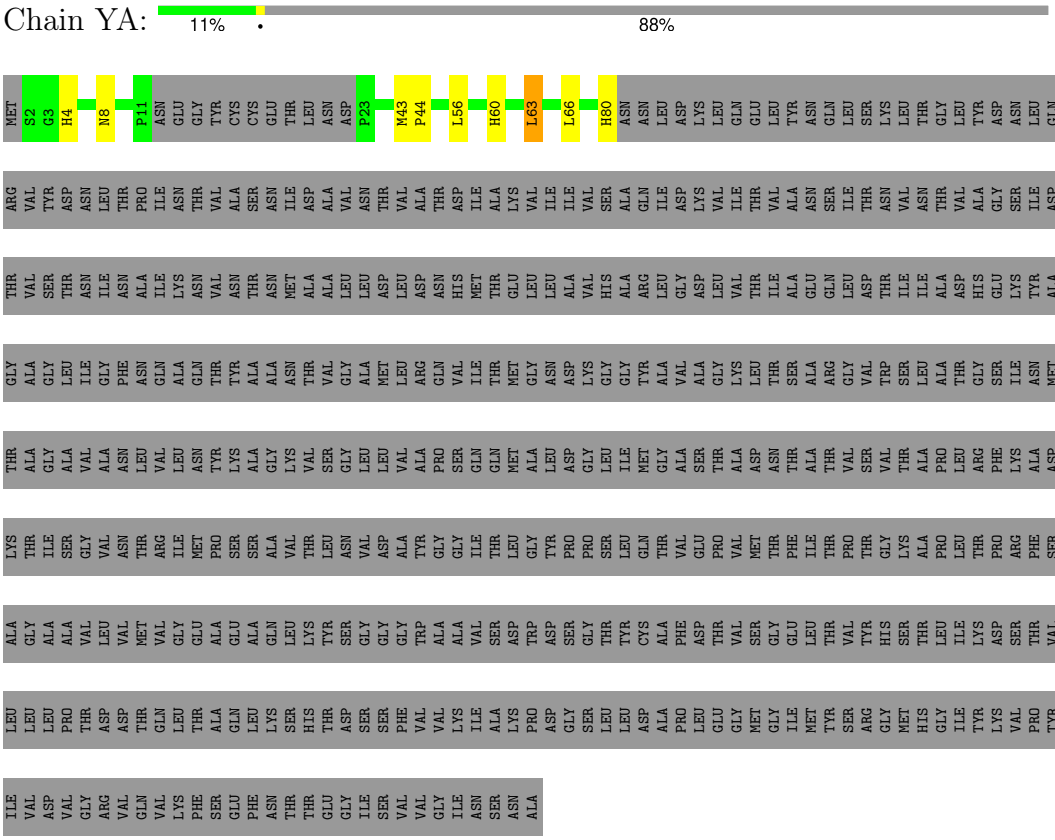


• Molecule 6: 60 kDa protein

Chain XB:

• Molecule 6: 60 kDa protein

Chain YA:

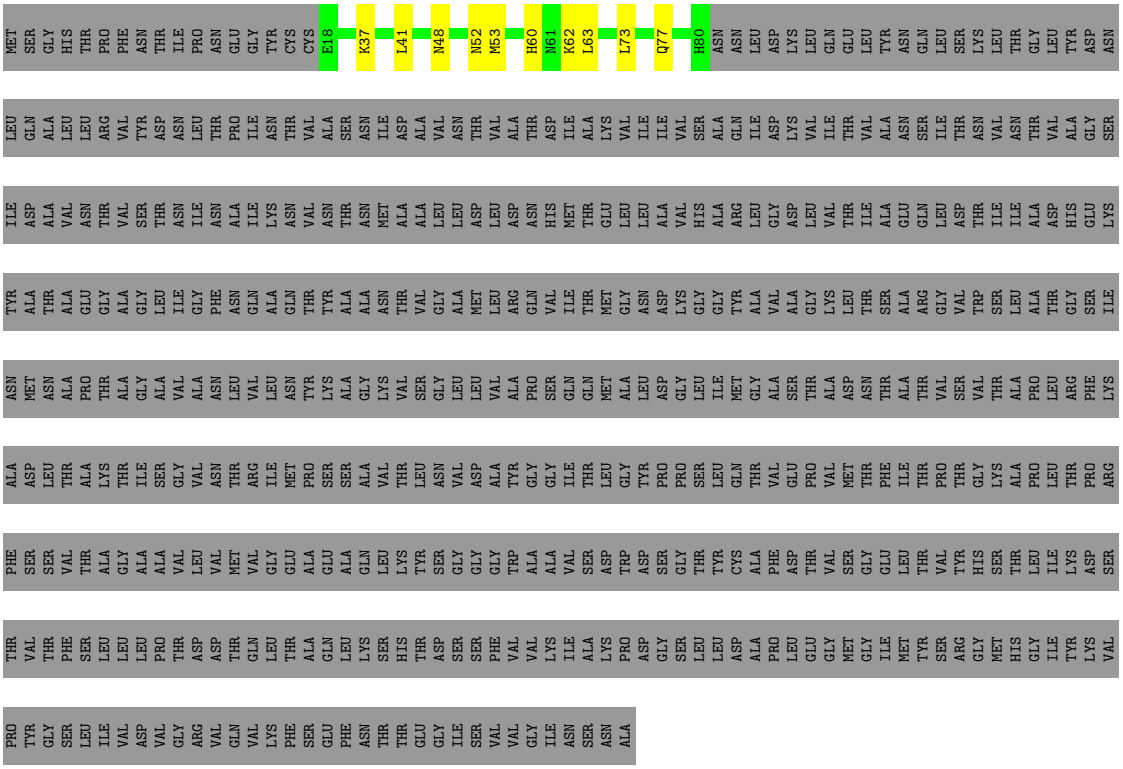


• Molecule 6: 60 kDa protein

Chain YB:

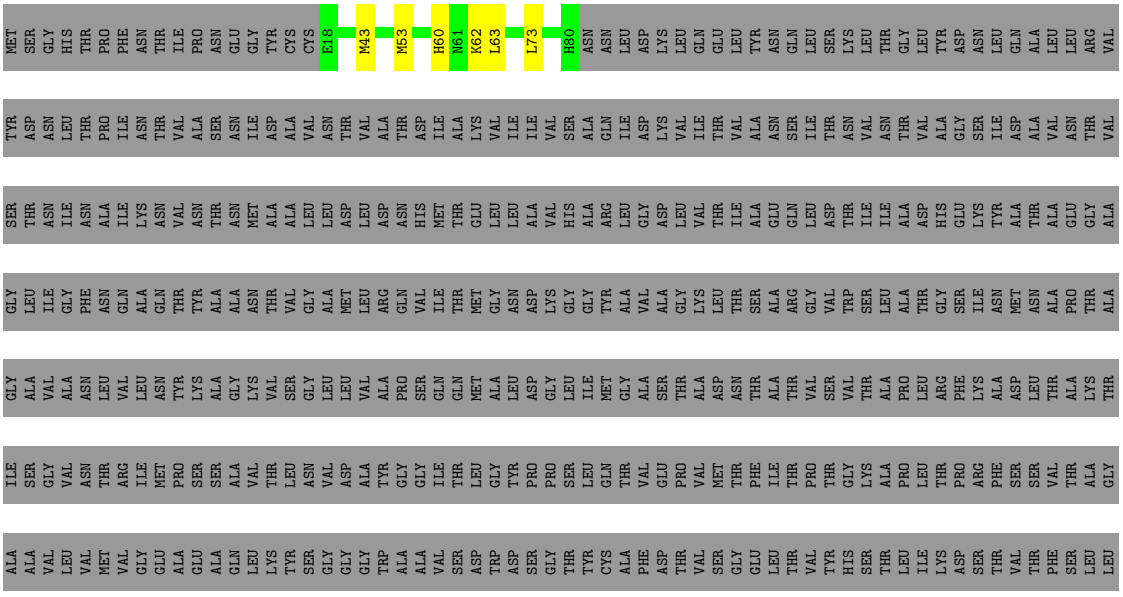
• Molecule 6: 60 kDa protein

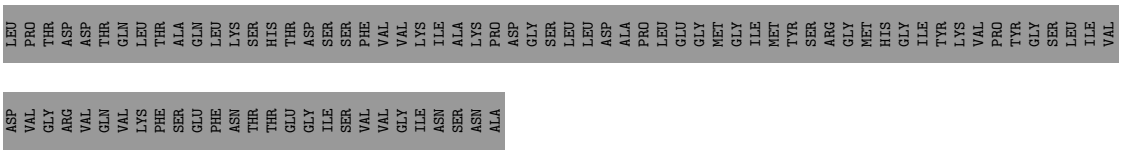
Chain ZA:



• Molecule 6: 60 kDa protein

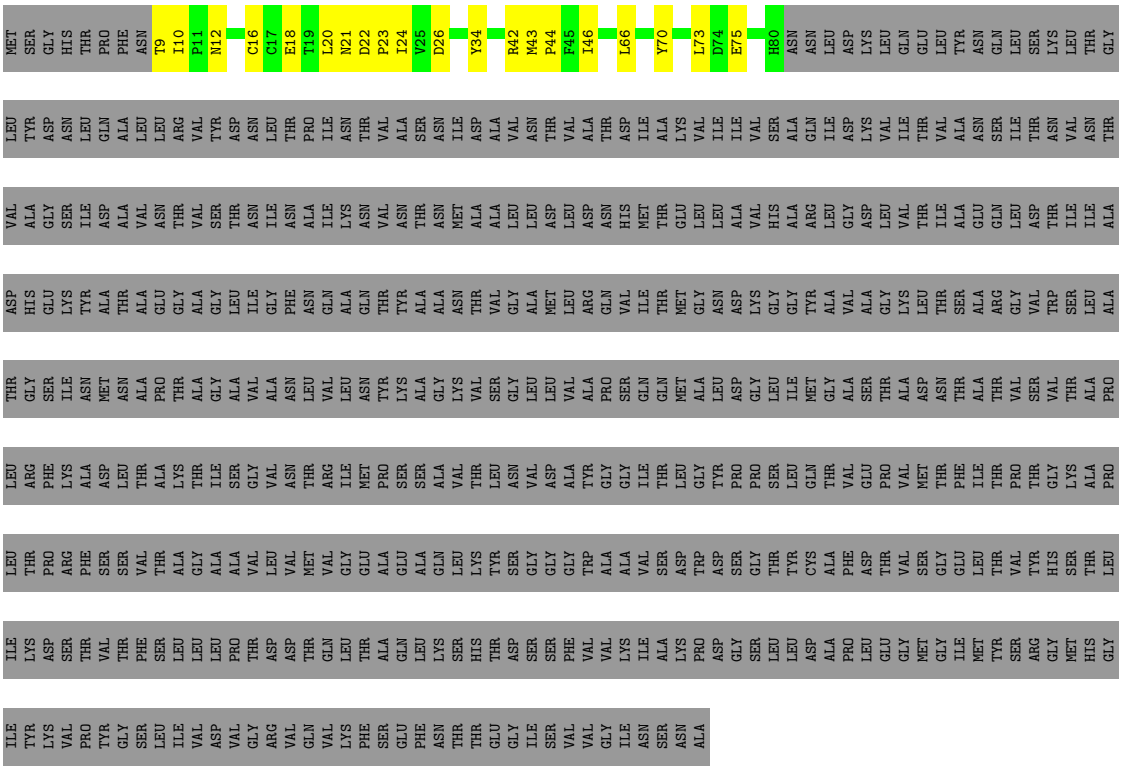
Chain ZB:





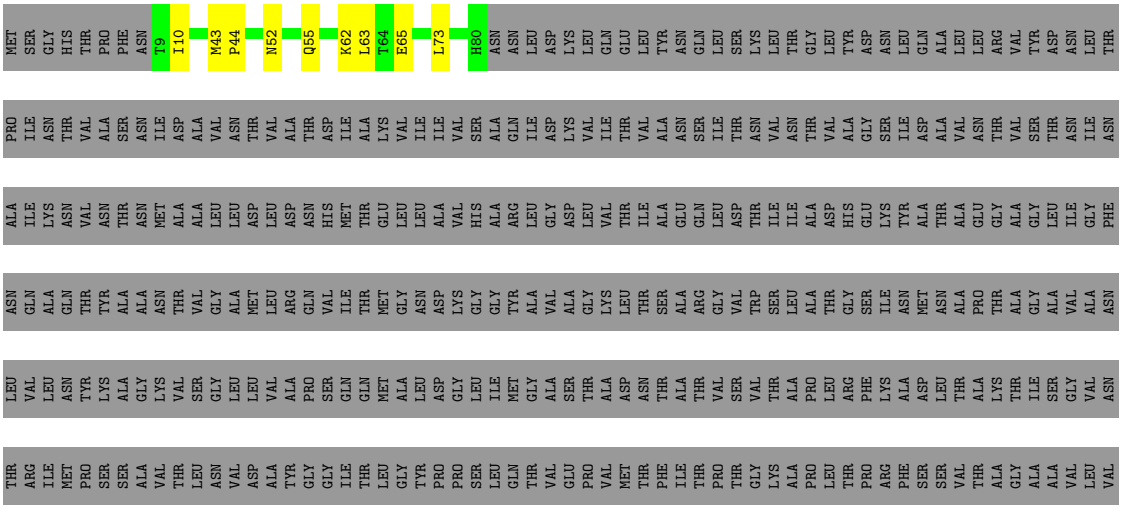
• Molecule 6: 60 kDa protein

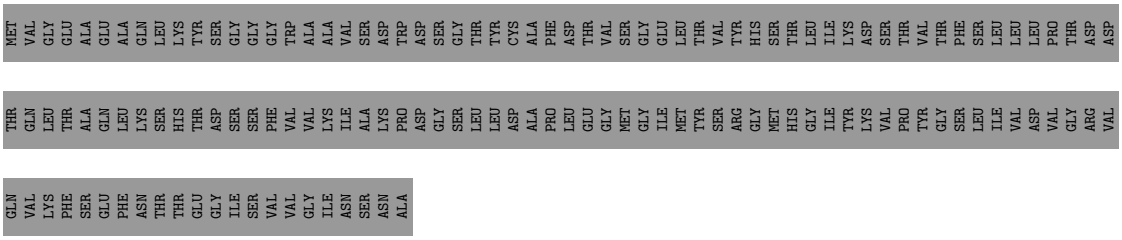
Chain XC:



• Molecule 6: 60 kDa protein

Chain XD:



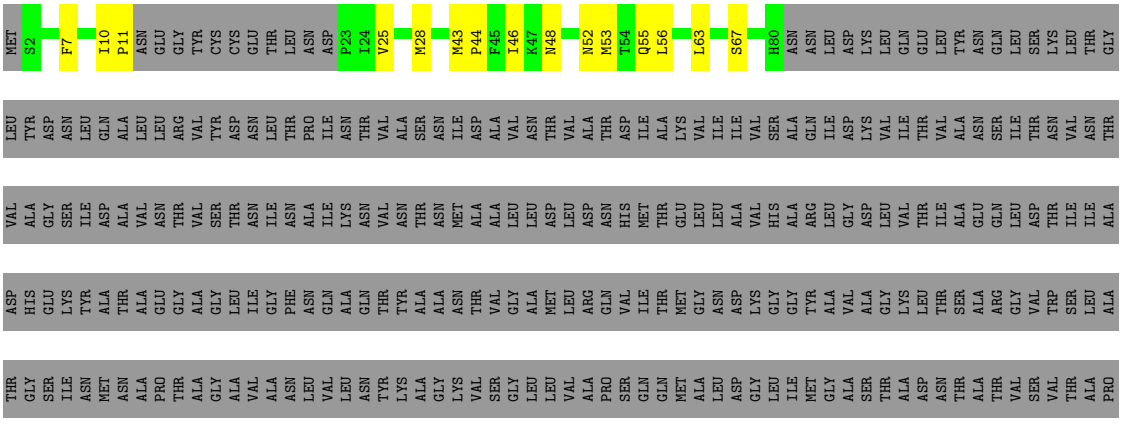


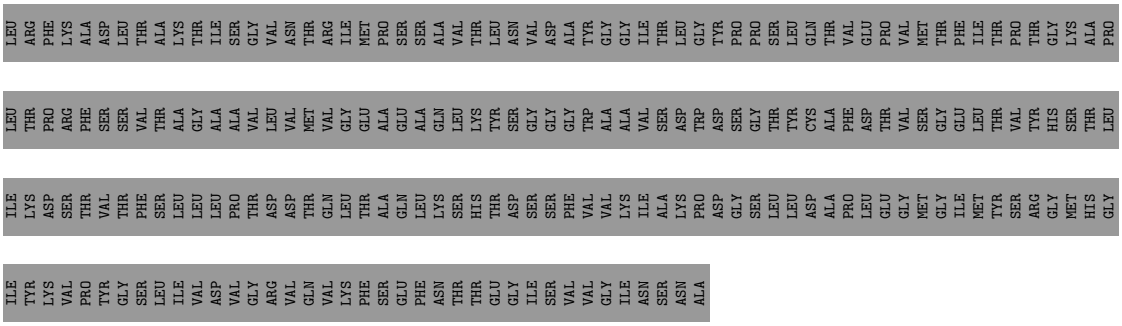
• Molecule 6: 60 kDa protein

Chain YC:

• Molecule 6: 60 kDa protein

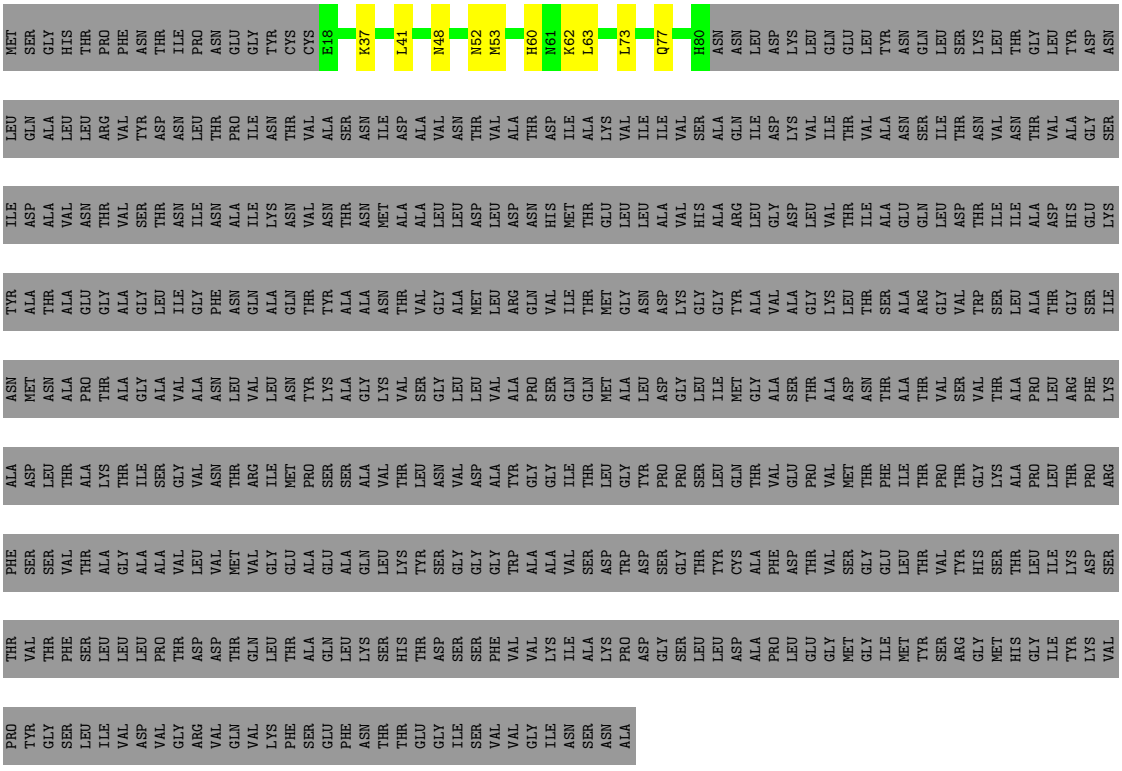
Chain YD:





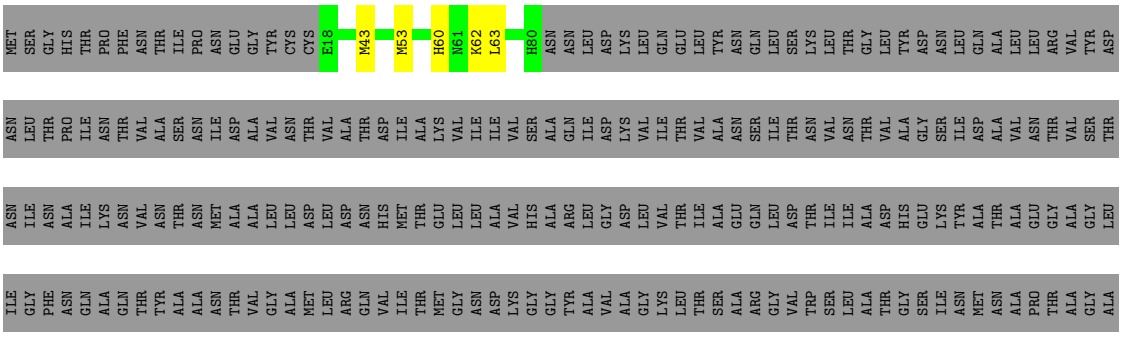
• Molecule 6: 60 kDa protein

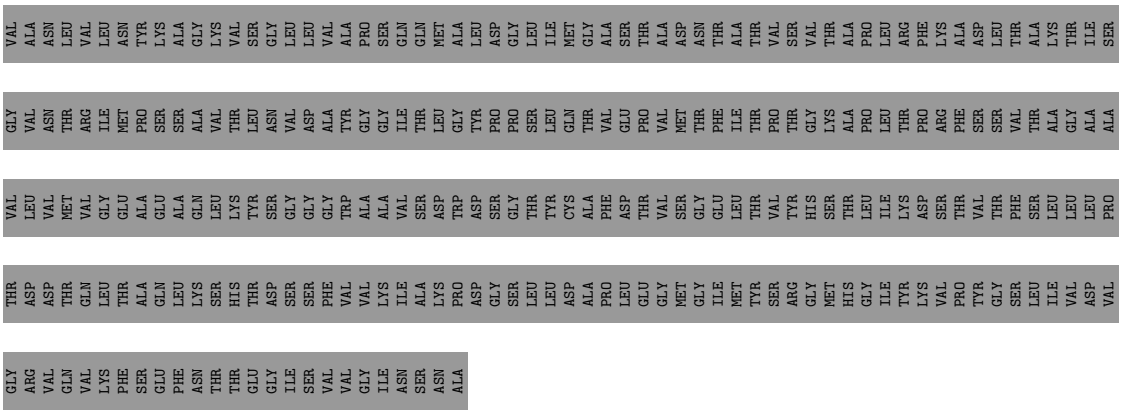
Chain ZC:



• Molecule 6: 60 kDa protein

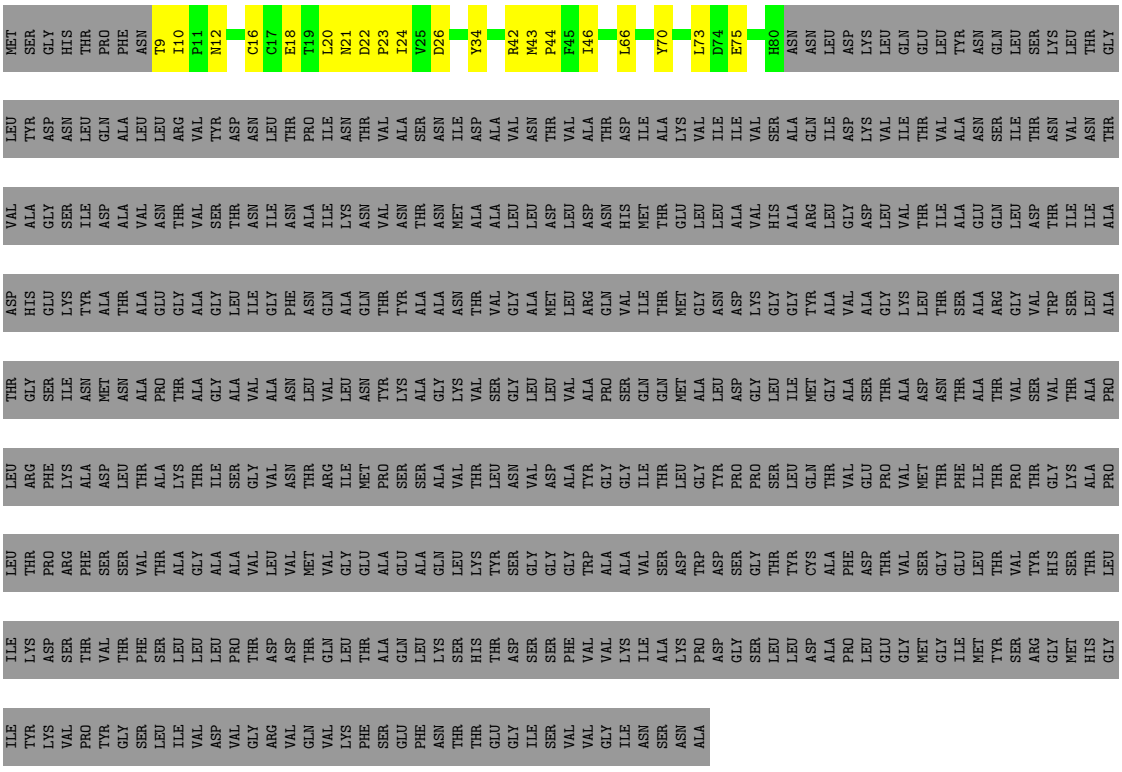
Chain ZD:





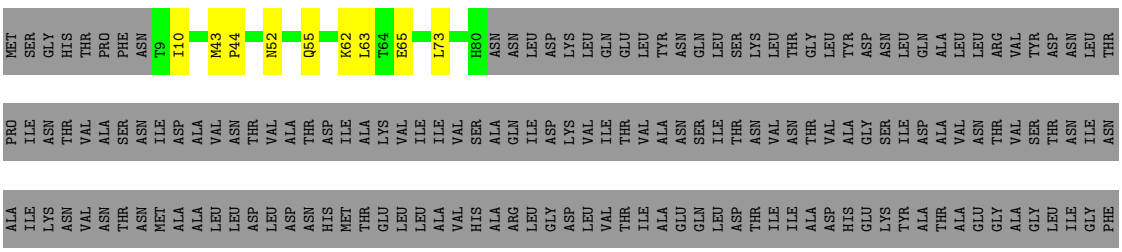
• Molecule 6: 60 kDa protein

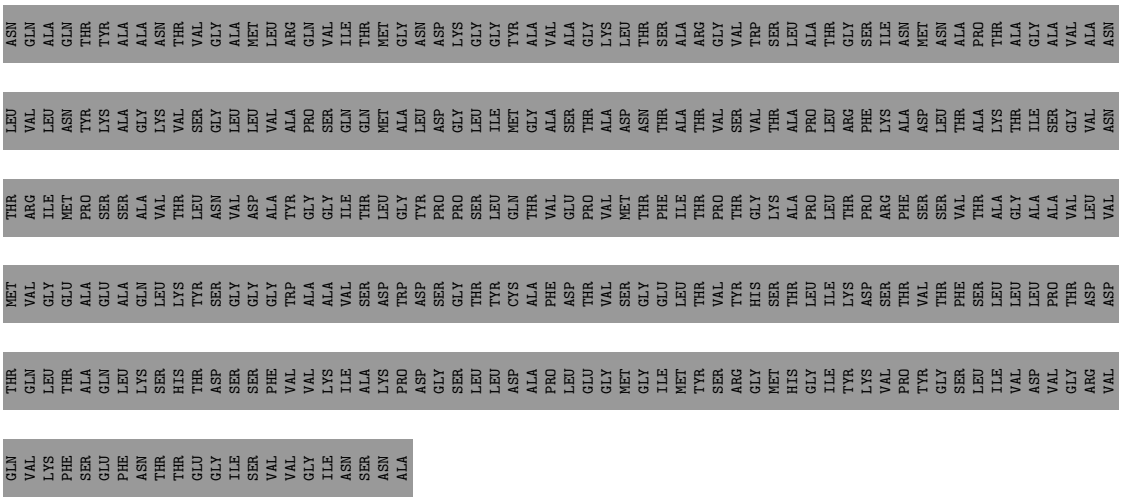
Chain XE:



• Molecule 6: 60 kDa protein

Chain XF:



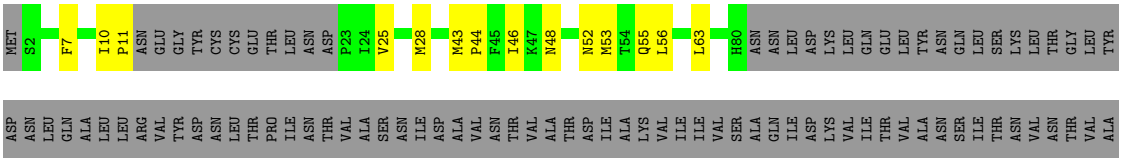


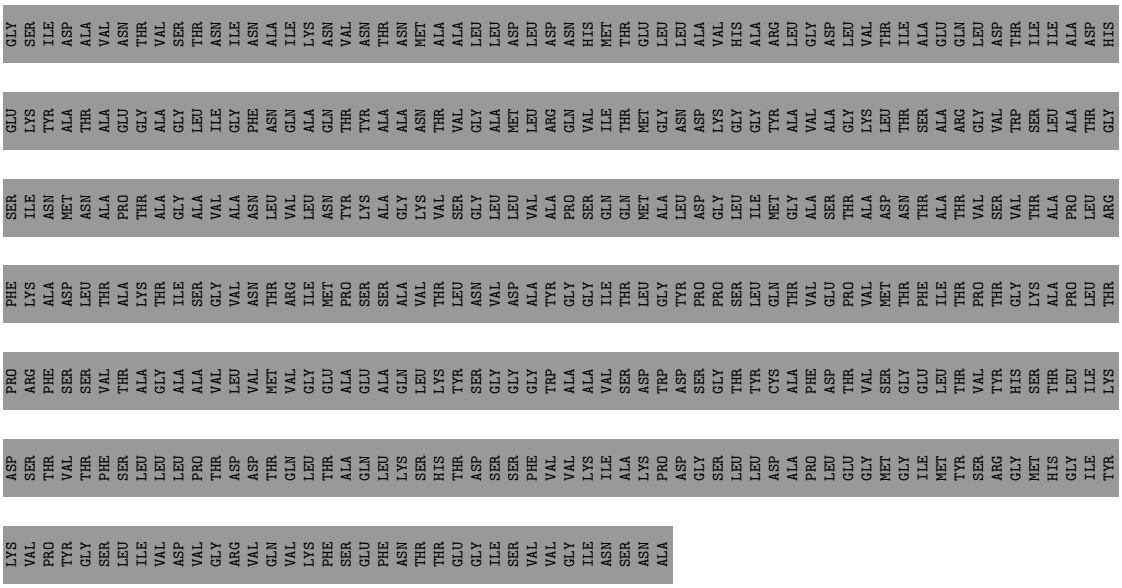
• Molecule 6: 60 kDa protein

Chain YE:

• Molecule 6: 60 kDa protein

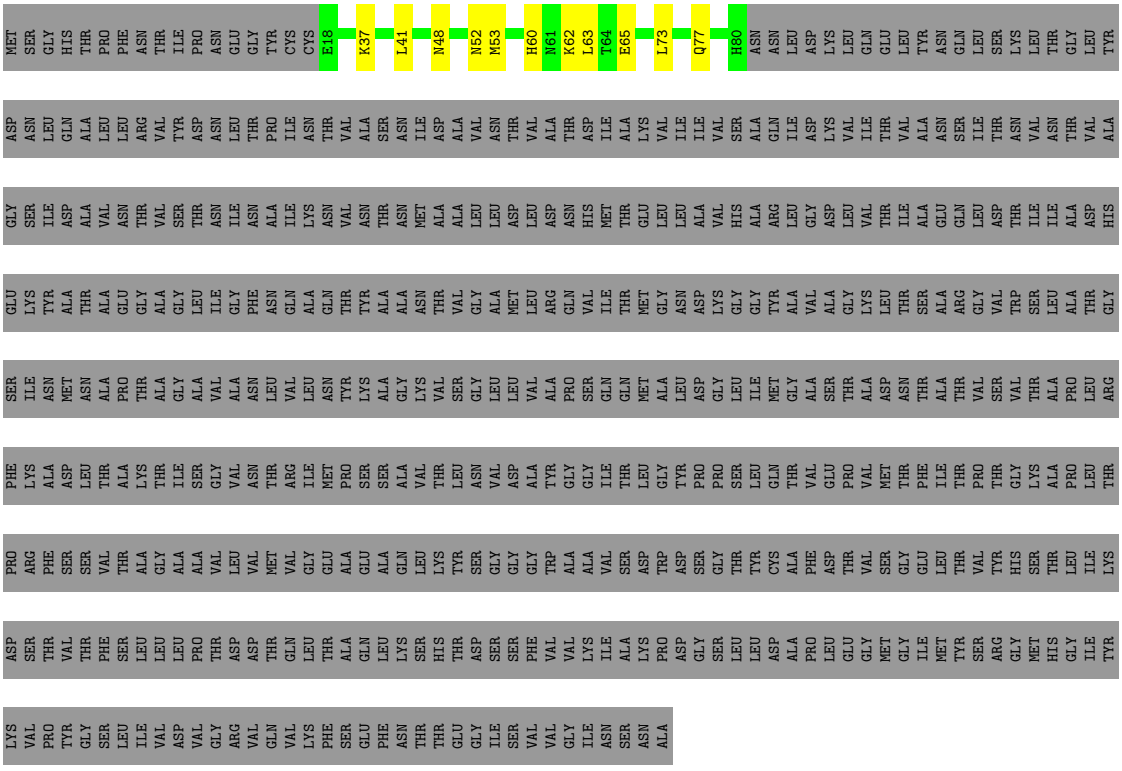
Chain YF:





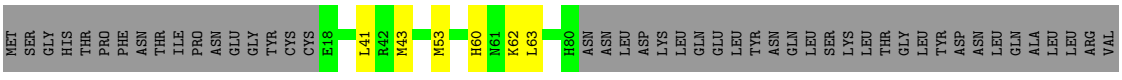
• Molecule 6: 60 kDa protein

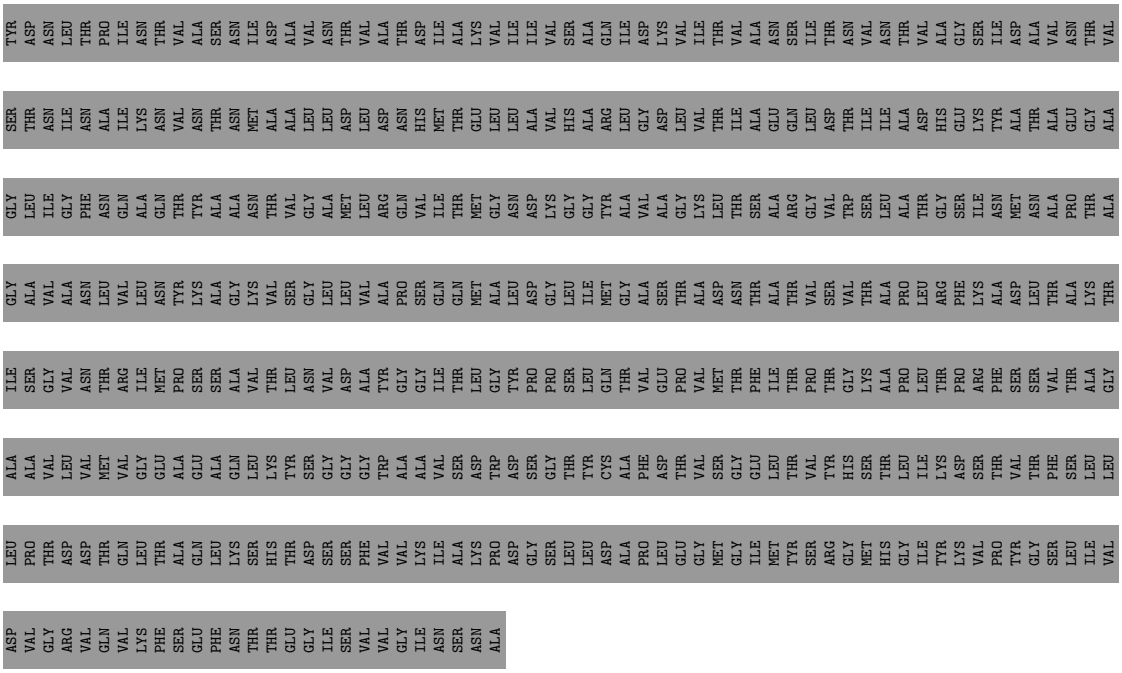
Chain ZE:



• Molecule 6: 60 kDa protein

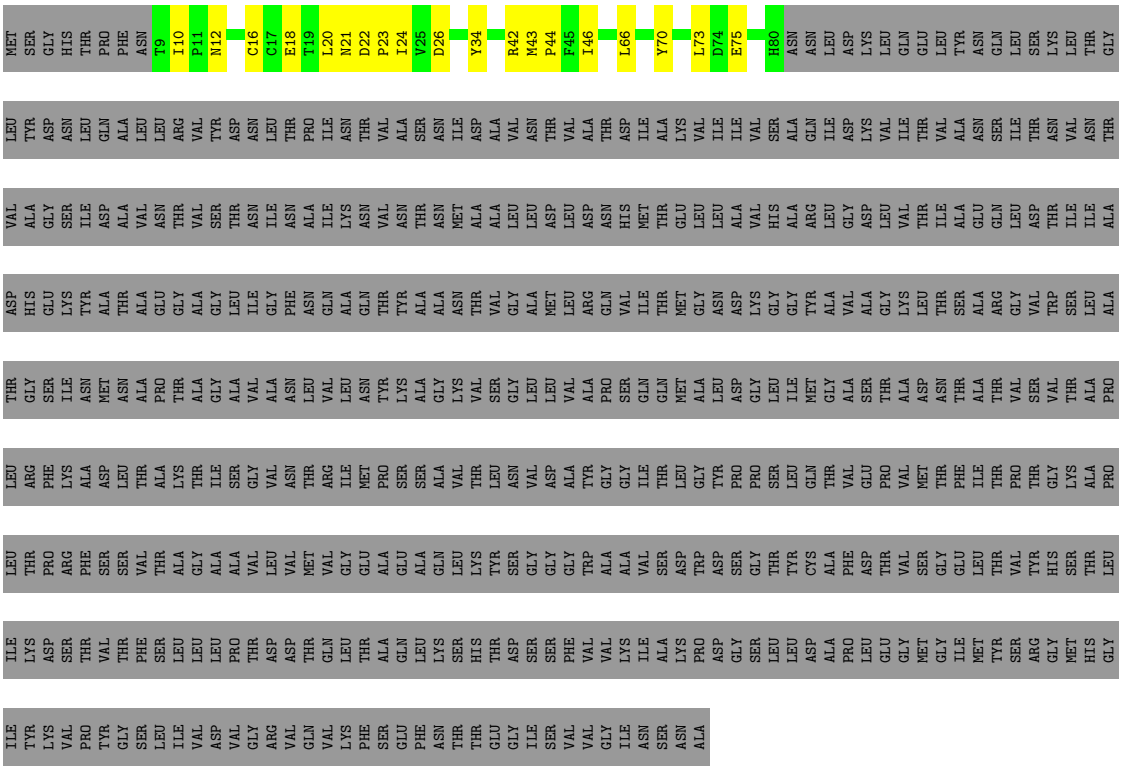
Chain ZF:





• Molecule 6: 60 kDa protein

Chain XG:



• Molecule 6: 60 kDa protein

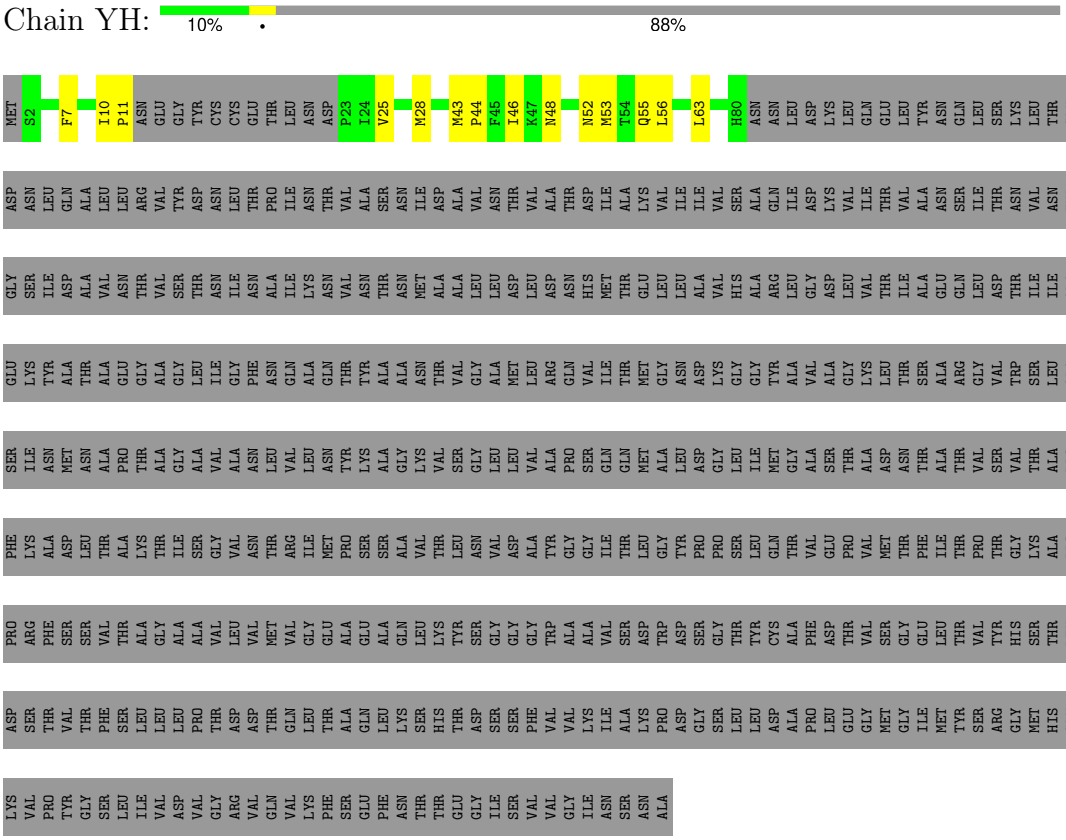
Chain XH:

- Molecule 6: 60 kDa protein

Chain YG:

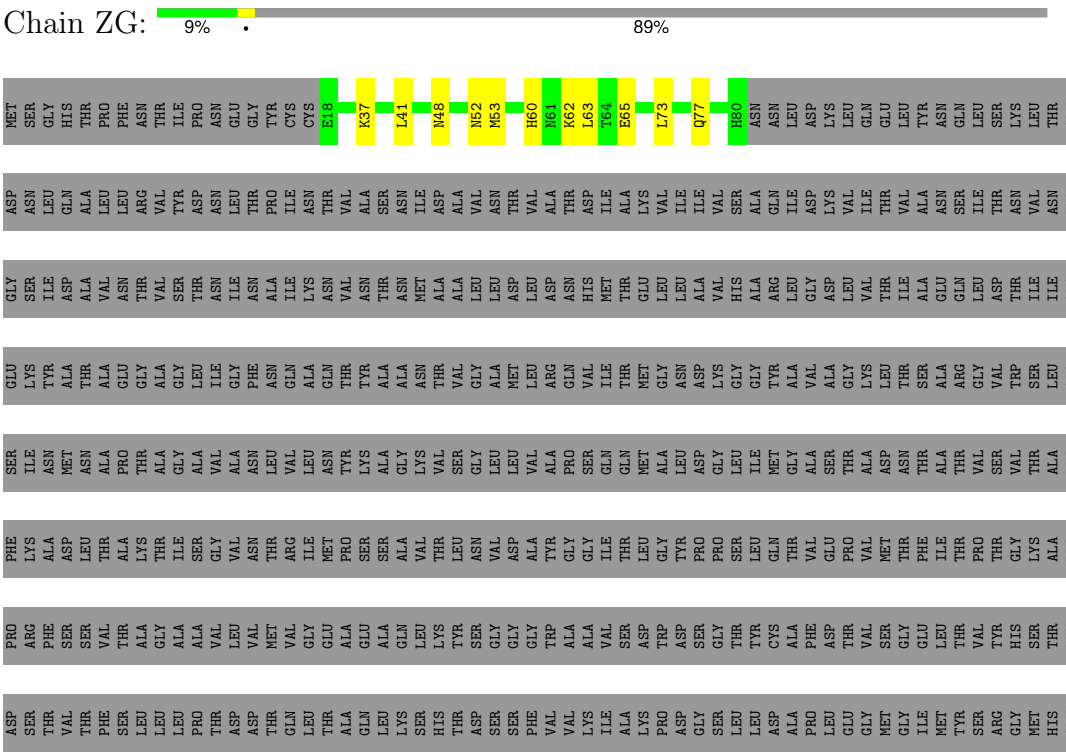
- Molecule 6: 60 kDa protein

Chain YH:



- Molecule 6: 60 kDa protein

Chain ZG:

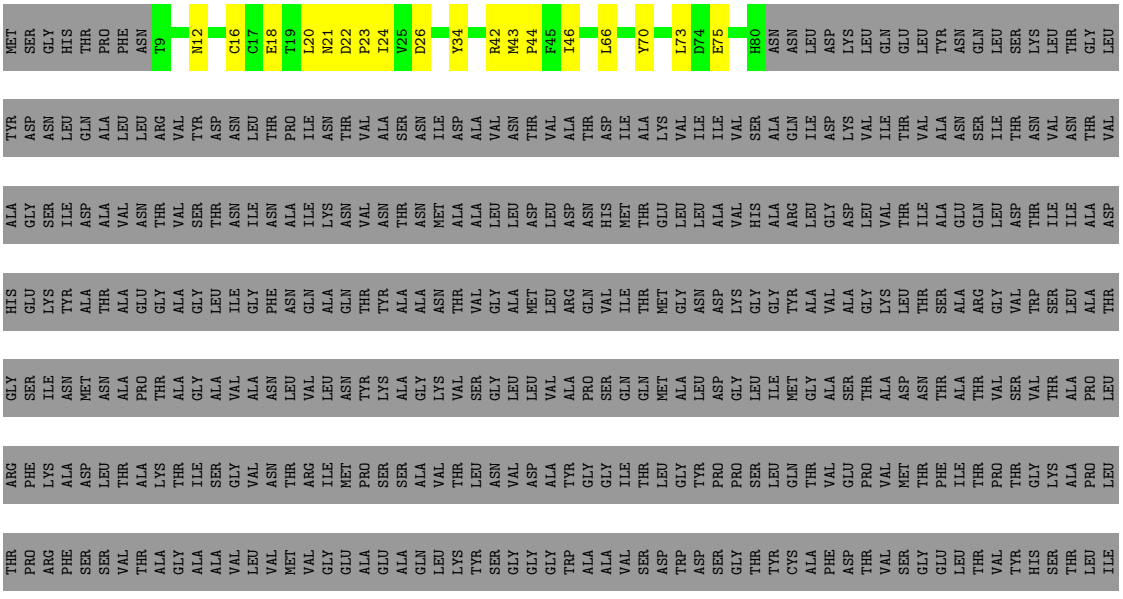


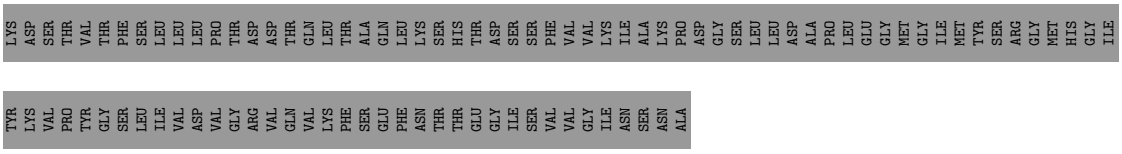
• Molecule 6: 60 kDa protein

Chain ZH:

• Molecule 6: 60 kDa protein

Chain XI:



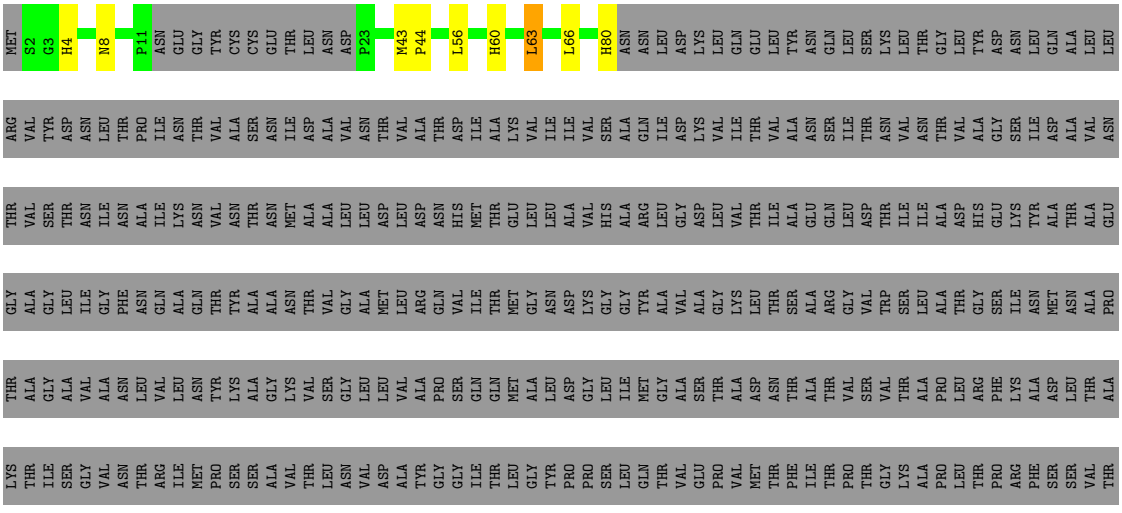


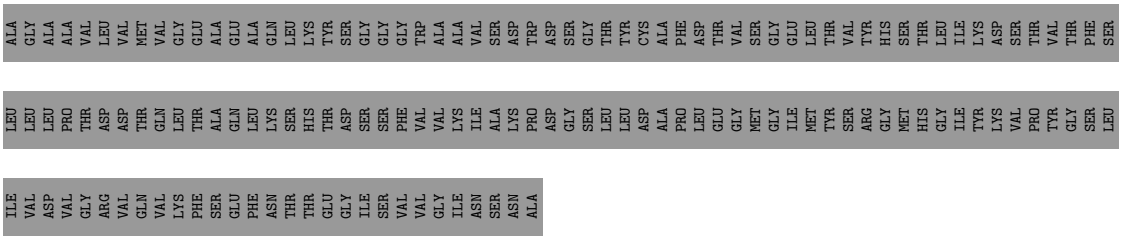
• Molecule 6: 60 kDa protein

Chain XJ:

• Molecule 6: 60 kDa protein

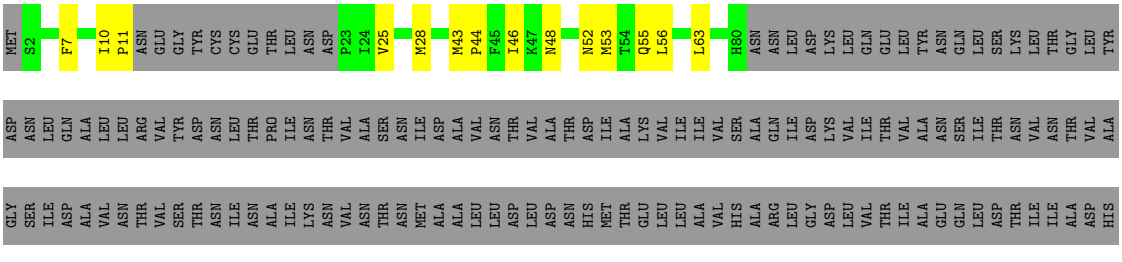
Chain YI:





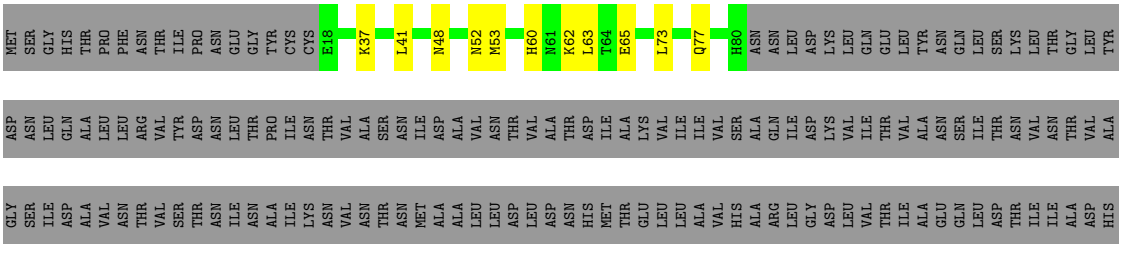
• Molecule 6: 60 kDa protein

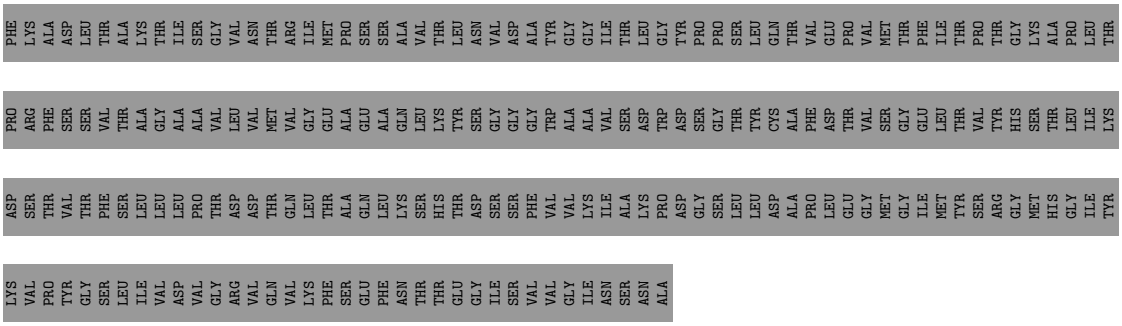
Chain YJ:



• Molecule 6: 60 kDa protein

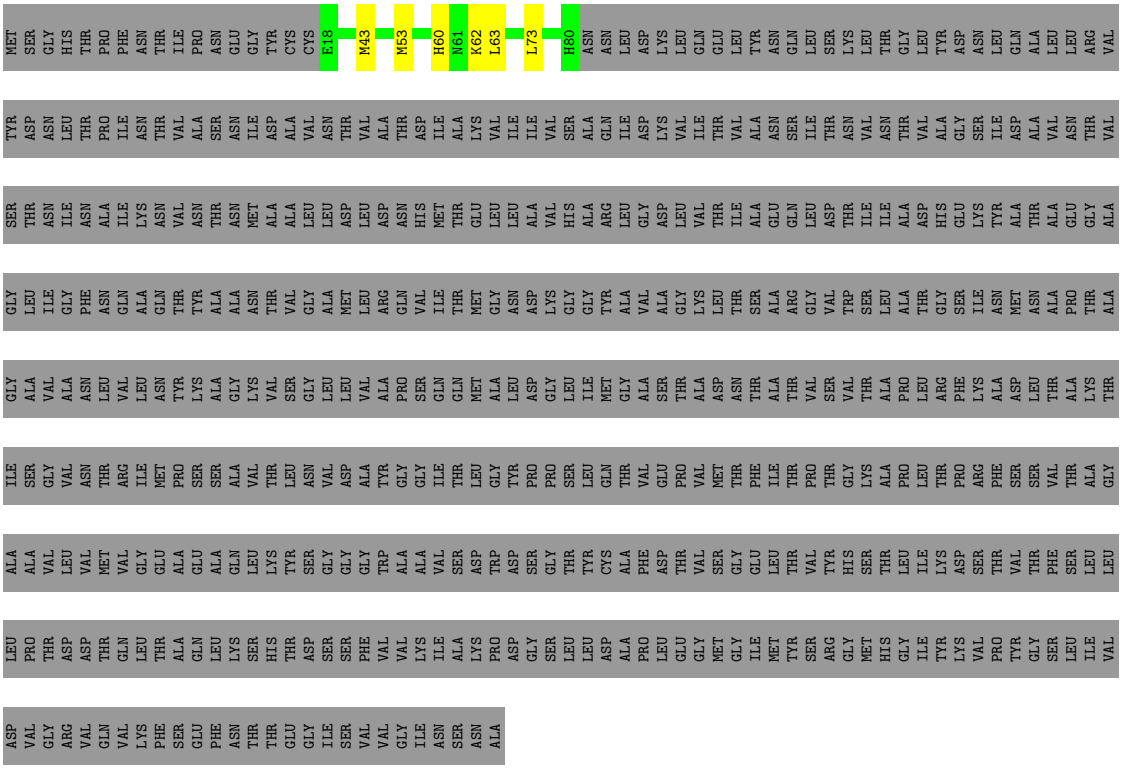
Chain ZI:





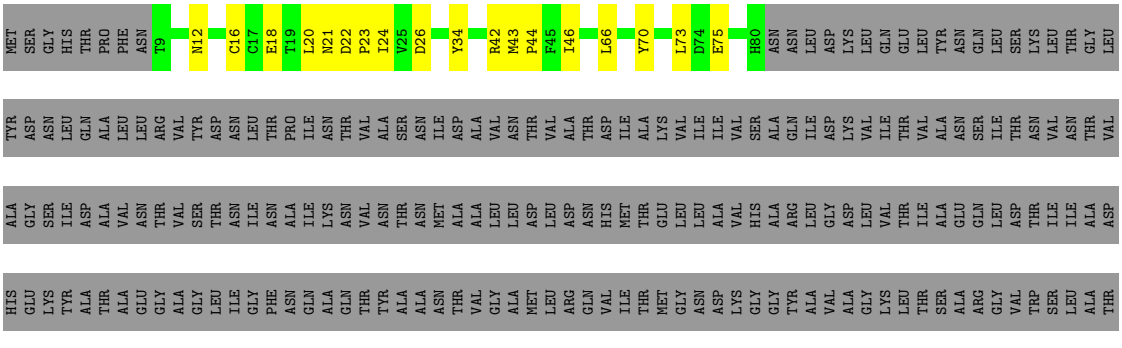
- Molecule 6: 60 kDa protein

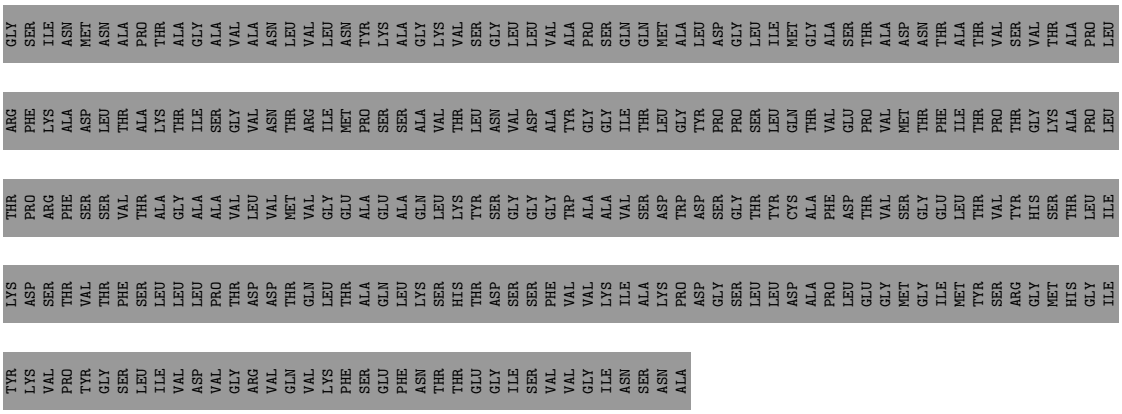
Chain ZJ:



- Molecule 6: 60 kDa protein

Chain XK:



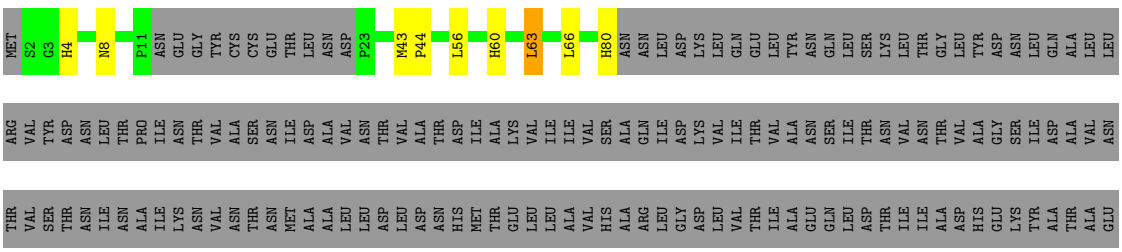


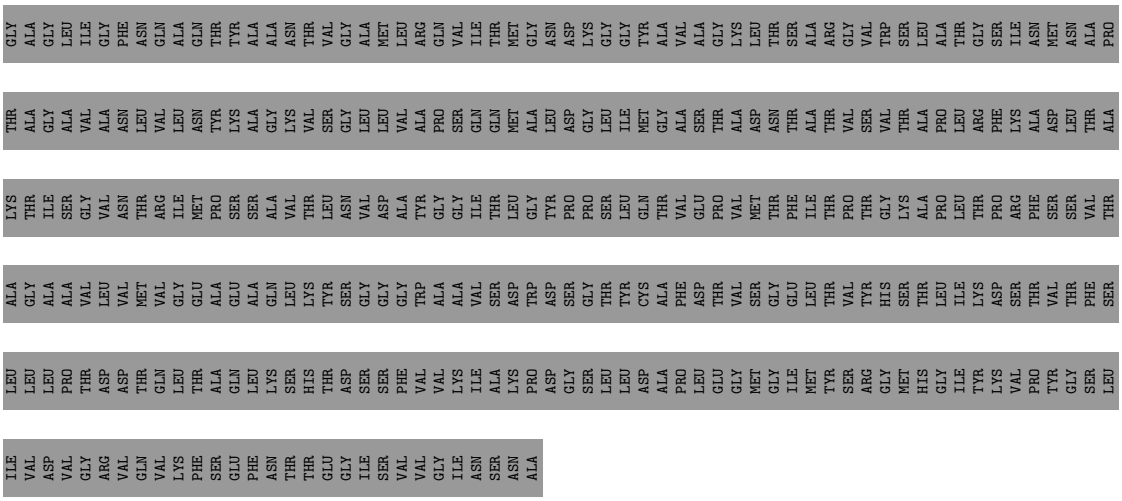
• Molecule 6: 60 kDa protein

Chain XL:

• Molecule 6: 60 kDa protein

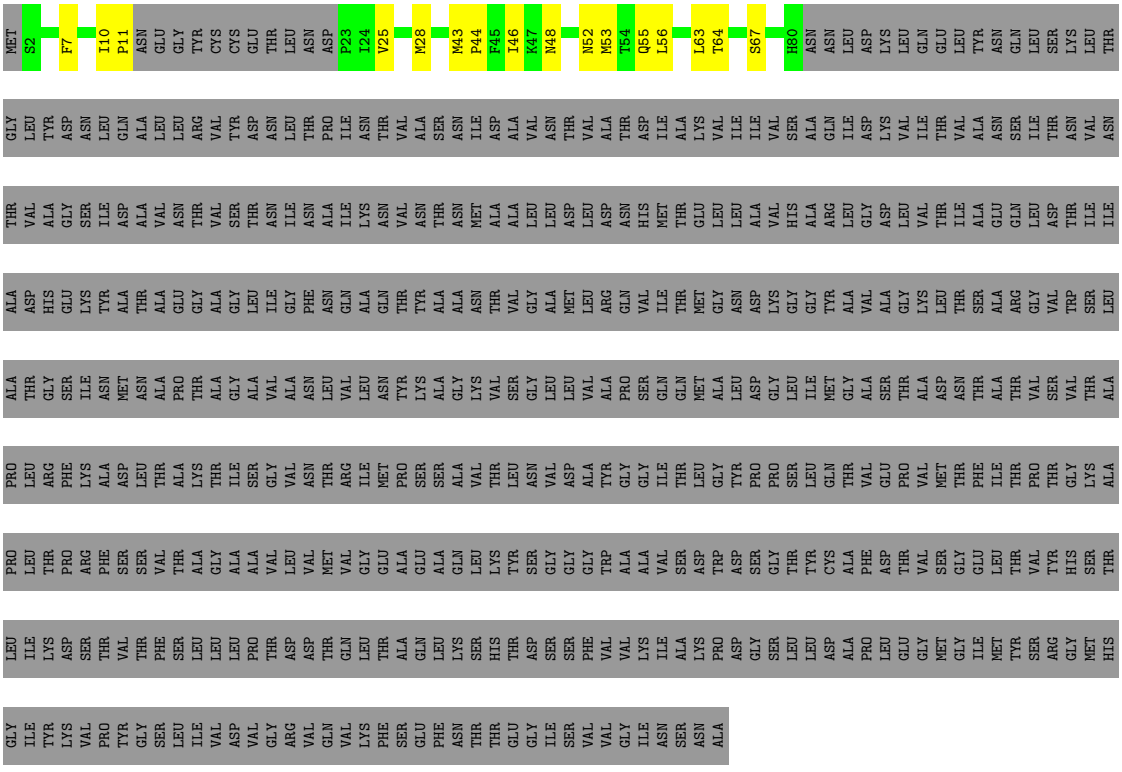
Chain YK:





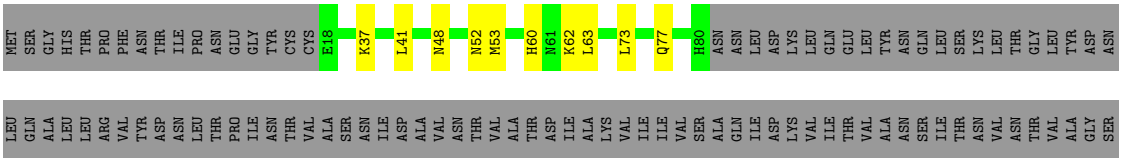
• Molecule 6: 60 kDa protein

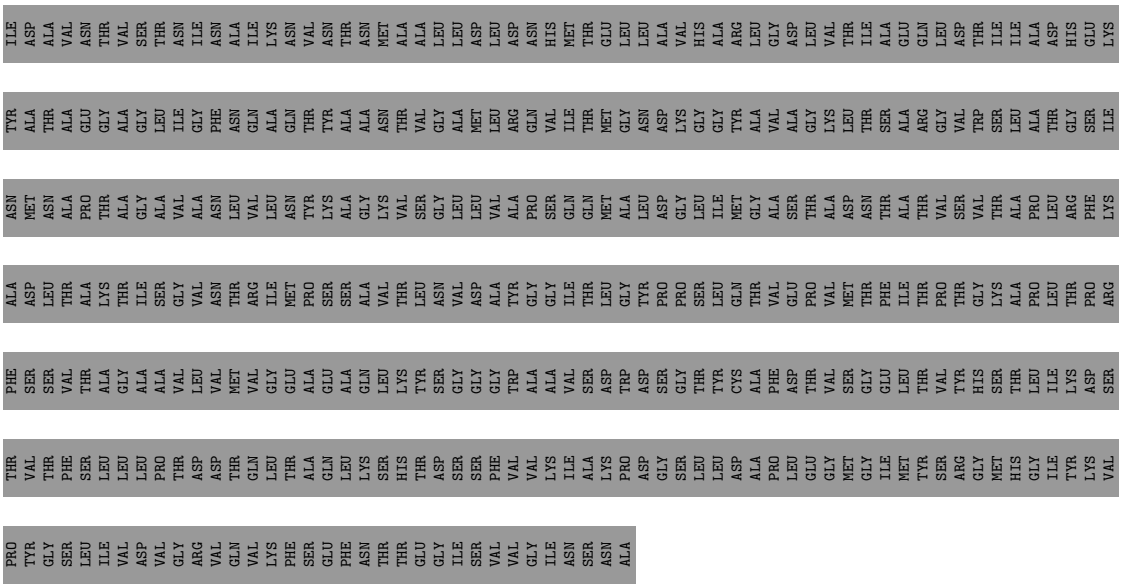
Chain YL:



• Molecule 6: 60 kDa protein

Chain ZK:



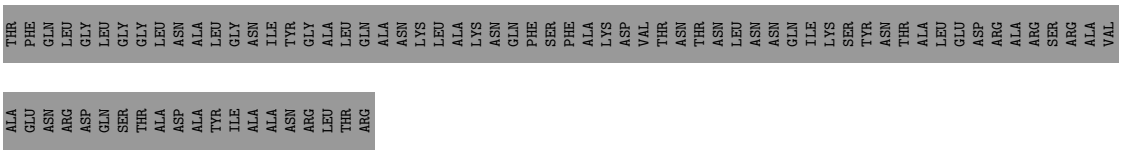


- Molecule 6: 60 kDa protein

Chain ZL:

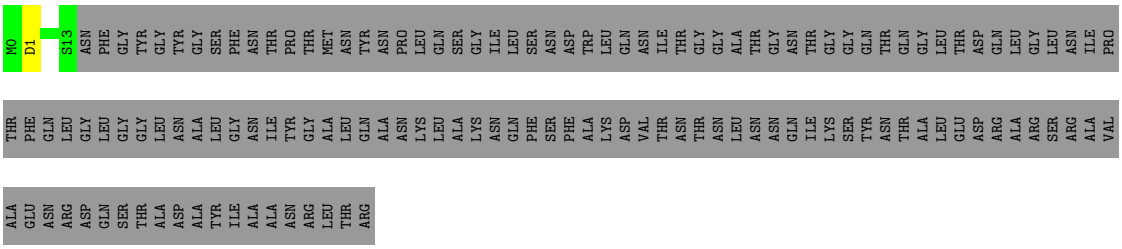
- Molecule 7: 16.5 kDa protein

Chain OA:



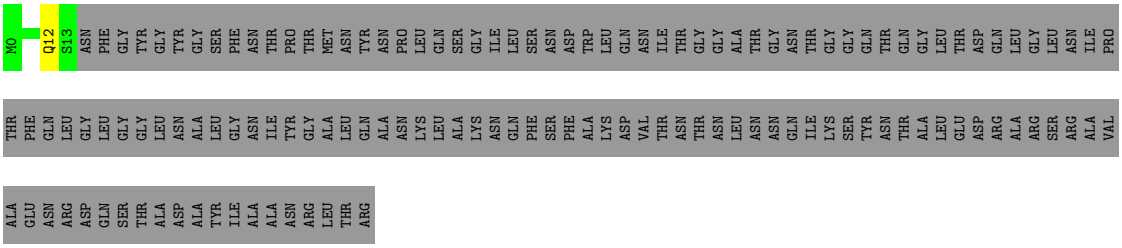
• Molecule 7: 16.5 kDa protein

Chain OB: 9% 91%



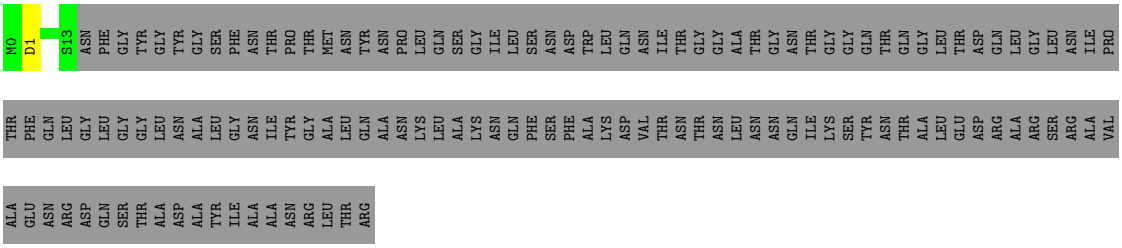
• Molecule 7: 16.5 kDa protein

Chain OC: 9% 91%



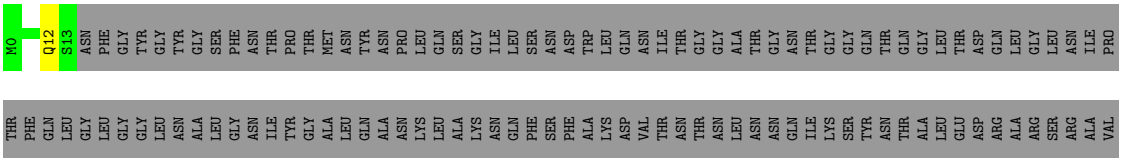
• Molecule 7: 16.5 kDa protein

Chain OD: 9% 91%



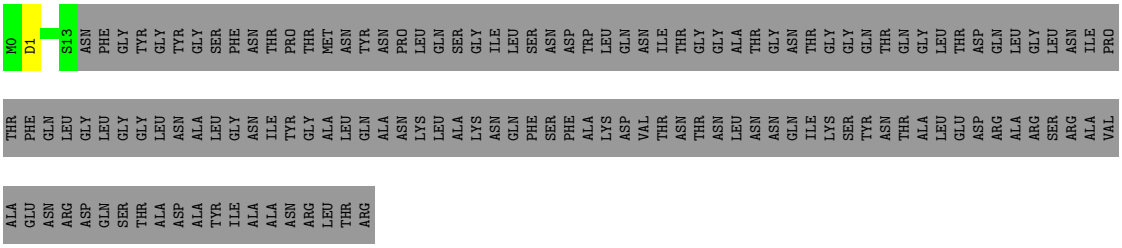
• Molecule 7: 16.5 kDa protein

Chain OE: 9% 91%



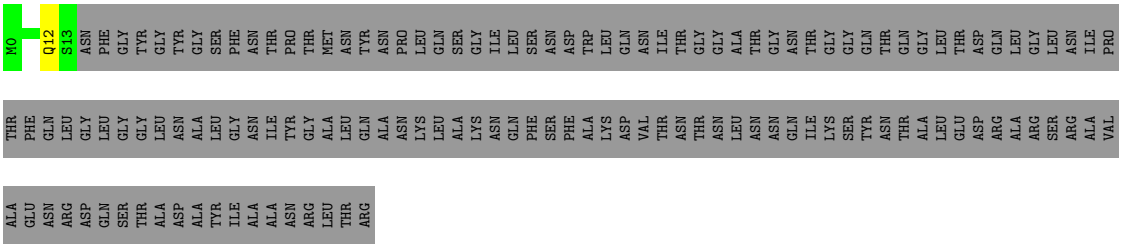
• Molecule 7: 16.5 kDa protein

Chain OF:



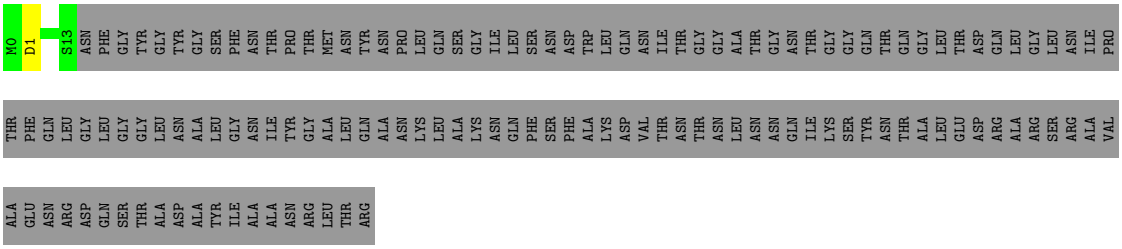
• Molecule 7: 16.5 kDa protein

Chain OG:



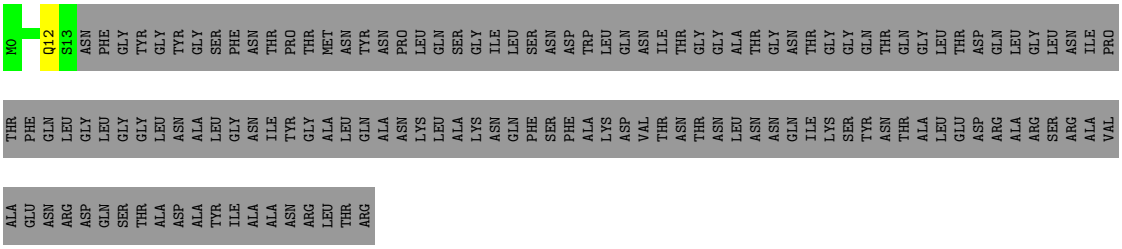
• Molecule 7: 16.5 kDa protein

Chain OH:



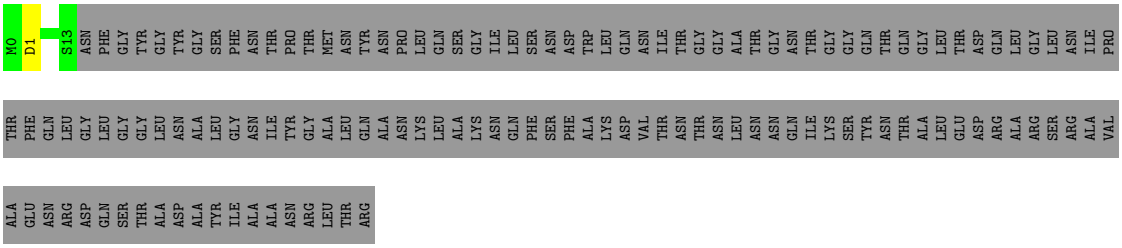
• Molecule 7: 16.5 kDa protein

Chain OI:



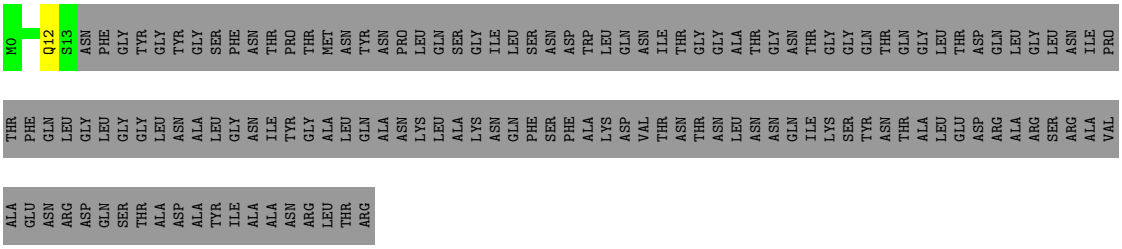
• Molecule 7: 16.5 kDa protein

Chain OJ:



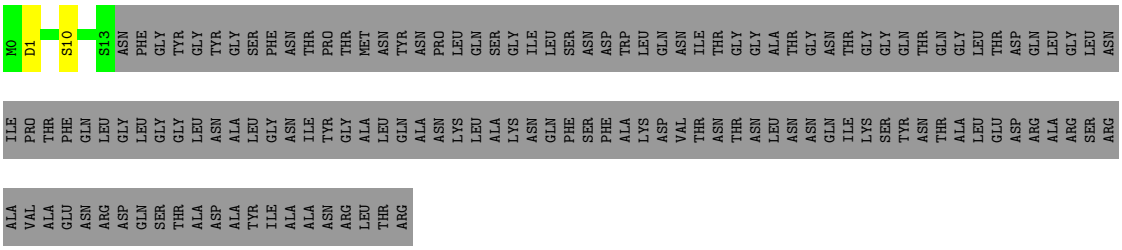
• Molecule 7: 16.5 kDa protein

Chain OK:



• Molecule 7: 16.5 kDa protein

Chain OL:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.694	Depositor
Minimum map value	-0.359	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.0693	Depositor
Map size (Å)	266.262, 265.068, 499.092	wwPDB
Map dimensions	418, 222, 223	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.194, 1.194, 1.194	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.08	0/1953	0.19	0/2654
1	AB	0.09	0/1953	0.20	0/2654
1	AC	0.08	0/1953	0.19	0/2654
1	AD	0.09	0/1953	0.20	0/2654
1	AE	0.08	0/1953	0.19	0/2654
1	AF	0.09	0/1953	0.20	0/2654
1	AG	0.08	0/1953	0.19	0/2654
1	AH	0.09	0/1953	0.20	0/2654
1	AI	0.08	0/1953	0.19	0/2654
1	AJ	0.09	0/1953	0.20	0/2654
1	AK	0.08	0/1953	0.19	0/2654
1	AL	0.09	0/1953	0.20	0/2654
2	LA	0.07	0/9606	0.22	0/13093
2	LB	0.07	0/9606	0.22	0/13093
2	LC	0.07	0/9606	0.22	0/13093
2	LD	0.07	0/9606	0.22	0/13093
2	LE	0.07	0/9606	0.22	0/13093
2	LF	0.07	0/9606	0.22	0/13093
3	PA	0.07	0/5453	0.19	0/7377
3	PB	0.08	0/5453	0.19	0/7377
3	PC	0.07	0/5453	0.18	0/7377
3	PD	0.07	0/5453	0.19	0/7377
3	PE	0.07	0/5453	0.18	0/7377
3	PF	0.07	0/5453	0.19	0/7377
3	PG	0.07	0/5453	0.19	0/7377
3	PH	0.07	0/5453	0.19	0/7377
3	PI	0.07	0/5453	0.18	0/7377
3	PJ	0.07	0/5453	0.19	0/7377
3	PK	0.07	0/5453	0.18	0/7377
3	PL	0.07	0/5453	0.19	0/7377
4	SA	0.08	0/3498	0.22	0/4781
4	SB	0.08	0/3498	0.22	0/4781
4	SC	0.08	0/3498	0.22	0/4781
4	SD	0.08	0/3498	0.22	0/4781

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	SE	0.08	0/3498	0.22	0/4781
4	SF	0.08	0/3498	0.22	0/4781
5	TA	0.07	0/2290	0.18	0/3103
5	TB	0.07	0/2290	0.18	0/3103
5	TC	0.07	0/2290	0.18	0/3103
5	TD	0.07	0/2290	0.19	0/3103
5	TE	0.07	0/2290	0.17	0/3103
5	TF	0.07	0/2290	0.18	0/3103
5	TG	0.07	0/2290	0.18	0/3103
5	TH	0.07	0/2290	0.18	0/3103
5	TI	0.07	0/2290	0.18	0/3103
5	TJ	0.07	0/2290	0.19	0/3103
5	TK	0.07	0/2290	0.17	0/3103
5	TL	0.07	0/2290	0.18	0/3103
6	XA	0.09	0/585	0.23	0/794
6	XB	0.08	0/585	0.20	0/794
6	XC	0.09	0/585	0.23	0/794
6	XD	0.08	0/585	0.20	0/794
6	XE	0.08	0/585	0.23	0/794
6	XF	0.08	0/585	0.20	0/794
6	XG	0.09	0/585	0.23	0/794
6	XH	0.08	0/585	0.20	0/794
6	XI	0.09	0/585	0.23	0/794
6	XJ	0.08	0/585	0.20	0/794
6	XK	0.09	0/585	0.23	0/794
6	XL	0.08	0/585	0.20	0/794
6	YA	0.08	0/554	0.25	0/750
6	YB	0.08	0/554	0.22	0/750
6	YC	0.09	0/554	0.25	0/750
6	YD	0.08	0/554	0.22	0/750
6	YE	0.09	0/554	0.25	0/750
6	YF	0.07	0/554	0.21	0/750
6	YG	0.09	0/554	0.25	0/750
6	YH	0.08	0/554	0.22	0/750
6	YI	0.09	0/554	0.25	0/750
6	YJ	0.09	0/554	0.22	0/750
6	YK	0.09	0/554	0.25	0/750
6	YL	0.08	0/554	0.21	0/750
6	ZA	0.08	0/516	0.21	0/699
6	ZB	0.08	0/516	0.22	0/699
6	ZC	0.08	0/516	0.21	0/699
6	ZD	0.08	0/516	0.22	0/699
6	ZE	0.08	0/516	0.21	0/699

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
6	ZF	0.08	0/516	0.21	0/699
6	ZG	0.08	0/516	0.21	0/699
6	ZH	0.08	0/516	0.22	0/699
6	ZI	0.08	0/516	0.21	0/699
6	ZJ	0.08	0/516	0.22	0/699
6	ZK	0.08	0/516	0.21	0/699
6	ZL	0.08	0/516	0.21	0/699
7	OA	0.09	0/107	0.28	0/144
7	OB	0.10	0/107	0.26	0/144
7	OC	0.09	0/107	0.28	0/144
7	OD	0.11	0/107	0.26	0/144
7	OE	0.10	0/107	0.29	0/144
7	OF	0.11	0/107	0.26	0/144
7	OG	0.09	0/107	0.28	0/144
7	OH	0.10	0/107	0.26	0/144
7	OI	0.09	0/107	0.28	0/144
7	OJ	0.11	0/107	0.26	0/144
7	OK	0.09	0/107	0.28	0/144
7	OL	0.11	0/107	0.26	0/144
All	All	0.07	0/216120	0.20	0/293496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1912	0	1842	14	0
1	AB	1912	0	1843	23	0
1	AC	1912	0	1842	14	0
1	AD	1912	0	1843	22	0
1	AE	1912	0	1842	15	0
1	AF	1912	0	1843	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AG	1912	0	1842	13	0
1	AH	1912	0	1843	24	0
1	AI	1912	0	1842	14	0
1	AJ	1912	0	1843	23	0
1	AK	1912	0	1842	14	0
1	AL	1912	0	1843	22	0
2	LA	9341	0	8931	116	0
2	LB	9341	0	8931	123	0
2	LC	9341	0	8931	118	0
2	LD	9341	0	8931	118	0
2	LE	9341	0	8931	115	0
2	LF	9341	0	8931	120	0
3	PA	5357	0	5339	80	0
3	PB	5357	0	5339	77	0
3	PC	5357	0	5339	78	0
3	PD	5357	0	5339	80	0
3	PE	5357	0	5339	79	0
3	PF	5357	0	5339	73	0
3	PG	5357	0	5339	80	0
3	PH	5357	0	5339	77	0
3	PI	5357	0	5339	79	0
3	PJ	5357	0	5339	75	0
3	PK	5357	0	5339	79	0
3	PL	5357	0	5339	73	0
4	SA	3383	0	3269	42	0
4	SB	3383	0	3269	42	0
4	SC	3383	0	3269	43	0
4	SD	3383	0	3269	44	0
4	SE	3383	0	3269	43	0
4	SF	3383	0	3269	42	0
5	TA	2263	0	2258	23	0
5	TB	2263	0	2258	26	0
5	TC	2263	0	2258	22	0
5	TD	2263	0	2258	24	0
5	TE	2263	0	2258	24	0
5	TF	2263	0	2258	26	0
5	TG	2263	0	2258	23	0
5	TH	2263	0	2258	27	0
5	TI	2263	0	2258	23	0
5	TJ	2263	0	2258	25	0
5	TK	2263	0	2258	24	0
5	TL	2263	0	2258	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	XA	575	0	586	12	0
6	XB	575	0	586	9	0
6	XC	575	0	586	13	0
6	XD	575	0	586	8	0
6	XE	575	0	586	14	0
6	XF	575	0	586	7	0
6	XG	575	0	586	13	0
6	XH	575	0	586	7	0
6	XI	575	0	586	12	0
6	XJ	575	0	586	8	0
6	XK	575	0	586	13	0
6	XL	575	0	586	9	0
6	YA	543	0	563	6	0
6	YB	543	0	563	12	0
6	YC	543	0	563	5	0
6	YD	543	0	563	11	0
6	YE	543	0	563	6	0
6	YF	543	0	563	10	0
6	YG	543	0	563	6	0
6	YH	543	0	563	10	0
6	YI	543	0	563	6	0
6	YJ	543	0	563	12	0
6	YK	543	0	563	6	0
6	YL	543	0	563	13	0
6	ZA	508	0	528	8	0
6	ZB	508	0	528	5	0
6	ZC	508	0	528	8	0
6	ZD	508	0	528	4	0
6	ZE	508	0	528	9	0
6	ZF	508	0	528	5	0
6	ZG	508	0	528	9	0
6	ZH	508	0	528	5	0
6	ZI	508	0	528	9	0
6	ZJ	508	0	528	4	0
6	ZK	508	0	528	8	0
6	ZL	508	0	528	5	0
7	OA	105	0	97	0	0
7	OB	105	0	97	2	0
7	OC	105	0	97	0	0
7	OD	105	0	97	2	0
7	OE	105	0	97	0	0
7	OF	105	0	97	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	OG	105	0	97	0	0
7	OH	105	0	97	2	0
7	OI	105	0	97	0	0
7	OJ	105	0	97	1	0
7	OK	105	0	97	0	0
7	OL	105	0	97	3	0
All	All	211500	0	207762	2269	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (2269) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LE:840:ALA:HA	2:LE:888:GLN:HB3	1.63	0.80
2:LF:840:ALA:HA	2:LF:888:GLN:HB3	1.63	0.79
2:LD:840:ALA:HA	2:LD:888:GLN:HB3	1.63	0.79
2:LA:840:ALA:HA	2:LA:888:GLN:HB3	1.63	0.79
2:LC:840:ALA:HA	2:LC:888:GLN:HB3	1.63	0.79
2:LB:840:ALA:HA	2:LB:888:GLN:HB3	1.63	0.78
2:LF:445:GLU:HG2	2:LF:551:ASP:HB2	1.70	0.73
2:LE:445:GLU:HG2	2:LE:551:ASP:HB2	1.71	0.73
2:LA:445:GLU:HG2	2:LA:551:ASP:HB2	1.71	0.73
2:LD:445:GLU:HG2	2:LD:551:ASP:HB2	1.71	0.72
2:LB:445:GLU:HG2	2:LB:551:ASP:HB2	1.70	0.72
2:LC:445:GLU:HG2	2:LC:551:ASP:HB2	1.70	0.72
2:LC:1130:TRP:NE1	2:LC:1132:SER:OG	2.25	0.70
2:LF:1130:TRP:NE1	2:LF:1132:SER:OG	2.25	0.69
2:LA:1130:TRP:NE1	2:LA:1132:SER:OG	2.25	0.69
2:LD:1130:TRP:NE1	2:LD:1132:SER:OG	2.25	0.69
2:LC:108:ASP:OD1	2:LC:391:ARG:NH1	2.27	0.68
2:LE:1130:TRP:NE1	2:LE:1132:SER:OG	2.25	0.68
2:LB:1130:TRP:NE1	2:LB:1132:SER:OG	2.25	0.68
2:LD:108:ASP:OD1	2:LD:391:ARG:NH1	2.27	0.68
3:PI:678:MET:SD	3:PI:678:MET:N	2.66	0.67
2:LB:108:ASP:OD1	2:LB:391:ARG:NH1	2.27	0.67
2:LF:108:ASP:OD1	2:LF:391:ARG:NH1	2.27	0.67
2:LE:108:ASP:OD1	2:LE:391:ARG:NH1	2.27	0.67
1:AA:13:ASN:ND2	4:SA:416:CYS:SG	2.68	0.67
1:AC:13:ASN:ND2	4:SB:416:CYS:SG	2.68	0.66
1:AE:13:ASN:ND2	4:SC:416:CYS:SG	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LA:108:ASP:OD1	2:LA:391:ARG:NH1	2.27	0.66
1:AK:13:ASN:ND2	4:SF:416:CYS:SG	2.69	0.66
1:AI:13:ASN:ND2	4:SE:416:CYS:SG	2.68	0.66
3:PG:678:MET:SD	3:PG:678:MET:N	2.67	0.66
1:AG:13:ASN:ND2	4:SD:416:CYS:SG	2.68	0.66
2:LF:738:VAL:HA	2:LF:838:ILE:HB	1.78	0.66
2:LC:738:VAL:HA	2:LC:838:ILE:HB	1.78	0.65
2:LE:738:VAL:HA	2:LE:838:ILE:HB	1.78	0.65
3:PI:535:ARG:NH1	3:PJ:548:ASP:OD2	2.28	0.65
3:PE:535:ARG:NH1	3:PF:548:ASP:OD2	2.28	0.65
2:LD:738:VAL:HA	2:LD:838:ILE:HB	1.77	0.65
4:SB:327:GLN:HG2	4:SB:361:HIS:HB2	1.79	0.65
4:SF:327:GLN:HG2	4:SF:361:HIS:HB2	1.79	0.65
3:PA:678:MET:SD	3:PA:678:MET:N	2.67	0.65
4:SA:327:GLN:HG2	4:SA:361:HIS:HB2	1.80	0.64
2:LB:738:VAL:HA	2:LB:838:ILE:HB	1.78	0.64
4:SA:279:ARG:NH1	4:SA:322:ASN:O	2.30	0.64
4:SB:279:ARG:NH1	4:SB:322:ASN:O	2.31	0.64
3:PD:514:SER:O	3:PD:518:ASN:ND2	2.30	0.64
4:SC:279:ARG:NH1	4:SC:322:ASN:O	2.31	0.64
4:SE:327:GLN:HG2	4:SE:361:HIS:HB2	1.79	0.64
4:SF:279:ARG:NH1	4:SF:322:ASN:O	2.31	0.64
2:LA:738:VAL:HA	2:LA:838:ILE:HB	1.77	0.64
4:SD:279:ARG:NH1	4:SD:322:ASN:O	2.30	0.64
3:PC:678:MET:SD	3:PC:678:MET:N	2.66	0.64
3:PH:572:LEU:HD12	3:PH:591:ILE:HG23	1.79	0.64
3:PF:514:SER:O	3:PF:518:ASN:ND2	2.30	0.64
3:PJ:514:SER:O	3:PJ:518:ASN:ND2	2.30	0.64
3:PE:514:SER:O	3:PE:518:ASN:ND2	2.31	0.64
4:SD:327:GLN:HG2	4:SD:361:HIS:HB2	1.80	0.64
4:SC:327:GLN:HG2	4:SC:361:HIS:HB2	1.79	0.64
3:PJ:271:CYS:SG	3:PJ:318:ARG:NH1	2.71	0.64
3:PL:514:SER:O	3:PL:518:ASN:ND2	2.30	0.64
2:LA:526:PRO:HB3	2:LA:530:LEU:HD23	1.81	0.63
3:PH:514:SER:O	3:PH:518:ASN:ND2	2.31	0.63
4:SE:279:ARG:NH1	4:SE:322:ASN:O	2.31	0.63
3:PA:514:SER:O	3:PA:518:ASN:ND2	2.31	0.63
3:PB:514:SER:O	3:PB:518:ASN:ND2	2.31	0.63
2:LD:526:PRO:HB3	2:LD:530:LEU:HD23	1.81	0.63
3:PG:514:SER:O	3:PG:518:ASN:ND2	2.31	0.63
2:LD:573:LYS:HE3	4:SD:24:ILE:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PJ:572:LEU:HD12	3:PJ:591:ILE:HG23	1.80	0.63
3:PK:514:SER:O	3:PK:518:ASN:ND2	2.31	0.63
3:PL:572:LEU:HD12	3:PL:591:ILE:HG23	1.80	0.63
3:PB:572:LEU:HD12	3:PB:591:ILE:HG23	1.79	0.63
3:PD:572:LEU:HD12	3:PD:591:ILE:HG23	1.80	0.63
2:LC:1109:GLN:HE21	2:LC:1133:GLU:HG3	1.64	0.63
3:PD:271:CYS:SG	3:PD:318:ARG:NH1	2.71	0.63
3:PH:271:CYS:SG	3:PH:318:ARG:NH1	2.72	0.63
3:PA:548:ASP:OD2	3:PD:535:ARG:NH1	2.31	0.63
2:LB:1109:GLN:HE21	2:LB:1133:GLU:HG3	1.64	0.63
3:PC:514:SER:O	3:PC:518:ASN:ND2	2.32	0.63
2:LF:1109:GLN:HE21	2:LF:1133:GLU:HG3	1.64	0.63
3:PL:271:CYS:SG	3:PL:318:ARG:NH1	2.72	0.63
2:LB:526:PRO:HB3	2:LB:530:LEU:HD23	1.81	0.63
3:PE:548:ASP:OD2	3:PH:535:ARG:NH1	2.31	0.63
2:LE:573:LYS:HE3	4:SE:24:ILE:HG23	1.81	0.63
3:PA:535:ARG:NH1	3:PB:548:ASP:OD2	2.28	0.62
3:PG:572:LEU:HD12	3:PG:591:ILE:HG23	1.81	0.62
3:PI:271:CYS:SG	3:PI:318:ARG:NH1	2.72	0.62
4:SE:276:ASN:OD1	4:SE:279:ARG:NH2	2.32	0.62
4:SF:276:ASN:OD1	4:SF:279:ARG:NH2	2.32	0.62
3:PB:271:CYS:SG	3:PB:318:ARG:NH1	2.72	0.62
3:PF:271:CYS:SG	3:PF:318:ARG:NH1	2.72	0.62
2:LA:573:LYS:HE3	4:SA:24:ILE:HG23	1.81	0.62
4:SB:276:ASN:OD1	4:SB:279:ARG:NH2	2.32	0.62
4:SC:276:ASN:OD1	4:SC:279:ARG:NH2	2.32	0.62
2:LC:573:LYS:HE3	4:SC:24:ILE:HG23	1.81	0.62
2:LD:1116:THR:HG23	2:LD:1157:ILE:HB	1.81	0.62
3:PG:535:ARG:NH1	3:PH:548:ASP:OD2	2.28	0.62
2:LC:526:PRO:HB3	2:LC:530:LEU:HD23	1.81	0.62
2:LE:526:PRO:HB3	2:LE:530:LEU:HD23	1.81	0.62
2:LF:526:PRO:HB3	2:LF:530:LEU:HD23	1.81	0.62
2:LC:1116:THR:HG23	2:LC:1157:ILE:HB	1.81	0.62
2:LA:1109:GLN:HE21	2:LA:1133:GLU:HG3	1.64	0.62
3:PC:271:CYS:SG	3:PC:318:ARG:NH1	2.72	0.62
3:PC:535:ARG:NH1	3:PD:548:ASP:OD2	2.28	0.62
1:AL:77:ALA:HA	1:AL:91:ILE:HB	1.82	0.62
3:PK:271:CYS:SG	3:PK:318:ARG:NH1	2.73	0.62
3:PE:271:CYS:SG	3:PE:318:ARG:NH1	2.73	0.62
3:PF:572:LEU:HD12	3:PF:591:ILE:HG23	1.80	0.62
2:LF:573:LYS:HE3	4:SF:24:ILE:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:77:ALA:HA	1:AF:91:ILE:HB	1.82	0.62
2:LD:1109:GLN:HE21	2:LD:1133:GLU:HG3	1.64	0.62
3:PA:572:LEU:HD12	3:PA:591:ILE:HG23	1.81	0.62
4:SA:276:ASN:OD1	4:SA:279:ARG:NH2	2.33	0.62
3:PE:572:LEU:HD12	3:PE:591:ILE:HG23	1.80	0.62
3:PI:514:SER:O	3:PI:518:ASN:ND2	2.32	0.62
3:PI:548:ASP:OD2	3:PL:535:ARG:NH1	2.31	0.62
3:PC:572:LEU:HD12	3:PC:591:ILE:HG23	1.81	0.61
4:SD:276:ASN:OD1	4:SD:279:ARG:NH2	2.33	0.61
3:PK:572:LEU:HD12	3:PK:591:ILE:HG23	1.80	0.61
2:LA:1116:THR:HG23	2:LA:1157:ILE:HB	1.81	0.61
3:PB:222:GLN:HE21	3:PB:224:GLY:H	1.48	0.61
2:LB:573:LYS:HE3	4:SB:24:ILE:HG23	1.81	0.61
3:PE:678:MET:SD	3:PE:678:MET:N	2.66	0.61
1:AD:77:ALA:HA	1:AD:91:ILE:HB	1.82	0.61
3:PD:222:GLN:HE21	3:PD:224:GLY:H	1.48	0.61
3:PI:572:LEU:HD12	3:PI:591:ILE:HG23	1.81	0.61
5:TA:213:LYS:HG3	5:TL:211:GLU:HG3	1.83	0.61
5:TF:261:THR:HG21	5:TG:259:LEU:HD12	1.81	0.61
5:TH:261:THR:HG21	5:TI:259:LEU:HD12	1.81	0.61
5:TJ:261:THR:HG21	5:TK:259:LEU:HD12	1.81	0.61
3:PK:535:ARG:NH1	3:PL:548:ASP:OD2	2.28	0.61
3:PA:520:ILE:HG22	3:PA:524:ASN:HD21	1.66	0.61
5:TA:259:LEU:HD12	5:TL:261:THR:HG21	1.81	0.61
5:TB:261:THR:HG21	5:TC:259:LEU:HD12	1.81	0.61
3:PC:520:ILE:HG22	3:PC:524:ASN:HD21	1.66	0.61
2:LE:1109:GLN:HE21	2:LE:1133:GLU:HG3	1.64	0.61
3:PL:222:GLN:HE21	3:PL:224:GLY:H	1.48	0.61
2:LA:1039:ASN:O	2:LA:1043:ASN:ND2	2.34	0.61
1:AH:77:ALA:HA	1:AH:91:ILE:HB	1.83	0.61
5:TL:102:ALA:O	5:TL:106:ASN:ND2	2.34	0.61
3:PB:520:ILE:O	3:PB:524:ASN:ND2	2.34	0.61
2:LB:1116:THR:HG23	2:LB:1157:ILE:HB	1.81	0.61
5:TE:261:THR:HG21	5:TF:259:LEU:HD12	1.83	0.61
1:AJ:77:ALA:HA	1:AJ:91:ILE:HB	1.82	0.61
5:TJ:211:GLU:HG3	5:TK:213:LYS:HG3	1.83	0.61
3:PK:222:GLN:HE21	3:PK:224:GLY:H	1.48	0.61
1:AB:77:ALA:HA	1:AB:91:ILE:HB	1.83	0.61
2:LA:1156:VAL:N	2:LA:1178:GLY:O	2.25	0.61
3:PB:535:ARG:NH1	3:PK:548:ASP:OD2	2.31	0.61
2:LC:280:GLN:HG3	2:LC:298:GLU:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PF:222:GLN:HE21	3:PF:224:GLY:H	1.48	0.61
2:LE:1039:ASN:O	2:LE:1043:ASN:ND2	2.34	0.61
3:PI:123:TYR:OH	3:PI:128:LYS:NZ	2.34	0.61
2:LF:1116:THR:HG23	2:LF:1157:ILE:HB	1.81	0.61
6:YL:46:ILE:HD11	6:ZL:43:MET:HE1	1.83	0.61
2:LB:1039:ASN:O	2:LB:1043:ASN:ND2	2.34	0.61
3:PJ:222:GLN:HE21	3:PJ:224:GLY:H	1.48	0.61
3:PA:222:GLN:HE21	3:PA:224:GLY:H	1.49	0.61
4:SA:399:SER:HB3	4:SA:402:GLN:HB2	1.83	0.61
5:TD:211:GLU:HG3	5:TE:213:LYS:HG3	1.83	0.61
5:TD:261:THR:HG21	5:TE:259:LEU:HD12	1.81	0.61
3:PF:520:ILE:O	3:PF:524:ASN:ND2	2.34	0.61
6:YG:56:LEU:HD11	6:ZG:53:MET:HE1	1.82	0.61
3:PH:520:ILE:O	3:PH:524:ASN:ND2	2.34	0.61
3:PL:520:ILE:O	3:PL:524:ASN:ND2	2.34	0.61
5:TB:102:ALA:O	5:TB:106:ASN:ND2	2.34	0.60
3:PD:520:ILE:O	3:PD:524:ASN:ND2	2.34	0.60
2:LD:280:GLN:HG3	2:LD:298:GLU:HG2	1.84	0.60
3:PG:123:TYR:OH	3:PG:128:LYS:NZ	2.34	0.60
3:PG:271:CYS:SG	3:PG:318:ARG:NH1	2.74	0.60
3:PH:222:GLN:HE21	3:PH:224:GLY:H	1.48	0.60
2:LE:1116:THR:HG23	2:LE:1157:ILE:HB	1.81	0.60
2:LA:280:GLN:HG3	2:LA:298:GLU:HG2	1.84	0.60
3:PB:520:ILE:HG22	3:PB:524:ASN:HD21	1.66	0.60
2:LB:280:GLN:HG3	2:LB:298:GLU:HG2	1.83	0.60
5:TC:261:THR:HG21	5:TD:259:LEU:HD12	1.83	0.60
6:YC:56:LEU:HD11	6:ZC:53:MET:HE1	1.82	0.60
2:LF:1039:ASN:O	2:LF:1043:ASN:ND2	2.34	0.60
3:PK:520:ILE:O	3:PK:524:ASN:ND2	2.34	0.60
3:PA:271:CYS:SG	3:PA:318:ARG:NH1	2.74	0.60
3:PC:222:GLN:HE21	3:PC:224:GLY:H	1.48	0.60
3:PI:222:GLN:HE21	3:PI:224:GLY:H	1.48	0.60
5:TJ:102:ALA:O	5:TJ:106:ASN:ND2	2.34	0.60
2:LF:280:GLN:HG3	2:LF:298:GLU:HG2	1.83	0.60
3:PA:520:ILE:O	3:PA:524:ASN:ND2	2.34	0.60
5:TB:211:GLU:HG3	5:TC:213:LYS:HG3	1.83	0.60
4:SB:399:SER:HB3	4:SB:402:GLN:HB2	1.83	0.60
4:SC:399:SER:HB3	4:SC:402:GLN:HB2	1.83	0.60
6:YE:56:LEU:HD11	6:ZE:53:MET:HE1	1.83	0.60
5:TH:211:GLU:HG3	5:TI:213:LYS:HG3	1.83	0.60
2:LE:280:GLN:HG3	2:LE:298:GLU:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PI:520:ILE:O	3:PI:524:ASN:ND2	2.35	0.60
5:TI:261:THR:HG21	5:TJ:259:LEU:HD12	1.83	0.60
3:PJ:520:ILE:O	3:PJ:524:ASN:ND2	2.34	0.60
6:YA:56:LEU:HD11	6:ZA:53:MET:HE1	1.82	0.60
2:LC:1039:ASN:O	2:LC:1043:ASN:ND2	2.34	0.60
5:TG:261:THR:HG21	5:TH:259:LEU:HD12	1.84	0.60
2:LF:1156:VAL:N	2:LF:1178:GLY:O	2.25	0.60
5:TA:211:GLU:HG3	5:TB:213:LYS:HG3	1.84	0.60
6:YB:28:MET:N	6:YB:28:MET:SD	2.75	0.60
5:TC:211:GLU:HG3	5:TD:213:LYS:HG3	1.84	0.60
3:PE:222:GLN:HE21	3:PE:224:GLY:H	1.48	0.60
5:TF:211:GLU:HG3	5:TG:213:LYS:HG3	1.83	0.60
3:PG:520:ILE:O	3:PG:524:ASN:ND2	2.34	0.60
5:TI:211:GLU:HG3	5:TJ:213:LYS:HG3	1.84	0.60
3:PK:520:ILE:HG22	3:PK:524:ASN:HD21	1.66	0.60
4:SF:399:SER:HB3	4:SF:402:GLN:HB2	1.83	0.60
5:TK:211:GLU:HG3	5:TL:213:LYS:HG3	1.84	0.60
6:YD:28:MET:N	6:YD:28:MET:SD	2.75	0.60
2:LD:1039:ASN:O	2:LD:1043:ASN:ND2	2.34	0.60
5:TK:261:THR:HG21	5:TL:259:LEU:HD12	1.83	0.60
6:XC:12:ASN:HD21	6:XC:18:GLU:HG2	1.67	0.60
3:PE:520:ILE:O	3:PE:524:ASN:ND2	2.34	0.60
3:PF:520:ILE:HG22	3:PF:524:ASN:HD21	1.67	0.60
6:XG:12:ASN:HD21	6:XG:18:GLU:HG2	1.66	0.60
3:PC:19:LYS:N	3:PC:26:GLU:OE1	2.35	0.60
3:PC:520:ILE:O	3:PC:524:ASN:ND2	2.35	0.60
3:PD:520:ILE:HG22	3:PD:524:ASN:HD21	1.67	0.60
3:PE:520:ILE:HG22	3:PE:524:ASN:HD21	1.66	0.60
3:PJ:678:MET:SD	3:PJ:678:MET:N	2.69	0.60
6:YD:46:ILE:HD11	6:ZD:43:MET:HE1	1.84	0.60
3:PG:222:GLN:HE21	3:PG:224:GLY:H	1.49	0.60
6:YF:28:MET:SD	6:YF:28:MET:N	2.75	0.59
6:XA:12:ASN:HD21	6:XA:18:GLU:HG2	1.66	0.59
3:PK:123:TYR:OH	3:PK:128:LYS:NZ	2.34	0.59
6:XE:12:ASN:HD21	6:XE:18:GLU:HG2	1.67	0.59
3:PH:19:LYS:N	3:PH:26:GLU:OE1	2.35	0.59
3:PH:520:ILE:HG22	3:PH:524:ASN:HD21	1.66	0.59
3:PI:520:ILE:HG22	3:PI:524:ASN:HD21	1.66	0.59
6:YL:28:MET:N	6:YL:28:MET:SD	2.75	0.59
3:PG:520:ILE:HG22	3:PG:524:ASN:HD21	1.66	0.59
3:PD:19:LYS:N	3:PD:26:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:YI:56:LEU:HD11	6:ZI:53:MET:HE1	1.82	0.59
3:PE:19:LYS:N	3:PE:26:GLU:OE1	2.36	0.59
3:PE:123:TYR:OH	3:PE:128:LYS:NZ	2.34	0.59
4:SD:399:SER:HB3	4:SD:402:GLN:HB2	1.83	0.59
5:TG:211:GLU:HG3	5:TH:213:LYS:HG3	1.84	0.59
6:YJ:46:ILE:HD11	6:ZJ:43:MET:HE1	1.84	0.59
6:YK:56:LEU:HD11	6:ZK:53:MET:HE1	1.83	0.59
2:LA:917:GLN:HA	2:LA:920:THR:HG22	1.85	0.59
5:TD:102:ALA:O	5:TD:106:ASN:ND2	2.34	0.59
2:LC:311:ASN:O	2:LC:476:ASN:ND2	2.36	0.59
6:YF:46:ILE:HD11	6:ZF:43:MET:HE1	1.83	0.59
1:AG:169:ASP:OD2	1:AH:132:ARG:NH2	2.36	0.59
2:LD:917:GLN:HA	2:LD:920:THR:HG22	1.85	0.59
3:PI:415:GLY:O	3:PI:434:ASN:ND2	2.36	0.59
3:PB:29:LEU:HD12	3:PB:348:LEU:HG	1.85	0.59
1:AC:169:ASP:OD2	1:AD:132:ARG:NH2	2.36	0.59
2:LB:917:GLN:HA	2:LB:920:THR:HG22	1.85	0.59
2:LC:681:THR:OG1	2:LC:775:ARG:NH2	2.36	0.59
5:TE:211:GLU:HG3	5:TF:213:LYS:HG3	1.84	0.59
2:LD:1156:VAL:N	2:LD:1178:GLY:O	2.25	0.59
6:YH:28:MET:N	6:YH:28:MET:SD	2.75	0.59
5:TH:102:ALA:O	5:TH:106:ASN:ND2	2.34	0.59
2:LE:917:GLN:HA	2:LE:920:THR:HG22	1.85	0.59
3:PL:520:ILE:HG22	3:PL:524:ASN:HD21	1.67	0.59
3:PB:19:LYS:N	3:PB:26:GLU:OE1	2.35	0.59
4:SE:399:SER:HB3	4:SE:402:GLN:HB2	1.83	0.59
3:PA:19:LYS:N	3:PA:26:GLU:OE1	2.36	0.59
3:PA:123:TYR:OH	3:PA:128:LYS:NZ	2.34	0.59
5:TA:261:THR:HG21	5:TB:259:LEU:HD12	1.84	0.59
6:YB:46:ILE:HD11	6:ZB:43:MET:HE1	1.84	0.59
2:LA:493:ASP:OD1	2:LA:494:ARG:N	2.36	0.58
1:AE:169:ASP:OD2	1:AF:132:ARG:NH2	2.36	0.58
2:LC:917:GLN:HA	2:LC:920:THR:HG22	1.85	0.58
3:PF:19:LYS:N	3:PF:26:GLU:OE1	2.36	0.58
3:PG:415:GLY:O	3:PG:434:ASN:ND2	2.36	0.58
3:PG:548:ASP:OD2	3:PJ:535:ARG:NH1	2.31	0.58
6:XI:12:ASN:HD21	6:XI:18:GLU:HG2	1.67	0.58
6:YJ:28:MET:N	6:YJ:28:MET:SD	2.75	0.58
2:LE:681:THR:OG1	2:LE:775:ARG:NH2	2.36	0.58
3:PI:19:LYS:N	3:PI:26:GLU:OE1	2.35	0.58
2:LF:917:GLN:HA	2:LF:920:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XK:12:ASN:HD21	6:XK:18:GLU:HG2	1.67	0.58
3:PL:29:LEU:HD12	3:PL:348:LEU:HG	1.84	0.58
3:PC:548:ASP:OD2	3:PF:535:ARG:NH1	2.31	0.58
2:LC:493:ASP:OD1	2:LC:494:ARG:N	2.36	0.58
3:PG:19:LYS:N	3:PG:26:GLU:OE1	2.36	0.58
2:LE:493:ASP:OD1	2:LE:494:ARG:N	2.36	0.58
3:PJ:520:ILE:HG22	3:PJ:524:ASN:HD21	1.67	0.58
2:LF:681:THR:OG1	2:LF:775:ARG:NH2	2.36	0.58
3:PK:19:LYS:N	3:PK:26:GLU:OE1	2.36	0.58
2:LC:622:ALA:HB3	2:LC:634:ARG:HB2	1.85	0.58
4:SC:156:ASN:HD21	4:SC:160:ASP:HB3	1.68	0.58
4:SE:156:ASN:HD21	4:SE:160:ASP:HB3	1.68	0.58
6:ZK:48:ASN:O	6:ZK:52:ASN:ND2	2.36	0.58
2:LB:493:ASP:OD1	2:LB:494:ARG:N	2.36	0.58
4:SB:156:ASN:HD21	4:SB:160:ASP:HB3	1.68	0.58
3:PE:415:GLY:O	3:PE:434:ASN:ND2	2.36	0.58
3:PC:123:TYR:OH	3:PC:128:LYS:NZ	2.34	0.58
1:AI:169:ASP:OD2	1:AJ:132:ARG:NH2	2.36	0.58
2:LF:493:ASP:OD1	2:LF:494:ARG:N	2.37	0.58
4:SF:156:ASN:HD21	4:SF:160:ASP:HB3	1.68	0.58
3:PC:415:GLY:O	3:PC:434:ASN:ND2	2.36	0.58
3:PJ:123:TYR:OH	3:PJ:128:LYS:NZ	2.37	0.58
3:PL:19:LYS:N	3:PL:26:GLU:OE1	2.36	0.58
1:AA:169:ASP:OD2	1:AB:132:ARG:NH2	2.36	0.58
2:LA:681:THR:OG1	2:LA:775:ARG:NH2	2.36	0.58
3:PD:29:LEU:HD12	3:PD:348:LEU:HG	1.85	0.58
5:TE:102:ALA:O	5:TE:106:ASN:ND2	2.35	0.58
4:SD:156:ASN:HD21	4:SD:160:ASP:HB3	1.67	0.58
3:PL:678:MET:SD	3:PL:678:MET:N	2.69	0.58
2:LA:622:ALA:HB3	2:LA:634:ARG:HB2	1.86	0.58
2:LB:1156:VAL:N	2:LB:1178:GLY:O	2.25	0.58
6:YH:46:ILE:HD11	6:ZH:43:MET:HE1	1.84	0.58
2:LE:1156:VAL:N	2:LE:1178:GLY:O	2.25	0.58
2:LB:681:THR:OG1	2:LB:775:ARG:NH2	2.36	0.58
3:PC:678:MET:SD	3:PF:677:LYS:NZ	2.77	0.58
2:LD:375:MET:HE2	4:SD:397:PRO:HD3	1.86	0.58
2:LD:622:ALA:HB3	2:LD:634:ARG:HB2	1.86	0.58
5:TI:102:ALA:O	5:TI:106:ASN:ND2	2.35	0.58
3:PK:415:GLY:O	3:PK:434:ASN:ND2	2.36	0.58
3:PB:678:MET:SD	3:PB:678:MET:N	2.69	0.57
2:LB:311:ASN:O	2:LB:476:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:622:ALA:HB3	2:LB:634:ARG:HB2	1.86	0.57
2:LD:681:THR:OG1	2:LD:775:ARG:NH2	2.36	0.57
6:ZG:48:ASN:O	6:ZG:52:ASN:ND2	2.36	0.57
3:PJ:19:LYS:N	3:PJ:26:GLU:OE1	2.36	0.57
4:SA:156:ASN:HD21	4:SA:160:ASP:HB3	1.67	0.57
2:LC:375:MET:HE2	4:SC:397:PRO:HD3	1.87	0.57
6:ZE:48:ASN:O	6:ZE:52:ASN:ND2	2.36	0.57
5:TF:102:ALA:O	5:TF:106:ASN:ND2	2.34	0.57
3:PL:123:TYR:OH	3:PL:128:LYS:NZ	2.37	0.57
5:TG:102:ALA:O	5:TG:106:ASN:ND2	2.36	0.57
1:AK:169:ASP:OD2	1:AL:132:ARG:NH2	2.36	0.57
5:TK:102:ALA:O	5:TK:106:ASN:ND2	2.35	0.57
4:SB:364:ILE:HG21	4:SB:380:VAL:HG13	1.87	0.57
2:LD:311:ASN:O	2:LD:476:ASN:ND2	2.36	0.57
2:LD:628:TRP:HB2	2:LD:790:MET:HG2	1.87	0.57
3:PF:29:LEU:HD12	3:PF:348:LEU:HG	1.84	0.57
2:LD:493:ASP:OD1	2:LD:494:ARG:N	2.36	0.57
2:LF:311:ASN:O	2:LF:476:ASN:ND2	2.36	0.57
3:PD:123:TYR:OH	3:PD:128:LYS:NZ	2.37	0.57
5:TD:268:LYS:NZ	5:TD:274:LEU:O	2.35	0.57
2:LC:628:TRP:HB2	2:LC:790:MET:HG2	1.86	0.57
3:PH:123:TYR:OH	3:PH:128:LYS:NZ	2.37	0.57
2:LB:375:MET:HE2	4:SB:397:PRO:HD3	1.87	0.57
3:PD:222:GLN:NE2	3:PD:224:GLY:O	2.38	0.57
3:PF:222:GLN:NE2	3:PF:224:GLY:O	2.38	0.57
2:LE:375:MET:HE2	4:SE:397:PRO:HD3	1.86	0.57
2:LE:628:TRP:HB2	2:LE:790:MET:HG2	1.87	0.57
2:LA:311:ASN:O	2:LA:476:ASN:ND2	2.36	0.57
4:SA:364:ILE:HG21	4:SA:380:VAL:HG13	1.86	0.57
5:TA:102:ALA:O	5:TA:106:ASN:ND2	2.36	0.57
3:PH:29:LEU:HD12	3:PH:348:LEU:HG	1.85	0.57
2:LF:622:ALA:HB3	2:LF:634:ARG:HB2	1.85	0.57
3:PL:222:GLN:NE2	3:PL:224:GLY:O	2.38	0.57
3:PB:222:GLN:NE2	3:PB:224:GLY:O	2.38	0.57
5:TG:251:ASP:OD2	5:TG:255:LYS:NZ	2.38	0.57
6:ZI:48:ASN:O	6:ZI:52:ASN:ND2	2.36	0.57
3:PC:222:GLN:NE2	3:PC:224:GLY:O	2.38	0.57
3:PF:123:TYR:OH	3:PF:128:LYS:NZ	2.37	0.57
3:PH:222:GLN:NE2	3:PH:224:GLY:O	2.38	0.57
2:LE:311:ASN:O	2:LE:476:ASN:ND2	2.36	0.57
3:PJ:29:LEU:HD12	3:PJ:348:LEU:HG	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XD:65:GLU:OE1	6:XD:65:GLU:N	2.37	0.56
3:PD:678:MET:SD	3:PD:678:MET:N	2.69	0.56
5:TF:268:LYS:NZ	5:TF:274:LEU:O	2.35	0.56
2:LE:622:ALA:HB3	2:LE:634:ARG:HB2	1.86	0.56
3:PJ:222:GLN:NE2	3:PJ:224:GLY:O	2.38	0.56
2:LF:494:ARG:HG2	2:LF:517:TRP:CD2	2.40	0.56
2:LB:628:TRP:HB2	2:LB:790:MET:HG2	1.87	0.56
2:LA:375:MET:HE2	4:SA:397:PRO:HD3	1.86	0.56
3:PA:222:GLN:NE2	3:PA:224:GLY:O	2.39	0.56
2:LB:649:ILE:HG12	2:LB:706:VAL:HG22	1.88	0.56
2:LC:649:ILE:HG12	2:LC:706:VAL:HG22	1.88	0.56
2:LD:494:ARG:HG2	2:LD:517:TRP:CD2	2.40	0.56
4:SD:364:ILE:HG21	4:SD:380:VAL:HG13	1.87	0.56
4:SE:364:ILE:HG21	4:SE:380:VAL:HG13	1.87	0.56
3:PJ:163:GLN:HE22	3:PJ:230:VAL:HB	1.71	0.56
5:TL:251:ASP:OD2	5:TL:255:LYS:NZ	2.38	0.56
3:PB:123:TYR:OH	3:PB:128:LYS:NZ	2.37	0.56
2:LC:494:ARG:HG2	2:LC:517:TRP:CD2	2.40	0.56
3:PE:29:LEU:HD12	3:PE:348:LEU:HG	1.87	0.56
5:TF:251:ASP:OD2	5:TF:255:LYS:NZ	2.38	0.56
3:PK:29:LEU:HD12	3:PK:348:LEU:HG	1.87	0.56
6:XL:65:GLU:OE1	6:XL:65:GLU:N	2.37	0.56
2:LA:649:ILE:HG12	2:LA:706:VAL:HG22	1.88	0.56
5:TE:251:ASP:OD2	5:TE:255:LYS:NZ	2.37	0.56
2:LD:649:ILE:HG12	2:LD:706:VAL:HG22	1.88	0.56
2:LE:494:ARG:HG2	2:LE:517:TRP:CD2	2.40	0.56
2:LF:375:MET:HE2	4:SF:397:PRO:HD3	1.87	0.56
6:ZC:48:ASN:O	6:ZC:52:ASN:ND2	2.36	0.56
3:PG:222:GLN:NE2	3:PG:224:GLY:O	2.39	0.56
3:PI:222:GLN:NE2	3:PI:224:GLY:O	2.38	0.56
4:SF:364:ILE:HG21	4:SF:380:VAL:HG13	1.87	0.56
5:TK:251:ASP:OD2	5:TK:255:LYS:NZ	2.37	0.56
3:PA:480:THR:OG1	3:PA:503:MET:SD	2.64	0.56
3:PG:29:LEU:HD12	3:PG:348:LEU:HG	1.87	0.56
3:PL:163:GLN:HE22	3:PL:230:VAL:HB	1.71	0.56
3:PA:29:LEU:HD12	3:PA:348:LEU:HG	1.87	0.56
5:TA:251:ASP:OD2	5:TA:255:LYS:NZ	2.38	0.56
3:PH:163:GLN:HE22	3:PH:230:VAL:HB	1.71	0.56
5:TH:251:ASP:OD2	5:TH:255:LYS:NZ	2.38	0.56
5:TH:268:LYS:NZ	5:TH:274:LEU:O	2.35	0.56
3:PI:480:THR:OG1	3:PI:503:MET:SD	2.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LF:628:TRP:HB2	2:LF:790:MET:HG2	1.86	0.56
3:PC:29:LEU:HD12	3:PC:348:LEU:HG	1.87	0.56
5:TC:102:ALA:O	5:TC:106:ASN:ND2	2.35	0.56
2:LC:1156:VAL:N	2:LC:1178:GLY:O	2.25	0.56
2:LE:649:ILE:HG12	2:LE:706:VAL:HG22	1.88	0.56
3:PI:29:LEU:HD12	3:PI:348:LEU:HG	1.87	0.56
2:LF:931:VAL:HG23	2:LF:934:SER:HB2	1.88	0.56
2:LA:628:TRP:HB2	2:LA:790:MET:HG2	1.87	0.56
2:LB:494:ARG:HG2	2:LB:517:TRP:CD2	2.40	0.56
2:LF:649:ILE:HG12	2:LF:706:VAL:HG22	1.88	0.56
2:LA:1115:ASN:O	2:LA:1125:ILE:N	2.39	0.55
3:PC:480:THR:OG1	3:PC:503:MET:SD	2.64	0.55
3:PE:107:THR:OG1	3:PE:110:ASP:OD2	2.24	0.55
3:PE:222:GLN:NE2	3:PE:224:GLY:O	2.39	0.55
3:PG:480:THR:OG1	3:PG:503:MET:SD	2.64	0.55
2:LE:93:ASN:ND2	2:LE:239:HIS:O	2.39	0.55
3:PK:222:GLN:NE2	3:PK:224:GLY:O	2.39	0.55
5:TB:251:ASP:OD2	5:TB:255:LYS:NZ	2.38	0.55
3:PE:480:THR:OG1	3:PE:503:MET:SD	2.64	0.55
2:LD:1115:ASN:O	2:LD:1125:ILE:N	2.39	0.55
3:PI:163:GLN:HE22	3:PI:230:VAL:HB	1.72	0.55
5:TI:251:ASP:OD2	5:TI:255:LYS:NZ	2.37	0.55
5:TJ:251:ASP:OD2	5:TJ:255:LYS:NZ	2.38	0.55
4:SF:317:GLU:O	4:SF:322:ASN:ND2	2.38	0.55
2:LA:931:VAL:HG23	2:LA:934:SER:HB2	1.88	0.55
2:LB:286:LEU:HB2	2:LB:325:ILE:HD11	1.88	0.55
4:SC:317:GLU:O	4:SC:322:ASN:ND2	2.38	0.55
4:SC:364:ILE:HG21	4:SC:380:VAL:HG13	1.87	0.55
3:PF:163:GLN:HE22	3:PF:230:VAL:HB	1.71	0.55
2:LD:93:ASN:ND2	2:LD:239:HIS:O	2.40	0.55
3:PI:107:THR:OG1	3:PI:110:ASP:OD2	2.24	0.55
1:AA:104:ILE:HD11	1:AA:154:LYS:HB3	1.88	0.55
2:LA:494:ARG:HG2	2:LA:517:TRP:CD2	2.40	0.55
3:PA:107:THR:OG1	3:PA:110:ASP:OD2	2.24	0.55
5:TC:251:ASP:OD2	5:TC:255:LYS:NZ	2.37	0.55
3:PD:163:GLN:HE22	3:PD:230:VAL:HB	1.71	0.55
3:PF:678:MET:SD	3:PF:678:MET:N	2.69	0.55
6:XH:65:GLU:OE1	6:XH:65:GLU:N	2.37	0.55
3:PK:107:THR:OG1	3:PK:110:ASP:OD2	2.24	0.55
3:PK:480:THR:OG1	3:PK:503:MET:SD	2.64	0.55
2:LA:93:ASN:ND2	2:LA:239:HIS:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SA:317:GLU:O	4:SA:322:ASN:ND2	2.38	0.55
6:ZA:48:ASN:O	6:ZA:52:ASN:ND2	2.36	0.55
6:XE:73:LEU:HD22	6:ZE:62:LYS:HZ1	1.71	0.55
6:XG:73:LEU:HD22	6:ZG:62:LYS:HZ1	1.71	0.55
6:XJ:65:GLU:OE1	6:XJ:65:GLU:N	2.37	0.55
3:PC:107:THR:OG1	3:PC:110:ASP:OD2	2.24	0.55
4:SB:351:ASN:OD1	4:SB:352:ARG:N	2.40	0.55
2:LC:286:LEU:HB2	2:LC:325:ILE:HD11	1.89	0.55
1:AG:104:ILE:HD11	1:AG:154:LYS:HB3	1.88	0.55
4:SD:351:ASN:OD1	4:SD:352:ARG:N	2.40	0.55
4:SA:351:ASN:OD1	4:SA:352:ARG:N	2.40	0.55
3:PG:107:THR:OG1	3:PG:110:ASP:OD2	2.24	0.55
3:PG:163:GLN:HE22	3:PG:230:VAL:HB	1.72	0.55
5:TJ:268:LYS:NZ	5:TJ:274:LEU:O	2.35	0.55
3:PL:147:THR:HG21	3:PL:376:TYR:HD1	1.71	0.55
3:PB:147:THR:HG21	3:PB:376:TYR:HD1	1.72	0.55
3:PB:413:PRO:HG3	3:PB:442:MET:HB3	1.88	0.55
2:LC:93:ASN:ND2	2:LC:239:HIS:O	2.40	0.55
3:PK:163:GLN:HE22	3:PK:230:VAL:HB	1.72	0.55
3:PB:163:GLN:HE22	3:PB:230:VAL:HB	1.71	0.55
1:AF:171:PRO:HG2	1:AF:174:LEU:HD23	1.88	0.55
4:SD:317:GLU:O	4:SD:322:ASN:ND2	2.38	0.55
1:AJ:43:GLU:OE2	1:AJ:185:ARG:NH2	2.40	0.55
1:AB:58:ASN:HB2	1:AB:148:ASN:HD21	1.72	0.55
1:AC:104:ILE:HD11	1:AC:154:LYS:HB3	1.89	0.55
2:LE:931:VAL:HG23	2:LE:934:SER:HB2	1.88	0.55
1:AL:171:PRO:HG2	1:AL:174:LEU:HD23	1.88	0.55
2:LF:446:SER:HB3	2:LF:488:GLY:HA2	1.89	0.55
4:SC:351:ASN:OD1	4:SC:352:ARG:N	2.40	0.54
1:AH:58:ASN:HB2	1:AH:148:ASN:HD21	1.72	0.54
2:LD:806:HIS:HB3	2:LD:819:ALA:HB2	1.90	0.54
4:SE:351:ASN:OD1	4:SE:352:ARG:N	2.40	0.54
2:LF:93:ASN:ND2	2:LF:239:HIS:O	2.40	0.54
4:SF:351:ASN:OD1	4:SF:352:ARG:N	2.40	0.54
2:LB:93:ASN:ND2	2:LB:239:HIS:O	2.39	0.54
3:PC:166:PRO:HA	3:PC:225:THR:HA	1.90	0.54
2:LC:931:VAL:HG23	2:LC:934:SER:HB2	1.88	0.54
1:AH:43:GLU:OE2	1:AH:185:ARG:NH2	2.40	0.54
3:PJ:118:GLU:O	3:PJ:122:ASN:ND2	2.34	0.54
1:AK:104:ILE:HD11	1:AK:154:LYS:HB3	1.87	0.54
3:PC:163:GLN:HE22	3:PC:230:VAL:HB	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:104:ILE:HD11	1:AE:154:LYS:HB3	1.87	0.54
3:PE:163:GLN:HE22	3:PE:230:VAL:HB	1.72	0.54
3:PE:166:PRO:HA	3:PE:225:THR:HA	1.89	0.54
3:PF:147:THR:HG21	3:PF:376:TYR:HD1	1.71	0.54
1:AI:104:ILE:HD11	1:AI:154:LYS:HB3	1.89	0.54
2:LE:806:HIS:HB3	2:LE:819:ALA:HB2	1.89	0.54
2:LB:931:VAL:HG23	2:LB:934:SER:HB2	1.88	0.54
3:PD:147:THR:HG21	3:PD:376:TYR:HD1	1.72	0.54
2:LC:245:ASP:OD2	2:LC:539:LYS:NZ	2.40	0.54
1:AJ:58:ASN:HB2	1:AJ:148:ASN:HD21	1.72	0.54
3:PA:166:PRO:HA	3:PA:225:THR:HA	1.90	0.54
1:AD:58:ASN:HB2	1:AD:148:ASN:HD21	1.72	0.54
2:LB:439:PRO:HB2	2:LB:542:PRO:HA	1.89	0.54
5:TD:251:ASP:OD2	5:TD:255:LYS:NZ	2.38	0.54
3:PH:118:GLU:O	3:PH:122:ASN:ND2	2.35	0.54
4:SF:223:ASN:HB3	4:SF:252:ILE:HG12	1.89	0.54
2:LA:286:LEU:HB2	2:LA:325:ILE:HD11	1.89	0.54
2:LB:891:THR:HG21	2:LB:950:TYR:HE1	1.73	0.54
3:PJ:147:THR:HG21	3:PJ:376:TYR:HD1	1.72	0.54
1:AL:43:GLU:OE2	1:AL:185:ARG:NH2	2.41	0.54
1:AL:58:ASN:HB2	1:AL:148:ASN:HD21	1.73	0.54
2:LF:1105:ARG:HD2	2:LF:1106:PRO:HD2	1.90	0.54
2:LA:806:HIS:HB3	2:LA:819:ALA:HB2	1.90	0.54
3:PB:480:THR:OG1	3:PB:503:MET:SD	2.66	0.54
2:LC:806:HIS:HB3	2:LC:819:ALA:HB2	1.90	0.54
2:LD:286:LEU:HB2	2:LD:325:ILE:HD11	1.89	0.54
3:PH:147:THR:HG21	3:PH:376:TYR:HD1	1.72	0.54
3:PK:55:ASP:OD1	3:PK:61:GLY:N	2.41	0.54
1:AB:43:GLU:OE2	1:AB:185:ARG:NH2	2.40	0.54
2:LA:446:SER:HB3	2:LA:488:GLY:HA2	1.89	0.54
1:AF:43:GLU:OE2	1:AF:185:ARG:NH2	2.41	0.54
2:LC:446:SER:HB3	2:LC:488:GLY:HA2	1.89	0.54
1:AH:65:GLU:OE2	6:ZG:37:LYS:NZ	2.39	0.54
4:SD:223:ASN:HB3	4:SD:252:ILE:HG12	1.89	0.54
2:LE:286:LEU:HB2	2:LE:325:ILE:HD11	1.88	0.54
4:SE:223:ASN:HB3	4:SE:252:ILE:HG12	1.89	0.54
2:LF:891:THR:HG21	2:LF:950:TYR:HE1	1.73	0.54
2:LA:891:THR:HG21	2:LA:950:TYR:HE1	1.73	0.54
3:PA:674:ASP:O	3:PD:677:LYS:NZ	2.41	0.54
2:LB:245:ASP:OD2	2:LB:539:LYS:NZ	2.41	0.54
3:PE:444:ILE:HD12	3:PH:440:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PL:480:THR:OG1	3:PL:503:MET:SD	2.66	0.54
1:AB:171:PRO:HG2	1:AB:174:LEU:HD23	1.90	0.54
2:LB:873:TRP:O	2:LB:877:ASN:ND2	2.28	0.54
3:PD:480:THR:OG1	3:PD:503:MET:SD	2.66	0.54
2:LC:423:ASP:OD1	2:LC:424:LYS:N	2.41	0.54
2:LC:1115:ASN:O	2:LC:1125:ILE:N	2.39	0.54
2:LD:931:VAL:HG23	2:LD:934:SER:HB2	1.88	0.54
3:PG:444:ILE:HD12	3:PJ:440:ALA:HB2	1.90	0.54
3:PG:674:ASP:O	3:PJ:677:LYS:NZ	2.41	0.54
2:LE:1105:ARG:HD2	2:LE:1106:PRO:HD2	1.90	0.54
2:LA:1105:ARG:HD2	2:LA:1106:PRO:HD2	1.90	0.53
3:PA:55:ASP:OD1	3:PA:61:GLY:N	2.41	0.53
1:AD:43:GLU:OE2	1:AD:185:ARG:NH2	2.40	0.53
3:PD:118:GLU:O	3:PD:122:ASN:ND2	2.34	0.53
2:LE:407:THR:HB	4:SE:135:PHE:HE1	1.74	0.53
4:SE:317:GLU:O	4:SE:322:ASN:ND2	2.38	0.53
2:LF:1115:ASN:O	2:LF:1125:ILE:N	2.39	0.53
3:PA:163:GLN:HE22	3:PA:230:VAL:HB	1.72	0.53
1:AF:58:ASN:HB2	1:AF:148:ASN:HD21	1.73	0.53
4:SC:223:ASN:HB3	4:SC:252:ILE:HG12	1.89	0.53
6:XF:65:GLU:OE1	6:XF:65:GLU:N	2.37	0.53
1:AH:171:PRO:HG2	1:AH:174:LEU:HD23	1.90	0.53
5:TH:59:ARG:NH1	5:TI:72:GLN:OE1	2.42	0.53
1:AL:211:ARG:HH22	7:OL:1:ASP:CB	2.22	0.53
2:LA:596:GLU:OE2	4:SA:41:THR:N	2.40	0.53
3:PF:480:THR:OG1	3:PF:503:MET:SD	2.66	0.53
3:PI:55:ASP:OD1	3:PI:61:GLY:N	2.41	0.53
3:PI:130:ASN:OD1	3:PJ:511:LYS:NZ	2.40	0.53
3:PK:166:PRO:HA	3:PK:225:THR:HA	1.89	0.53
5:TL:268:LYS:NZ	5:TL:274:LEU:O	2.35	0.53
2:LA:423:ASP:OD1	2:LA:424:LYS:N	2.41	0.53
2:LA:1138:THR:HG23	2:LA:1141:GLU:HG2	1.91	0.53
2:LB:1004:ASN:OD1	2:LB:1005:ARG:N	2.41	0.53
3:PG:147:THR:HG21	3:PG:376:TYR:HD1	1.73	0.53
3:PG:166:PRO:HA	3:PG:225:THR:HA	1.90	0.53
2:LF:286:LEU:HB2	2:LF:325:ILE:HD11	1.89	0.53
2:LF:407:THR:HB	4:SF:135:PHE:HE1	1.74	0.53
3:PD:166:PRO:HA	3:PD:225:THR:HA	1.91	0.53
2:LC:891:THR:HG21	2:LC:950:TYR:HE1	1.73	0.53
3:PF:166:PRO:HA	3:PF:225:THR:HA	1.91	0.53
2:LD:39:GLU:HA	4:SD:412:VAL:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LD:1138:THR:HG23	2:LD:1141:GLU:HG2	1.91	0.53
3:PG:442:MET:O	3:PJ:433:TYR:OH	2.27	0.53
2:LB:423:ASP:OD1	2:LB:424:LYS:N	2.41	0.53
5:TD:59:ARG:NH1	5:TE:72:GLN:OE1	2.41	0.53
2:LC:1138:THR:HG23	2:LC:1141:GLU:HG2	1.91	0.53
2:LD:446:SER:HB3	2:LD:488:GLY:HA2	1.89	0.53
2:LE:439:PRO:HB2	2:LE:542:PRO:HA	1.89	0.53
2:LF:423:ASP:OD1	2:LF:424:LYS:N	2.41	0.53
2:LF:1138:THR:HG23	2:LF:1141:GLU:HG2	1.91	0.53
5:TK:204:GLU:HG3	5:TL:206:ILE:HG23	1.90	0.53
2:LB:596:GLU:OE2	4:SB:41:THR:N	2.40	0.53
2:LB:806:HIS:HB3	2:LB:819:ALA:HB2	1.89	0.53
2:LD:891:THR:HG21	2:LD:950:TYR:HE1	1.73	0.53
3:PH:480:THR:OG1	3:PH:503:MET:SD	2.66	0.53
5:TJ:59:ARG:NH1	5:TK:72:GLN:OE1	2.41	0.53
3:PK:664:GLU:HB3	3:PK:669:THR:HB	1.91	0.53
2:LA:245:ASP:OD2	2:LA:539:LYS:NZ	2.41	0.53
2:LA:1004:ASN:OD1	2:LA:1005:ARG:N	2.41	0.53
4:SA:223:ASN:HB3	4:SA:252:ILE:HG12	1.89	0.53
5:TA:204:GLU:HG3	5:TB:206:ILE:HG23	1.91	0.53
2:LB:1138:THR:HG23	2:LB:1141:GLU:HG2	1.91	0.53
1:AF:211:ARG:HH22	7:OF:1:ASP:CB	2.22	0.53
3:PE:674:ASP:O	3:PH:677:LYS:NZ	2.42	0.53
3:PI:664:GLU:HB3	3:PI:669:THR:HB	1.91	0.53
1:AL:65:GLU:OE2	6:ZK:37:LYS:NZ	2.39	0.53
2:LF:922:ASN:OD1	2:LF:923:ILE:N	2.42	0.53
3:PK:678:MET:SD	3:PK:678:MET:N	2.66	0.53
3:PA:444:ILE:HD12	3:PD:440:ALA:HB2	1.90	0.53
6:XC:73:LEU:HD22	6:ZC:62:LYS:HZ1	1.73	0.53
5:TE:59:ARG:NH1	5:TF:72:GLN:OE1	2.42	0.53
5:TE:204:GLU:HG3	5:TF:206:ILE:HG23	1.90	0.53
2:LD:423:ASP:OD1	2:LD:424:LYS:N	2.41	0.53
2:LD:1018:VAL:HG13	2:LD:1019:THR:HG23	1.91	0.53
2:LD:1105:ARG:HD2	2:LD:1106:PRO:HD2	1.90	0.53
1:AJ:171:PRO:HG2	1:AJ:174:LEU:HD23	1.91	0.53
2:LE:1138:THR:HG23	2:LE:1141:GLU:HG2	1.91	0.53
3:PI:166:PRO:HA	3:PI:225:THR:HA	1.90	0.53
3:PJ:480:THR:OG1	3:PJ:503:MET:SD	2.66	0.53
2:LF:245:ASP:OD2	2:LF:539:LYS:NZ	2.40	0.53
5:TL:222:ASP:OD1	5:TL:238:LYS:NZ	2.34	0.53
1:AB:65:GLU:OE2	6:ZA:37:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PA:147:THR:HG21	3:PA:376:TYR:HD1	1.73	0.53
3:PA:678:MET:SD	3:PD:677:LYS:NZ	2.77	0.53
1:AD:171:PRO:HG2	1:AD:174:LEU:HD23	1.91	0.53
2:LB:1018:VAL:HG13	2:LB:1019:THR:HG23	1.90	0.53
2:LB:1105:ARG:HD2	2:LB:1106:PRO:HD2	1.90	0.53
4:SB:317:GLU:O	4:SB:322:ASN:ND2	2.38	0.53
5:TF:59:ARG:NH1	5:TG:72:GLN:OE1	2.42	0.53
1:AJ:211:ARG:HH22	7:OJ:1:ASP:CB	2.22	0.53
3:PI:674:ASP:O	3:PL:677:LYS:NZ	2.42	0.53
3:PB:677:LYS:NZ	3:PK:674:ASP:O	2.42	0.52
2:LB:446:SER:HB3	2:LB:488:GLY:HA2	1.90	0.52
2:LB:968:LEU:O	2:LB:969:ASN:ND2	2.43	0.52
2:LC:1004:ASN:OD1	2:LC:1005:ARG:N	2.41	0.52
3:PF:107:THR:OG1	3:PF:110:ASP:OD2	2.27	0.52
2:LD:245:ASP:OD2	2:LD:539:LYS:NZ	2.41	0.52
2:LD:922:ASN:OD1	2:LD:923:ILE:N	2.42	0.52
3:PG:664:GLU:HB3	3:PG:669:THR:HB	1.91	0.52
2:LF:806:HIS:HB3	2:LF:819:ALA:HB2	1.90	0.52
2:LF:1004:ASN:OD1	2:LF:1005:ARG:N	2.41	0.52
3:PL:55:ASP:OD1	3:PL:61:GLY:N	2.42	0.52
3:PC:674:ASP:O	3:PF:677:LYS:NZ	2.42	0.52
4:SB:223:ASN:HB3	4:SB:252:ILE:HG12	1.89	0.52
3:PF:118:GLU:O	3:PF:122:ASN:ND2	2.35	0.52
3:PJ:55:ASP:OD1	3:PJ:61:GLY:N	2.42	0.52
3:PB:166:PRO:HA	3:PB:225:THR:HA	1.91	0.52
2:LB:128:ARG:HG2	2:LB:204:ILE:HG22	1.92	0.52
3:PC:55:ASP:OD1	3:PC:61:GLY:N	2.41	0.52
2:LC:1105:ARG:HD2	2:LC:1106:PRO:HD2	1.90	0.52
3:PG:55:ASP:OD1	3:PG:61:GLY:N	2.41	0.52
4:SE:347:ASP:OD1	4:SE:351:ASN:ND2	2.42	0.52
2:LF:968:LEU:O	2:LF:969:ASN:ND2	2.43	0.52
5:TC:59:ARG:NH1	5:TD:72:GLN:OE1	2.43	0.52
5:TG:59:ARG:NH1	5:TH:72:GLN:OE1	2.43	0.52
2:LE:423:ASP:OD1	2:LE:424:LYS:N	2.41	0.52
2:LE:446:SER:HB3	2:LE:488:GLY:HA2	1.90	0.52
6:XI:73:LEU:HD13	6:ZI:62:LYS:HZ1	1.74	0.52
6:XK:73:LEU:HD22	6:ZK:62:LYS:HZ1	1.74	0.52
5:TB:59:ARG:NH1	5:TC:72:GLN:OE1	2.42	0.52
3:PC:454:SER:HB2	3:PF:451:LEU:HG	1.92	0.52
2:LC:128:ARG:HG2	2:LC:204:ILE:HG22	1.92	0.52
2:LC:439:PRO:HB2	2:LC:542:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LC:1018:VAL:HG13	2:LC:1019:THR:HG23	1.91	0.52
3:PH:166:PRO:HA	3:PH:225:THR:HA	1.91	0.52
2:LF:128:ARG:HG2	2:LF:204:ILE:HG22	1.92	0.52
1:AB:211:ARG:HH22	7:OB:1:ASP:CB	2.23	0.52
4:SA:347:ASP:OD1	4:SA:351:ASN:ND2	2.42	0.52
6:XB:65:GLU:OE1	6:XB:65:GLU:N	2.37	0.52
2:LB:165:GLU:HG2	2:LB:176:THR:HG22	1.92	0.52
3:PE:147:THR:HG21	3:PE:376:TYR:HD1	1.74	0.52
3:PF:134:PHE:HE2	3:PF:513:MET:HE1	1.75	0.52
5:TG:204:GLU:HG3	5:TH:206:ILE:HG23	1.91	0.52
2:LE:891:THR:HG21	2:LE:950:TYR:HE1	1.73	0.52
3:PI:454:SER:HB2	3:PL:451:LEU:HG	1.92	0.52
2:LA:128:ARG:HG2	2:LA:204:ILE:HG22	1.92	0.52
2:LA:407:THR:HB	4:SA:135:PHE:HE1	1.74	0.52
3:PA:664:GLU:HB3	3:PA:669:THR:HB	1.91	0.52
3:PC:444:ILE:HD12	3:PF:440:ALA:HB2	1.91	0.52
1:AE:23:THR:OG1	1:AE:28:ASP:O	2.27	0.52
2:LC:499:ASN:HB3	2:LC:514:GLY:HA2	1.92	0.52
5:TF:208:MET:HE3	5:TG:209:THR:HG23	1.92	0.52
2:LD:407:THR:HB	4:SD:135:PHE:HE1	1.74	0.52
2:LE:922:ASN:OD1	2:LE:923:ILE:N	2.42	0.52
2:LA:922:ASN:OD1	2:LA:923:ILE:N	2.42	0.52
3:PA:130:ASN:OD1	3:PB:511:LYS:NZ	2.40	0.52
6:YA:60:HIS:HA	6:YA:63:LEU:HD23	1.92	0.52
2:LC:39:GLU:HA	4:SC:412:VAL:HA	1.91	0.52
3:PE:55:ASP:OD1	3:PE:61:GLY:N	2.41	0.52
5:TF:278:ASN:HA	5:TF:281:THR:HG23	1.92	0.52
1:AH:211:ARG:HH22	7:OH:1:ASP:CB	2.23	0.52
3:PH:107:THR:OG1	3:PH:110:ASP:OD2	2.28	0.52
3:PH:678:MET:SD	3:PH:678:MET:N	2.69	0.52
2:LE:128:ARG:HG2	2:LE:204:ILE:HG22	1.92	0.52
3:PI:677:LYS:NZ	3:PJ:678:MET:SD	2.83	0.52
2:LF:1018:VAL:HG13	2:LF:1019:THR:HG23	1.91	0.52
3:PL:664:GLU:HB3	3:PL:669:THR:HB	1.92	0.52
4:SA:29:ILE:HG23	4:SA:36:HIS:HB2	1.92	0.52
5:TA:72:GLN:OE1	5:TL:59:ARG:NH1	2.42	0.52
6:XA:73:LEU:HD13	6:ZA:62:LYS:HZ1	1.75	0.52
1:AD:211:ARG:HH22	7:OD:1:ASP:CB	2.22	0.52
3:PC:664:GLU:HB3	3:PC:669:THR:HB	1.91	0.52
2:LE:873:TRP:O	2:LE:877:ASN:ND2	2.28	0.52
3:PJ:664:GLU:HB3	3:PJ:669:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LF:39:GLU:HA	4:SF:412:VAL:HA	1.91	0.52
6:YK:60:HIS:HA	6:YK:63:LEU:HD23	1.92	0.52
5:TA:59:ARG:NH1	5:TB:72:GLN:OE1	2.43	0.52
4:SB:29:ILE:HG23	4:SB:36:HIS:HB2	1.92	0.52
2:LC:922:ASN:OD1	2:LC:923:ILE:N	2.42	0.52
4:SC:347:ASP:OD1	4:SC:351:ASN:ND2	2.42	0.52
2:LD:499:ASN:HB3	2:LD:514:GLY:HA2	1.92	0.52
2:LD:873:TRP:O	2:LD:877:ASN:ND2	2.28	0.52
2:LE:1018:VAL:HG13	2:LE:1019:THR:HG23	1.90	0.52
3:PI:147:THR:HG21	3:PI:376:TYR:HD1	1.74	0.52
5:TJ:208:MET:HE3	5:TK:209:THR:HG23	1.92	0.52
3:PK:677:LYS:NZ	3:PL:678:MET:SD	2.83	0.52
3:PL:166:PRO:HA	3:PL:225:THR:HA	1.91	0.52
2:LA:1018:VAL:HG13	2:LA:1019:THR:HG23	1.91	0.51
6:YC:60:HIS:HA	6:YC:63:LEU:HD23	1.92	0.51
2:LD:1004:ASN:OD1	2:LD:1005:ARG:N	2.41	0.51
1:AJ:214:VAL:O	3:PK:414:LYS:NZ	2.35	0.51
2:LE:1004:ASN:OD1	2:LE:1005:ARG:N	2.41	0.51
5:TI:59:ARG:NH1	5:TJ:72:GLN:OE1	2.43	0.51
1:AK:43:GLU:OE2	1:AK:181:TYR:OH	2.26	0.51
3:PK:147:THR:HG21	3:PK:376:TYR:HD1	1.74	0.51
3:PB:55:ASP:OD1	3:PB:61:GLY:N	2.42	0.51
3:PC:147:THR:HG21	3:PC:376:TYR:HD1	1.74	0.51
3:PD:107:THR:OG1	3:PD:110:ASP:OD2	2.27	0.51
3:PG:130:ASN:OD1	3:PH:511:LYS:NZ	2.40	0.51
3:PJ:166:PRO:HA	3:PJ:225:THR:HA	1.91	0.51
2:LF:439:PRO:HB2	2:LF:542:PRO:HA	1.91	0.51
2:LA:39:GLU:HA	4:SA:412:VAL:HA	1.91	0.51
3:PA:118:GLU:O	3:PA:122:ASN:ND2	2.34	0.51
3:PA:442:MET:O	3:PD:433:TYR:OH	2.27	0.51
5:TA:209:THR:HG23	5:TL:208:MET:HE3	1.92	0.51
5:TB:268:LYS:NZ	5:TB:274:LEU:O	2.35	0.51
2:LB:499:ASN:HB3	2:LB:514:GLY:HA2	1.92	0.51
3:PD:134:PHE:HE2	3:PD:513:MET:HE1	1.75	0.51
5:TD:208:MET:HE3	5:TE:209:THR:HG23	1.92	0.51
2:LC:968:LEU:O	2:LC:969:ASN:ND2	2.43	0.51
2:LD:128:ARG:HG2	2:LD:204:ILE:HG22	1.92	0.51
5:TH:278:ASN:HA	5:TH:281:THR:HG23	1.92	0.51
2:LE:245:ASP:OD2	2:LE:539:LYS:NZ	2.41	0.51
2:LE:968:LEU:O	2:LE:969:ASN:ND2	2.44	0.51
5:TK:59:ARG:NH1	5:TL:72:GLN:OE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PB:664:GLU:HB3	3:PB:669:THR:HB	1.92	0.51
2:LB:922:ASN:OD1	2:LB:923:ILE:N	2.42	0.51
2:LB:1115:ASN:O	2:LB:1125:ILE:N	2.39	0.51
3:PD:55:ASP:OD1	3:PD:61:GLY:N	2.42	0.51
5:TD:278:ASN:HA	5:TD:281:THR:HG23	1.92	0.51
2:LC:596:GLU:OE2	4:SC:41:THR:N	2.39	0.51
6:YE:60:HIS:HA	6:YE:63:LEU:HD23	1.92	0.51
3:PG:451:LEU:HG	3:PH:454:SER:HB2	1.92	0.51
3:PG:677:LYS:NZ	3:PH:678:MET:SD	2.83	0.51
4:SD:29:ILE:HG23	4:SD:36:HIS:HB2	1.92	0.51
1:AJ:65:GLU:OE2	6:ZI:37:LYS:NZ	2.39	0.51
2:LE:39:GLU:HA	4:SE:412:VAL:HA	1.91	0.51
5:TI:204:GLU:HG3	5:TJ:206:ILE:HG23	1.91	0.51
2:LB:39:GLU:HA	4:SB:412:VAL:HA	1.91	0.51
1:AI:43:GLU:OE2	1:AI:181:TYR:OH	2.26	0.51
3:PL:118:GLU:O	3:PL:122:ASN:ND2	2.35	0.51
2:LA:439:PRO:HB2	2:LA:542:PRO:HA	1.92	0.51
3:PA:164:GLU:HA	3:PA:227:THR:HA	1.92	0.51
3:PH:55:ASP:OD1	3:PH:61:GLY:N	2.42	0.51
3:PJ:107:THR:OG1	3:PJ:110:ASP:OD2	2.27	0.51
3:PA:451:LEU:HG	3:PB:454:SER:HB2	1.92	0.51
2:LB:407:THR:HB	4:SB:135:PHE:HE1	1.74	0.51
2:LC:165:GLU:HG2	2:LC:176:THR:HG22	1.92	0.51
3:PI:444:ILE:HD12	3:PL:440:ALA:HB2	1.91	0.51
6:YI:60:HIS:HA	6:YI:63:LEU:HD23	1.92	0.51
5:TL:278:ASN:HA	5:TL:281:THR:HG23	1.92	0.51
3:PA:454:SER:HB2	3:PD:451:LEU:HG	1.93	0.51
3:PA:677:LYS:NZ	3:PB:678:MET:SD	2.83	0.51
6:XA:73:LEU:HD22	6:ZA:62:LYS:HZ1	1.76	0.51
3:PB:107:THR:OG1	3:PB:110:ASP:OD2	2.28	0.51
5:TC:204:GLU:HG3	5:TD:206:ILE:HG23	1.91	0.51
3:PE:664:GLU:HB3	3:PE:669:THR:HB	1.91	0.51
3:PE:677:LYS:NZ	3:PF:678:MET:SD	2.83	0.51
1:AG:23:THR:OG1	1:AG:28:ASP:O	2.27	0.51
5:TH:208:MET:HE3	5:TI:209:THR:HG23	1.93	0.51
2:LE:165:GLU:HG2	2:LE:176:THR:HG22	1.92	0.51
2:LE:1115:ASN:O	2:LE:1125:ILE:N	2.39	0.51
3:PI:442:MET:O	3:PL:433:TYR:OH	2.28	0.51
4:SF:29:ILE:HG23	4:SF:36:HIS:HB2	1.93	0.51
5:TB:208:MET:HE3	5:TC:209:THR:HG23	1.93	0.51
6:XD:10:ILE:HD11	6:ZC:41:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XF:10:ILE:HD11	6:ZE:41:LEU:HA	1.92	0.51
2:LD:968:LEU:O	2:LD:969:ASN:ND2	2.44	0.51
3:PG:164:GLU:HA	3:PG:227:THR:HA	1.92	0.51
3:PG:454:SER:HB2	3:PJ:451:LEU:HG	1.93	0.51
4:SE:29:ILE:HG23	4:SE:36:HIS:HB2	1.92	0.51
1:AL:87:LYS:HE3	2:LF:15:SER:HB3	1.93	0.51
6:XB:10:ILE:HD11	6:ZA:41:LEU:HA	1.93	0.51
3:PC:134:PHE:HE2	3:PC:513:MET:HE1	1.76	0.51
3:PC:164:GLU:HA	3:PC:227:THR:HA	1.92	0.51
2:LA:165:GLU:HG2	2:LA:176:THR:HG22	1.93	0.50
5:TA:222:ASP:OD1	5:TA:238:LYS:NZ	2.35	0.50
3:PC:130:ASN:OD1	3:PD:511:LYS:NZ	2.40	0.50
1:AH:87:LYS:HE3	2:LD:15:SER:HB3	1.92	0.50
2:LD:439:PRO:HB2	2:LD:542:PRO:HA	1.92	0.50
6:XG:66:LEU:HD11	6:YG:66:LEU:HD13	1.93	0.50
3:PI:134:PHE:HE2	3:PI:513:MET:HE1	1.76	0.50
3:PK:164:GLU:HA	3:PK:227:THR:HA	1.93	0.50
3:PL:107:THR:OG1	3:PL:110:ASP:OD2	2.27	0.50
3:PL:134:PHE:HE2	3:PL:513:MET:HE1	1.75	0.50
2:LA:499:ASN:HB3	2:LA:514:GLY:HA2	1.92	0.50
2:LA:968:LEU:O	2:LA:969:ASN:ND2	2.44	0.50
3:PD:664:GLU:HB3	3:PD:669:THR:HB	1.92	0.50
6:YG:60:HIS:HA	6:YG:63:LEU:HD23	1.92	0.50
2:LE:499:ASN:HB3	2:LE:514:GLY:HA2	1.92	0.50
5:TJ:278:ASN:HA	5:TJ:281:THR:HG23	1.92	0.50
2:LF:165:GLU:HG2	2:LF:176:THR:HG22	1.92	0.50
2:LF:596:GLU:OE2	4:SF:41:THR:N	2.39	0.50
6:XK:73:LEU:HD13	6:ZK:62:LYS:HZ1	1.77	0.50
3:PA:134:PHE:HE2	3:PA:513:MET:HE1	1.76	0.50
1:AD:87:LYS:HE3	2:LB:15:SER:HB3	1.92	0.50
1:AF:87:LYS:HE3	2:LC:15:SER:HB3	1.93	0.50
3:PE:130:ASN:OD1	3:PF:511:LYS:NZ	2.40	0.50
3:PF:664:GLU:HB3	3:PF:669:THR:HB	1.92	0.50
3:PH:664:GLU:HB3	3:PH:669:THR:HB	1.92	0.50
5:TB:278:ASN:HA	5:TB:281:THR:HG23	1.92	0.50
1:AE:43:GLU:OE2	1:AE:181:TYR:OH	2.26	0.50
4:SD:341:LEU:HA	4:SD:344:LEU:HD13	1.93	0.50
6:XH:10:ILE:HD11	6:ZG:41:LEU:HA	1.93	0.50
1:AJ:87:LYS:HE3	2:LE:15:SER:HB3	1.92	0.50
3:PI:164:GLU:HA	3:PI:227:THR:HA	1.92	0.50
4:SF:341:LEU:HA	4:SF:344:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XL:10:ILE:HD11	6:ZK:41:LEU:HA	1.92	0.50
3:PC:677:LYS:NZ	3:PD:678:MET:SD	2.83	0.50
2:LC:407:THR:HB	4:SC:135:PHE:HE1	1.74	0.50
3:PF:55:ASP:OD1	3:PF:61:GLY:N	2.42	0.50
3:PI:678:MET:SD	3:PL:677:LYS:NZ	2.77	0.50
1:AD:65:GLU:OE2	6:ZC:37:LYS:NZ	2.39	0.50
3:PE:164:GLU:HA	3:PE:227:THR:HA	1.93	0.50
4:SC:341:LEU:HA	4:SC:344:LEU:HD13	1.94	0.50
3:PA:158:ILE:HD11	3:PA:231:GLU:HB3	1.94	0.50
3:PB:134:PHE:HE2	3:PB:513:MET:HE1	1.76	0.50
3:PH:134:PHE:HE2	3:PH:513:MET:HE1	1.76	0.50
2:LF:499:ASN:HB3	2:LF:514:GLY:HA2	1.92	0.50
1:AB:87:LYS:HE3	2:LA:15:SER:HB3	1.92	0.50
6:XE:66:LEU:HD11	6:YE:66:LEU:HD13	1.93	0.50
5:TG:268:LYS:NZ	5:TG:274:LEU:O	2.43	0.50
6:XJ:10:ILE:HD11	6:ZI:41:LEU:HA	1.93	0.50
3:PE:451:LEU:HG	3:PF:454:SER:HB2	1.94	0.50
3:PG:134:PHE:HE2	3:PG:513:MET:HE1	1.76	0.50
1:AA:23:THR:OG1	1:AA:28:ASP:O	2.27	0.49
2:LA:740:ILE:HD11	2:LA:808:TRP:CG	2.47	0.49
3:PC:158:ILE:HD11	3:PC:231:GLU:HB3	1.94	0.49
5:TC:200:LYS:O	5:TC:203:THR:OG1	2.29	0.49
6:XC:66:LEU:HD11	6:YC:66:LEU:HD13	1.93	0.49
4:SE:341:LEU:HA	4:SE:344:LEU:HD13	1.93	0.49
3:PJ:344:ILE:O	3:PJ:347:THR:OG1	2.29	0.49
1:AK:23:THR:OG1	1:AK:28:ASP:O	2.27	0.49
2:LD:740:ILE:HD11	2:LD:808:TRP:CG	2.47	0.49
3:PG:158:ILE:HD11	3:PG:231:GLU:HB3	1.94	0.49
4:SD:228:TYR:CZ	4:SD:248:TRP:HB3	2.48	0.49
6:XI:73:LEU:HD22	6:ZI:62:LYS:HZ1	1.77	0.49
3:PK:134:PHE:HE2	3:PK:513:MET:HE1	1.76	0.49
3:PA:440:ALA:HB2	3:PB:444:ILE:HD12	1.94	0.49
4:SA:341:LEU:HA	4:SA:344:LEU:HD13	1.93	0.49
3:PC:442:MET:O	3:PF:433:TYR:OH	2.28	0.49
6:XC:73:LEU:HD13	6:ZC:62:LYS:HZ1	1.77	0.49
2:LC:740:ILE:HD11	2:LC:808:TRP:CG	2.48	0.49
4:SC:228:TYR:CZ	4:SC:248:TRP:HB3	2.48	0.49
2:LD:887:PHE:O	2:LD:928:GLY:N	2.43	0.49
3:PI:677:LYS:NZ	3:PJ:674:ASP:O	2.46	0.49
3:PJ:134:PHE:HE2	3:PJ:513:MET:HE1	1.75	0.49
3:PK:451:LEU:HG	3:PL:454:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:142:GLN:HB3	2:LB:230:MET:HG2	1.94	0.49
4:SC:29:ILE:HG23	4:SC:36:HIS:HB2	1.93	0.49
1:AI:23:THR:OG1	1:AI:28:ASP:O	2.28	0.49
2:LE:400:GLY:HA2	2:LE:402:ARG:HE	1.78	0.49
6:XA:66:LEU:HD11	6:YA:66:LEU:HD13	1.93	0.49
2:LB:740:ILE:HD11	2:LB:808:TRP:CG	2.48	0.49
5:TD:293:LYS:O	2:LE:1042:GLN:NE2	2.45	0.49
3:PE:118:GLU:O	3:PE:122:ASN:ND2	2.34	0.49
3:PG:118:GLU:O	3:PG:122:ASN:ND2	2.34	0.49
4:SF:228:TYR:CZ	4:SF:248:TRP:HB3	2.48	0.49
6:XK:66:LEU:HD11	6:YK:66:LEU:HD13	1.93	0.49
2:LA:400:GLY:HA2	2:LA:402:ARG:HE	1.77	0.49
3:PB:164:GLU:HA	3:PB:227:THR:HA	1.94	0.49
2:LC:318:GLY:O	2:LD:162:ARG:NH1	2.46	0.49
3:PE:134:PHE:HE2	3:PE:513:MET:HE1	1.76	0.49
2:LE:740:ILE:HD11	2:LE:808:TRP:CG	2.48	0.49
2:LF:740:ILE:HD11	2:LF:808:TRP:CG	2.48	0.49
2:LA:681:THR:OG1	2:LA:682:VAL:N	2.46	0.49
3:PE:158:ILE:HD11	3:PE:231:GLU:HB3	1.94	0.49
3:PI:158:ILE:HD11	3:PI:231:GLU:HB3	1.94	0.49
4:SE:228:TYR:CZ	4:SE:248:TRP:HB3	2.47	0.49
5:TI:278:ASN:HA	5:TI:281:THR:HG23	1.95	0.49
3:PL:77:LYS:HB3	3:PL:80:ARG:HB3	1.95	0.49
2:LA:142:GLN:HB3	2:LA:230:MET:HG2	1.95	0.49
2:LB:681:THR:OG1	2:LB:682:VAL:N	2.46	0.49
4:SB:228:TYR:CZ	4:SB:248:TRP:HB3	2.47	0.49
5:TC:278:ASN:HA	5:TC:281:THR:HG23	1.95	0.49
2:LC:142:GLN:HB3	2:LC:230:MET:HG2	1.95	0.49
5:TE:268:LYS:NZ	5:TE:274:LEU:O	2.44	0.49
2:LD:681:THR:OG1	2:LD:682:VAL:N	2.46	0.49
4:SD:128:LEU:HG	4:SD:133:MET:HE3	1.95	0.49
2:LE:681:THR:OG1	2:LE:682:VAL:N	2.46	0.49
2:LF:400:GLY:HA2	2:LF:402:ARG:HE	1.77	0.49
4:SF:347:ASP:OD1	4:SF:351:ASN:ND2	2.42	0.49
2:LA:318:GLY:O	2:LB:162:ARG:NH1	2.45	0.49
3:PA:677:LYS:NZ	3:PB:674:ASP:O	2.46	0.49
3:PB:130:ASN:OD1	3:PK:511:LYS:NZ	2.40	0.49
3:PD:164:GLU:HA	3:PD:227:THR:HA	1.94	0.49
3:PE:442:MET:O	3:PH:433:TYR:OH	2.28	0.49
3:PE:677:LYS:NZ	3:PF:674:ASP:O	2.46	0.49
2:LD:165:GLU:HG2	2:LD:176:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PH:164:GLU:HA	3:PH:227:THR:HA	1.94	0.49
2:LF:253:ASN:HA	2:LF:260:PHE:HB2	1.94	0.49
2:LA:1042:GLN:NE2	5:TH:293:LYS:O	2.45	0.49
4:SA:128:LEU:HG	4:SA:133:MET:HE3	1.95	0.49
4:SA:343:PRO:HA	4:SA:346:PHE:HD2	1.78	0.49
3:PB:374:ASP:OD1	3:PB:375:MET:N	2.46	0.49
3:PB:433:TYR:OH	3:PK:442:MET:O	2.29	0.49
6:XC:75:GLU:OE2	6:YC:80:HIS:NE2	2.41	0.49
2:LC:400:GLY:HA2	2:LC:402:ARG:HE	1.77	0.49
4:SC:128:LEU:HG	4:SC:133:MET:HE3	1.95	0.49
2:LD:400:GLY:HA2	2:LD:402:ARG:HE	1.77	0.49
4:SD:347:ASP:OD1	4:SD:351:ASN:ND2	2.42	0.49
4:SF:343:PRO:HA	4:SF:346:PHE:HD2	1.78	0.49
2:LA:162:ARG:NH1	2:LF:318:GLY:O	2.46	0.48
3:PB:118:GLU:O	3:PB:122:ASN:ND2	2.35	0.48
3:PE:374:ASP:OD1	3:PE:375:MET:N	2.46	0.48
4:SC:343:PRO:HA	4:SC:346:PHE:HD2	1.78	0.48
6:XE:26:ASP:OD1	6:XE:34:TYR:OH	2.28	0.48
3:PF:158:ILE:HD11	3:PF:231:GLU:HB3	1.95	0.48
3:PF:374:ASP:OD1	3:PF:375:MET:N	2.46	0.48
2:LD:318:GLY:O	2:LE:162:ARG:NH1	2.45	0.48
6:XG:75:GLU:OE2	6:YG:80:HIS:NE2	2.41	0.48
4:SE:343:PRO:HA	4:SE:346:PHE:HD2	1.78	0.48
6:XI:66:LEU:HD11	6:YI:66:LEU:HD13	1.93	0.48
2:LA:114:TYR:HA	2:LA:365:GLN:HA	1.96	0.48
4:SA:228:TYR:CZ	4:SA:248:TRP:HB3	2.48	0.48
4:SB:341:LEU:HA	4:SB:344:LEU:HD13	1.93	0.48
3:PH:344:ILE:O	3:PH:347:THR:OG1	2.30	0.48
5:TI:197:GLU:HG3	5:TJ:199:THR:HG23	1.96	0.48
3:PJ:77:LYS:HB3	3:PJ:80:ARG:HB3	1.96	0.48
3:PL:174:GLN:NE2	3:PL:217:ALA:O	2.47	0.48
3:PA:35:ASP:OD2	3:PD:316:ARG:NH2	2.46	0.48
2:LB:436:LEU:HD11	4:SB:87:SER:HB3	1.96	0.48
3:PC:677:LYS:NZ	3:PD:674:ASP:O	2.46	0.48
5:TC:222:ASP:OD1	5:TC:238:LYS:NZ	2.35	0.48
6:XC:43:MET:HE3	6:XC:46:ILE:HB	1.95	0.48
2:LC:681:THR:OG1	2:LC:682:VAL:N	2.46	0.48
3:PG:677:LYS:NZ	3:PH:674:ASP:O	2.46	0.48
3:PI:35:ASP:OD2	3:PL:316:ARG:NH2	2.46	0.48
4:SE:128:LEU:HG	4:SE:133:MET:HE3	1.95	0.48
6:XI:43:MET:HE3	6:XI:46:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PJ:164:GLU:HA	3:PJ:227:THR:HA	1.94	0.48
3:PB:158:ILE:HD11	3:PB:231:GLU:HB3	1.95	0.48
3:PB:316:ARG:NH2	3:PK:35:ASP:OD2	2.46	0.48
3:PC:35:ASP:OD2	3:PF:316:ARG:NH2	2.46	0.48
3:PC:451:LEU:HG	3:PD:454:SER:HB2	1.96	0.48
3:PE:454:SER:HB2	3:PH:451:LEU:HG	1.95	0.48
3:PE:678:MET:SD	3:PH:677:LYS:NZ	2.77	0.48
2:LD:253:ASN:HA	2:LD:260:PHE:HB2	1.94	0.48
6:XG:73:LEU:HD13	6:ZG:62:LYS:HZ1	1.79	0.48
3:PH:374:ASP:OD1	3:PH:375:MET:N	2.46	0.48
2:LE:253:ASN:HA	2:LE:260:PHE:HB2	1.95	0.48
2:LE:887:PHE:O	2:LE:928:GLY:N	2.43	0.48
3:PI:451:LEU:HG	3:PJ:454:SER:HB2	1.96	0.48
3:PJ:374:ASP:OD1	3:PJ:375:MET:N	2.46	0.48
2:LF:114:TYR:HA	2:LF:365:GLN:HA	1.96	0.48
3:PK:677:LYS:NZ	3:PL:674:ASP:O	2.46	0.48
4:SF:128:LEU:HG	4:SF:133:MET:HE3	1.95	0.48
5:TA:197:GLU:HG3	5:TB:199:THR:HG23	1.96	0.48
3:PB:451:LEU:HG	3:PK:454:SER:HB2	1.95	0.48
2:LB:650:GLU:OE1	2:LB:705:ARG:NH2	2.43	0.48
4:SB:128:LEU:HG	4:SB:133:MET:HE3	1.95	0.48
1:AF:173:THR:HG23	1:AF:174:LEU:HD22	1.96	0.48
2:LC:253:ASN:HA	2:LC:260:PHE:HB2	1.94	0.48
6:XF:73:LEU:HD11	6:ZF:62:LYS:HD2	1.95	0.48
3:PF:174:GLN:NE2	3:PF:217:ALA:O	2.47	0.48
3:PG:374:ASP:OD1	3:PG:375:MET:N	2.47	0.48
2:LE:142:GLN:HB3	2:LE:230:MET:HG2	1.94	0.48
2:LE:521:LEU:HD12	2:LE:571:ARG:HG3	1.96	0.48
3:PJ:174:GLN:NE2	3:PJ:217:ALA:O	2.47	0.48
2:LF:373:MET:HE1	2:LF:400:GLY:HA3	1.96	0.48
5:TK:278:ASN:HA	5:TK:281:THR:HG23	1.95	0.48
6:XK:26:ASP:OD1	6:XK:34:TYR:OH	2.28	0.48
3:PL:374:ASP:OD1	3:PL:375:MET:N	2.46	0.48
3:PA:432:GLU:HB3	3:PB:414:LYS:HG2	1.96	0.48
6:YB:48:ASN:O	6:YB:52:ASN:ND2	2.40	0.48
1:AD:176:PRO:HG3	1:AE:43:GLU:HG3	1.96	0.48
2:LB:253:ASN:HA	2:LB:260:PHE:HB2	1.95	0.48
4:SB:343:PRO:HA	4:SB:346:PHE:HD2	1.78	0.48
5:TC:197:GLU:HG3	5:TD:199:THR:HG23	1.96	0.48
1:AF:176:PRO:HG3	1:AG:43:GLU:HG3	1.96	0.48
2:LC:873:TRP:O	2:LC:877:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:43:GLU:OE2	1:AG:181:TYR:OH	2.26	0.48
1:AH:173:THR:HG23	1:AH:174:LEU:HD22	1.96	0.48
2:LD:521:LEU:HD12	2:LD:571:ARG:HG3	1.96	0.48
2:LE:373:MET:HE1	2:LE:400:GLY:HA3	1.96	0.48
3:PL:158:ILE:HD11	3:PL:231:GLU:HB3	1.95	0.48
2:LA:253:ASN:HA	2:LA:260:PHE:HB2	1.94	0.48
6:XA:43:MET:HE3	6:XA:46:ILE:HB	1.95	0.48
5:TB:204:GLU:HG3	5:TC:206:ILE:HG23	1.96	0.48
2:LB:114:TYR:HA	2:LB:365:GLN:HA	1.95	0.48
2:LC:436:LEU:HD11	4:SC:87:SER:HB3	1.95	0.48
2:LC:475:ILE:HD12	2:LC:479:GLY:HA3	1.96	0.48
5:TE:200:LYS:O	5:TE:203:THR:OG1	2.30	0.48
6:YF:48:ASN:O	6:YF:52:ASN:ND2	2.39	0.48
2:LD:114:TYR:HA	2:LD:365:GLN:HA	1.96	0.48
5:TG:197:GLU:HG3	5:TH:199:THR:HG23	1.96	0.48
5:TG:278:ASN:HA	5:TG:281:THR:HG23	1.95	0.48
1:AJ:176:PRO:HG3	1:AK:43:GLU:HG3	1.96	0.48
2:LF:142:GLN:HB3	2:LF:230:MET:HG2	1.95	0.48
3:PK:158:ILE:HD11	3:PK:231:GLU:HB3	1.94	0.48
5:TK:197:GLU:HG3	5:TL:199:THR:HG23	1.96	0.48
2:LA:436:LEU:HD11	4:SA:87:SER:HB3	1.96	0.48
5:TA:278:ASN:HA	5:TA:281:THR:HG23	1.95	0.48
3:PD:374:ASP:OD1	3:PD:375:MET:N	2.46	0.48
3:PE:35:ASP:OD2	3:PH:316:ARG:NH2	2.46	0.48
5:TE:278:ASN:HA	5:TE:281:THR:HG23	1.95	0.48
2:LD:142:GLN:HB3	2:LD:230:MET:HG2	1.95	0.48
2:LF:284:ARG:NH1	2:LF:328:ASP:OD1	2.47	0.48
2:LA:887:PHE:O	2:LA:928:GLY:N	2.43	0.48
2:LB:400:GLY:HA2	2:LB:402:ARG:HE	1.78	0.48
6:XG:43:MET:HE3	6:XG:46:ILE:HB	1.95	0.48
6:XH:73:LEU:HD11	6:ZH:62:LYS:HD2	1.96	0.48
3:PH:77:LYS:HB3	3:PH:80:ARG:HB3	1.96	0.48
2:LE:284:ARG:NH1	2:LE:328:ASP:OD1	2.47	0.48
3:PK:118:GLU:O	3:PK:122:ASN:ND2	2.34	0.48
3:PK:374:ASP:OD1	3:PK:375:MET:N	2.46	0.48
3:PL:288:ILE:HG22	3:PL:290:TRP:H	1.79	0.48
2:LA:1157:ILE:HD13	2:LA:1178:GLY:H	1.79	0.48
3:PA:511:LYS:NZ	3:PD:130:ASN:OD1	2.40	0.48
3:PB:77:LYS:HB3	3:PB:80:ARG:HB3	1.96	0.48
3:PB:174:GLN:NE2	3:PB:217:ALA:O	2.47	0.48
2:LB:284:ARG:NH1	2:LB:328:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:373:MET:HE1	2:LB:400:GLY:HA3	1.96	0.48
2:LB:891:THR:HG21	2:LB:950:TYR:CE1	2.49	0.48
2:LB:995:THR:OG1	2:LB:997:ASP:OD1	2.27	0.48
3:PC:77:LYS:HB3	3:PC:80:ARG:HB3	1.96	0.48
2:LC:143:THR:HG23	2:LC:146:LYS:H	1.79	0.48
3:PE:77:LYS:HB3	3:PE:80:ARG:HB3	1.96	0.48
3:PG:35:ASP:OD2	3:PJ:316:ARG:NH2	2.46	0.48
4:SD:343:PRO:HA	4:SD:346:PHE:HD2	1.78	0.48
2:LE:475:ILE:HD12	2:LE:479:GLY:HA3	1.96	0.48
1:AA:43:GLU:HG3	1:AL:176:PRO:HG3	1.96	0.47
2:LA:466:GLN:NE2	2:LA:477:TYR:O	2.37	0.47
5:TA:200:LYS:O	5:TA:203:THR:OG1	2.29	0.47
5:TF:222:ASP:OD1	5:TF:238:LYS:NZ	2.34	0.47
4:SD:102:LEU:HB3	4:SD:106:PRO:HB3	1.96	0.47
4:SD:163:LEU:HD22	4:SD:169:PRO:HB2	1.96	0.47
6:XG:26:ASP:OD1	6:XG:34:TYR:OH	2.27	0.47
3:PH:158:ILE:HD11	3:PH:231:GLU:HB3	1.95	0.47
3:PJ:398:MET:HE3	3:PJ:451:LEU:HD13	1.96	0.47
6:XL:73:LEU:HD11	6:ZL:62:LYS:HD2	1.95	0.47
6:YL:48:ASN:O	6:YL:52:ASN:ND2	2.39	0.47
2:LA:373:MET:HE1	2:LA:400:GLY:HA3	1.96	0.47
2:LA:891:THR:HG21	2:LA:950:TYR:CE1	2.49	0.47
3:PA:77:LYS:HB3	3:PA:80:ARG:HB3	1.96	0.47
2:LB:1082:MET:HB2	2:LB:1171:SER:HB3	1.96	0.47
4:SB:347:ASP:OD1	4:SB:351:ASN:ND2	2.42	0.47
3:PD:162:LYS:HA	3:PD:229:GLU:HA	1.96	0.47
3:PD:174:GLN:NE2	3:PD:217:ALA:O	2.47	0.47
1:AF:54:MET:HG2	1:AF:219:THR:HG21	1.96	0.47
2:LC:114:TYR:HA	2:LC:365:GLN:HA	1.95	0.47
5:TE:197:GLU:HG3	5:TF:199:THR:HG23	1.96	0.47
6:XE:73:LEU:HD13	6:ZE:62:LYS:HZ1	1.79	0.47
6:YF:56:LEU:HD21	6:ZF:53:MET:HE1	1.97	0.47
3:PF:77:LYS:HB3	3:PF:80:ARG:HB3	1.95	0.47
3:PF:164:GLU:HA	3:PF:227:THR:HA	1.95	0.47
2:LE:114:TYR:HA	2:LE:365:GLN:HA	1.95	0.47
3:PI:374:ASP:OD1	3:PI:375:MET:N	2.47	0.47
3:PJ:162:LYS:HA	3:PJ:229:GLU:HA	1.97	0.47
2:LF:436:LEU:HD11	4:SF:87:SER:HB3	1.96	0.47
6:XK:43:MET:HE3	6:XK:46:ILE:HB	1.95	0.47
2:LA:845:THR:HG22	2:LA:911:VAL:HG21	1.97	0.47
1:AC:23:THR:OG1	1:AC:28:ASP:O	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:148:ASN:HB2	6:YD:7:PHE:CD2	2.50	0.47
2:LB:887:PHE:O	2:LB:928:GLY:N	2.43	0.47
3:PC:374:ASP:OD1	3:PC:375:MET:N	2.47	0.47
3:PD:158:ILE:HD11	3:PD:231:GLU:HB3	1.96	0.47
1:AH:176:PRO:HG3	1:AI:43:GLU:HG3	1.96	0.47
2:LD:143:THR:HG23	2:LD:146:LYS:H	1.79	0.47
3:PH:398:MET:HE3	3:PH:451:LEU:HD13	1.96	0.47
5:TH:204:GLU:HG3	5:TI:206:ILE:HG23	1.96	0.47
5:TI:208:MET:HE3	5:TJ:209:THR:HG23	1.97	0.47
3:PJ:288:ILE:HG22	3:PJ:290:TRP:H	1.79	0.47
1:AL:54:MET:HG2	1:AL:219:THR:HG21	1.96	0.47
2:LF:475:ILE:HD12	2:LF:479:GLY:HA3	1.96	0.47
4:SF:102:LEU:HB3	4:SF:106:PRO:HB3	1.96	0.47
1:AB:148:ASN:HB2	6:YB:7:PHE:CD2	2.49	0.47
3:PA:344:ILE:O	3:PA:347:THR:OG1	2.31	0.47
1:AD:54:MET:HG2	1:AD:219:THR:HG21	1.97	0.47
2:LB:1042:GLN:NE2	5:TJ:293:LYS:O	2.45	0.47
2:LB:1157:ILE:HD13	2:LB:1178:GLY:H	1.79	0.47
6:XD:73:LEU:HD11	6:ZD:62:LYS:HD2	1.96	0.47
3:PD:398:MET:HE3	3:PD:451:LEU:HD13	1.96	0.47
2:LC:887:PHE:O	2:LC:928:GLY:N	2.44	0.47
3:PF:288:ILE:HG22	3:PF:290:TRP:H	1.79	0.47
2:LD:596:GLU:OE2	4:SD:41:THR:N	2.40	0.47
5:TG:200:LYS:O	5:TG:203:THR:OG1	2.29	0.47
2:LF:873:TRP:O	2:LF:877:ASN:ND2	2.28	0.47
3:PK:77:LYS:HB3	3:PK:80:ARG:HB3	1.96	0.47
3:PK:150:VAL:HG11	3:PK:516:ILE:HD11	1.96	0.47
3:PK:344:ILE:O	3:PK:347:THR:OG1	2.31	0.47
2:LA:284:ARG:NH1	2:LA:328:ASP:OD1	2.48	0.47
2:LA:848:MET:HA	2:LA:851:VAL:HG22	1.97	0.47
2:LA:1082:MET:HB2	2:LA:1171:SER:HB3	1.96	0.47
2:LB:38:ARG:HG2	2:LB:40:HIS:CE1	2.50	0.47
2:LB:521:LEU:HD12	2:LB:571:ARG:HG3	1.96	0.47
2:LC:373:MET:HE1	2:LC:400:GLY:HA3	1.96	0.47
2:LD:373:MET:HE1	2:LD:400:GLY:HA3	1.96	0.47
3:PG:77:LYS:HB3	3:PG:80:ARG:HB3	1.96	0.47
6:YH:56:LEU:HD21	6:ZH:53:MET:HE1	1.97	0.47
3:PH:288:ILE:HG22	3:PH:290:TRP:H	1.79	0.47
3:PI:77:LYS:HB3	3:PI:80:ARG:HB3	1.96	0.47
3:PI:150:VAL:HG11	3:PI:516:ILE:HD11	1.97	0.47
3:PL:164:GLU:HA	3:PL:227:THR:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PA:374:ASP:OD1	3:PA:375:MET:N	2.47	0.47
5:TB:200:LYS:O	5:TB:203:THR:OG1	2.32	0.47
3:PD:77:LYS:HB3	3:PD:80:ARG:HB3	1.96	0.47
3:PD:366:ILE:HG21	3:PD:509:LEU:HD23	1.96	0.47
4:SC:102:LEU:HB3	4:SC:106:PRO:HB3	1.96	0.47
1:AH:148:ASN:HB2	6:YH:7:PHE:CD2	2.49	0.47
2:LD:475:ILE:HD12	2:LD:479:GLY:HA3	1.96	0.47
1:AI:28:ASP:OD1	1:AI:29:ILE:N	2.48	0.47
3:PJ:158:ILE:HD11	3:PJ:231:GLU:HB3	1.96	0.47
2:LF:143:THR:HG23	2:LF:146:LYS:H	1.79	0.47
2:LF:1157:ILE:HD13	2:LF:1178:GLY:H	1.79	0.47
1:AB:173:THR:HG23	1:AB:174:LEU:HD22	1.95	0.47
3:PB:150:VAL:HG11	3:PB:516:ILE:HD11	1.97	0.47
3:PB:517:GLY:HA3	3:PB:557:VAL:HG11	1.97	0.47
1:AD:173:THR:HG23	1:AD:174:LEU:HD22	1.96	0.47
2:LB:143:THR:HG23	2:LB:146:LYS:H	1.79	0.47
2:LB:475:ILE:HD12	2:LB:479:GLY:HA3	1.96	0.47
3:PD:150:VAL:HG11	3:PD:516:ILE:HD11	1.96	0.47
2:LC:284:ARG:NH1	2:LC:328:ASP:OD1	2.47	0.47
2:LC:377:MET:HE3	2:LC:378:THR:H	1.80	0.47
2:LC:521:LEU:HD12	2:LC:571:ARG:HG3	1.97	0.47
2:LC:1157:ILE:HD13	2:LC:1178:GLY:H	1.79	0.47
3:PE:554:ASP:OD2	3:PH:194:ARG:NH2	2.48	0.47
3:PF:162:LYS:HA	3:PF:229:GLU:HA	1.97	0.47
3:PF:398:MET:HE3	3:PF:451:LEU:HD13	1.95	0.47
1:AG:28:ASP:OD1	1:AG:29:ILE:N	2.48	0.47
1:AH:54:MET:HG2	1:AH:219:THR:HG21	1.97	0.47
2:LD:848:MET:HA	2:LD:851:VAL:HG22	1.97	0.47
2:LD:1082:MET:HB2	2:LD:1171:SER:HB3	1.96	0.47
5:TG:208:MET:HE3	5:TH:209:THR:HG23	1.97	0.47
3:PH:162:LYS:HA	3:PH:229:GLU:HA	1.96	0.47
1:AJ:148:ASN:HB2	6:YJ:7:PHE:CD2	2.50	0.47
2:LE:377:MET:HE3	2:LE:378:THR:H	1.80	0.47
2:LE:891:THR:HG21	2:LE:950:TYR:CE1	2.49	0.47
4:SE:102:LEU:HB3	4:SE:106:PRO:HB3	1.97	0.47
4:SE:163:LEU:HD22	4:SE:169:PRO:HB2	1.97	0.47
2:LF:279:LEU:HD22	2:LF:332:GLY:HA2	1.97	0.47
4:SF:150:ASP:HA	4:SF:153:LYS:HE2	1.97	0.47
3:PL:398:MET:HE3	3:PL:451:LEU:HD13	1.95	0.47
1:AB:54:MET:HG2	1:AB:219:THR:HG21	1.97	0.47
2:LA:143:THR:HG23	2:LA:146:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:TA:206:ILE:HG23	5:TL:204:GLU:HG3	1.97	0.47
3:PB:398:MET:HE3	3:PB:451:LEU:HD13	1.96	0.47
2:LD:414:TYR:HD2	4:SD:113:ILE:HG12	1.80	0.47
2:LD:1157:ILE:HD13	2:LD:1178:GLY:H	1.79	0.47
3:PH:174:GLN:NE2	3:PH:217:ALA:O	2.47	0.47
2:LE:414:TYR:HD2	4:SE:113:ILE:HG12	1.80	0.47
2:LE:650:GLU:OE1	2:LE:705:ARG:NH2	2.43	0.47
5:TI:268:LYS:NZ	5:TI:274:LEU:O	2.43	0.47
1:AK:28:ASP:OD1	1:AK:29:ILE:N	2.48	0.47
3:PL:150:VAL:HG11	3:PL:516:ILE:HD11	1.97	0.47
3:PL:162:LYS:HA	3:PL:229:GLU:HA	1.97	0.47
1:AB:176:PRO:HG3	1:AC:43:GLU:HG3	1.96	0.47
2:LA:521:LEU:HD12	2:LA:571:ARG:HG3	1.96	0.47
3:PA:160:LYS:NZ	3:PA:229:GLU:OE2	2.39	0.47
2:LB:253:ASN:HD21	2:LB:320:LEU:HB2	1.80	0.47
2:LB:377:MET:HE3	2:LB:378:THR:H	1.80	0.47
2:LB:845:THR:HG22	2:LB:911:VAL:HG21	1.97	0.47
2:LB:848:MET:HA	2:LB:851:VAL:HG22	1.97	0.47
6:XC:26:ASP:OD1	6:XC:34:TYR:OH	2.27	0.47
6:YD:56:LEU:HD21	6:ZD:53:MET:HE1	1.97	0.47
5:TE:208:MET:HE3	5:TF:209:THR:HG23	1.97	0.47
2:LD:38:ARG:HG2	2:LD:40:HIS:CE1	2.50	0.47
2:LD:845:THR:HG22	2:LD:911:VAL:HG21	1.97	0.47
2:LE:143:THR:HG23	2:LE:146:LYS:H	1.79	0.47
3:PJ:150:VAL:HG11	3:PJ:516:ILE:HD11	1.96	0.47
1:AL:104:ILE:HD11	1:AL:154:LYS:HB3	1.97	0.47
1:AL:173:THR:HG23	1:AL:174:LEU:HD22	1.96	0.47
2:LF:521:LEU:HD12	2:LF:571:ARG:HG3	1.97	0.47
2:LF:681:THR:OG1	2:LF:682:VAL:N	2.46	0.47
3:PL:344:ILE:O	3:PL:347:THR:OG1	2.29	0.47
2:LA:38:ARG:HG2	2:LA:40:HIS:CE1	2.50	0.47
3:PB:162:LYS:HA	3:PB:229:GLU:HA	1.96	0.47
3:PB:288:ILE:HG22	3:PB:290:TRP:H	1.79	0.47
2:LB:414:TYR:HD2	4:SB:113:ILE:HG12	1.80	0.47
3:PD:288:ILE:HG22	3:PD:290:TRP:H	1.79	0.47
2:LC:891:THR:HG21	2:LC:950:TYR:CE1	2.49	0.47
4:SC:150:ASP:HA	4:SC:153:LYS:HE2	1.97	0.47
4:SC:163:LEU:HD22	4:SC:169:PRO:HB2	1.97	0.47
2:LD:734:LYS:HB2	2:LD:789:VAL:HG12	1.96	0.47
2:LD:891:THR:HG21	2:LD:950:TYR:CE1	2.49	0.47
3:PH:517:GLY:HA3	3:PH:557:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:54:MET:HG2	1:AJ:219:THR:HG21	1.97	0.47
2:LE:596:GLU:OE2	4:SE:41:THR:N	2.40	0.47
2:LE:734:LYS:HB2	2:LE:789:VAL:HG12	1.97	0.47
2:LE:1157:ILE:HD13	2:LE:1178:GLY:H	1.79	0.47
3:PJ:366:ILE:HG21	3:PJ:509:LEU:HD23	1.96	0.47
2:LF:248:ILE:HG21	2:LF:251:MET:HE3	1.97	0.47
2:LA:475:ILE:HD12	2:LA:479:GLY:HA3	1.96	0.46
2:LA:650:GLU:OE1	2:LA:705:ARG:NH2	2.43	0.46
5:TB:293:LYS:O	2:LD:1042:GLN:NE2	2.45	0.46
1:AF:65:GLU:OE2	6:ZE:37:LYS:NZ	2.39	0.46
2:LC:551:ASP:OD1	4:SC:18:ARG:NH1	2.41	0.46
2:LC:845:THR:HG22	2:LC:911:VAL:HG21	1.97	0.46
2:LD:436:LEU:HD11	4:SD:87:SER:HB3	1.96	0.46
2:LE:436:LEU:HD11	4:SE:87:SER:HB3	1.96	0.46
4:SE:236:TYR:O	4:SE:240:THR:OG1	2.27	0.46
6:YJ:56:LEU:HD21	6:ZJ:53:MET:HE1	1.97	0.46
2:LF:38:ARG:HG2	2:LF:40:HIS:CE1	2.50	0.46
2:LF:414:TYR:HD2	4:SF:113:ILE:HG12	1.80	0.46
2:LF:845:THR:HG22	2:LF:911:VAL:HG21	1.97	0.46
2:LF:891:THR:HG21	2:LF:950:TYR:CE1	2.49	0.46
5:TK:208:MET:HE3	5:TL:209:THR:HG23	1.97	0.46
2:LA:377:MET:HE3	2:LA:378:THR:H	1.80	0.46
4:SA:102:LEU:HB3	4:SA:106:PRO:HB3	1.96	0.46
4:SA:150:ASP:HA	4:SA:153:LYS:HE2	1.97	0.46
2:LB:551:ASP:OD1	4:SB:18:ARG:NH1	2.41	0.46
5:TC:208:MET:HE3	5:TD:209:THR:HG23	1.97	0.46
3:PD:371:VAL:HB	3:PD:374:ASP:HB3	1.97	0.46
2:LC:38:ARG:HG2	2:LC:40:HIS:CE1	2.50	0.46
3:PE:150:VAL:HG11	3:PE:516:ILE:HD11	1.96	0.46
2:LD:253:ASN:HD21	2:LD:320:LEU:HB2	1.80	0.46
2:LE:38:ARG:HG2	2:LE:40:HIS:CE1	2.50	0.46
2:LE:279:LEU:HD22	2:LE:332:GLY:HA2	1.97	0.46
3:PI:118:GLU:O	3:PI:122:ASN:ND2	2.34	0.46
3:PI:511:LYS:NZ	3:PL:130:ASN:OD1	2.40	0.46
5:TJ:204:GLU:HG3	5:TK:206:ILE:HG23	1.97	0.46
2:LA:734:LYS:HB2	2:LA:789:VAL:HG12	1.96	0.46
6:YB:56:LEU:HD21	6:ZB:53:MET:HE1	1.97	0.46
3:PB:194:ARG:NH2	3:PK:554:ASP:OD2	2.48	0.46
3:PC:371:VAL:HB	3:PC:374:ASP:HB3	1.97	0.46
6:YD:10:ILE:HD12	6:YD:11:PRO:HD2	1.97	0.46
5:TD:204:GLU:HG3	5:TE:206:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LC:248:ILE:HG21	2:LC:251:MET:HE3	1.98	0.46
6:XE:43:MET:HE3	6:XE:46:ILE:HB	1.95	0.46
2:LD:284:ARG:NH1	2:LD:328:ASP:OD1	2.48	0.46
3:PG:150:VAL:HG11	3:PG:516:ILE:HD11	1.96	0.46
3:PI:554:ASP:OD2	3:PL:194:ARG:NH2	2.48	0.46
6:YJ:10:ILE:HD12	6:YJ:11:PRO:HD2	1.97	0.46
3:PL:366:ILE:HG21	3:PL:509:LEU:HD23	1.96	0.46
5:TL:200:LYS:O	5:TL:203:THR:OG1	2.31	0.46
1:AB:104:ILE:HD11	1:AB:154:LYS:HB3	1.97	0.46
3:PA:150:VAL:HG11	3:PA:516:ILE:HD11	1.96	0.46
5:TA:268:LYS:NZ	5:TA:274:LEU:O	2.43	0.46
2:LB:1155:HIS:ND1	2:LB:1179:GLN:HG3	2.31	0.46
5:TD:200:LYS:O	5:TD:203:THR:OG1	2.31	0.46
1:AE:28:ASP:OD1	1:AE:29:ILE:N	2.48	0.46
2:LC:848:MET:HA	2:LC:851:VAL:HG22	1.96	0.46
1:AH:45:LEU:HD23	1:AH:155:HIS:CG	2.51	0.46
2:LF:253:ASN:HD21	2:LF:320:LEU:HB2	1.80	0.46
2:LA:414:TYR:HD2	4:SA:113:ILE:HG12	1.80	0.46
4:SA:163:LEU:HD22	4:SA:169:PRO:HB2	1.96	0.46
6:XB:73:LEU:HD11	6:ZB:62:LYS:HD2	1.96	0.46
2:LB:610:ASN:O	2:LB:610:ASN:ND2	2.44	0.46
3:PC:150:VAL:HG11	3:PC:516:ILE:HD11	1.97	0.46
3:PC:554:ASP:OD2	3:PF:194:ARG:NH2	2.48	0.46
1:AF:148:ASN:HB2	6:YF:7:PHE:CD2	2.50	0.46
2:LC:414:TYR:HD2	4:SC:113:ILE:HG12	1.80	0.46
2:LC:734:LYS:HB2	2:LC:789:VAL:HG12	1.97	0.46
3:PF:366:ILE:HG21	3:PF:509:LEU:HD23	1.96	0.46
2:LE:845:THR:HG22	2:LE:911:VAL:HG21	1.97	0.46
2:LE:1082:MET:HB2	2:LE:1171:SER:HB3	1.96	0.46
3:PI:517:GLY:HA3	3:PI:557:VAL:HG11	1.97	0.46
6:XJ:73:LEU:HD11	6:ZJ:62:LYS:HD2	1.96	0.46
1:AL:148:ASN:HB2	6:YL:7:PHE:CD2	2.50	0.46
2:LF:734:LYS:HB2	2:LF:789:VAL:HG12	1.97	0.46
6:YL:56:LEU:HD21	6:ZL:53:MET:HE1	1.97	0.46
2:LA:251:MET:HE2	2:LA:262:MET:HE2	1.98	0.46
5:TA:26:ASP:OD1	5:TA:26:ASP:N	2.49	0.46
3:PB:366:ILE:HG21	3:PB:509:LEU:HD23	1.98	0.46
1:AD:104:ILE:HD11	1:AD:154:LYS:HB3	1.97	0.46
2:LB:734:LYS:HB2	2:LB:789:VAL:HG12	1.97	0.46
4:SB:163:LEU:HD22	4:SB:169:PRO:HB2	1.96	0.46
2:LC:253:ASN:HD21	2:LC:320:LEU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LC:1082:MET:HB2	2:LC:1171:SER:HB3	1.96	0.46
5:TF:197:GLU:HG3	5:TG:199:THR:HG23	1.98	0.46
3:PG:554:ASP:OD2	3:PJ:194:ARG:NH2	2.49	0.46
1:AJ:173:THR:HG23	1:AJ:174:LEU:HD22	1.96	0.46
2:LE:251:MET:HE2	2:LE:262:MET:HE2	1.98	0.46
2:LE:253:ASN:HD21	2:LE:320:LEU:HB2	1.80	0.46
2:LE:848:MET:HA	2:LE:851:VAL:HG22	1.97	0.46
6:XK:75:GLU:OE2	6:YK:80:HIS:NE2	2.41	0.46
6:YL:10:ILE:HD12	6:YL:11:PRO:HD2	1.98	0.46
1:AA:28:ASP:OD1	1:AA:29:ILE:N	2.48	0.46
2:LA:253:ASN:HD21	2:LA:320:LEU:HB2	1.80	0.46
2:LA:1155:HIS:ND1	2:LA:1179:GLN:HG3	2.31	0.46
5:TA:208:MET:HE3	5:TB:209:THR:HG23	1.97	0.46
3:PB:371:VAL:HB	3:PB:374:ASP:HB3	1.97	0.46
3:PE:162:LYS:HA	3:PE:229:GLU:HA	1.98	0.46
1:AH:104:ILE:HD11	1:AH:154:LYS:HB3	1.97	0.46
2:LD:377:MET:HE3	2:LD:378:THR:H	1.80	0.46
4:SD:150:ASP:HA	4:SD:153:LYS:HE2	1.97	0.46
2:LE:927:LEU:HD21	2:LE:930:PHE:CZ	2.51	0.46
2:LF:927:LEU:HD21	2:LF:930:PHE:CZ	2.51	0.46
3:PC:517:GLY:HA3	3:PC:557:VAL:HG11	1.97	0.46
2:LC:279:LEU:HD22	2:LC:332:GLY:HA2	1.97	0.46
4:SC:236:TYR:O	4:SC:240:THR:OG1	2.27	0.46
6:YF:10:ILE:HD12	6:YF:11:PRO:HD2	1.98	0.46
3:PF:150:VAL:HG11	3:PF:516:ILE:HD11	1.97	0.46
2:LD:927:LEU:HD21	2:LD:930:PHE:CZ	2.51	0.46
1:AJ:45:LEU:HD23	1:AJ:155:HIS:CG	2.51	0.46
2:LF:377:MET:HE3	2:LF:378:THR:H	1.80	0.46
3:PB:344:ILE:O	3:PB:347:THR:OG1	2.30	0.46
5:TB:197:GLU:HG3	5:TC:199:THR:HG23	1.98	0.46
4:SB:239:GLU:OE2	4:SB:266:TRP:NE1	2.45	0.46
3:PD:344:ILE:O	3:PD:347:THR:OG1	2.29	0.46
5:TD:197:GLU:HG3	5:TE:199:THR:HG23	1.98	0.46
5:TG:26:ASP:OD1	5:TG:26:ASP:N	2.49	0.46
3:PH:366:ILE:HG21	3:PH:509:LEU:HD23	1.98	0.46
3:PK:371:VAL:HB	3:PK:374:ASP:HB3	1.98	0.46
4:SF:163:LEU:HD22	4:SF:169:PRO:HB2	1.97	0.46
1:AB:45:LEU:HD23	1:AB:155:HIS:CG	2.51	0.46
2:LA:927:LEU:HD21	2:LA:930:PHE:CZ	2.51	0.46
6:XB:55:GLN:OE1	6:XB:55:GLN:N	2.43	0.46
1:AF:45:LEU:HD23	1:AF:155:HIS:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LC:1155:HIS:ND1	2:LC:1179:GLN:HG3	2.31	0.46
3:PE:344:ILE:O	3:PE:347:THR:OG1	2.31	0.46
3:PG:162:LYS:HA	3:PG:229:GLU:HA	1.98	0.46
3:PH:150:VAL:HG11	3:PH:516:ILE:HD11	1.97	0.46
2:LE:995:THR:OG1	2:LE:997:ASP:OD1	2.27	0.46
2:LE:1155:HIS:ND1	2:LE:1179:GLN:HG3	2.31	0.46
3:PJ:517:GLY:HA3	3:PJ:557:VAL:HG11	1.98	0.46
2:LF:1155:HIS:ND1	2:LF:1179:GLN:HG3	2.31	0.46
1:AA:10:ARG:NH1	1:AA:179:ASP:OD2	2.49	0.45
3:PC:67:LYS:NZ	3:PC:73:GLN:HE22	2.14	0.45
4:SB:102:LEU:HB3	4:SB:106:PRO:HB3	1.97	0.45
4:SB:150:ASP:HA	4:SB:153:LYS:HE2	1.97	0.45
3:PE:398:MET:HE3	3:PE:451:LEU:HD13	1.98	0.45
5:TF:204:GLU:HG3	5:TG:206:ILE:HG23	1.97	0.45
4:SD:247:PRO:O	4:SD:260:GLN:NE2	2.49	0.45
2:LF:848:MET:HA	2:LF:851:VAL:HG22	1.97	0.45
3:PK:162:LYS:HA	3:PK:229:GLU:HA	1.98	0.45
3:PA:554:ASP:OD2	3:PD:194:ARG:NH2	2.49	0.45
2:LB:251:MET:HE2	2:LB:262:MET:HE2	1.98	0.45
2:LB:318:GLY:O	2:LC:162:ARG:NH1	2.47	0.45
6:XE:21:ASN:O	6:XE:42:ARG:NH1	2.50	0.45
6:YJ:55:GLN:OE1	6:YJ:55:GLN:N	2.48	0.45
2:LF:551:ASP:OD1	4:SF:18:ARG:NH1	2.41	0.45
2:LF:1082:MET:HB2	2:LF:1171:SER:HB3	1.96	0.45
5:TK:268:LYS:NZ	5:TK:274:LEU:O	2.44	0.45
3:PA:371:VAL:HB	3:PA:374:ASP:HB3	1.98	0.45
5:TA:199:THR:HG23	5:TL:197:GLU:HG3	1.98	0.45
3:PB:151:ARG:HB2	3:PB:243:LEU:HD11	1.99	0.45
3:PC:50:VAL:O	3:PC:54:ASN:ND2	2.43	0.45
3:PC:162:LYS:HA	3:PC:229:GLU:HA	1.98	0.45
6:XD:52:ASN:ND2	6:YD:53:MET:SD	2.90	0.45
3:PD:517:GLY:HA3	3:PD:557:VAL:HG11	1.98	0.45
2:LC:610:ASN:O	2:LC:610:ASN:ND2	2.44	0.45
2:LC:927:LEU:HD21	2:LC:930:PHE:CZ	2.51	0.45
3:PE:517:GLY:HA3	3:PE:557:VAL:HG11	1.99	0.45
5:TE:26:ASP:OD1	5:TE:26:ASP:N	2.49	0.45
3:PF:517:GLY:HA3	3:PF:557:VAL:HG11	1.98	0.45
5:TF:293:LYS:O	2:LF:1042:GLN:NE2	2.45	0.45
1:AG:10:ARG:NH1	1:AG:179:ASP:OD2	2.49	0.45
2:LD:1155:HIS:ND1	2:LD:1179:GLN:HG3	2.31	0.45
3:PG:50:VAL:O	3:PG:54:ASN:ND2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PG:517:GLY:HA3	3:PG:557:VAL:HG11	1.98	0.45
6:YH:48:ASN:O	6:YH:52:ASN:ND2	2.40	0.45
5:TH:197:GLU:HG3	5:TI:199:THR:HG23	1.98	0.45
3:PJ:371:VAL:HB	3:PJ:374:ASP:HB3	1.98	0.45
1:AK:128:LEU:HD23	1:AK:136:LEU:HD11	1.99	0.45
3:PK:517:GLY:HA3	3:PK:557:VAL:HG11	1.99	0.45
2:LA:979:TRP:CD1	2:LA:979:TRP:H	2.34	0.45
3:PA:538:ASN:ND2	3:PB:109:GLU:OE1	2.50	0.45
1:AC:28:ASP:OD1	1:AC:29:ILE:N	2.48	0.45
3:PE:288:ILE:HG22	3:PE:290:TRP:H	1.82	0.45
3:PE:371:VAL:HB	3:PE:374:ASP:HB3	1.98	0.45
4:SC:247:PRO:O	4:SC:260:GLN:NE2	2.50	0.45
2:LD:935:ASN:OD1	2:LD:935:ASN:N	2.50	0.45
2:LD:979:TRP:CD1	2:LD:979:TRP:H	2.34	0.45
6:YH:10:ILE:HD12	6:YH:11:PRO:HD2	1.98	0.45
5:TH:26:ASP:OD1	5:TH:26:ASP:N	2.50	0.45
2:LF:887:PHE:O	2:LF:928:GLY:N	2.44	0.45
3:PA:162:LYS:HA	3:PA:229:GLU:HA	1.98	0.45
3:PA:662:TYR:CD1	3:PD:660:LEU:HD11	2.52	0.45
2:LB:927:LEU:HD21	2:LB:930:PHE:CZ	2.51	0.45
4:SB:247:PRO:O	4:SB:260:GLN:NE2	2.50	0.45
1:AE:225:ASP:N	1:AE:225:ASP:OD1	2.50	0.45
2:LC:979:TRP:CD1	2:LC:979:TRP:H	2.34	0.45
5:TF:200:LYS:O	5:TF:203:THR:OG1	2.31	0.45
1:AH:19:THR:OG1	1:AH:186:TYR:OH	2.33	0.45
2:LD:466:GLN:NE2	2:LD:477:TYR:O	2.37	0.45
1:AJ:104:ILE:HD11	1:AJ:154:LYS:HB3	1.97	0.45
4:SE:150:ASP:HA	4:SE:153:LYS:HE2	1.97	0.45
4:SE:247:PRO:O	4:SE:260:GLN:NE2	2.50	0.45
1:AL:45:LEU:HD23	1:AL:155:HIS:CG	2.51	0.45
2:LF:54:THR:HG23	2:LF:365:GLN:HB3	1.98	0.45
2:LF:251:MET:HE2	2:LF:262:MET:HE2	1.99	0.45
2:LF:543:LYS:HA	2:LF:590:ILE:HG21	1.99	0.45
5:TL:26:ASP:OD1	5:TL:26:ASP:N	2.50	0.45
2:LA:279:LEU:HD22	2:LA:332:GLY:HA2	1.98	0.45
2:LA:935:ASN:OD1	2:LA:935:ASN:N	2.50	0.45
2:LA:995:THR:OG1	2:LA:997:ASP:OD1	2.27	0.45
2:LB:279:LEU:HD22	2:LB:332:GLY:HA2	1.97	0.45
2:LB:979:TRP:H	2:LB:979:TRP:CD1	2.34	0.45
5:TC:268:LYS:NZ	5:TC:274:LEU:O	2.43	0.45
1:AE:10:ARG:NH1	1:AE:179:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PE:418:ASP:OD1	3:PE:421:ASN:ND2	2.49	0.45
3:PG:288:ILE:HG22	3:PG:290:TRP:H	1.81	0.45
6:XG:21:ASN:O	6:XG:42:ARG:NH1	2.50	0.45
5:TI:222:ASP:OD1	5:TI:238:LYS:NZ	2.35	0.45
2:LF:650:GLU:OE1	2:LF:705:ARG:NH2	2.43	0.45
3:PL:517:GLY:HA3	3:PL:557:VAL:HG11	1.98	0.45
3:PA:50:VAL:O	3:PA:54:ASN:ND2	2.43	0.45
3:PA:67:LYS:NZ	3:PA:73:GLN:HE22	2.14	0.45
3:PA:366:ILE:HG21	3:PA:509:LEU:HD23	1.99	0.45
6:XB:52:ASN:ND2	6:YB:53:MET:SD	2.90	0.45
3:PC:468:SER:HB3	3:PF:81:ARG:HD2	1.99	0.45
1:AF:104:ILE:HD11	1:AF:154:LYS:HB3	1.97	0.45
3:PE:67:LYS:NZ	3:PE:73:GLN:HE22	2.14	0.45
3:PF:344:ILE:O	3:PF:347:THR:OG1	2.29	0.45
2:LD:551:ASP:OD1	4:SD:18:ARG:NH1	2.41	0.45
2:LE:318:GLY:O	2:LF:162:ARG:NH1	2.47	0.45
2:LE:543:LYS:HA	2:LE:590:ILE:HG21	1.99	0.45
3:PI:398:MET:HE3	3:PI:451:LEU:HD13	1.98	0.45
1:AK:10:ARG:NH1	1:AK:179:ASP:OD2	2.49	0.45
2:LF:979:TRP:CD1	2:LF:979:TRP:H	2.34	0.45
4:SF:247:PRO:O	4:SF:260:GLN:NE2	2.50	0.45
4:SA:247:PRO:O	4:SA:260:GLN:NE2	2.49	0.45
6:YB:10:ILE:HD12	6:YB:11:PRO:HD2	1.98	0.45
3:PB:660:LEU:HD11	3:PK:662:TYR:CD1	2.52	0.45
1:AC:10:ARG:NH1	1:AC:179:ASP:OD2	2.50	0.45
3:PC:118:GLU:O	3:PC:122:ASN:ND2	2.34	0.45
4:SB:229:ASP:O	4:SB:232:THR:OG1	2.29	0.45
3:PF:371:VAL:HB	3:PF:374:ASP:HB3	1.97	0.45
2:LD:78:PRO:HA	2:LD:84:PHE:HA	1.99	0.45
3:PG:366:ILE:HG21	3:PG:509:LEU:HD23	1.99	0.45
3:PH:371:VAL:HB	3:PH:374:ASP:HB3	1.97	0.45
3:PI:67:LYS:NZ	3:PI:73:GLN:HE22	2.14	0.45
4:SE:48:ASP:HB3	4:SE:64:THR:HG21	1.99	0.45
6:XI:21:ASN:O	6:XI:42:ARG:NH1	2.50	0.45
3:PK:50:VAL:O	3:PK:54:ASN:ND2	2.44	0.45
1:AA:225:ASP:OD1	1:AA:225:ASP:N	2.50	0.45
1:AB:19:THR:OG1	1:AB:186:TYR:OH	2.33	0.45
3:PA:288:ILE:HG22	3:PA:290:TRP:H	1.81	0.45
1:AD:45:LEU:HD23	1:AD:155:HIS:CG	2.51	0.45
2:LB:445:GLU:HB2	2:LB:549:GLN:HA	1.99	0.45
5:TD:26:ASP:OD1	5:TD:26:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LC:935:ASN:OD1	2:LC:935:ASN:N	2.50	0.45
3:PE:468:SER:HB3	3:PH:81:ARG:HD2	1.99	0.45
3:PE:662:TYR:CD1	3:PH:660:LEU:HD11	2.52	0.45
3:PG:398:MET:HE3	3:PG:451:LEU:HD13	1.99	0.45
3:PG:511:LYS:NZ	3:PJ:130:ASN:OD1	2.40	0.45
4:SD:48:ASP:HB3	4:SD:64:THR:HG21	1.99	0.45
3:PI:538:ASN:ND2	3:PJ:109:GLU:OE1	2.50	0.45
1:AL:19:THR:OG1	1:AL:186:TYR:OH	2.34	0.45
2:LF:834:PRO:O	2:LF:880:ASN:ND2	2.36	0.45
3:PA:517:GLY:HA3	3:PA:557:VAL:HG11	1.98	0.45
3:PC:288:ILE:HG22	3:PC:290:TRP:H	1.82	0.45
1:AF:124:ASN:HB3	1:AF:127:SER:HB2	1.99	0.45
2:LC:54:THR:HG23	2:LC:365:GLN:HB3	1.98	0.45
2:LC:1042:GLN:NE2	5:TL:293:LYS:O	2.45	0.45
3:PE:327:PHE:HB3	3:PE:336:LEU:HB3	1.99	0.45
3:PG:371:VAL:HB	3:PG:374:ASP:HB3	1.98	0.45
3:PI:162:LYS:HA	3:PI:229:GLU:HA	1.98	0.45
3:PI:371:VAL:HB	3:PI:374:ASP:HB3	1.97	0.45
3:PI:662:TYR:CD1	3:PL:660:LEU:HD11	2.52	0.45
5:TI:200:LYS:O	5:TI:203:THR:OG1	2.29	0.45
3:PK:288:ILE:HG22	3:PK:290:TRP:H	1.82	0.45
3:PL:371:VAL:HB	3:PL:374:ASP:HB3	1.97	0.45
3:PC:194:ARG:NH2	3:PD:554:ASP:OD2	2.51	0.44
3:PC:662:TYR:CD1	3:PF:660:LEU:HD11	2.52	0.44
6:XC:21:ASN:O	6:XC:42:ARG:NH1	2.50	0.44
2:LC:405:TRP:CD1	2:LC:407:THR:HG1	2.35	0.44
3:PE:194:ARG:NH2	3:PF:554:ASP:OD2	2.50	0.44
4:SC:174:GLN:NE2	4:SC:229:ASP:OD2	2.50	0.44
2:LD:54:THR:HG23	2:LD:365:GLN:HB3	1.99	0.44
2:LD:251:MET:HE2	2:LD:262:MET:HE2	1.98	0.44
4:SD:229:ASP:O	4:SD:232:THR:OG1	2.29	0.44
2:LE:935:ASN:OD1	2:LE:935:ASN:N	2.50	0.44
1:AL:124:ASN:HB3	1:AL:127:SER:HB2	1.99	0.44
2:LF:801:MET:SD	2:LF:801:MET:N	2.80	0.44
3:PL:151:ARG:HB2	3:PL:243:LEU:HD11	1.99	0.44
2:LB:1092:LYS:NZ	2:LB:1096:GLY:O	2.50	0.44
3:PC:511:LYS:NZ	3:PF:130:ASN:OD1	2.40	0.44
3:PC:538:ASN:ND2	3:PD:109:GLU:OE1	2.50	0.44
2:LC:466:GLN:NE2	2:LC:477:TYR:O	2.36	0.44
3:PG:418:ASP:OD1	3:PG:421:ASN:ND2	2.50	0.44
4:SD:236:TYR:O	4:SD:240:THR:OG1	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:225:ASP:N	1:AI:225:ASP:OD1	2.50	0.44
2:LE:54:THR:HG23	2:LE:365:GLN:HB3	2.00	0.44
2:LE:78:PRO:HA	2:LE:84:PHE:HA	1.99	0.44
5:TJ:197:GLU:HG3	5:TK:199:THR:HG23	1.98	0.44
3:PK:194:ARG:NH2	3:PL:554:ASP:OD2	2.50	0.44
6:XL:55:GLN:OE1	6:XL:55:GLN:N	2.43	0.44
2:LA:610:ASN:O	2:LA:610:ASN:ND2	2.44	0.44
2:LA:657:LEU:HB3	2:LA:703:LYS:HE2	2.00	0.44
1:AC:225:ASP:N	1:AC:225:ASP:OD1	2.50	0.44
3:PC:671:HIS:CG	3:PF:673:ARG:HD2	2.53	0.44
2:LC:543:LYS:HA	2:LC:590:ILE:HG21	1.99	0.44
3:PE:558:ASP:OD1	3:PE:559:ILE:N	2.51	0.44
3:PF:67:LYS:NZ	3:PF:73:GLN:HE22	2.15	0.44
2:LD:279:LEU:HD22	2:LD:332:GLY:HA2	1.98	0.44
6:XH:52:ASN:ND2	6:YH:53:MET:SD	2.90	0.44
3:PI:468:SER:HB3	3:PL:81:ARG:HD2	1.99	0.44
3:PK:398:MET:HE3	3:PK:451:LEU:HD13	1.98	0.44
4:SF:48:ASP:HB3	4:SF:64:THR:HG21	1.99	0.44
2:LA:54:THR:HG23	2:LA:365:GLN:HB3	1.99	0.44
3:PA:671:HIS:CG	3:PD:673:ARG:HD2	2.53	0.44
4:SA:48:ASP:HB3	4:SA:64:THR:HG21	1.99	0.44
6:XA:21:ASN:O	6:XA:42:ARG:NH1	2.50	0.44
6:XA:75:GLU:OE2	6:YA:80:HIS:NE2	2.41	0.44
3:PC:327:PHE:HB3	3:PC:336:LEU:HB3	1.99	0.44
3:PC:558:ASP:OD1	3:PC:559:ILE:N	2.51	0.44
2:LC:445:GLU:HB2	2:LC:549:GLN:HA	1.99	0.44
3:PE:538:ASN:ND2	3:PF:109:GLU:OE1	2.50	0.44
6:XF:52:ASN:ND2	6:YF:53:MET:SD	2.91	0.44
2:LE:979:TRP:CD1	2:LE:979:TRP:H	2.34	0.44
3:PK:327:PHE:HB3	3:PK:336:LEU:HB3	1.99	0.44
3:PK:679:LYS:HA	3:PK:679:LYS:HD3	1.86	0.44
2:LA:873:TRP:O	2:LA:877:ASN:ND2	2.28	0.44
3:PB:677:LYS:HZ2	3:PK:675:LEU:HA	1.82	0.44
1:AE:128:LEU:HD23	1:AE:136:LEU:HD11	1.99	0.44
6:XE:75:GLU:OE2	6:YE:80:HIS:NE2	2.41	0.44
1:AH:124:ASN:HB3	1:AH:127:SER:HB2	2.00	0.44
2:LD:543:LYS:HA	2:LD:590:ILE:HG21	1.99	0.44
3:PG:67:LYS:NZ	3:PG:73:GLN:HE22	2.14	0.44
3:PI:194:ARG:NH2	3:PJ:554:ASP:OD2	2.51	0.44
6:XJ:52:ASN:ND2	6:YJ:53:MET:SD	2.90	0.44
4:SF:174:GLN:NE2	4:SF:229:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:TK:222:ASP:OD1	5:TK:238:LYS:NZ	2.35	0.44
6:XK:21:ASN:O	6:XK:42:ARG:NH1	2.50	0.44
2:LA:445:GLU:HB2	2:LA:549:GLN:HA	2.00	0.44
2:LB:54:THR:HG23	2:LB:365:GLN:HB3	2.00	0.44
6:YD:48:ASN:O	6:YD:52:ASN:ND2	2.39	0.44
3:PD:679:LYS:HA	3:PD:679:LYS:HD3	1.86	0.44
2:LC:251:MET:HE2	2:LC:262:MET:HE2	1.99	0.44
2:LC:621:LEU:HD13	2:LC:635:TRP:HB3	2.00	0.44
3:PG:662:TYR:CD1	3:PJ:660:LEU:HD11	2.52	0.44
1:AI:10:ARG:NH1	1:AI:179:ASP:OD2	2.50	0.44
2:LE:466:GLN:NE2	2:LE:477:TYR:O	2.36	0.44
3:PI:288:ILE:HG22	3:PI:290:TRP:H	1.82	0.44
2:LF:78:PRO:HA	2:LF:84:PHE:HA	1.98	0.44
3:PK:366:ILE:HG21	3:PK:509:LEU:HD23	1.99	0.44
7:OL:1:ASP:OD2	7:OL:10:SER:OG	2.31	0.44
2:LA:248:ILE:HG21	2:LA:251:MET:HE3	2.00	0.44
3:PB:50:VAL:O	3:PB:54:ASN:ND2	2.45	0.44
3:PC:344:ILE:O	3:PC:347:THR:OG1	2.32	0.44
4:SB:196:GLN:HG3	4:SB:202:LEU:HD11	2.00	0.44
3:PD:67:LYS:NZ	3:PD:73:GLN:HE22	2.16	0.44
3:PD:660:LEU:H	3:PD:660:LEU:HD12	1.83	0.44
2:LC:78:PRO:HA	2:LC:84:PHE:HA	1.98	0.44
2:LD:248:ILE:HG21	2:LD:251:MET:HE3	2.00	0.44
3:PG:327:PHE:HB3	3:PG:336:LEU:HB3	2.00	0.44
3:PG:675:LEU:HA	3:PJ:677:LYS:HZ2	1.82	0.44
3:PH:151:ARG:HB2	3:PH:243:LEU:HD11	1.99	0.44
2:LE:737:LEU:O	2:LE:838:ILE:N	2.48	0.44
4:SE:229:ASP:O	4:SE:232:THR:OG1	2.29	0.44
4:SE:366:PHE:CE2	4:SE:368:LEU:HB2	2.53	0.44
1:AK:176:PRO:HG3	1:AL:43:GLU:HG3	2.00	0.44
2:LF:445:GLU:HB2	2:LF:549:GLN:HA	1.99	0.44
2:LF:610:ASN:O	2:LF:610:ASN:ND2	2.44	0.44
3:PK:130:ASN:OD1	3:PL:511:LYS:NZ	2.40	0.44
4:SF:366:PHE:CE2	4:SF:368:LEU:HB2	2.53	0.44
2:LA:551:ASP:OD1	4:SA:18:ARG:NH1	2.41	0.44
3:PA:194:ARG:NH2	3:PB:554:ASP:OD2	2.51	0.44
3:PB:637:LEU:O	3:PB:641:ILE:HG12	2.18	0.44
3:PC:398:MET:HE3	3:PC:451:LEU:HD13	1.98	0.44
4:SB:174:GLN:NE2	4:SB:229:ASP:OD2	2.50	0.44
3:PD:495:LEU:HB3	3:PD:499:SER:HB2	2.00	0.44
2:LC:132:ASP:OD2	2:LC:238:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PE:671:HIS:CG	3:PH:673:ARG:HD2	2.52	0.44
3:PG:671:HIS:CG	3:PJ:673:ARG:HD2	2.53	0.44
1:AJ:19:THR:OG1	1:AJ:186:TYR:OH	2.34	0.44
3:PI:675:LEU:HA	3:PL:677:LYS:HZ2	1.83	0.44
4:SE:174:GLN:NE2	4:SE:229:ASP:OD2	2.50	0.44
2:LF:657:LEU:HB3	2:LF:703:LYS:HE2	2.00	0.44
1:AD:124:ASN:HB3	1:AD:127:SER:HB2	2.00	0.44
2:LC:582:TYR:O	2:LC:585:SER:OG	2.30	0.44
4:SC:196:GLN:HG3	4:SC:202:LEU:HD11	2.00	0.44
2:LE:801:MET:HA	2:LE:808:TRP:HB3	2.00	0.44
2:LE:860:MET:HB3	2:LE:914:LYS:HE3	2.00	0.44
3:PI:327:PHE:HB3	3:PI:336:LEU:HB3	1.99	0.44
2:LF:860:MET:HB3	2:LF:914:LYS:HE3	2.00	0.44
6:YL:55:GLN:OE1	6:YL:55:GLN:N	2.48	0.44
1:AB:49:HIS:CE1	1:AB:155:HIS:HB2	2.53	0.43
1:AB:124:ASN:HB3	1:AB:127:SER:HB2	2.00	0.43
3:PD:637:LEU:O	3:PD:641:ILE:HG12	2.18	0.43
3:PE:366:ILE:HG21	3:PE:509:LEU:HD23	1.99	0.43
4:SC:366:PHE:CE2	4:SC:368:LEU:HB2	2.53	0.43
3:PF:495:LEU:HB3	3:PF:499:SER:HB2	2.00	0.43
3:PG:468:SER:HB3	3:PJ:81:ARG:HD2	2.00	0.43
4:SD:174:GLN:NE2	4:SD:229:ASP:OD2	2.50	0.43
4:SD:366:PHE:CE2	4:SD:368:LEU:HB2	2.53	0.43
1:AI:128:LEU:HD23	1:AI:136:LEU:HD11	2.00	0.43
3:PI:344:ILE:O	3:PI:347:THR:OG1	2.32	0.43
6:XJ:62:LYS:HZ2	6:YJ:63:LEU:HG	1.82	0.43
3:PJ:327:PHE:HB3	3:PJ:336:LEU:HB3	2.01	0.43
2:LF:894:TRP:CD1	2:LF:899:PRO:HG2	2.53	0.43
3:PK:67:LYS:NZ	3:PK:73:GLN:HE22	2.14	0.43
6:XL:73:LEU:HD21	6:ZL:62:LYS:HZ3	1.83	0.43
2:LA:1092:LYS:NZ	2:LA:1096:GLY:O	2.50	0.43
3:PA:558:ASP:OD1	3:PA:559:ILE:N	2.51	0.43
3:PB:673:ARG:HD2	3:PK:671:HIS:CG	2.52	0.43
1:AD:43:GLU:OE1	1:AD:185:ARG:NH1	2.51	0.43
2:LB:657:LEU:HB3	2:LB:703:LYS:HE2	2.00	0.43
6:XE:70:TYR:HA	6:XE:73:LEU:HD21	2.01	0.43
2:LD:650:GLU:OE1	2:LD:705:ARG:NH2	2.43	0.43
1:AJ:124:ASN:HB3	1:AJ:127:SER:HB2	2.00	0.43
2:LE:551:ASP:OD1	4:SE:18:ARG:NH1	2.41	0.43
3:PI:151:ARG:HB2	3:PI:243:LEU:HD11	2.00	0.43
2:LF:621:LEU:HD13	2:LF:635:TRP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XL:52:ASN:ND2	6:YL:53:MET:SD	2.91	0.43
3:PL:637:LEU:O	3:PL:641:ILE:HG12	2.18	0.43
2:LA:801:MET:HA	2:LA:808:TRP:HB3	2.00	0.43
3:PA:151:ARG:HB2	3:PA:243:LEU:HD11	2.00	0.43
6:ZA:60:HIS:HA	6:ZA:63:LEU:HB2	2.00	0.43
3:PB:81:ARG:HD2	3:PK:468:SER:HB3	1.99	0.43
5:TB:294:ASN:HB3	2:LD:1046:ASN:O	2.19	0.43
2:LB:543:LYS:HA	2:LB:590:ILE:HG21	1.99	0.43
1:AE:176:PRO:HG3	1:AF:43:GLU:HG3	2.00	0.43
2:LC:1179:GLN:N	2:LC:1179:GLN:CD	2.77	0.43
3:PE:50:VAL:O	3:PE:54:ASN:ND2	2.44	0.43
3:PF:151:ARG:HB2	3:PF:243:LEU:HD11	1.99	0.43
2:LD:801:MET:SD	2:LD:801:MET:N	2.80	0.43
3:PG:194:ARG:NH2	3:PH:554:ASP:OD2	2.51	0.43
3:PG:558:ASP:OD1	3:PG:559:ILE:N	2.51	0.43
6:XG:70:TYR:HA	6:XG:73:LEU:HD21	2.01	0.43
3:PH:495:LEU:HB3	3:PH:499:SER:HB2	2.00	0.43
2:LE:657:LEU:HB3	2:LE:703:LYS:HE2	2.00	0.43
3:PI:671:HIS:CG	3:PL:673:ARG:HD2	2.53	0.43
3:PJ:67:LYS:NZ	3:PJ:73:GLN:HE22	2.16	0.43
3:PK:558:ASP:OD1	3:PK:559:ILE:N	2.51	0.43
5:TK:200:LYS:O	5:TK:203:THR:OG1	2.30	0.43
3:PL:67:LYS:NZ	3:PL:73:GLN:HE22	2.15	0.43
3:PL:175:THR:OG1	3:PL:176:GLN:N	2.51	0.43
2:LA:1046:ASN:O	5:TH:294:ASN:HB3	2.19	0.43
3:PD:327:PHE:HB3	3:PD:336:LEU:HB3	2.00	0.43
2:LC:275:ALA:O	2:LC:336:GLN:NE2	2.46	0.43
2:LC:894:TRP:CD1	2:LC:899:PRO:HG2	2.53	0.43
3:PE:495:LEU:HB3	3:PE:499:SER:HB2	2.00	0.43
4:SC:48:ASP:HB3	4:SC:64:THR:HG21	1.99	0.43
2:LD:219:ASN:O	5:TH:41:ASN:ND2	2.52	0.43
2:LD:801:MET:HA	2:LD:808:TRP:HB3	2.00	0.43
2:LD:894:TRP:CD1	2:LD:899:PRO:HG2	2.54	0.43
2:LF:737:LEU:O	2:LF:838:ILE:N	2.48	0.43
2:LF:1179:GLN:CD	2:LF:1179:GLN:N	2.77	0.43
2:LA:219:ASN:O	5:TB:41:ASN:ND2	2.52	0.43
2:LA:543:LYS:HA	2:LA:590:ILE:HG21	1.99	0.43
2:LA:894:TRP:CD1	2:LA:899:PRO:HG2	2.54	0.43
3:PA:398:MET:HE3	3:PA:451:LEU:HD13	1.99	0.43
6:XB:62:LYS:NZ	6:YB:63:LEU:HG	2.34	0.43
3:PB:175:THR:OG1	3:PB:176:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PB:268:PHE:HE1	3:PB:323:GLU:HG3	1.83	0.43
5:TB:24:LEU:HD11	5:TC:150:LEU:HD13	2.01	0.43
2:LB:1120:ASP:OD1	2:LB:1123:THR:OG1	2.32	0.43
4:SB:340:ASP:OD1	4:SB:340:ASP:N	2.52	0.43
6:XD:62:LYS:NZ	6:YD:63:LEU:HG	2.34	0.43
5:TD:294:ASN:HB3	2:LE:1046:ASN:O	2.19	0.43
3:PE:414:LYS:HG2	3:PH:432:GLU:OE1	2.19	0.43
4:SC:229:ASP:O	4:SC:232:THR:OG1	2.29	0.43
1:AG:128:LEU:HD23	1:AG:136:LEU:HD11	2.00	0.43
2:LD:132:ASP:OD2	2:LD:238:ALA:N	2.52	0.43
2:LD:621:LEU:HD13	2:LD:635:TRP:HB3	2.00	0.43
3:PG:414:LYS:HG2	3:PJ:432:GLU:OE1	2.19	0.43
4:SE:249:ILE:HD11	4:SE:260:GLN:HG3	2.01	0.43
6:XI:26:ASP:OD1	6:XI:34:TYR:OH	2.27	0.43
3:PK:174:GLN:NE2	3:PK:217:ALA:O	2.52	0.43
3:PA:327:PHE:HB3	3:PA:336:LEU:HB3	2.00	0.43
2:LB:78:PRO:HA	2:LB:84:PHE:HA	1.99	0.43
2:LB:132:ASP:OD2	2:LB:238:ALA:N	2.52	0.43
3:PC:151:ARG:HB2	3:PC:243:LEU:HD11	2.00	0.43
6:XC:70:TYR:HA	6:XC:73:LEU:HD21	2.01	0.43
6:XD:55:GLN:OE1	6:XD:55:GLN:N	2.43	0.43
4:SC:340:ASP:OD1	4:SC:340:ASP:N	2.52	0.43
3:PH:67:LYS:NZ	3:PH:73:GLN:HE22	2.16	0.43
6:XI:20:LEU:O	6:XI:23:PRO:HD2	2.19	0.43
6:XJ:62:LYS:NZ	6:YJ:63:LEU:HG	2.34	0.43
3:PJ:175:THR:OG1	3:PJ:176:GLN:N	2.51	0.43
3:PJ:314:PRO:HA	3:PJ:317:LYS:HG3	2.00	0.43
6:ZK:60:HIS:HA	6:ZK:63:LEU:HB2	2.01	0.43
4:SA:174:GLN:NE2	4:SA:229:ASP:OD2	2.50	0.43
2:LB:1046:ASN:O	5:TJ:294:ASN:HB3	2.19	0.43
2:LB:1105:ARG:HD2	2:LB:1105:ARG:HA	1.89	0.43
3:PC:414:LYS:HG2	3:PF:432:GLU:OE1	2.19	0.43
2:LC:801:MET:HA	2:LC:808:TRP:HB3	2.00	0.43
6:ZE:60:HIS:HA	6:ZE:63:LEU:HB2	2.01	0.43
6:ZG:60:HIS:HA	6:ZG:63:LEU:HB2	2.00	0.43
2:LE:132:ASP:OD2	2:LE:238:ALA:N	2.52	0.43
2:LE:445:GLU:HB2	2:LE:549:GLN:HA	1.99	0.43
2:LE:1179:GLN:CD	2:LE:1179:GLN:N	2.77	0.43
3:PI:174:GLN:NE2	3:PI:217:ALA:O	2.52	0.43
3:PI:414:LYS:HG2	3:PL:432:GLU:OE1	2.19	0.43
2:LF:102:MET:HE1	2:LF:230:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SF:229:ASP:O	4:SF:232:THR:OG1	2.29	0.43
2:LA:78:PRO:HA	2:LA:84:PHE:HA	1.99	0.43
2:LA:102:MET:HE1	2:LA:230:MET:HE2	2.01	0.43
3:PA:414:LYS:HG2	3:PD:432:GLU:OE1	2.19	0.43
4:SA:366:PHE:CE2	4:SA:368:LEU:HB2	2.53	0.43
2:LB:737:LEU:O	2:LB:838:ILE:N	2.48	0.43
6:ZC:60:HIS:HA	6:ZC:63:LEU:HB2	2.01	0.43
3:PD:151:ARG:HB2	3:PD:243:LEU:HD11	2.00	0.43
1:AF:225:ASP:N	1:AF:225:ASP:OD1	2.52	0.43
2:LC:1092:LYS:NZ	2:LC:1096:GLY:O	2.49	0.43
3:PF:637:LEU:O	3:PF:641:ILE:HG12	2.18	0.43
1:AH:233:ARG:HA	1:AH:233:ARG:HD3	1.92	0.43
4:SD:213:ASP:HA	4:SD:225:PRO:HA	2.01	0.43
6:XG:20:LEU:O	6:XG:23:PRO:HD2	2.19	0.43
3:PH:327:PHE:HB3	3:PH:336:LEU:HB3	2.01	0.43
5:TH:277:PRO:HD2	5:TH:280:PHE:HD2	1.84	0.43
1:AI:176:PRO:HG3	1:AJ:43:GLU:HG3	2.00	0.43
2:LF:132:ASP:OD2	2:LF:238:ALA:N	2.51	0.43
2:LF:1050:LEU:HG	2:LF:1075:VAL:HG23	2.01	0.43
3:PL:314:PRO:HA	3:PL:317:LYS:HG3	2.00	0.43
1:AA:128:LEU:HD23	1:AA:136:LEU:HD11	2.00	0.43
2:LA:1179:GLN:CD	2:LA:1179:GLN:N	2.77	0.43
3:PB:67:LYS:NZ	3:PB:73:GLN:HE22	2.16	0.43
5:TB:277:PRO:HD2	5:TB:280:PHE:HD2	1.84	0.43
2:LB:248:ILE:HG21	2:LB:251:MET:HE3	2.01	0.43
2:LB:801:MET:HA	2:LB:808:TRP:HB3	2.00	0.43
2:LB:1179:GLN:CD	2:LB:1179:GLN:N	2.77	0.43
3:PC:418:ASP:OD1	3:PC:421:ASN:ND2	2.50	0.43
3:PC:495:LEU:HB3	3:PC:499:SER:HB2	2.01	0.43
4:SC:249:ILE:HD11	4:SC:260:GLN:HG3	2.01	0.43
2:LD:657:LEU:HB3	2:LD:703:LYS:HE2	2.00	0.43
3:PG:538:ASN:ND2	3:PH:109:GLU:OE1	2.50	0.43
4:SD:83:TYR:HA	4:SD:84:PRO:HD3	1.91	0.43
3:PH:50:VAL:O	3:PH:54:ASN:ND2	2.45	0.43
2:LE:801:MET:SD	2:LE:801:MET:N	2.80	0.43
2:LE:894:TRP:CD1	2:LE:899:PRO:HG2	2.54	0.43
2:LF:801:MET:HA	2:LF:808:TRP:HB3	2.00	0.43
3:PK:538:ASN:ND2	3:PL:109:GLU:OE1	2.50	0.43
2:LA:860:MET:HB3	2:LA:914:LYS:HE3	2.00	0.43
3:PA:468:SER:HB3	3:PD:81:ARG:HD2	2.00	0.43
2:LB:860:MET:HB3	2:LB:914:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:894:TRP:CD1	2:LB:899:PRO:HG2	2.54	0.43
2:LB:1088:LEU:HD13	2:LB:1102:TRP:HB3	2.01	0.43
3:PC:174:GLN:NE2	3:PC:217:ALA:O	2.52	0.43
4:SB:48:ASP:HB3	4:SB:64:THR:HG21	1.99	0.43
4:SB:249:ILE:HD11	4:SB:260:GLN:HG3	2.01	0.43
2:LC:657:LEU:HB3	2:LC:703:LYS:HE2	2.00	0.43
2:LC:860:MET:HB3	2:LC:914:LYS:HE3	2.00	0.43
2:LC:1050:LEU:HG	2:LC:1075:VAL:HG23	2.01	0.43
5:TF:294:ASN:HB3	2:LF:1046:ASN:O	2.19	0.43
6:XH:73:LEU:HD21	6:ZH:62:LYS:HZ3	1.84	0.43
5:TH:200:LYS:O	5:TH:203:THR:OG1	2.32	0.43
3:PI:50:VAL:O	3:PI:54:ASN:ND2	2.43	0.43
4:SE:340:ASP:OD1	4:SE:340:ASP:N	2.52	0.43
2:LF:51:THR:O	2:LF:368:TYR:OH	2.36	0.43
3:PK:268:PHE:HE1	3:PK:323:GLU:HG3	1.84	0.43
6:XK:20:LEU:O	6:XK:23:PRO:HD2	2.19	0.43
6:XL:62:LYS:NZ	6:YL:63:LEU:HG	2.34	0.43
3:PB:660:LEU:H	3:PB:660:LEU:HD12	1.84	0.42
3:PD:268:PHE:HE1	3:PD:323:GLU:HG3	1.83	0.42
3:PD:314:PRO:HA	3:PD:317:LYS:HG3	2.00	0.42
2:LC:219:ASN:O	5:TF:41:ASN:ND2	2.52	0.42
3:PE:511:LYS:NZ	3:PH:130:ASN:OD1	2.40	0.42
2:LD:610:ASN:O	2:LD:610:ASN:ND2	2.44	0.42
3:PG:151:ARG:HB2	3:PG:243:LEU:HD11	2.00	0.42
6:XH:43:MET:N	6:XH:44:PRO:HD2	2.34	0.42
2:LE:102:MET:HE1	2:LE:230:MET:HE2	2.01	0.42
2:LE:219:ASN:O	5:TJ:41:ASN:ND2	2.52	0.42
2:LE:248:ILE:HG21	2:LE:251:MET:HE3	2.01	0.42
3:PJ:151:ARG:HB2	3:PJ:243:LEU:HD11	2.00	0.42
3:PJ:495:LEU:HB3	3:PJ:499:SER:HB2	2.00	0.42
3:PJ:660:LEU:H	3:PJ:660:LEU:HD12	1.83	0.42
4:SF:249:ILE:HD11	4:SF:260:GLN:HG3	2.01	0.42
6:XL:43:MET:N	6:XL:44:PRO:HD2	2.34	0.42
5:TL:277:PRO:HD2	5:TL:280:PHE:HD2	1.84	0.42
2:LA:132:ASP:OD2	2:LA:238:ALA:N	2.52	0.42
3:PA:675:LEU:HA	3:PD:677:LYS:HZ2	1.84	0.42
4:SA:196:GLN:HG3	4:SA:202:LEU:HD11	2.01	0.42
6:XB:43:MET:N	6:XB:44:PRO:HD2	2.34	0.42
3:PB:495:LEU:HB3	3:PB:499:SER:HB2	2.00	0.42
1:AC:128:LEU:HD23	1:AC:136:LEU:HD11	2.00	0.42
2:LB:935:ASN:OD1	2:LB:935:ASN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:366:PHE:CE2	4:SB:368:LEU:HB2	2.53	0.42
3:PD:50:VAL:O	3:PD:54:ASN:ND2	2.45	0.42
3:PE:174:GLN:NE2	3:PE:217:ALA:O	2.52	0.42
1:AH:49:HIS:CE1	1:AH:155:HIS:HB2	2.53	0.42
2:LD:445:GLU:HB2	2:LD:549:GLN:HA	2.00	0.42
2:LD:1088:LEU:HD13	2:LD:1102:TRP:HB3	2.01	0.42
3:PH:314:PRO:HA	3:PH:317:LYS:HG3	2.00	0.42
2:LE:749:THR:OG1	2:LE:762:ALA:O	2.31	0.42
3:PI:418:ASP:OD1	3:PI:421:ASN:ND2	2.50	0.42
4:SE:196:GLN:HG3	4:SE:202:LEU:HD11	2.00	0.42
3:PK:413:PRO:HG3	3:PK:442:MET:HB3	2.01	0.42
3:PK:495:LEU:HB3	3:PK:499:SER:HB2	2.00	0.42
3:PL:50:VAL:O	3:PL:54:ASN:ND2	2.45	0.42
2:LA:621:LEU:HD13	2:LA:635:TRP:HB3	2.00	0.42
2:LA:1179:GLN:NE2	5:TJ:275:SER:OG	2.48	0.42
3:PB:645:ASP:OD1	3:PB:646:ALA:N	2.53	0.42
2:LB:219:ASN:O	5:TD:41:ASN:ND2	2.52	0.42
2:LB:621:LEU:HD13	2:LB:635:TRP:HB3	2.00	0.42
6:XD:43:MET:N	6:XD:44:PRO:HD2	2.34	0.42
2:LC:737:LEU:O	2:LC:838:ILE:N	2.48	0.42
2:LC:1046:ASN:O	5:TL:294:ASN:HB3	2.19	0.42
6:XF:43:MET:N	6:XF:44:PRO:HD2	2.34	0.42
3:PF:175:THR:OG1	3:PF:176:GLN:N	2.51	0.42
3:PF:660:LEU:HD12	3:PF:660:LEU:H	1.84	0.42
5:TF:277:PRO:HD2	5:TF:280:PHE:HD2	1.84	0.42
3:PH:268:PHE:HE1	3:PH:323:GLU:HG3	1.83	0.42
5:TH:275:SER:OG	2:LF:1179:GLN:NE2	2.48	0.42
2:LE:621:LEU:HD13	2:LE:635:TRP:HB3	2.00	0.42
2:LE:1088:LEU:HD13	2:LE:1102:TRP:HB3	2.01	0.42
6:XI:70:TYR:HA	6:XI:73:LEU:HD21	2.01	0.42
3:PJ:546:ARG:HA	3:PJ:549:LEU:HD23	2.01	0.42
3:PJ:645:ASP:OD1	3:PJ:646:ALA:N	2.53	0.42
2:LF:219:ASN:O	5:TL:41:ASN:ND2	2.52	0.42
3:PK:151:ARG:HB2	3:PK:243:LEU:HD11	2.02	0.42
3:PL:268:PHE:HE1	3:PL:323:GLU:HG3	1.84	0.42
3:PL:495:LEU:HB3	3:PL:499:SER:HB2	2.00	0.42
3:PA:418:ASP:OD1	3:PA:421:ASN:ND2	2.50	0.42
3:PA:625:LEU:HB3	3:PB:634:ASN:HD21	1.84	0.42
3:PA:634:ASN:HD21	3:PD:625:LEU:HB3	1.85	0.42
5:TA:150:LEU:HD13	5:TL:24:LEU:HD11	2.02	0.42
1:AD:19:THR:OG1	1:AD:186:TYR:OH	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:1130:TRP:HE1	2:LB:1132:SER:HG	1.65	0.42
3:PD:645:ASP:OD1	3:PD:646:ALA:N	2.53	0.42
5:TD:24:LEU:HD11	5:TE:150:LEU:HD13	2.01	0.42
6:XF:62:LYS:NZ	6:YF:63:LEU:HG	2.34	0.42
3:PF:645:ASP:OD1	3:PF:646:ALA:N	2.53	0.42
4:SD:196:GLN:HG3	4:SD:202:LEU:HD11	2.01	0.42
6:XI:75:GLU:OE2	6:YI:80:HIS:NE2	2.41	0.42
6:XJ:43:MET:N	6:XJ:44:PRO:HD2	2.34	0.42
1:AK:225:ASP:N	1:AK:225:ASP:OD1	2.50	0.42
2:LF:582:TYR:O	2:LF:585:SER:OG	2.30	0.42
6:XK:70:TYR:HA	6:XK:73:LEU:HD21	2.01	0.42
3:PA:174:GLN:NE2	3:PA:217:ALA:O	2.52	0.42
3:PA:413:PRO:HG3	3:PA:442:MET:HB3	2.01	0.42
6:XA:26:ASP:OD1	6:XA:34:TYR:OH	2.27	0.42
2:LB:283:TRP:CZ3	2:LB:285:TYR:HB3	2.55	0.42
3:PC:268:PHE:HE1	3:PC:323:GLU:HG3	1.83	0.42
4:SB:213:ASP:HA	4:SB:225:PRO:HA	2.01	0.42
6:XC:20:LEU:O	6:XC:23:PRO:HD2	2.19	0.42
6:YD:55:GLN:HG3	6:ZD:60:HIS:CD2	2.55	0.42
3:PD:561:THR:HB	3:PD:564:VAL:HG12	2.02	0.42
5:TD:277:PRO:HD2	5:TD:280:PHE:HD2	1.84	0.42
2:LC:834:PRO:O	2:LC:880:ASN:ND2	2.36	0.42
2:LC:1105:ARG:HD2	2:LC:1105:ARG:HA	1.89	0.42
2:LD:1179:GLN:CD	2:LD:1179:GLN:N	2.77	0.42
3:PG:174:GLN:NE2	3:PG:217:ALA:O	2.52	0.42
3:PG:344:ILE:O	3:PG:347:THR:OG1	2.31	0.42
3:PG:413:PRO:HG3	3:PG:442:MET:HB3	2.01	0.42
4:SD:249:ILE:HD11	4:SD:260:GLN:HG3	2.02	0.42
6:XH:62:LYS:NZ	6:YH:63:LEU:HG	2.34	0.42
2:LE:283:TRP:CZ3	2:LE:285:TYR:HB3	2.55	0.42
3:PI:558:ASP:OD1	3:PI:559:ILE:N	2.51	0.42
6:ZI:60:HIS:HA	6:ZI:63:LEU:HB2	2.01	0.42
3:PJ:268:PHE:HE1	3:PJ:323:GLU:HG3	1.83	0.42
5:TJ:222:ASP:OD1	5:TJ:238:LYS:NZ	2.34	0.42
2:LF:1088:LEU:HD13	2:LF:1102:TRP:HB3	2.01	0.42
4:SF:196:GLN:HG3	4:SF:202:LEU:HD11	2.00	0.42
1:AB:43:GLU:OE1	1:AB:185:ARG:NH1	2.52	0.42
4:SA:213:ASP:HA	4:SA:225:PRO:HA	2.01	0.42
3:PB:327:PHE:HB3	3:PB:336:LEU:HB3	2.01	0.42
3:PB:432:GLU:OE1	3:PK:414:LYS:HG2	2.19	0.42
3:PB:561:THR:HB	3:PB:564:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PE:660:LEU:HD11	3:PF:662:TYR:CE1	2.55	0.42
3:PF:327:PHE:HB3	3:PF:336:LEU:HB3	2.01	0.42
2:LD:1050:LEU:HG	2:LD:1075:VAL:HG23	2.01	0.42
3:PG:149:ILE:HG21	3:PG:248:ILE:HD13	2.02	0.42
2:LE:51:THR:O	2:LE:368:TYR:OH	2.36	0.42
2:LE:1092:LYS:NZ	2:LE:1096:GLY:O	2.50	0.42
5:TJ:24:LEU:HD11	5:TK:150:LEU:HD13	2.01	0.42
2:LF:995:THR:OG1	2:LF:997:ASP:OD1	2.27	0.42
6:XA:20:LEU:O	6:XA:23:PRO:HD2	2.19	0.42
6:XA:70:TYR:HA	6:XA:73:LEU:HD21	2.01	0.42
3:PB:625:LEU:HB3	3:PK:634:ASN:HD21	1.85	0.42
3:PC:366:ILE:HG21	3:PC:509:LEU:HD23	2.01	0.42
3:PE:268:PHE:HE1	3:PE:323:GLU:HG3	1.84	0.42
5:TE:269:THR:HG23	5:TE:270:ILE:HG12	2.02	0.42
6:XE:20:LEU:O	6:XE:23:PRO:HD2	2.19	0.42
1:AG:176:PRO:HG3	1:AH:43:GLU:HG3	2.01	0.42
3:PH:637:LEU:O	3:PH:641:ILE:HG12	2.18	0.42
3:PI:268:PHE:HE1	3:PI:323:GLU:HG3	1.83	0.42
3:PI:495:LEU:HB3	3:PI:499:SER:HB2	2.01	0.42
3:PJ:637:LEU:O	3:PJ:641:ILE:HG12	2.18	0.42
3:PK:149:ILE:HG21	3:PK:248:ILE:HD13	2.01	0.42
3:PK:175:THR:OG1	3:PK:176:GLN:N	2.53	0.42
3:PK:625:LEU:HB3	3:PL:634:ASN:HD21	1.84	0.42
3:PL:327:PHE:HB3	3:PL:336:LEU:HB3	2.01	0.42
2:LA:1050:LEU:HG	2:LA:1075:VAL:HG23	2.01	0.42
3:PA:268:PHE:HE1	3:PA:323:GLU:HG3	1.84	0.42
3:PB:314:PRO:HA	3:PB:317:LYS:HG3	2.00	0.42
1:AC:43:GLU:OE2	1:AC:181:TYR:OH	2.26	0.42
2:LB:498:VAL:HG11	2:LB:509:GLN:HE22	1.85	0.42
2:LB:1137:TRP:CE2	2:LB:1142:GLN:HG2	2.55	0.42
3:PC:679:LYS:HA	3:PC:679:LYS:HD3	1.86	0.42
3:PD:175:THR:OG1	3:PD:176:GLN:N	2.51	0.42
2:LC:283:TRP:CZ3	2:LC:285:TYR:HB3	2.55	0.42
3:PF:50:VAL:O	3:PF:54:ASN:ND2	2.45	0.42
3:PF:268:PHE:HE1	3:PF:323:GLU:HG3	1.84	0.42
2:LD:102:MET:HE1	2:LD:230:MET:HE2	2.01	0.42
2:LD:1137:TRP:CE2	2:LD:1142:GLN:HG2	2.55	0.42
3:PH:415:GLY:O	3:PH:434:ASN:ND2	2.53	0.42
2:LE:1050:LEU:HG	2:LE:1075:VAL:HG23	2.01	0.42
5:TI:269:THR:HG23	5:TI:270:ILE:HG12	2.02	0.42
3:PK:660:LEU:HD11	3:PL:662:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PL:645:ASP:OD1	3:PL:646:ALA:N	2.53	0.42
4:SA:229:ASP:O	4:SA:232:THR:OG1	2.29	0.42
1:AC:176:PRO:HG3	1:AD:43:GLU:HG3	2.00	0.42
2:LC:1088:LEU:HD13	2:LC:1102:TRP:HB3	2.01	0.42
3:PE:149:ILE:HG21	3:PE:248:ILE:HD13	2.01	0.42
3:PE:535:ARG:HA	3:PE:535:ARG:HD2	1.90	0.42
2:LD:834:PRO:O	2:LD:880:ASN:ND2	2.36	0.42
3:PH:546:ARG:HA	3:PH:549:LEU:HD23	2.01	0.42
2:LE:749:THR:OG1	2:LE:750:ASP:N	2.53	0.42
3:PI:660:LEU:HD11	3:PJ:662:TYR:CE1	2.55	0.42
2:LF:907:ALA:O	2:LF:910:THR:OG1	2.33	0.42
3:PK:637:LEU:O	3:PK:641:ILE:HG12	2.20	0.42
4:SF:340:ASP:OD1	4:SF:340:ASP:N	2.52	0.42
3:PA:495:LEU:HB3	3:PA:499:SER:HB2	2.01	0.42
6:YA:4:HIS:NE2	6:YA:8:ASN:OD1	2.53	0.42
6:YB:55:GLN:HG3	6:ZB:60:HIS:CD2	2.55	0.42
5:TB:222:ASP:OD1	5:TB:238:LYS:NZ	2.34	0.42
2:LB:907:ALA:O	2:LB:910:THR:OG1	2.33	0.42
3:PC:149:ILE:HG21	3:PC:248:ILE:HD13	2.01	0.42
3:PC:561:THR:HB	3:PC:564:VAL:HG12	2.02	0.42
3:PC:634:ASN:HD21	3:PF:625:LEU:HB3	1.85	0.42
4:SC:327:GLN:HB3	4:SC:363:PHE:HE1	1.85	0.42
6:YF:55:GLN:HG3	6:ZF:60:HIS:CD2	2.55	0.42
1:AG:49:HIS:O	1:AG:152:GLN:NE2	2.52	0.42
2:LD:283:TRP:CZ3	2:LD:285:TYR:HB3	2.55	0.42
3:PG:495:LEU:HB3	3:PG:499:SER:HB2	2.01	0.42
3:PG:634:ASN:HD21	3:PJ:625:LEU:HB3	1.85	0.42
4:SD:340:ASP:OD1	4:SD:340:ASP:N	2.52	0.42
3:PH:645:ASP:OD1	3:PH:646:ALA:N	2.53	0.42
5:TH:24:LEU:HD11	5:TI:150:LEU:HD13	2.01	0.42
2:LE:1137:TRP:CE2	2:LE:1142:GLN:HG2	2.55	0.42
3:PI:314:PRO:HA	3:PI:317:LYS:HG3	2.02	0.42
3:PI:366:ILE:HG21	3:PI:509:LEU:HD23	2.01	0.42
3:PI:546:ARG:HA	3:PI:549:LEU:HD23	2.02	0.42
3:PI:637:LEU:O	3:PI:641:ILE:HG12	2.20	0.42
1:AL:49:HIS:CE1	1:AL:155:HIS:HB2	2.55	0.42
2:LF:283:TRP:CZ3	2:LF:285:TYR:HB3	2.55	0.42
3:PL:660:LEU:H	3:PL:660:LEU:HD12	1.84	0.42
1:AB:233:ARG:HA	1:AB:233:ARG:HD3	1.92	0.41
2:LA:283:TRP:CZ3	2:LA:285:TYR:HB3	2.55	0.41
2:LA:737:LEU:O	2:LA:838:ILE:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LA:1088:LEU:HD13	2:LA:1102:TRP:HB3	2.01	0.41
6:YB:55:GLN:OE1	6:YB:55:GLN:N	2.48	0.41
2:LB:102:MET:HE1	2:LB:230:MET:HE2	2.01	0.41
2:LB:275:ALA:O	2:LB:336:GLN:NE2	2.46	0.41
2:LB:582:TYR:O	2:LB:585:SER:OG	2.30	0.41
3:PC:660:LEU:HD11	3:PD:662:TYR:CE1	2.55	0.41
1:AE:49:HIS:O	1:AE:152:GLN:NE2	2.53	0.41
2:LC:1137:TRP:CE2	2:LC:1142:GLN:HG2	2.55	0.41
3:PE:625:LEU:HB3	3:PF:634:ASN:HD21	1.84	0.41
3:PF:314:PRO:HA	3:PF:317:LYS:HG3	2.00	0.41
1:AG:225:ASP:OD1	1:AG:225:ASP:N	2.50	0.41
3:PG:660:LEU:HD11	3:PH:662:TYR:CE1	2.55	0.41
4:SD:327:GLN:HB3	4:SD:363:PHE:HE1	1.85	0.41
6:YH:55:GLN:HG3	6:ZH:60:HIS:CD2	2.55	0.41
3:PH:558:ASP:OD1	3:PH:559:ILE:N	2.53	0.41
1:AI:172:ASP:OD1	1:AI:172:ASP:N	2.53	0.41
4:SE:213:ASP:HA	4:SE:225:PRO:HA	2.01	0.41
5:TJ:26:ASP:OD1	5:TJ:26:ASP:N	2.50	0.41
5:TJ:147:ILE:HD13	5:TK:153:LYS:HB2	2.02	0.41
2:LF:1092:LYS:NZ	2:LF:1096:GLY:O	2.49	0.41
6:YL:43:MET:N	6:YL:44:PRO:HD2	2.35	0.41
3:PL:546:ARG:HA	3:PL:549:LEU:HD23	2.02	0.41
1:AB:34:LYS:O	1:AB:38:ILE:HG12	2.20	0.41
2:LA:465:PHE:HB2	4:SA:69:CYS:HB3	2.02	0.41
3:PA:149:ILE:HG21	3:PA:248:ILE:HD13	2.02	0.41
4:SA:249:ILE:HD11	4:SA:260:GLN:HG3	2.02	0.41
2:LB:834:PRO:O	2:LB:880:ASN:ND2	2.36	0.41
3:PC:298:GLU:HG3	3:PC:320:VAL:HG11	2.02	0.41
6:YC:43:MET:N	6:YC:44:PRO:HD2	2.35	0.41
4:SC:213:ASP:HA	4:SC:225:PRO:HA	2.02	0.41
1:AH:34:LYS:O	1:AH:38:ILE:HG12	2.20	0.41
2:LD:749:THR:OG1	2:LD:762:ALA:O	2.31	0.41
5:TH:147:ILE:HD13	5:TI:153:LYS:HB2	2.03	0.41
3:PJ:679:LYS:HA	3:PJ:679:LYS:HD3	1.86	0.41
5:TJ:277:PRO:HD2	5:TJ:280:PHE:HD2	1.84	0.41
2:LF:1137:TRP:CE2	2:LF:1142:GLN:HG2	2.55	0.41
5:TK:26:ASP:OD1	5:TK:26:ASP:N	2.49	0.41
2:LA:1137:TRP:CE2	2:LA:1142:GLN:HG2	2.55	0.41
6:ZA:73:LEU:O	6:ZA:77:GLN:HG2	2.21	0.41
2:LB:465:PHE:HB2	4:SB:69:CYS:HB3	2.02	0.41
4:SB:342:VAL:N	4:SB:343:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PD:546:ARG:HA	3:PD:549:LEU:HD23	2.01	0.41
2:LC:102:MET:HE1	2:LC:230:MET:HE2	2.01	0.41
3:PF:149:ILE:HG21	3:PF:248:ILE:HD13	2.03	0.41
2:LD:275:ALA:O	2:LD:336:GLN:NE2	2.46	0.41
3:PG:171:PHE:HB2	3:PG:219:TYR:HB2	2.02	0.41
3:PG:175:THR:OG1	3:PG:176:GLN:N	2.53	0.41
4:SD:229:ASP:HB3	4:SD:232:THR:HG23	2.02	0.41
6:YG:43:MET:N	6:YG:44:PRO:HD2	2.36	0.41
1:AJ:34:LYS:O	1:AJ:38:ILE:HG12	2.20	0.41
1:AJ:225:ASP:N	1:AJ:225:ASP:OD1	2.52	0.41
3:PI:634:ASN:HD21	3:PL:625:LEU:HB3	1.84	0.41
4:SE:367:VAL:HG21	4:SE:377:TRP:CE2	2.56	0.41
6:XJ:55:GLN:OE1	6:XJ:55:GLN:N	2.43	0.41
6:YJ:43:MET:N	6:YJ:44:PRO:HD2	2.35	0.41
6:YJ:48:ASN:O	6:YJ:52:ASN:ND2	2.39	0.41
1:AL:34:LYS:O	1:AL:38:ILE:HG12	2.20	0.41
2:LF:710:TYR:O	2:LF:711:GLN:HG3	2.20	0.41
3:PK:314:PRO:HA	3:PK:317:LYS:HG3	2.02	0.41
1:AA:49:HIS:O	1:AA:152:GLN:NE2	2.52	0.41
6:YA:43:MET:N	6:YA:44:PRO:HD2	2.36	0.41
1:AC:49:HIS:O	1:AC:152:GLN:NE2	2.52	0.41
3:PC:535:ARG:HA	3:PC:535:ARG:HD2	1.90	0.41
3:PC:637:LEU:O	3:PC:641:ILE:HG12	2.20	0.41
3:PC:658:LYS:NZ	3:PF:654:GLU:OE1	2.53	0.41
5:TC:269:THR:HG23	5:TC:270:ILE:HG12	2.02	0.41
6:YD:43:MET:N	6:YD:44:PRO:HD2	2.35	0.41
3:PD:558:ASP:OD1	3:PD:559:ILE:N	2.53	0.41
1:AF:49:HIS:CE1	1:AF:155:HIS:HB2	2.55	0.41
3:PE:679:LYS:HA	3:PE:679:LYS:HD3	1.86	0.41
4:SC:342:VAL:N	4:SC:343:PRO:HD2	2.36	0.41
2:LD:860:MET:HB3	2:LD:914:LYS:HE3	2.00	0.41
3:PG:314:PRO:HA	3:PG:317:LYS:HG3	2.02	0.41
6:YG:4:HIS:NE2	6:YG:8:ASN:OD1	2.53	0.41
6:YH:43:MET:N	6:YH:44:PRO:HD2	2.35	0.41
3:PI:149:ILE:HG21	3:PI:248:ILE:HD13	2.01	0.41
4:SE:342:VAL:N	4:SE:343:PRO:HD2	2.36	0.41
6:ZI:73:LEU:O	6:ZI:77:GLN:HG2	2.21	0.41
3:PK:418:ASP:OD1	3:PK:421:ASN:ND2	2.49	0.41
6:YL:55:GLN:HG3	6:ZL:60:HIS:CD2	2.55	0.41
3:PL:149:ILE:HG21	3:PL:248:ILE:HD13	2.03	0.41
1:AA:176:PRO:HG3	1:AB:43:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PA:109:GLU:OE1	3:PD:538:ASN:ND2	2.54	0.41
3:PA:671:HIS:NE2	3:PD:673:ARG:O	2.53	0.41
4:SA:342:VAL:N	4:SA:343:PRO:HD2	2.35	0.41
3:PB:546:ARG:HA	3:PB:549:LEU:HD23	2.01	0.41
3:PB:654:GLU:OE1	3:PK:658:LYS:NZ	2.53	0.41
1:AD:225:ASP:OD1	1:AD:225:ASP:N	2.52	0.41
2:LB:466:GLN:NE2	2:LB:477:TYR:O	2.36	0.41
2:LB:749:THR:OG1	2:LB:750:ASP:N	2.53	0.41
3:PC:171:PHE:HB2	3:PC:219:TYR:HB2	2.02	0.41
3:PC:625:LEU:HB3	3:PD:634:ASN:HD21	1.84	0.41
1:AF:19:THR:OG1	1:AF:186:TYR:OH	2.34	0.41
1:AF:211:ARG:HH22	7:OF:1:ASP:HB3	1.85	0.41
2:LC:498:VAL:HG11	2:LC:509:GLN:HE22	1.85	0.41
3:PE:151:ARG:HB2	3:PE:243:LEU:HD11	2.02	0.41
3:PE:413:PRO:HG3	3:PE:442:MET:HB3	2.01	0.41
3:PE:546:ARG:HA	3:PE:549:LEU:HD23	2.02	0.41
3:PE:634:ASN:HD21	3:PH:625:LEU:HB3	1.85	0.41
3:PH:298:GLU:HG3	3:PH:320:VAL:HG11	2.02	0.41
3:PH:660:LEU:H	3:PH:660:LEU:HD12	1.84	0.41
2:LE:610:ASN:O	2:LE:610:ASN:ND2	2.44	0.41
3:PI:658:LYS:NZ	3:PL:654:GLU:OE1	2.53	0.41
3:PI:679:LYS:HA	3:PI:679:LYS:HD3	1.86	0.41
3:PJ:561:THR:HB	3:PJ:564:VAL:HG12	2.02	0.41
3:PK:561:THR:HB	3:PK:564:VAL:HG12	2.02	0.41
3:PK:645:ASP:OD1	3:PK:646:ALA:N	2.54	0.41
4:SF:213:ASP:HA	4:SF:225:PRO:HA	2.02	0.41
4:SF:367:VAL:HG21	4:SF:377:TRP:CE2	2.56	0.41
1:AA:172:ASP:OD1	1:AA:172:ASP:N	2.54	0.41
1:AD:49:HIS:CE1	1:AD:155:HIS:HB2	2.56	0.41
6:ZC:73:LEU:O	6:ZC:77:GLN:HG2	2.21	0.41
3:PD:415:GLY:O	3:PD:434:ASN:ND2	2.53	0.41
3:PE:645:ASP:OD1	3:PE:646:ALA:N	2.54	0.41
6:YF:43:MET:N	6:YF:44:PRO:HD2	2.35	0.41
3:PF:546:ARG:HA	3:PF:549:LEU:HD23	2.02	0.41
3:PH:561:THR:HB	3:PH:564:VAL:HG12	2.02	0.41
2:LE:498:VAL:HG11	2:LE:509:GLN:HE22	1.85	0.41
2:LE:682:VAL:HA	2:LE:685:TRP:CD1	2.56	0.41
3:PI:298:GLU:HG3	3:PI:320:VAL:HG11	2.02	0.41
3:PI:561:THR:HB	3:PI:564:VAL:HG12	2.02	0.41
4:SE:229:ASP:HB3	4:SE:232:THR:HG23	2.03	0.41
6:YI:43:MET:N	6:YI:44:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:225:ASP:OD1	1:AL:225:ASP:N	2.52	0.41
2:LF:1120:ASP:OD1	2:LF:1123:THR:OG1	2.32	0.41
3:PK:546:ARG:HA	3:PK:549:LEU:HD23	2.02	0.41
5:TK:269:THR:HG23	5:TK:270:ILE:HG12	2.02	0.41
2:LA:498:VAL:HG11	2:LA:509:GLN:HE22	1.85	0.41
2:LA:710:TYR:O	2:LA:711:GLN:HG3	2.20	0.41
5:TA:24:LEU:HD11	5:TB:150:LEU:HD13	2.03	0.41
3:PB:558:ASP:OD1	3:PB:559:ILE:N	2.53	0.41
2:LB:254:ASN:OD1	2:LB:261:GLN:HG2	2.21	0.41
3:PC:645:ASP:OD1	3:PC:646:ALA:N	2.54	0.41
6:XC:22:ASP:HB2	6:XC:23:PRO:HD3	2.03	0.41
3:PD:664:GLU:HB2	3:PD:670:LYS:NZ	2.36	0.41
2:LC:77:ILE:HD11	4:SC:120:PHE:HA	2.02	0.41
3:PE:561:THR:HB	3:PE:564:VAL:HG12	2.02	0.41
6:XE:12:ASN:ND2	6:XE:18:GLU:HG2	2.34	0.41
3:PF:558:ASP:OD1	3:PF:559:ILE:N	2.54	0.41
5:TF:147:ILE:HD13	5:TG:153:LYS:HB2	2.03	0.41
3:PG:268:PHE:HE1	3:PG:323:GLU:HG3	1.84	0.41
3:PG:637:LEU:O	3:PG:641:ILE:HG12	2.20	0.41
4:SD:342:VAL:N	4:SD:343:PRO:HD2	2.35	0.41
1:AI:49:HIS:O	1:AI:152:GLN:NE2	2.52	0.41
3:PI:171:PHE:HB2	3:PI:219:TYR:HB2	2.02	0.41
3:PI:625:LEU:HB3	3:PJ:634:ASN:HD21	1.84	0.41
5:TI:277:PRO:HD2	5:TI:280:PHE:HD2	1.86	0.41
6:YJ:55:GLN:HG3	6:ZJ:60:HIS:CD2	2.55	0.41
3:PJ:171:PHE:HB2	3:PJ:219:TYR:HB2	2.03	0.41
1:AK:172:ASP:OD1	1:AK:172:ASP:N	2.53	0.41
4:SF:342:VAL:N	4:SF:343:PRO:HD2	2.36	0.41
6:YK:4:HIS:NE2	6:YK:8:ASN:OD1	2.54	0.41
2:LA:275:ALA:O	2:LA:336:GLN:NE2	2.46	0.41
2:LA:643:ALA:HA	2:LA:669:THR:H	1.86	0.41
2:LA:984:PRO:HD3	2:LA:1068:ALA:HB3	2.03	0.41
3:PA:561:THR:HB	3:PA:564:VAL:HG12	2.03	0.41
3:PA:645:ASP:OD1	3:PA:646:ALA:N	2.54	0.41
4:SA:367:VAL:HG21	4:SA:377:TRP:CE2	2.56	0.41
6:XA:43:MET:N	6:XA:44:PRO:HD2	2.36	0.41
2:LB:494:ARG:NH2	2:LB:500:PRO:O	2.41	0.41
2:LB:682:VAL:HA	2:LB:685:TRP:CD1	2.56	0.41
2:LB:984:PRO:HD3	2:LB:1068:ALA:HB3	2.03	0.41
2:LB:1050:LEU:HG	2:LB:1075:VAL:HG23	2.01	0.41
3:PC:314:PRO:HA	3:PC:317:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XC:9:THR:OG1	6:XC:10:ILE:N	2.53	0.41
6:XC:43:MET:N	6:XC:44:PRO:HD2	2.35	0.41
3:PD:298:GLU:HG3	3:PD:320:VAL:HG11	2.02	0.41
2:LC:465:PHE:HB2	4:SC:69:CYS:HB3	2.03	0.41
2:LC:886:TRP:HE3	2:LC:928:GLY:HA2	1.86	0.41
3:PE:658:LYS:NZ	3:PH:654:GLU:OE1	2.53	0.41
5:TF:24:LEU:HD11	5:TG:150:LEU:HD13	2.02	0.41
2:LD:984:PRO:HD3	2:LD:1068:ALA:HB3	2.03	0.41
3:PG:546:ARG:HA	3:PG:549:LEU:HD23	2.03	0.41
3:PG:645:ASP:OD1	3:PG:646:ALA:N	2.54	0.41
6:ZG:73:LEU:O	6:ZG:77:GLN:HG2	2.21	0.41
2:LE:710:TYR:O	2:LE:711:GLN:HG3	2.20	0.41
2:LE:984:PRO:HD3	2:LE:1068:ALA:HB3	2.03	0.41
6:XI:22:ASP:HB2	6:XI:23:PRO:HD3	2.03	0.41
2:LF:254:ASN:OD1	2:LF:261:GLN:HG2	2.21	0.41
2:LF:465:PHE:HB2	4:SF:69:CYS:HB3	2.03	0.41
6:ZK:73:LEU:O	6:ZK:77:GLN:HG2	2.20	0.41
3:PL:561:THR:HB	3:PL:564:VAL:HG12	2.03	0.41
3:PA:298:GLU:HG3	3:PA:320:VAL:HG11	2.03	0.41
3:PA:637:LEU:O	3:PA:641:ILE:HG12	2.20	0.41
3:PA:658:LYS:NZ	3:PD:654:GLU:OE1	2.54	0.41
4:SA:83:TYR:HA	4:SA:84:PRO:HD3	1.91	0.41
4:SA:229:ASP:HB3	4:SA:232:THR:HG23	2.02	0.41
4:SA:340:ASP:OD1	4:SA:340:ASP:N	2.52	0.41
6:XA:22:ASP:HB2	6:XA:23:PRO:HD3	2.03	0.41
6:YB:43:MET:N	6:YB:44:PRO:HD2	2.35	0.41
3:PB:664:GLU:HB2	3:PB:670:LYS:NZ	2.36	0.41
1:AD:34:LYS:O	1:AD:38:ILE:HG12	2.20	0.41
3:PC:175:THR:OG1	3:PC:176:GLN:N	2.53	0.41
3:PD:171:PHE:HB2	3:PD:219:TYR:HB2	2.03	0.41
1:AF:34:LYS:O	1:AF:38:ILE:HG12	2.20	0.41
2:LC:682:VAL:HA	2:LC:685:TRP:CD1	2.56	0.41
2:LC:801:MET:SD	2:LC:801:MET:N	2.80	0.41
2:LC:984:PRO:HD3	2:LC:1068:ALA:HB3	2.03	0.41
3:PE:298:GLU:HG3	3:PE:320:VAL:HG11	2.02	0.41
3:PE:314:PRO:HA	3:PE:317:LYS:HG3	2.02	0.41
3:PE:637:LEU:O	3:PE:641:ILE:HG12	2.20	0.41
6:XE:22:ASP:HB2	6:XE:23:PRO:HD3	2.03	0.41
6:XE:43:MET:N	6:XE:44:PRO:HD2	2.35	0.41
6:YE:4:HIS:NE2	6:YE:8:ASN:OD1	2.54	0.41
3:PF:561:THR:HB	3:PF:564:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:58:ASN:HB2	1:AH:148:ASN:ND2	2.35	0.41
1:AH:225:ASP:N	1:AH:225:ASP:OD1	2.52	0.41
2:LD:254:ASN:OD1	2:LD:261:GLN:HG2	2.21	0.41
2:LD:749:THR:OG1	2:LD:750:ASP:N	2.53	0.41
3:PG:81:ARG:HD2	3:PH:468:SER:HB3	2.03	0.41
3:PG:317:LYS:HE3	3:PG:317:LYS:HB3	1.95	0.41
3:PG:343:TRP:HB3	3:PG:348:LEU:HD23	2.03	0.41
3:PG:625:LEU:HB3	3:PH:634:ASN:HD21	1.84	0.41
5:TG:269:THR:HG23	5:TG:270:ILE:HG12	2.02	0.41
5:TH:269:THR:HG23	5:TH:270:ILE:HG12	2.03	0.41
3:PI:175:THR:OG1	3:PI:176:GLN:N	2.53	0.41
3:PI:645:ASP:OD1	3:PI:646:ALA:N	2.54	0.41
6:XI:43:MET:N	6:XI:44:PRO:HD2	2.35	0.41
3:PJ:664:GLU:HB2	3:PJ:670:LYS:NZ	2.36	0.41
1:AK:49:HIS:O	1:AK:152:GLN:NE2	2.53	0.41
3:PK:171:PHE:HB2	3:PK:219:TYR:HB2	2.02	0.41
2:LA:749:THR:OG1	2:LA:750:ASP:N	2.53	0.41
3:PA:660:LEU:HD11	3:PB:662:TYR:CE1	2.55	0.41
5:TA:153:LYS:HB2	5:TL:147:ILE:HD13	2.03	0.41
3:PB:298:GLU:HG3	3:PB:320:VAL:HG11	2.02	0.41
4:SB:327:GLN:HB3	4:SB:363:PHE:HE1	1.85	0.41
5:TD:147:ILE:HD13	5:TE:153:LYS:HB2	2.02	0.41
2:LC:254:ASN:OD1	2:LC:261:GLN:HG2	2.21	0.41
3:PE:171:PHE:HB2	3:PE:219:TYR:HB2	2.02	0.41
1:AG:85:GLU:OE1	1:AG:85:GLU:N	2.54	0.41
2:LD:886:TRP:HE3	2:LD:928:GLY:HA2	1.86	0.41
3:PG:298:GLU:HG3	3:PG:320:VAL:HG11	2.03	0.41
3:PG:658:LYS:NZ	3:PJ:654:GLU:OE1	2.54	0.41
4:SD:367:VAL:HG21	4:SD:377:TRP:CE2	2.56	0.41
2:LE:254:ASN:OD1	2:LE:261:GLN:HG2	2.21	0.41
2:LF:984:PRO:HD3	2:LF:1068:ALA:HB3	2.03	0.41
1:AA:85:GLU:OE1	1:AA:85:GLU:N	2.54	0.40
3:PA:175:THR:OG1	3:PA:176:GLN:N	2.53	0.40
5:TA:277:PRO:HD2	5:TA:280:PHE:HD2	1.86	0.40
6:XB:62:LYS:NZ	6:YB:67:SER:HB3	2.37	0.40
3:PB:538:ASN:ND2	3:PK:109:GLU:OE1	2.54	0.40
1:AC:45:LEU:HD23	1:AC:155:HIS:CG	2.56	0.40
1:AC:172:ASP:OD1	1:AC:172:ASP:N	2.53	0.40
2:LB:643:ALA:HA	2:LB:669:THR:H	1.86	0.40
3:PC:546:ARG:HA	3:PC:549:LEU:HD23	2.02	0.40
6:XD:62:LYS:NZ	6:YD:67:SER:HB3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:45:LEU:HD23	1:AE:155:HIS:CG	2.56	0.40
5:TE:276:PRO:HA	5:TE:277:PRO:HD3	1.99	0.40
5:TF:269:THR:HG23	5:TF:270:ILE:HG12	2.03	0.40
1:AH:43:GLU:OE1	1:AH:185:ARG:NH1	2.52	0.40
2:LD:338:ASP:OD1	2:LD:339:GLY:N	2.53	0.40
2:LD:465:PHE:HB2	4:SD:69:CYS:HB3	2.02	0.40
2:LD:682:VAL:HA	2:LD:685:TRP:CD1	2.56	0.40
2:LD:932:PRO:HG2	2:LD:957:ALA:HB1	2.03	0.40
2:LD:1089:LYS:HE2	2:LD:1089:LYS:HB2	1.92	0.40
5:TG:24:LEU:HD11	5:TH:150:LEU:HD13	2.03	0.40
6:XG:22:ASP:HB2	6:XG:23:PRO:HD3	2.03	0.40
6:ZG:62:LYS:HB2	6:ZG:65:GLU:CD	2.47	0.40
3:PH:664:GLU:HB2	3:PH:670:LYS:NZ	2.36	0.40
2:LE:465:PHE:HB2	4:SE:69:CYS:HB3	2.02	0.40
5:TI:26:ASP:OD1	5:TI:26:ASP:N	2.48	0.40
1:AL:211:ARG:HH22	7:OL:1:ASP:HB3	1.86	0.40
6:XK:43:MET:N	6:XK:44:PRO:HD2	2.36	0.40
1:AA:45:LEU:HD23	1:AA:155:HIS:CG	2.56	0.40
1:AB:225:ASP:OD1	1:AB:225:ASP:N	2.52	0.40
2:LA:77:ILE:HD11	4:SA:120:PHE:HA	2.03	0.40
3:PA:660:LEU:HD12	3:PA:660:LEU:H	1.86	0.40
2:LB:790:MET:HE3	2:LB:790:MET:HB3	1.99	0.40
4:SB:367:VAL:HG21	4:SB:377:TRP:CE2	2.56	0.40
2:LC:1089:LYS:HE2	2:LC:1089:LYS:HB2	1.92	0.40
5:TE:277:PRO:HD2	5:TE:280:PHE:HD2	1.86	0.40
6:XF:55:GLN:OE1	6:XF:55:GLN:N	2.43	0.40
6:YE:43:MET:N	6:YE:44:PRO:HD2	2.35	0.40
5:TG:226:ASP:N	5:TG:226:ASP:OD1	2.54	0.40
6:XG:43:MET:N	6:XG:44:PRO:HD2	2.36	0.40
2:LE:741:ASN:HA	2:LE:796:ALA:O	2.21	0.40
3:PI:343:TRP:HB3	3:PI:348:LEU:HD23	2.04	0.40
4:SE:327:GLN:HB3	4:SE:363:PHE:HE1	1.85	0.40
6:ZI:62:LYS:HB2	6:ZI:65:GLU:CD	2.46	0.40
1:AK:45:LEU:HD23	1:AK:155:HIS:CG	2.56	0.40
2:LF:77:ILE:HD11	4:SF:120:PHE:HA	2.02	0.40
2:LF:466:GLN:NE2	2:LF:477:TYR:O	2.36	0.40
2:LF:469:MET:HE2	2:LF:473:TRP:CH2	2.57	0.40
3:PK:298:GLU:HG3	3:PK:320:VAL:HG11	2.02	0.40
4:SF:327:GLN:HB3	4:SF:363:PHE:HE1	1.85	0.40
6:YK:43:MET:N	6:YK:44:PRO:HD2	2.35	0.40
3:PL:664:GLU:HB2	3:PL:670:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:211:ARG:HH22	7:OB:1:ASP:HB3	1.87	0.40
2:LA:682:VAL:HA	2:LA:685:TRP:CD1	2.56	0.40
2:LA:886:TRP:HE3	2:LA:928:GLY:HA2	1.86	0.40
2:LB:469:MET:HE2	2:LB:473:TRP:CH2	2.57	0.40
2:LB:710:TYR:O	2:LB:711:GLN:HG3	2.20	0.40
2:LB:886:TRP:HE3	2:LB:928:GLY:HA2	1.86	0.40
1:AE:172:ASP:OD1	1:AE:172:ASP:N	2.53	0.40
4:SC:229:ASP:HB3	4:SC:232:THR:HG23	2.02	0.40
6:ZE:73:LEU:O	6:ZE:77:GLN:HG2	2.20	0.40
3:PF:664:GLU:HB2	3:PF:670:LYS:NZ	2.36	0.40
2:LD:498:VAL:HG11	2:LD:509:GLN:HE22	1.85	0.40
3:PG:175:THR:HG23	3:PG:177:GLU:HG3	2.04	0.40
3:PH:171:PHE:HB2	3:PH:219:TYR:HB2	2.03	0.40
3:PH:175:THR:OG1	3:PH:176:GLN:N	2.52	0.40
1:AJ:43:GLU:OE2	1:AJ:181:TYR:OH	2.33	0.40
3:PJ:149:ILE:HG21	3:PJ:248:ILE:HD13	2.03	0.40
2:LF:643:ALA:HA	2:LF:669:THR:H	1.86	0.40
2:LF:682:VAL:HA	2:LF:685:TRP:CD1	2.56	0.40
5:TK:226:ASP:OD1	5:TK:226:ASP:N	2.54	0.40
6:XK:22:ASP:HB2	6:XK:23:PRO:HD3	2.03	0.40
6:XL:62:LYS:NZ	6:YL:67:SER:HB3	2.37	0.40
6:YL:64:THR:O	6:YL:67:SER:OG	2.31	0.40
2:LA:1157:ILE:HD12	2:LA:1177:THR:HB	2.04	0.40
6:XB:73:LEU:HD21	6:ZB:62:LYS:HZ3	1.87	0.40
3:PB:171:PHE:HB2	3:PB:219:TYR:HB2	2.03	0.40
5:TB:147:ILE:HD13	5:TC:153:LYS:HB2	2.03	0.40
2:LB:110:HIS:HA	2:LB:113:ARG:HH11	1.87	0.40
4:SB:229:ASP:HB3	4:SB:232:THR:HG23	2.03	0.40
5:TC:277:PRO:HD2	5:TC:280:PHE:HD2	1.86	0.40
2:LC:92:THR:OG1	2:LC:95:ASP:OD1	2.39	0.40
2:LC:682:VAL:HA	2:LC:685:TRP:NE1	2.37	0.40
3:PE:109:GLU:OE1	3:PH:538:ASN:ND2	2.54	0.40
3:PE:175:THR:OG1	3:PE:176:GLN:N	2.53	0.40
6:XE:9:THR:OG1	6:XE:10:ILE:N	2.52	0.40
6:ZE:62:LYS:HB2	6:ZE:65:GLU:CD	2.47	0.40
1:AH:211:ARG:HH22	7:OH:1:ASP:HB3	1.87	0.40
2:LD:77:ILE:HD11	4:SD:120:PHE:HA	2.03	0.40
1:AI:85:GLU:OE1	1:AI:85:GLU:N	2.54	0.40
1:AJ:49:HIS:CE1	1:AJ:155:HIS:HB2	2.56	0.40
1:AJ:233:ARG:HA	1:AJ:233:ARG:HD3	1.91	0.40
4:SE:151:GLU:HG2	4:SE:152:TRP:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:YI:4:HIS:NE2	6:YI:8:ASN:OD1	2.55	0.40
3:PJ:298:GLU:HG3	3:PJ:320:VAL:HG11	2.02	0.40
3:PJ:558:ASP:OD1	3:PJ:559:ILE:N	2.53	0.40
1:AL:43:GLU:OE1	1:AL:185:ARG:NH1	2.52	0.40
2:LF:338:ASP:OD1	2:LF:339:GLY:N	2.53	0.40
2:LF:901:ASN:CG	2:LF:905:SER:HB3	2.47	0.40
3:PK:343:TRP:HB3	3:PK:348:LEU:HD23	2.03	0.40
4:SF:229:ASP:HB3	4:SF:232:THR:HG23	2.02	0.40
2:LA:940:TYR:HA	2:LA:950:TYR:HA	2.04	0.40
3:PA:343:TRP:HB3	3:PA:348:LEU:HD23	2.03	0.40
5:TB:101:GLU:H	5:TB:101:GLU:CD	2.30	0.40
1:AD:211:ARG:HH22	7:OD:1:ASP:HB3	1.86	0.40
3:PC:660:LEU:HD12	3:PC:660:LEU:H	1.86	0.40
3:PD:317:LYS:HE3	3:PD:317:LYS:HB3	1.96	0.40
1:AE:85:GLU:OE1	1:AE:85:GLU:N	2.55	0.40
2:LC:901:ASN:CG	2:LC:905:SER:HB3	2.47	0.40
4:SC:367:VAL:HG21	4:SC:377:TRP:CE2	2.56	0.40
5:TE:24:LEU:HD11	5:TF:150:LEU:HD13	2.03	0.40
6:ZF:41:LEU:HD23	6:XG:10:ILE:HD11	2.04	0.40
2:LD:110:HIS:HA	2:LD:113:ARG:HH11	1.87	0.40
2:LD:710:TYR:O	2:LD:711:GLN:HG3	2.20	0.40
2:LD:1130:TRP:HE1	2:LD:1132:SER:HG	1.65	0.40
3:PG:561:THR:HB	3:PG:564:VAL:HG12	2.03	0.40
2:LE:1157:ILE:HD12	2:LE:1177:THR:HB	2.04	0.40
3:PI:175:THR:HG23	3:PI:177:GLU:HG3	2.04	0.40
2:LF:940:TYR:HA	2:LF:950:TYR:HA	2.04	0.40
5:TK:24:LEU:HD11	5:TL:150:LEU:HD13	2.03	0.40
6:XK:12:ASN:ND2	6:XK:18:GLU:HG2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	234/236 (99%)	234 (100%)	0	0	100	100
1	AB	234/236 (99%)	232 (99%)	2 (1%)	0	100	100
1	AC	234/236 (99%)	234 (100%)	0	0	100	100
1	AD	234/236 (99%)	232 (99%)	2 (1%)	0	100	100
1	AE	234/236 (99%)	233 (100%)	1 (0%)	0	100	100
1	AF	234/236 (99%)	232 (99%)	2 (1%)	0	100	100
1	AG	234/236 (99%)	234 (100%)	0	0	100	100
1	AH	234/236 (99%)	232 (99%)	2 (1%)	0	100	100
1	AI	234/236 (99%)	234 (100%)	0	0	100	100
1	AJ	234/236 (99%)	232 (99%)	2 (1%)	0	100	100
1	AK	234/236 (99%)	233 (100%)	1 (0%)	0	100	100
1	AL	234/236 (99%)	232 (99%)	2 (1%)	0	100	100
2	LA	1179/1382 (85%)	1150 (98%)	29 (2%)	0	100	100
2	LB	1179/1382 (85%)	1147 (97%)	32 (3%)	0	100	100
2	LC	1179/1382 (85%)	1147 (97%)	32 (3%)	0	100	100
2	LD	1179/1382 (85%)	1150 (98%)	29 (2%)	0	100	100
2	LE	1179/1382 (85%)	1147 (97%)	32 (3%)	0	100	100
2	LF	1179/1382 (85%)	1148 (97%)	31 (3%)	0	100	100
3	PA	673/763 (88%)	665 (99%)	8 (1%)	0	100	100
3	PB	673/763 (88%)	663 (98%)	10 (2%)	0	100	100
3	PC	673/763 (88%)	665 (99%)	8 (1%)	0	100	100
3	PD	673/763 (88%)	664 (99%)	9 (1%)	0	100	100
3	PE	673/763 (88%)	665 (99%)	8 (1%)	0	100	100
3	PF	673/763 (88%)	664 (99%)	9 (1%)	0	100	100
3	PG	673/763 (88%)	665 (99%)	8 (1%)	0	100	100
3	PH	673/763 (88%)	664 (99%)	9 (1%)	0	100	100
3	PI	673/763 (88%)	665 (99%)	8 (1%)	0	100	100
3	PJ	673/763 (88%)	664 (99%)	9 (1%)	0	100	100
3	PK	673/763 (88%)	665 (99%)	8 (1%)	0	100	100
3	PL	673/763 (88%)	664 (99%)	9 (1%)	0	100	100
4	SA	413/417 (99%)	404 (98%)	9 (2%)	0	100	100
4	SB	413/417 (99%)	403 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SC	413/417 (99%)	404 (98%)	9 (2%)	0	100	100
4	SD	413/417 (99%)	404 (98%)	9 (2%)	0	100	100
4	SE	413/417 (99%)	403 (98%)	10 (2%)	0	100	100
4	SF	413/417 (99%)	404 (98%)	9 (2%)	0	100	100
5	TA	296/299 (99%)	292 (99%)	4 (1%)	0	100	100
5	TB	296/299 (99%)	291 (98%)	5 (2%)	0	100	100
5	TC	296/299 (99%)	292 (99%)	4 (1%)	0	100	100
5	TD	296/299 (99%)	291 (98%)	5 (2%)	0	100	100
5	TE	296/299 (99%)	292 (99%)	4 (1%)	0	100	100
5	TF	296/299 (99%)	291 (98%)	5 (2%)	0	100	100
5	TG	296/299 (99%)	292 (99%)	4 (1%)	0	100	100
5	TH	296/299 (99%)	291 (98%)	5 (2%)	0	100	100
5	TI	296/299 (99%)	292 (99%)	4 (1%)	0	100	100
5	TJ	296/299 (99%)	291 (98%)	5 (2%)	0	100	100
5	TK	296/299 (99%)	292 (99%)	4 (1%)	0	100	100
5	TL	296/299 (99%)	291 (98%)	5 (2%)	0	100	100
6	XA	70/556 (13%)	67 (96%)	3 (4%)	0	100	100
6	XB	70/556 (13%)	68 (97%)	2 (3%)	0	100	100
6	XC	70/556 (13%)	67 (96%)	3 (4%)	0	100	100
6	XD	70/556 (13%)	68 (97%)	2 (3%)	0	100	100
6	XE	70/556 (13%)	67 (96%)	3 (4%)	0	100	100
6	XF	70/556 (13%)	68 (97%)	2 (3%)	0	100	100
6	XG	70/556 (13%)	67 (96%)	3 (4%)	0	100	100
6	XH	70/556 (13%)	68 (97%)	2 (3%)	0	100	100
6	XI	70/556 (13%)	67 (96%)	3 (4%)	0	100	100
6	XJ	70/556 (13%)	68 (97%)	2 (3%)	0	100	100
6	XK	70/556 (13%)	67 (96%)	3 (4%)	0	100	100
6	XL	70/556 (13%)	68 (97%)	2 (3%)	0	100	100
6	YA	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YB	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YC	64/556 (12%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	YD	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YE	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YF	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YG	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YH	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YI	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YJ	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YK	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	YL	64/556 (12%)	63 (98%)	1 (2%)	0	100	100
6	ZA	61/556 (11%)	61 (100%)	0	0	100	100
6	ZB	61/556 (11%)	61 (100%)	0	0	100	100
6	ZC	61/556 (11%)	61 (100%)	0	0	100	100
6	ZD	61/556 (11%)	61 (100%)	0	0	100	100
6	ZE	61/556 (11%)	61 (100%)	0	0	100	100
6	ZF	61/556 (11%)	61 (100%)	0	0	100	100
6	ZG	61/556 (11%)	61 (100%)	0	0	100	100
6	ZH	61/556 (11%)	61 (100%)	0	0	100	100
6	ZI	61/556 (11%)	61 (100%)	0	0	100	100
6	ZJ	61/556 (11%)	61 (100%)	0	0	100	100
6	ZK	61/556 (11%)	61 (100%)	0	0	100	100
6	ZL	61/556 (11%)	61 (100%)	0	0	100	100
7	OA	12/150 (8%)	12 (100%)	0	0	100	100
7	OB	12/150 (8%)	12 (100%)	0	0	100	100
7	OC	12/150 (8%)	12 (100%)	0	0	100	100
7	OD	12/150 (8%)	12 (100%)	0	0	100	100
7	OE	12/150 (8%)	12 (100%)	0	0	100	100
7	OF	12/150 (8%)	12 (100%)	0	0	100	100
7	OG	12/150 (8%)	12 (100%)	0	0	100	100
7	OH	12/150 (8%)	12 (100%)	0	0	100	100
7	OI	12/150 (8%)	12 (100%)	0	0	100	100
7	OJ	12/150 (8%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	OK	12/150 (8%)	12 (100%)	0	0	100	100
7	OL	12/150 (8%)	12 (100%)	0	0	100	100
All	All	26472/48186 (55%)	26018 (98%)	454 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	209/209 (100%)	208 (100%)	1 (0%)	81	83
1	AB	209/209 (100%)	206 (99%)	3 (1%)	59	74
1	AC	209/209 (100%)	208 (100%)	1 (0%)	81	83
1	AD	209/209 (100%)	206 (99%)	3 (1%)	59	74
1	AE	209/209 (100%)	208 (100%)	1 (0%)	81	83
1	AF	209/209 (100%)	206 (99%)	3 (1%)	59	74
1	AG	209/209 (100%)	208 (100%)	1 (0%)	81	83
1	AH	209/209 (100%)	206 (99%)	3 (1%)	59	74
1	AI	209/209 (100%)	208 (100%)	1 (0%)	81	83
1	AJ	209/209 (100%)	206 (99%)	3 (1%)	59	74
1	AK	209/209 (100%)	208 (100%)	1 (0%)	81	83
1	AL	209/209 (100%)	206 (99%)	3 (1%)	59	74
2	LA	989/1155 (86%)	972 (98%)	17 (2%)	53	71
2	LB	989/1155 (86%)	972 (98%)	17 (2%)	53	71
2	LC	989/1155 (86%)	971 (98%)	18 (2%)	51	70
2	LD	989/1155 (86%)	972 (98%)	17 (2%)	53	71
2	LE	989/1155 (86%)	972 (98%)	17 (2%)	53	71
2	LF	989/1155 (86%)	971 (98%)	18 (2%)	51	70
3	PA	579/652 (89%)	572 (99%)	7 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	PB	579/652 (89%)	568 (98%)	11 (2%)	50	69
3	PC	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PD	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PE	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PF	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PG	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PH	579/652 (89%)	571 (99%)	8 (1%)	59	74
3	PI	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PJ	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PK	579/652 (89%)	572 (99%)	7 (1%)	63	75
3	PL	579/652 (89%)	572 (99%)	7 (1%)	63	75
4	SA	369/371 (100%)	365 (99%)	4 (1%)	65	76
4	SB	369/371 (100%)	366 (99%)	3 (1%)	73	79
4	SC	369/371 (100%)	366 (99%)	3 (1%)	73	79
4	SD	369/371 (100%)	365 (99%)	4 (1%)	65	76
4	SE	369/371 (100%)	366 (99%)	3 (1%)	73	79
4	SF	369/371 (100%)	366 (99%)	3 (1%)	73	79
5	TA	243/244 (100%)	240 (99%)	3 (1%)	63	75
5	TB	243/244 (100%)	239 (98%)	4 (2%)	55	72
5	TC	243/244 (100%)	240 (99%)	3 (1%)	63	75
5	TD	243/244 (100%)	239 (98%)	4 (2%)	55	72
5	TE	243/244 (100%)	240 (99%)	3 (1%)	63	75
5	TF	243/244 (100%)	239 (98%)	4 (2%)	55	72
5	TG	243/244 (100%)	240 (99%)	3 (1%)	63	75
5	TH	243/244 (100%)	239 (98%)	4 (2%)	55	72
5	TI	243/244 (100%)	240 (99%)	3 (1%)	63	75
5	TJ	243/244 (100%)	239 (98%)	4 (2%)	55	72
5	TK	243/244 (100%)	240 (99%)	3 (1%)	63	75
5	TL	243/244 (100%)	239 (98%)	4 (2%)	55	72
6	XA	66/455 (14%)	64 (97%)	2 (3%)	36	61
6	XB	66/455 (14%)	65 (98%)	1 (2%)	57	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	XC	66/455 (14%)	64 (97%)	2 (3%)	36	61
6	XD	66/455 (14%)	65 (98%)	1 (2%)	57	73
6	XE	66/455 (14%)	64 (97%)	2 (3%)	36	61
6	XF	66/455 (14%)	65 (98%)	1 (2%)	57	73
6	XG	66/455 (14%)	64 (97%)	2 (3%)	36	61
6	XH	66/455 (14%)	65 (98%)	1 (2%)	57	73
6	XI	66/455 (14%)	64 (97%)	2 (3%)	36	61
6	XJ	66/455 (14%)	65 (98%)	1 (2%)	57	73
6	XK	66/455 (14%)	64 (97%)	2 (3%)	36	61
6	XL	66/455 (14%)	65 (98%)	1 (2%)	57	73
6	YA	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YB	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YC	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YD	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YE	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YF	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YG	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YH	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YI	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YJ	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YK	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	YL	62/455 (14%)	61 (98%)	1 (2%)	55	72
6	ZA	58/455 (13%)	58 (100%)	0	100	100
6	ZB	58/455 (13%)	56 (97%)	2 (3%)	32	59
6	ZC	58/455 (13%)	58 (100%)	0	100	100
6	ZD	58/455 (13%)	57 (98%)	1 (2%)	53	71
6	ZE	58/455 (13%)	58 (100%)	0	100	100
6	ZF	58/455 (13%)	57 (98%)	1 (2%)	53	71
6	ZG	58/455 (13%)	58 (100%)	0	100	100
6	ZH	58/455 (13%)	56 (97%)	2 (3%)	32	59
6	ZI	58/455 (13%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	ZJ	58/455 (13%)	56 (97%)	2 (3%)	32 59
6	ZK	58/455 (13%)	58 (100%)	0	100 100
6	ZL	58/455 (13%)	56 (97%)	2 (3%)	32 59
7	OA	12/118 (10%)	11 (92%)	1 (8%)	10 35
7	OB	12/118 (10%)	12 (100%)	0	100 100
7	OC	12/118 (10%)	11 (92%)	1 (8%)	10 35
7	OD	12/118 (10%)	12 (100%)	0	100 100
7	OE	12/118 (10%)	11 (92%)	1 (8%)	10 35
7	OF	12/118 (10%)	12 (100%)	0	100 100
7	OG	12/118 (10%)	11 (92%)	1 (8%)	10 35
7	OH	12/118 (10%)	12 (100%)	0	100 100
7	OI	12/118 (10%)	11 (92%)	1 (8%)	10 35
7	OJ	12/118 (10%)	12 (100%)	0	100 100
7	OK	12/118 (10%)	11 (92%)	1 (8%)	10 35
7	OL	12/118 (10%)	12 (100%)	0	100 100
All	All	22896/40212 (57%)	22571 (99%)	325 (1%)	57 74

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	23	THR
1	AB	148	ASN
1	AB	178	LEU
1	AB	219	THR
2	LA	28	ARG
2	LA	46	THR
2	LA	139	VAL
2	LA	183	VAL
2	LA	319	MET
2	LA	341	ILE
2	LA	592	ILE
2	LA	610	ASN
2	LA	611	VAL
2	LA	699	TRP
2	LA	707	VAL
2	LA	1038	LEU
2	LA	1113	VAL

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Mol	Chain	Res	Type
2	LA	1116	THR
2	LA	1135	LEU
2	LA	1176	VAL
2	LA	1179	GLN
3	PA	150	VAL
3	PA	219	TYR
3	PA	304	THR
3	PA	340	VAL
3	PA	351	LEU
3	PA	487	VAL
3	PA	675	LEU
4	SA	35	VAL
4	SA	102	LEU
4	SA	144	LEU
4	SA	328	ILE
5	TA	17	VAL
5	TA	113	THR
5	TA	282	ASN
6	XA	16	CYS
6	XA	24	ILE
6	XB	63	LEU
6	YA	63	LEU
6	YB	25	VAL
6	ZB	63	LEU
6	ZB	73	LEU
3	PB	111	VAL
3	PB	150	VAL
3	PB	219	TYR
3	PB	304	THR
3	PB	340	VAL
3	PB	351	LEU
3	PB	414	LYS
3	PB	437	GLN
3	PB	441	GLN
3	PB	487	VAL
3	PB	675	LEU
5	TB	17	VAL
5	TB	113	THR
5	TB	254	VAL
5	TB	282	ASN
1	AC	23	THR
1	AD	148	ASN

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Mol	Chain	Res	Type
1	AD	178	LEU
1	AD	219	THR
2	LB	28	ARG
2	LB	46	THR
2	LB	139	VAL
2	LB	183	VAL
2	LB	319	MET
2	LB	341	ILE
2	LB	592	ILE
2	LB	610	ASN
2	LB	611	VAL
2	LB	699	TRP
2	LB	707	VAL
2	LB	1038	LEU
2	LB	1113	VAL
2	LB	1116	THR
2	LB	1135	LEU
2	LB	1176	VAL
2	LB	1179	GLN
3	PC	150	VAL
3	PC	219	TYR
3	PC	304	THR
3	PC	340	VAL
3	PC	351	LEU
3	PC	487	VAL
3	PC	675	LEU
4	SB	102	LEU
4	SB	144	LEU
4	SB	328	ILE
5	TC	17	VAL
5	TC	113	THR
5	TC	282	ASN
6	XC	16	CYS
6	XC	24	ILE
6	XD	63	LEU
6	YC	63	LEU
6	YD	25	VAL
6	ZD	63	LEU
3	PD	150	VAL
3	PD	219	TYR
3	PD	304	THR
3	PD	340	VAL

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Mol	Chain	Res	Type
3	PD	351	LEU
3	PD	487	VAL
3	PD	675	LEU
5	TD	17	VAL
5	TD	113	THR
5	TD	254	VAL
5	TD	282	ASN
1	AE	23	THR
1	AF	148	ASN
1	AF	178	LEU
1	AF	219	THR
2	LC	28	ARG
2	LC	46	THR
2	LC	139	VAL
2	LC	183	VAL
2	LC	319	MET
2	LC	341	ILE
2	LC	355	VAL
2	LC	592	ILE
2	LC	610	ASN
2	LC	611	VAL
2	LC	699	TRP
2	LC	707	VAL
2	LC	1038	LEU
2	LC	1113	VAL
2	LC	1116	THR
2	LC	1135	LEU
2	LC	1176	VAL
2	LC	1179	GLN
3	PE	150	VAL
3	PE	219	TYR
3	PE	304	THR
3	PE	340	VAL
3	PE	351	LEU
3	PE	487	VAL
3	PE	675	LEU
4	SC	102	LEU
4	SC	144	LEU
4	SC	328	ILE
5	TE	17	VAL
5	TE	113	THR
5	TE	282	ASN

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Mol	Chain	Res	Type
6	XE	16	CYS
6	XE	24	ILE
6	XF	63	LEU
6	YE	63	LEU
6	YF	25	VAL
6	ZF	63	LEU
3	PF	150	VAL
3	PF	219	TYR
3	PF	304	THR
3	PF	340	VAL
3	PF	351	LEU
3	PF	487	VAL
3	PF	675	LEU
5	TF	17	VAL
5	TF	113	THR
5	TF	254	VAL
5	TF	282	ASN
1	AG	23	THR
1	AH	148	ASN
1	AH	178	LEU
1	AH	219	THR
2	LD	28	ARG
2	LD	46	THR
2	LD	139	VAL
2	LD	183	VAL
2	LD	319	MET
2	LD	341	ILE
2	LD	592	ILE
2	LD	610	ASN
2	LD	611	VAL
2	LD	699	TRP
2	LD	707	VAL
2	LD	1038	LEU
2	LD	1113	VAL
2	LD	1116	THR
2	LD	1135	LEU
2	LD	1176	VAL
2	LD	1179	GLN
3	PG	150	VAL
3	PG	219	TYR
3	PG	304	THR
3	PG	340	VAL

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Mol	Chain	Res	Type
3	PG	351	LEU
3	PG	487	VAL
3	PG	675	LEU
4	SD	35	VAL
4	SD	102	LEU
4	SD	144	LEU
4	SD	328	ILE
5	TG	17	VAL
5	TG	113	THR
5	TG	282	ASN
6	XG	16	CYS
6	XG	24	ILE
6	XH	63	LEU
6	YG	63	LEU
6	YH	25	VAL
6	ZH	63	LEU
6	ZH	73	LEU
3	PH	111	VAL
3	PH	150	VAL
3	PH	219	TYR
3	PH	304	THR
3	PH	340	VAL
3	PH	351	LEU
3	PH	487	VAL
3	PH	675	LEU
5	TH	17	VAL
5	TH	113	THR
5	TH	254	VAL
5	TH	282	ASN
1	AI	23	THR
1	AJ	148	ASN
1	AJ	178	LEU
1	AJ	219	THR
2	LE	28	ARG
2	LE	46	THR
2	LE	139	VAL
2	LE	183	VAL
2	LE	319	MET
2	LE	341	ILE
2	LE	592	ILE
2	LE	610	ASN
2	LE	611	VAL

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Mol	Chain	Res	Type
2	LE	699	TRP
2	LE	707	VAL
2	LE	1038	LEU
2	LE	1113	VAL
2	LE	1116	THR
2	LE	1135	LEU
2	LE	1176	VAL
2	LE	1179	GLN
3	PI	150	VAL
3	PI	219	TYR
3	PI	304	THR
3	PI	340	VAL
3	PI	351	LEU
3	PI	487	VAL
3	PI	675	LEU
4	SE	102	LEU
4	SE	144	LEU
4	SE	328	ILE
5	TI	17	VAL
5	TI	113	THR
5	TI	282	ASN
6	XI	16	CYS
6	XI	24	ILE
6	XJ	63	LEU
6	YI	63	LEU
6	YJ	25	VAL
6	ZJ	63	LEU
6	ZJ	73	LEU
3	PJ	150	VAL
3	PJ	219	TYR
3	PJ	304	THR
3	PJ	340	VAL
3	PJ	351	LEU
3	PJ	487	VAL
3	PJ	675	LEU
5	TJ	17	VAL
5	TJ	113	THR
5	TJ	254	VAL
5	TJ	282	ASN
1	AK	23	THR
1	AL	148	ASN
1	AL	178	LEU

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Mol	Chain	Res	Type
1	AL	219	THR
2	LF	28	ARG
2	LF	46	THR
2	LF	139	VAL
2	LF	183	VAL
2	LF	319	MET
2	LF	341	ILE
2	LF	355	VAL
2	LF	592	ILE
2	LF	610	ASN
2	LF	611	VAL
2	LF	699	TRP
2	LF	707	VAL
2	LF	1038	LEU
2	LF	1113	VAL
2	LF	1116	THR
2	LF	1135	LEU
2	LF	1176	VAL
2	LF	1179	GLN
3	PK	150	VAL
3	PK	219	TYR
3	PK	304	THR
3	PK	340	VAL
3	PK	351	LEU
3	PK	487	VAL
3	PK	675	LEU
4	SF	102	LEU
4	SF	144	LEU
4	SF	328	ILE
5	TK	17	VAL
5	TK	113	THR
5	TK	282	ASN
6	XK	16	CYS
6	XK	24	ILE
6	XL	63	LEU
6	YK	63	LEU
6	YL	25	VAL
6	ZL	63	LEU
6	ZL	73	LEU
3	PL	150	VAL
3	PL	219	TYR
3	PL	304	THR

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Mol	Chain	Res	Type
3	PL	340	VAL
3	PL	351	LEU
3	PL	487	VAL
3	PL	675	LEU
5	TL	17	VAL
5	TL	113	THR
5	TL	254	VAL
5	TL	282	ASN
7	OA	12	GLN
7	OC	12	GLN
7	OE	12	GLN
7	OG	12	GLN
7	OI	12	GLN
7	OK	12	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (372) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	58	ASN
1	AA	69	ASN
1	AA	191	ASN
1	AB	13	ASN
1	AB	53	ASN
1	AB	56	ASN
1	AB	58	ASN
1	AB	64	GLN
1	AB	134	ASN
1	AB	148	ASN
1	AB	227	ASN
2	LA	93	ASN
2	LA	159	ASN
2	LA	219	ASN
2	LA	311	ASN
2	LA	362	GLN
2	LA	422	GLN
2	LA	447	GLN
2	LA	481	HIS
2	LA	509	GLN
2	LA	532	HIS
2	LA	882	ASN
2	LA	969	ASN
2	LA	1093	GLN

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Mol	Chain	Res	Type
2	LA	1109	GLN
3	PA	73	GLN
3	PA	75	GLN
3	PA	187	GLN
3	PA	222	GLN
3	PA	310	GLN
3	PA	388	GLN
3	PA	437	GLN
3	PA	567	GLN
3	PA	614	GLN
4	SA	57	GLN
4	SA	93	HIS
4	SA	205	GLN
4	SA	217	ASN
5	TA	116	GLN
5	TA	148	GLN
5	TA	194	GLN
6	XA	12	ASN
6	XA	80	HIS
6	ZB	60	HIS
6	ZB	61	ASN
3	PB	73	GLN
3	PB	75	GLN
3	PB	187	GLN
3	PB	222	GLN
3	PB	259	ASN
3	PB	310	GLN
3	PB	388	GLN
3	PB	441	GLN
3	PB	614	GLN
5	TB	116	GLN
5	TB	148	GLN
5	TB	194	GLN
5	TB	198	GLN
5	TB	282	ASN
5	TB	295	ASN
5	TB	296	ASN
1	AC	58	ASN
1	AD	13	ASN
1	AD	53	ASN
1	AD	56	ASN
1	AD	58	ASN

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Mol	Chain	Res	Type
1	AD	64	GLN
1	AD	134	ASN
1	AD	148	ASN
1	AD	227	ASN
2	LB	93	ASN
2	LB	159	ASN
2	LB	219	ASN
2	LB	311	ASN
2	LB	362	GLN
2	LB	447	GLN
2	LB	481	HIS
2	LB	509	GLN
2	LB	532	HIS
2	LB	564	ASN
2	LB	662	HIS
2	LB	882	ASN
2	LB	969	ASN
2	LB	1093	GLN
2	LB	1109	GLN
3	PC	73	GLN
3	PC	75	GLN
3	PC	187	GLN
3	PC	222	GLN
3	PC	259	ASN
3	PC	310	GLN
3	PC	388	GLN
3	PC	437	GLN
3	PC	567	GLN
3	PC	614	GLN
4	SB	57	GLN
4	SB	205	GLN
4	SB	217	ASN
5	TC	116	GLN
5	TC	148	GLN
5	TC	194	GLN
6	XC	12	ASN
6	XC	80	HIS
6	XD	77	GLN
6	ZD	60	HIS
6	ZD	61	ASN
3	PD	73	GLN
3	PD	75	GLN

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Mol	Chain	Res	Type
3	PD	124	GLN
3	PD	187	GLN
3	PD	222	GLN
3	PD	259	ASN
3	PD	310	GLN
3	PD	388	GLN
3	PD	524	ASN
3	PD	567	GLN
3	PD	614	GLN
5	TD	116	GLN
5	TD	148	GLN
5	TD	194	GLN
5	TD	198	GLN
5	TD	282	ASN
5	TD	295	ASN
5	TD	296	ASN
1	AE	13	ASN
1	AE	58	ASN
1	AF	13	ASN
1	AF	53	ASN
1	AF	56	ASN
1	AF	58	ASN
1	AF	64	GLN
1	AF	134	ASN
1	AF	148	ASN
1	AF	227	ASN
2	LC	93	ASN
2	LC	159	ASN
2	LC	219	ASN
2	LC	311	ASN
2	LC	362	GLN
2	LC	447	GLN
2	LC	481	HIS
2	LC	509	GLN
2	LC	532	HIS
2	LC	882	ASN
2	LC	969	ASN
2	LC	1093	GLN
2	LC	1109	GLN
3	PE	73	GLN
3	PE	75	GLN
3	PE	187	GLN

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Mol	Chain	Res	Type
3	PE	222	GLN
3	PE	259	ASN
3	PE	310	GLN
3	PE	388	GLN
3	PE	437	GLN
3	PE	567	GLN
3	PE	614	GLN
4	SC	57	GLN
4	SC	93	HIS
4	SC	205	GLN
4	SC	217	ASN
5	TE	116	GLN
5	TE	148	GLN
5	TE	194	GLN
6	XE	12	ASN
6	XE	80	HIS
6	ZE	77	GLN
6	ZF	60	HIS
6	ZF	61	ASN
3	PF	73	GLN
3	PF	75	GLN
3	PF	187	GLN
3	PF	222	GLN
3	PF	259	ASN
3	PF	283	HIS
3	PF	310	GLN
3	PF	388	GLN
3	PF	567	GLN
3	PF	614	GLN
5	TF	41	ASN
5	TF	116	GLN
5	TF	148	GLN
5	TF	194	GLN
5	TF	282	ASN
5	TF	295	ASN
5	TF	296	ASN
1	AG	58	ASN
1	AG	191	ASN
1	AH	13	ASN
1	AH	53	ASN
1	AH	56	ASN
1	AH	58	ASN

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Mol	Chain	Res	Type
1	AH	64	GLN
1	AH	134	ASN
1	AH	148	ASN
1	AH	227	ASN
2	LD	93	ASN
2	LD	159	ASN
2	LD	219	ASN
2	LD	311	ASN
2	LD	362	GLN
2	LD	447	GLN
2	LD	481	HIS
2	LD	509	GLN
2	LD	532	HIS
2	LD	882	ASN
2	LD	969	ASN
2	LD	1093	GLN
2	LD	1109	GLN
3	PG	73	GLN
3	PG	75	GLN
3	PG	187	GLN
3	PG	222	GLN
3	PG	259	ASN
3	PG	310	GLN
3	PG	388	GLN
3	PG	437	GLN
3	PG	567	GLN
3	PG	614	GLN
4	SD	57	GLN
4	SD	205	GLN
4	SD	217	ASN
5	TG	116	GLN
5	TG	148	GLN
5	TG	194	GLN
6	XG	12	ASN
6	XG	80	HIS
6	XH	77	GLN
6	ZG	77	GLN
6	ZH	60	HIS
6	ZH	61	ASN
3	PH	73	GLN
3	PH	75	GLN
3	PH	187	GLN

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Mol	Chain	Res	Type
3	PH	222	GLN
3	PH	259	ASN
3	PH	310	GLN
3	PH	388	GLN
3	PH	567	GLN
3	PH	614	GLN
5	TH	116	GLN
5	TH	148	GLN
5	TH	194	GLN
5	TH	198	GLN
5	TH	282	ASN
5	TH	295	ASN
5	TH	296	ASN
1	AI	58	ASN
1	AI	191	ASN
1	AJ	13	ASN
1	AJ	53	ASN
1	AJ	56	ASN
1	AJ	58	ASN
1	AJ	134	ASN
1	AJ	148	ASN
1	AJ	227	ASN
2	LE	45	ASN
2	LE	93	ASN
2	LE	159	ASN
2	LE	219	ASN
2	LE	311	ASN
2	LE	362	GLN
2	LE	447	GLN
2	LE	481	HIS
2	LE	509	GLN
2	LE	532	HIS
2	LE	882	ASN
2	LE	969	ASN
2	LE	1093	GLN
2	LE	1109	GLN
3	PI	73	GLN
3	PI	75	GLN
3	PI	187	GLN
3	PI	222	GLN
3	PI	259	ASN
3	PI	310	GLN

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Mol	Chain	Res	Type
3	PI	388	GLN
3	PI	437	GLN
3	PI	567	GLN
3	PI	614	GLN
4	SE	93	HIS
4	SE	205	GLN
4	SE	217	ASN
5	TI	116	GLN
5	TI	148	GLN
5	TI	194	GLN
6	XI	12	ASN
6	XI	80	HIS
6	XJ	77	GLN
6	ZI	77	GLN
6	ZJ	60	HIS
6	ZJ	61	ASN
3	PJ	73	GLN
3	PJ	75	GLN
3	PJ	187	GLN
3	PJ	222	GLN
3	PJ	259	ASN
3	PJ	283	HIS
3	PJ	310	GLN
3	PJ	388	GLN
3	PJ	567	GLN
3	PJ	614	GLN
5	TJ	116	GLN
5	TJ	148	GLN
5	TJ	194	GLN
5	TJ	198	GLN
5	TJ	282	ASN
5	TJ	295	ASN
5	TJ	296	ASN
1	AK	58	ASN
1	AK	191	ASN
1	AL	13	ASN
1	AL	53	ASN
1	AL	56	ASN
1	AL	58	ASN
1	AL	64	GLN
1	AL	134	ASN
1	AL	148	ASN

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Mol	Chain	Res	Type
1	AL	227	ASN
2	LF	93	ASN
2	LF	159	ASN
2	LF	219	ASN
2	LF	311	ASN
2	LF	362	GLN
2	LF	447	GLN
2	LF	481	HIS
2	LF	509	GLN
2	LF	532	HIS
2	LF	882	ASN
2	LF	888	GLN
2	LF	969	ASN
2	LF	1093	GLN
2	LF	1109	GLN
2	LF	1179	GLN
3	PK	73	GLN
3	PK	75	GLN
3	PK	187	GLN
3	PK	222	GLN
3	PK	259	ASN
3	PK	310	GLN
3	PK	388	GLN
3	PK	437	GLN
3	PK	567	GLN
3	PK	614	GLN
4	SF	57	GLN
4	SF	93	HIS
4	SF	205	GLN
4	SF	217	ASN
5	TK	116	GLN
5	TK	148	GLN
5	TK	194	GLN
6	XK	12	ASN
6	XK	80	HIS
6	XL	77	GLN
6	ZK	77	GLN
6	ZL	60	HIS
6	ZL	61	ASN
3	PL	73	GLN
3	PL	75	GLN
3	PL	187	GLN

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Mol	Chain	Res	Type
3	PL	222	GLN
3	PL	259	ASN
3	PL	310	GLN
3	PL	567	GLN
3	PL	614	GLN
5	TL	116	GLN
5	TL	148	GLN
5	TL	194	GLN
5	TL	198	GLN
5	TL	282	ASN
5	TL	295	ASN
5	TL	296	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

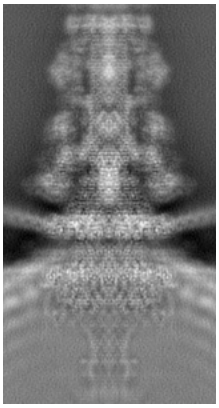
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72876. These allow visual inspection of the internal detail of the map and identification of artifacts.

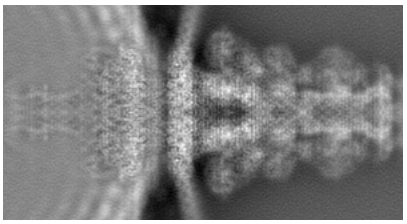
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

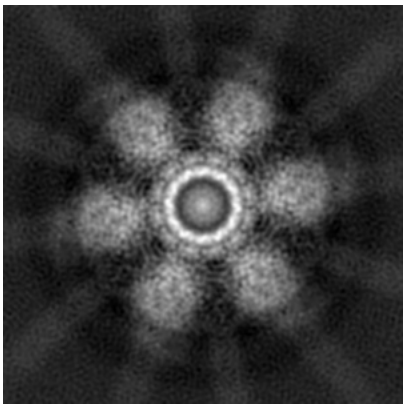
6.1.1 Primary map



X

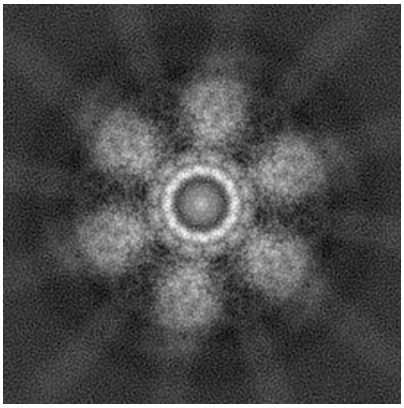


Y

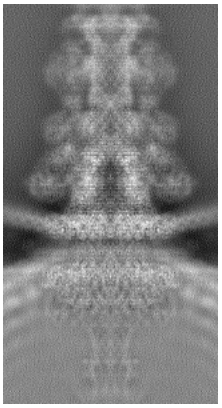


Z

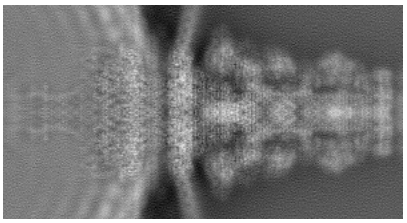
6.1.2 Raw map



X



Y

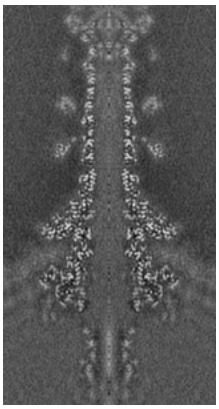


Z

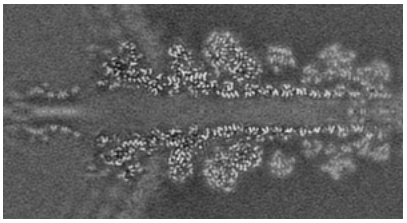
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

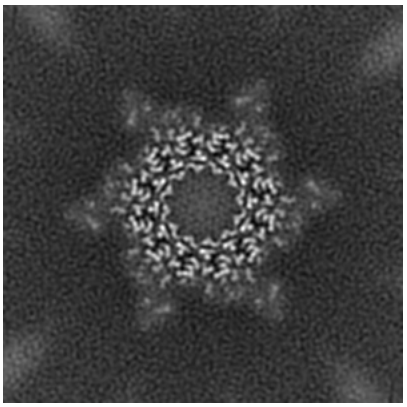
6.2.1 Primary map



X Index: 111

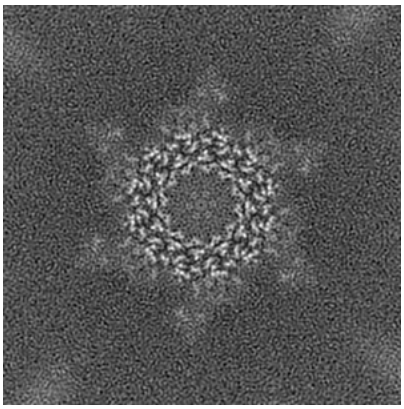


Y Index: 111

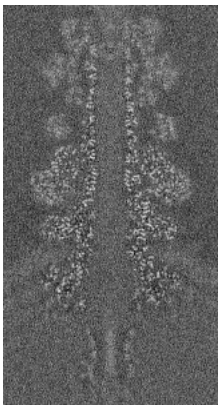


Z Index: 209

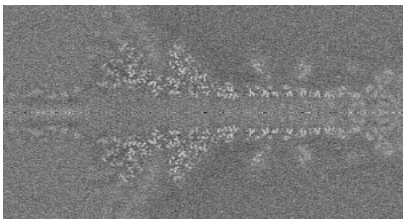
6.2.2 Raw map



X Index: 209



Y Index: 111

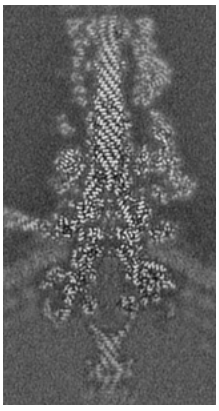


Z Index: 111

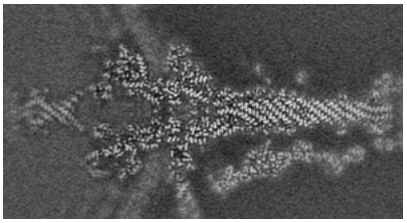
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

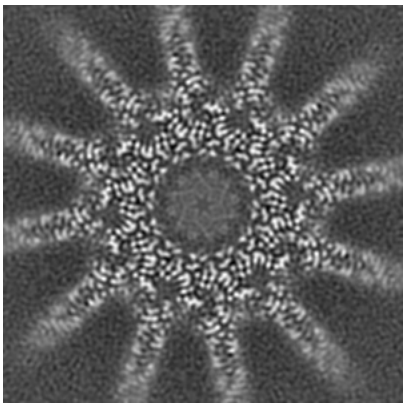
6.3.1 Primary map



X Index: 129

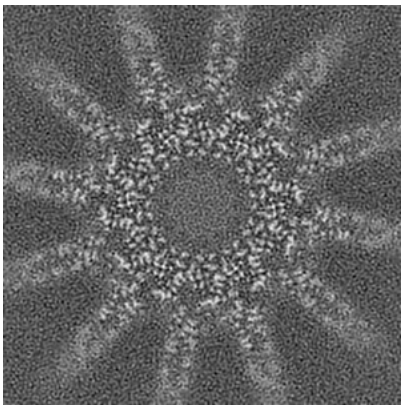


Y Index: 92

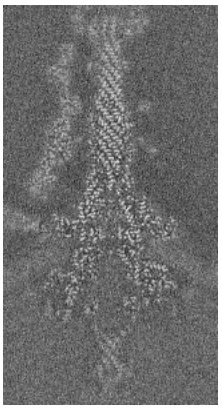


Z Index: 189

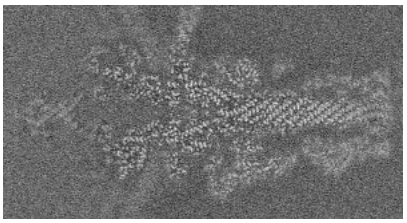
6.3.2 Raw map



X Index: 189



Y Index: 92

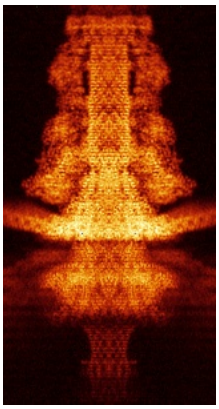


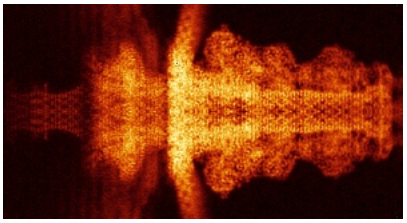
Z Index: 93

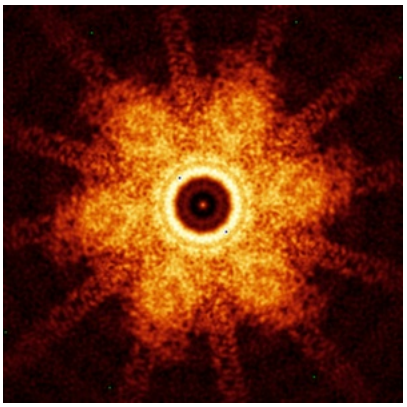
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

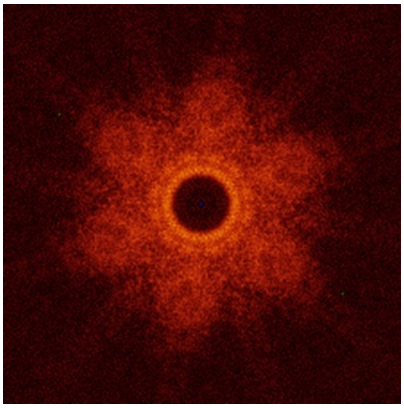
6.4.1 Primary map

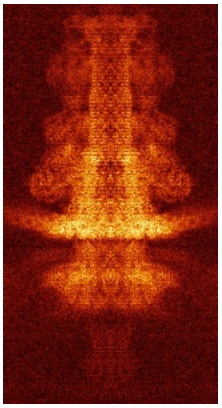

X

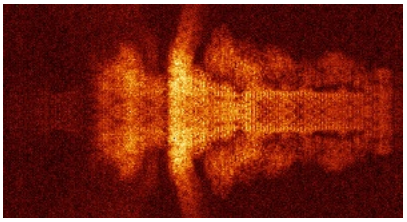

Y


Z

6.4.2 Raw map


X

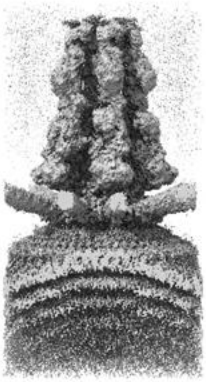

Y


Z

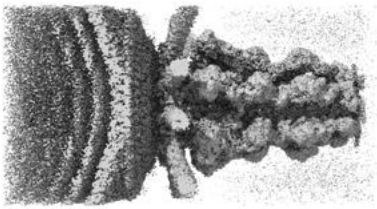
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

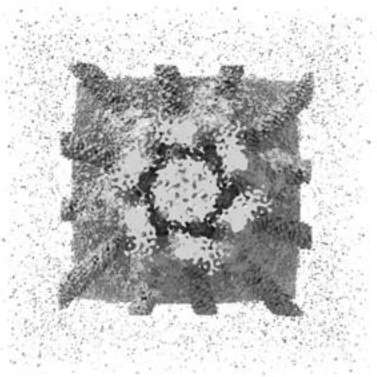
6.5.1 Primary map



X



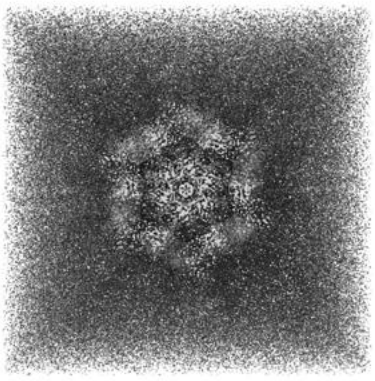
Y



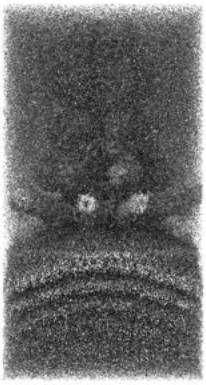
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0693. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

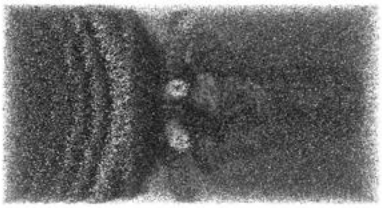
6.5.2 Raw map



X



Y



Z

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

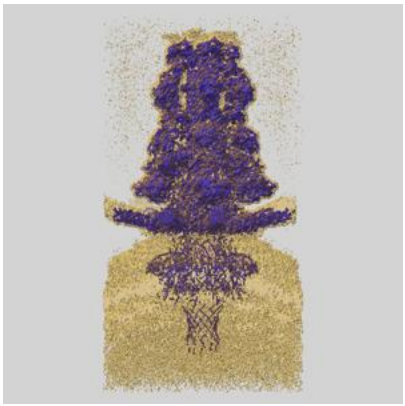
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

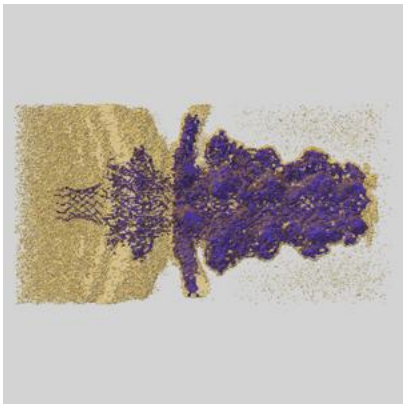
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

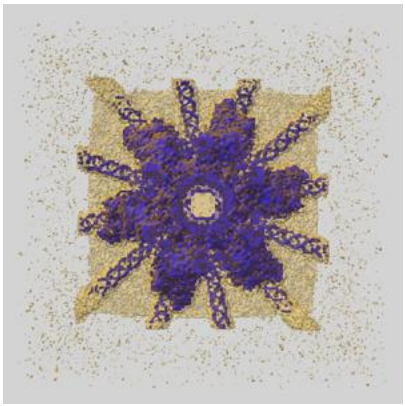
6.6.1 emd_72876_msk_1.map (i)



X



Y

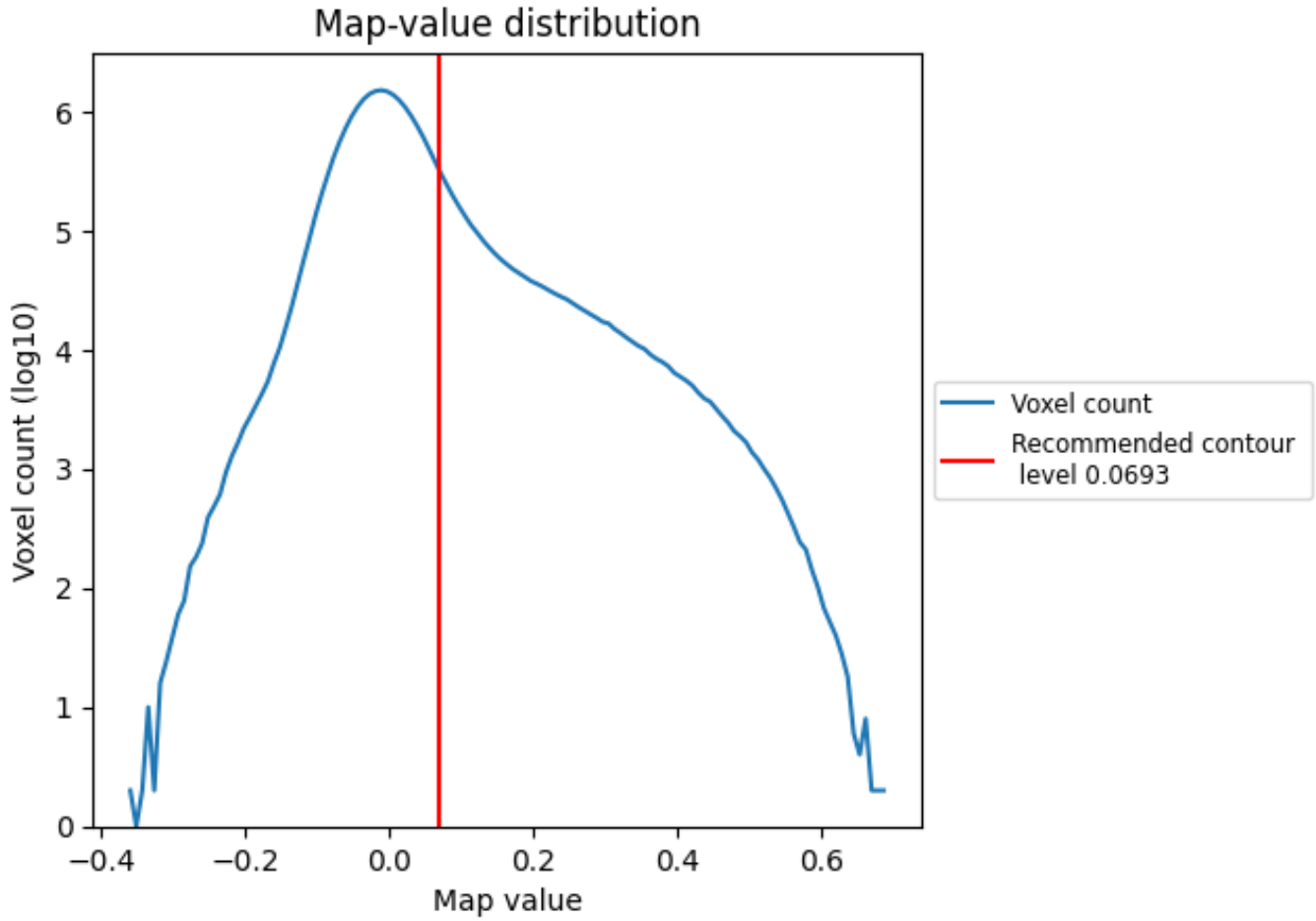


Z

7 Map analysis

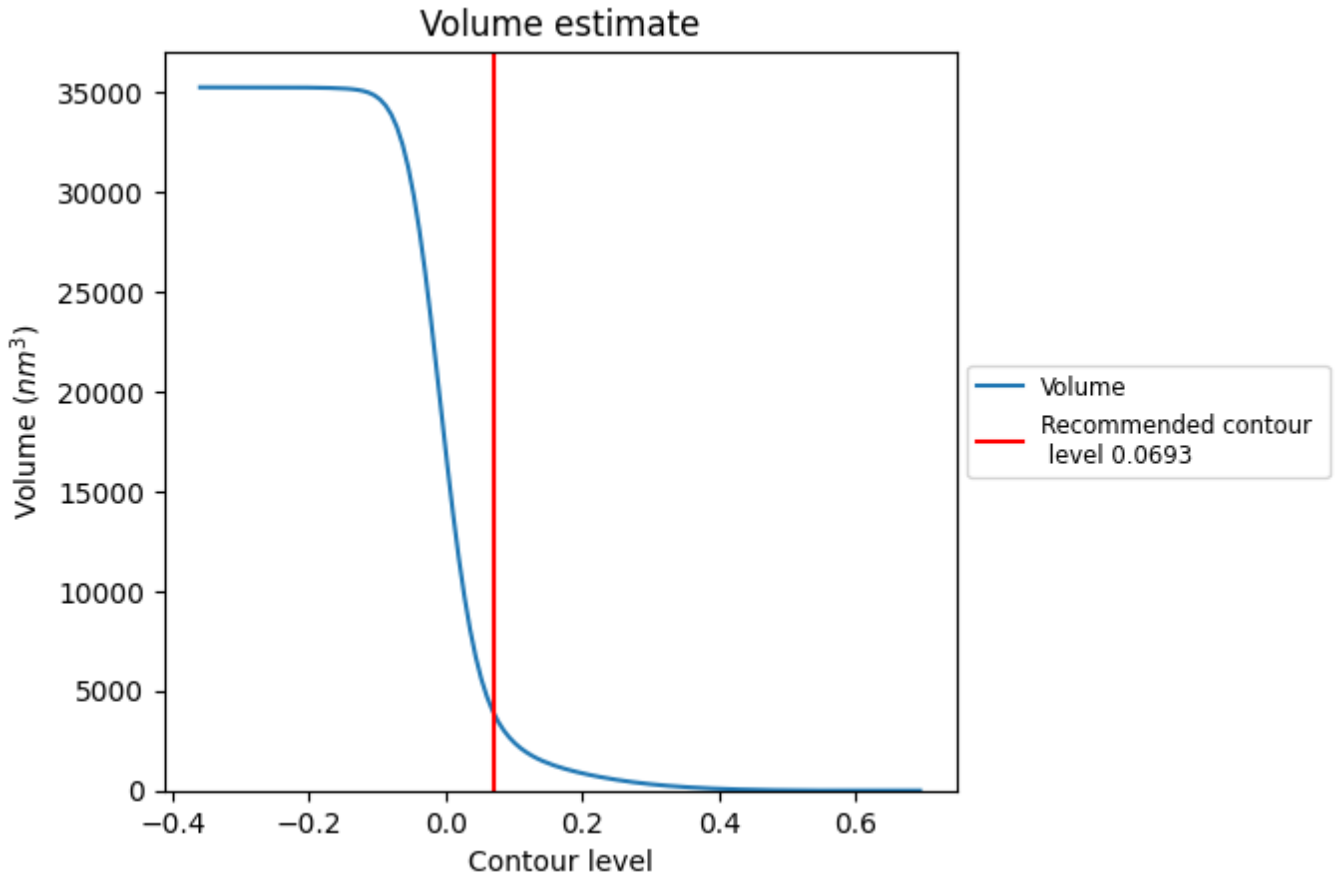
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 3953 nm^3; this corresponds to an approximate mass of 3571 kDa.

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

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

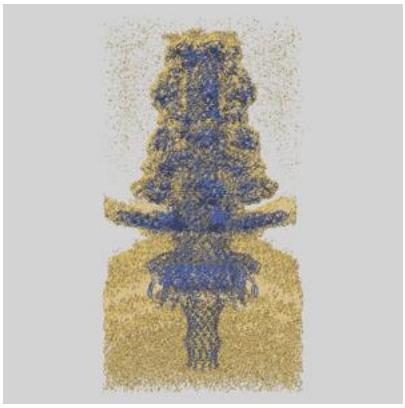
8 Fourier-Shell correlation

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

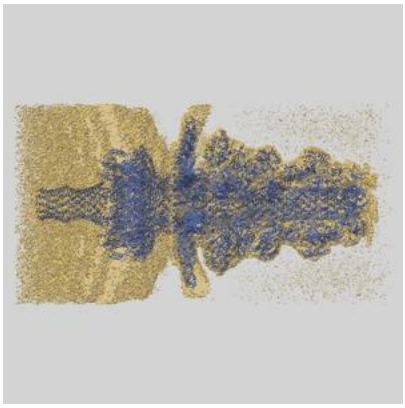
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72876 and PDB model 9YF4. Per-residue inclusion information can be found in section 3 on page 13.

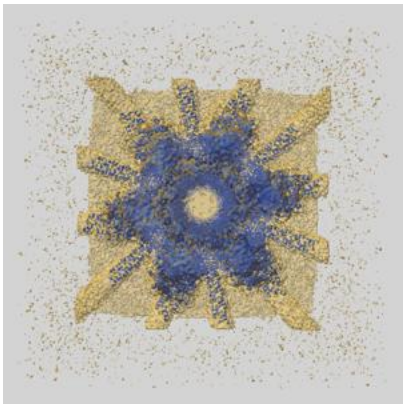
9.1 Map-model overlay



X



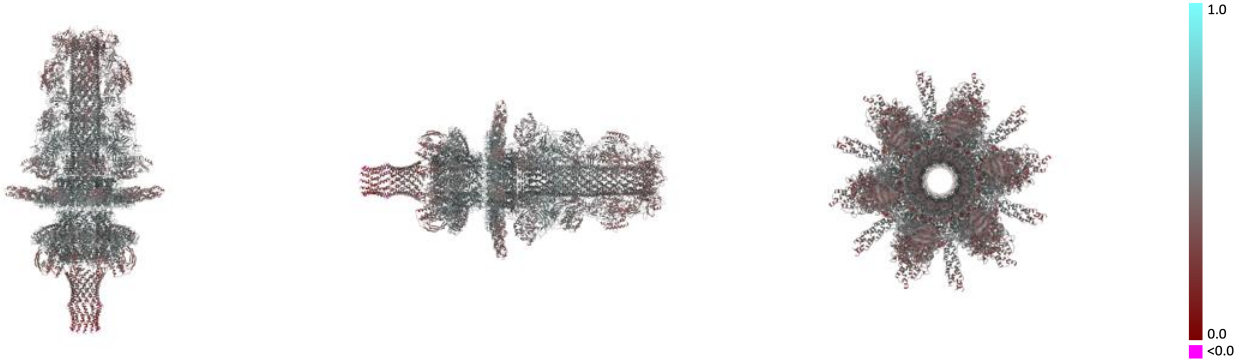
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0693 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

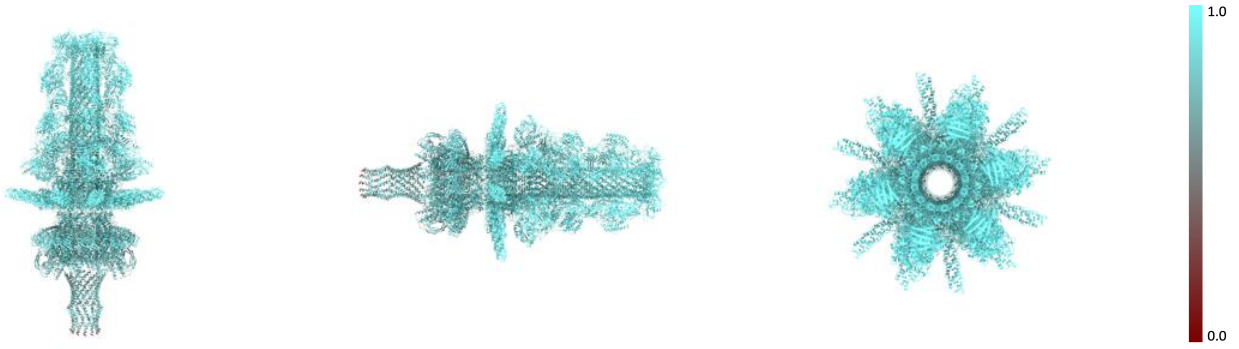
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

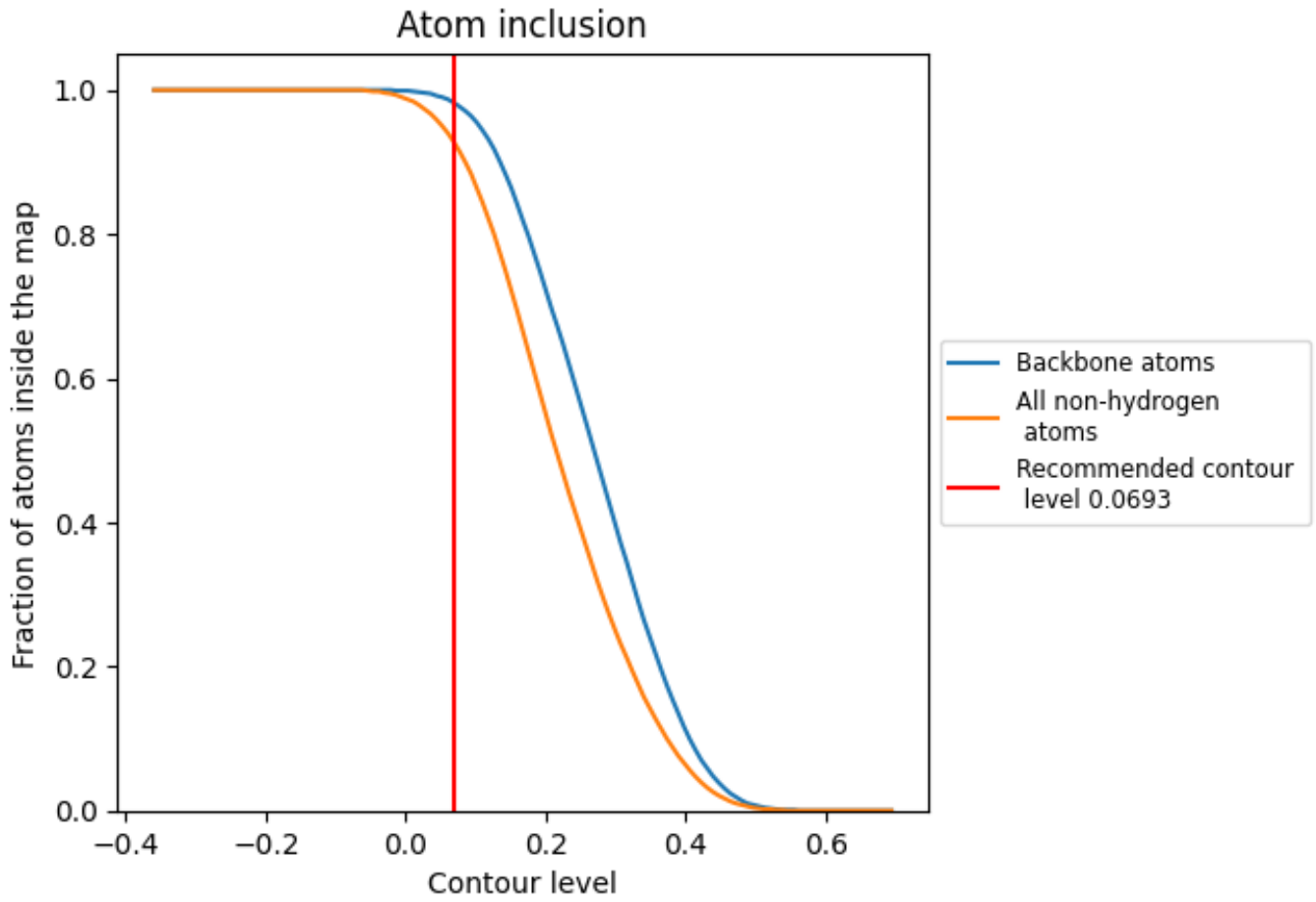
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0693).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0693) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9270	0.4620
AA	0.9570	0.5230
AB	0.9610	0.5240
AC	0.9560	0.5220
AD	0.9600	0.5260
AE	0.9570	0.5210
AF	0.9610	0.5270
AG	0.9570	0.5230
AH	0.9610	0.5250
AI	0.9560	0.5210
AJ	0.9600	0.5270
AK	0.9570	0.5220
AL	0.9610	0.5270
LA	0.9800	0.4510
LB	0.9810	0.4510
LC	0.9800	0.4510
LD	0.9800	0.4520
LE	0.9810	0.4510
LF	0.9800	0.4500
OA	0.9140	0.5080
OB	0.8670	0.4740
OC	0.8950	0.4980
OD	0.8670	0.4740
OE	0.9050	0.5060
OF	0.8670	0.4720
OG	0.9140	0.5090
OH	0.8670	0.4750
OI	0.8950	0.5030
OJ	0.8670	0.4730
OK	0.9050	0.5030
OL	0.8670	0.4780
PA	0.8270	0.4580
PB	0.8190	0.4480
PC	0.8240	0.4570
PD	0.8190	0.4470

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Chain	Atom inclusion	Q-score
PE	0.8260	0.4560
PF	0.8180	0.4450
PG	0.8270	0.4570
PH	0.8190	0.4460
PI	0.8240	0.4580
PJ	0.8190	0.4460
PK	0.8260	0.4580
PL	0.8180	0.4470
SA	0.9810	0.4550
SB	0.9810	0.4530
SC	0.9810	0.4530
SD	0.9810	0.4540
SE	0.9810	0.4530
SF	0.9810	0.4520
TA	0.9680	0.4790
TB	0.9640	0.4700
TC	0.9690	0.4790
TD	0.9660	0.4690
TE	0.9690	0.4780
TF	0.9650	0.4690
TG	0.9680	0.4780
TH	0.9640	0.4690
TI	0.9690	0.4780
TJ	0.9660	0.4710
TK	0.9690	0.4790
TL	0.9650	0.4710
XA	0.9790	0.4570
XB	0.9600	0.4390
XC	0.9810	0.4570
XD	0.9610	0.4450
XE	0.9810	0.4540
XF	0.9600	0.4440
XG	0.9790	0.4560
XH	0.9600	0.4420
XI	0.9810	0.4540
XJ	0.9610	0.4410
XK	0.9810	0.4540
XL	0.9600	0.4400
YA	0.9850	0.4590
YB	0.9670	0.4530
YC	0.9870	0.4620
YD	0.9680	0.4540

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Chain	Atom inclusion	Q-score
YE	0.9810	0.4610
YF	0.9670	0.4540
YG	0.9850	0.4590
YH	0.9670	0.4540
YI	0.9870	0.4600
YJ	0.9680	0.4500
YK	0.9810	0.4590
YL	0.9670	0.4520
ZA	0.9800	0.4370
ZB	0.9820	0.4310
ZC	0.9800	0.4360
ZD	0.9800	0.4320
ZE	0.9800	0.4420
ZF	0.9800	0.4310
ZG	0.9800	0.4370
ZH	0.9820	0.4340
ZI	0.9800	0.4370
ZJ	0.9800	0.4330
ZK	0.9800	0.4390
ZL	0.9800	0.4290