Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 09:26 AM EST

PDB ID	:	4EO2
Title	:	Structure of the bacteriophage C1 tail knob protein, gp12
Authors	:	Aksyuk, A.A.; Rossmann, M.G.
Deposited on	:	2012-04-13
Resolution	:	3.01 Å(reported)

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

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

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

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

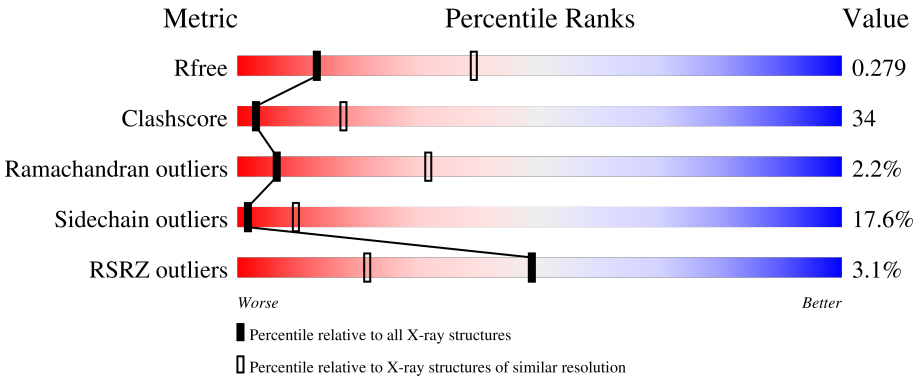
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	583	2% 42% 30% 11% • 16%
1	B	583	% 42% 31% 10% • 16%
1	C	583	3% 42% 30% 11% • 16%
1	D	583	4% 39% 34% 11% 16%
1	E	583	3% 39% 33% 11% • 16%

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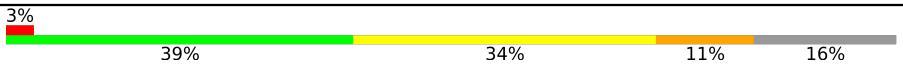
Mol	Chain	Length	Quality of chain
1	F	583	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major tail protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	B	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	C	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	D	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	E	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	F	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP Q7Y3F0
A	576	LEU	-	expression tag	UNP Q7Y3F0
A	577	GLU	-	expression tag	UNP Q7Y3F0
A	578	HIS	-	expression tag	UNP Q7Y3F0
A	579	HIS	-	expression tag	UNP Q7Y3F0
A	580	HIS	-	expression tag	UNP Q7Y3F0
A	581	HIS	-	expression tag	UNP Q7Y3F0
A	582	HIS	-	expression tag	UNP Q7Y3F0
A	583	HIS	-	expression tag	UNP Q7Y3F0
B	575	SER	-	expression tag	UNP Q7Y3F0
B	576	LEU	-	expression tag	UNP Q7Y3F0
B	577	GLU	-	expression tag	UNP Q7Y3F0
B	578	HIS	-	expression tag	UNP Q7Y3F0
B	579	HIS	-	expression tag	UNP Q7Y3F0
B	580	HIS	-	expression tag	UNP Q7Y3F0
B	581	HIS	-	expression tag	UNP Q7Y3F0
B	582	HIS	-	expression tag	UNP Q7Y3F0

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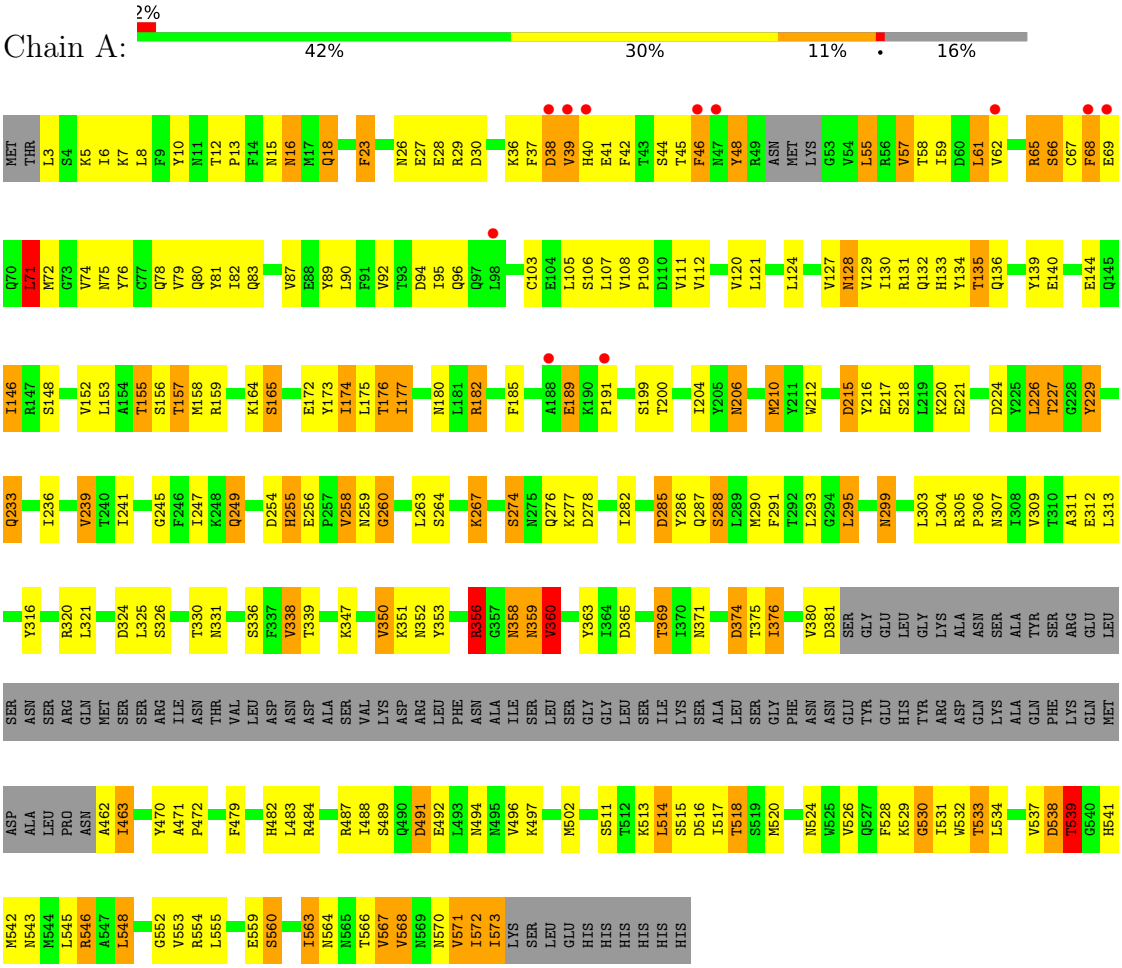
Chain	Residue	Modelled	Actual	Comment	Reference
B	583	HIS	-	expression tag	UNP Q7Y3F0
C	575	SER	-	expression tag	UNP Q7Y3F0
C	576	LEU	-	expression tag	UNP Q7Y3F0
C	577	GLU	-	expression tag	UNP Q7Y3F0
C	578	HIS	-	expression tag	UNP Q7Y3F0
C	579	HIS	-	expression tag	UNP Q7Y3F0
C	580	HIS	-	expression tag	UNP Q7Y3F0
C	581	HIS	-	expression tag	UNP Q7Y3F0
C	582	HIS	-	expression tag	UNP Q7Y3F0
C	583	HIS	-	expression tag	UNP Q7Y3F0
D	575	SER	-	expression tag	UNP Q7Y3F0
D	576	LEU	-	expression tag	UNP Q7Y3F0
D	577	GLU	-	expression tag	UNP Q7Y3F0
D	578	HIS	-	expression tag	UNP Q7Y3F0
D	579	HIS	-	expression tag	UNP Q7Y3F0
D	580	HIS	-	expression tag	UNP Q7Y3F0
D	581	HIS	-	expression tag	UNP Q7Y3F0
D	582	HIS	-	expression tag	UNP Q7Y3F0
D	583	HIS	-	expression tag	UNP Q7Y3F0
E	575	SER	-	expression tag	UNP Q7Y3F0
E	576	LEU	-	expression tag	UNP Q7Y3F0
E	577	GLU	-	expression tag	UNP Q7Y3F0
E	578	HIS	-	expression tag	UNP Q7Y3F0
E	579	HIS	-	expression tag	UNP Q7Y3F0
E	580	HIS	-	expression tag	UNP Q7Y3F0
E	581	HIS	-	expression tag	UNP Q7Y3F0
E	582	HIS	-	expression tag	UNP Q7Y3F0
E	583	HIS	-	expression tag	UNP Q7Y3F0
F	575	SER	-	expression tag	UNP Q7Y3F0
F	576	LEU	-	expression tag	UNP Q7Y3F0
F	577	GLU	-	expression tag	UNP Q7Y3F0
F	578	HIS	-	expression tag	UNP Q7Y3F0
F	579	HIS	-	expression tag	UNP Q7Y3F0
F	580	HIS	-	expression tag	UNP Q7Y3F0
F	581	HIS	-	expression tag	UNP Q7Y3F0
F	582	HIS	-	expression tag	UNP Q7Y3F0
F	583	HIS	-	expression tag	UNP Q7Y3F0

3 Residue-property plots (i)

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

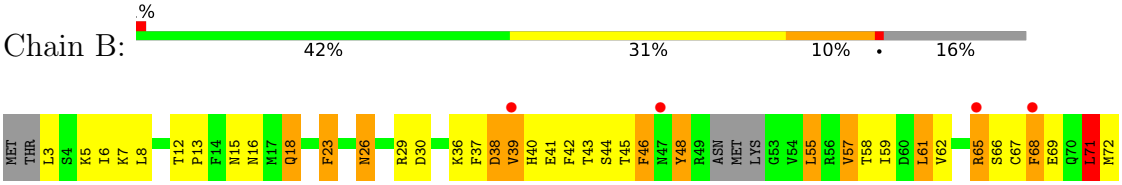
• Molecule 1: Major tail protein

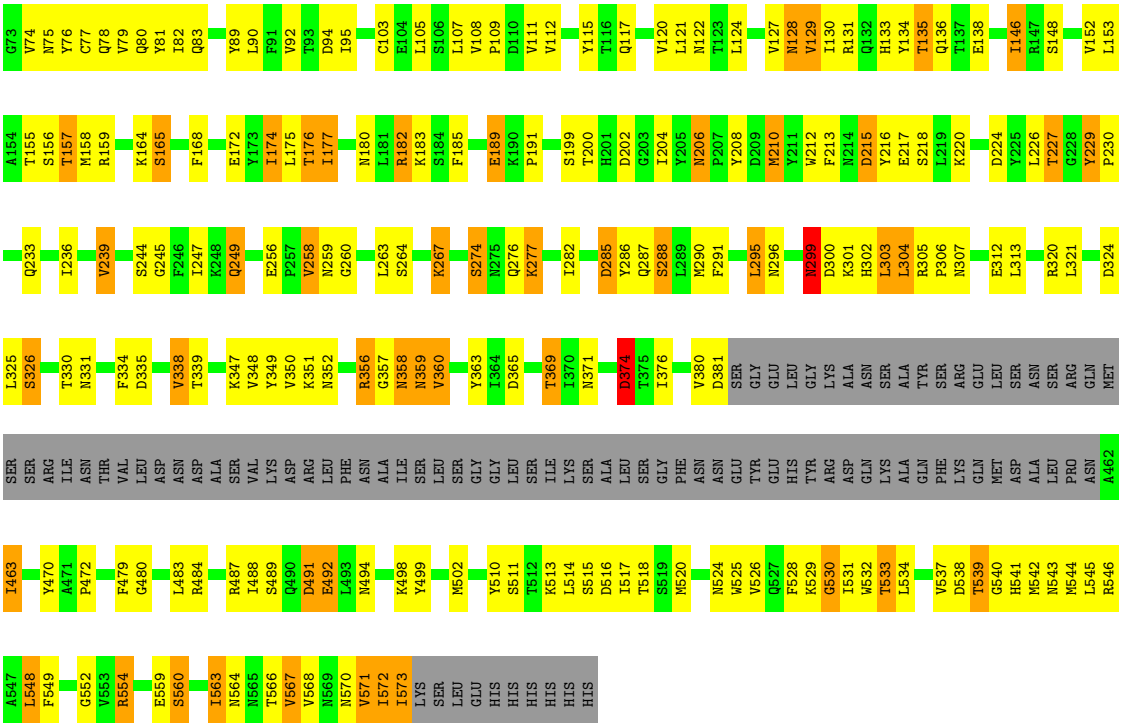
Chain A:



• Molecule 1: Major tail protein

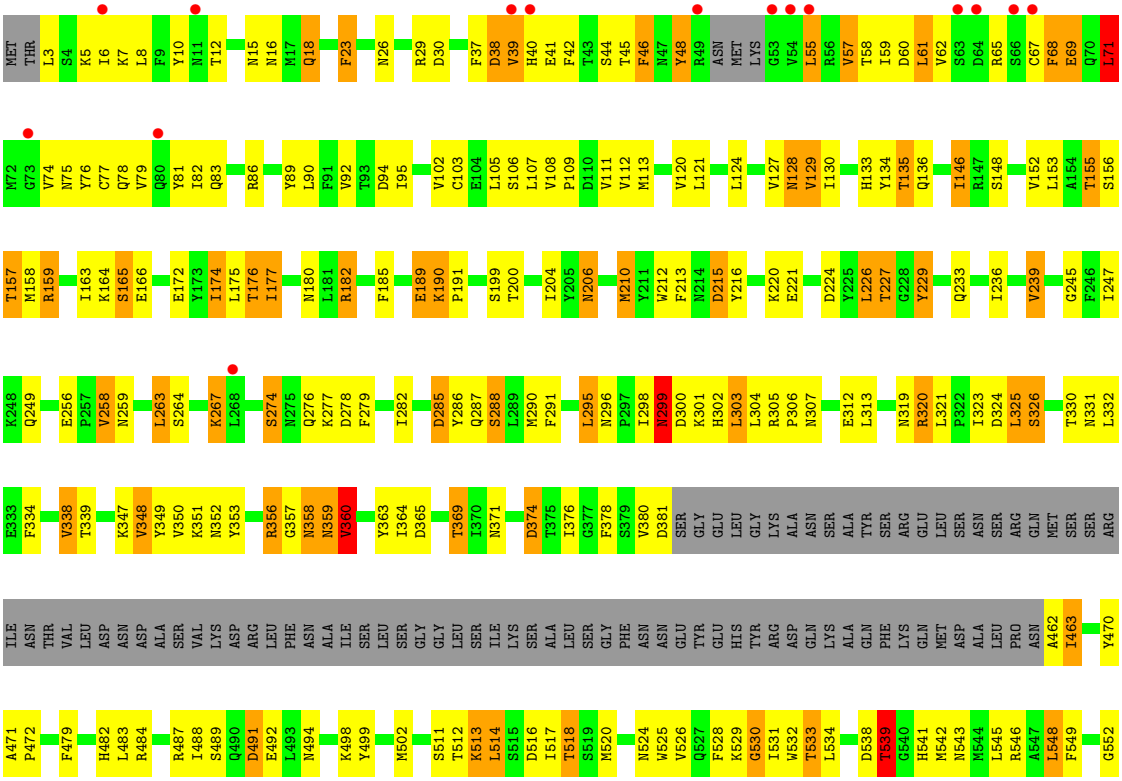
Chain B:

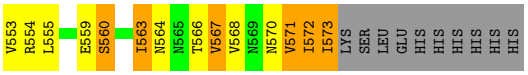




• Molecule 1: Major tail protein

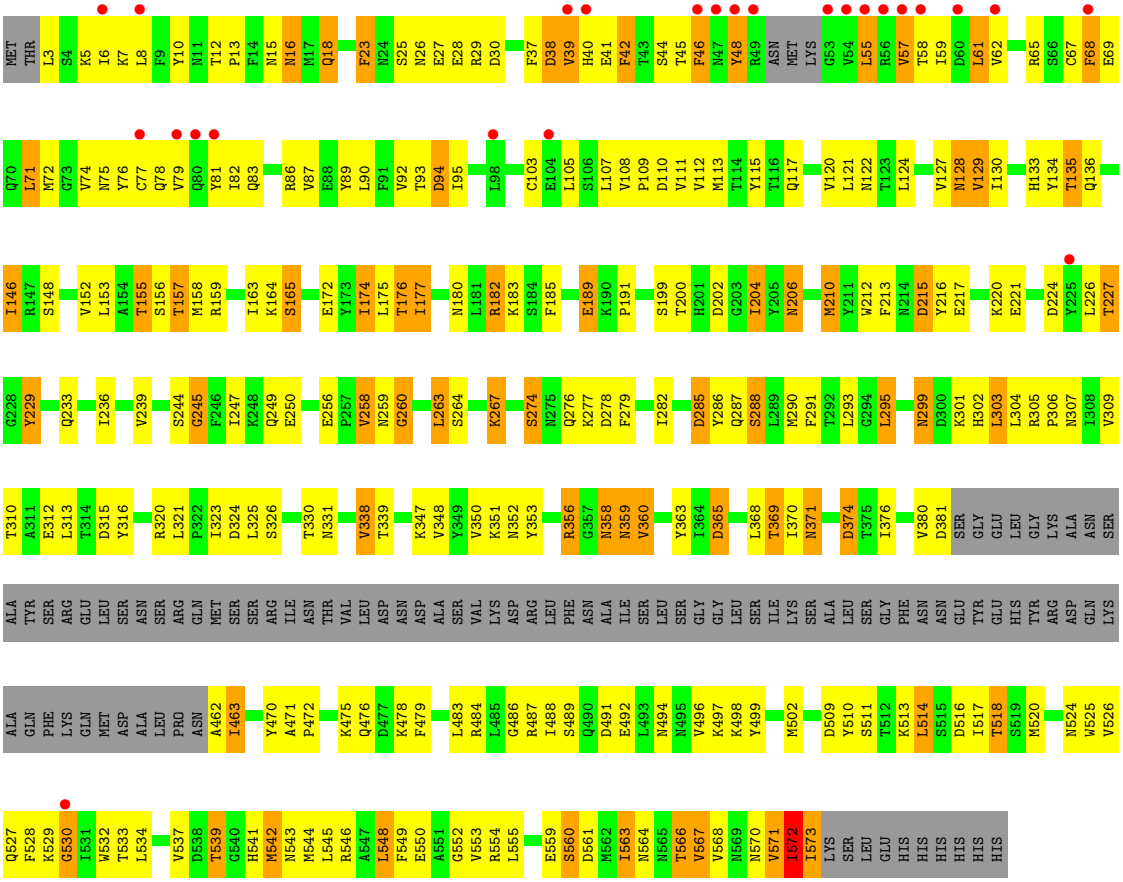
Chain C:





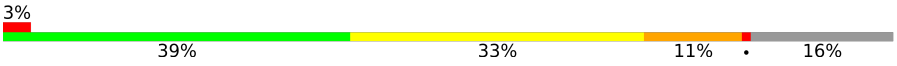
• Molecule 1: Major tail protein

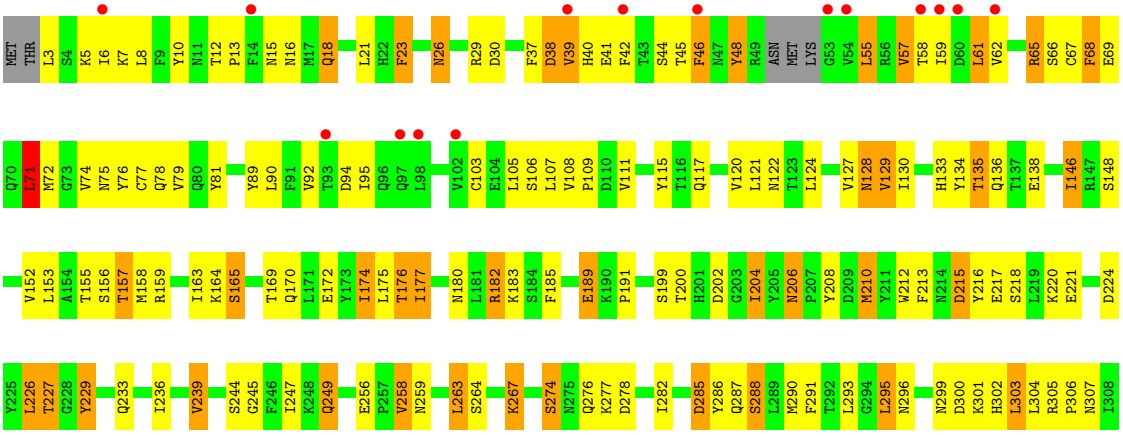
Chain D:

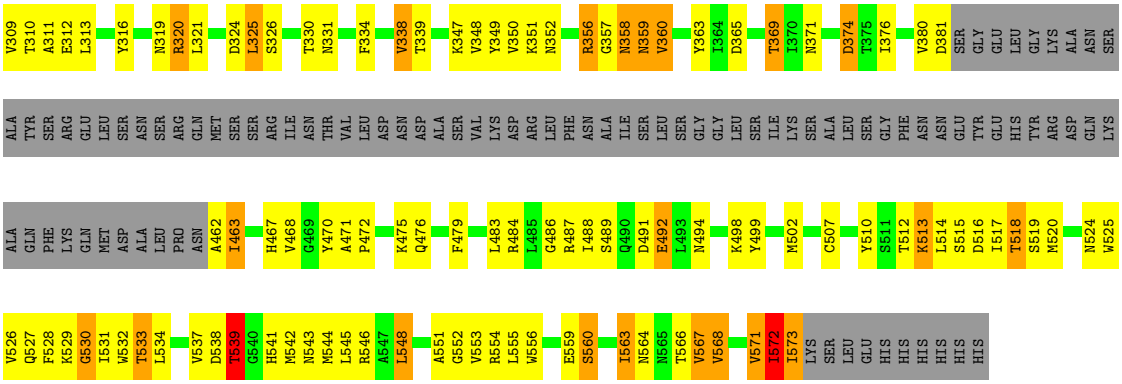


• Molecule 1: Major tail protein

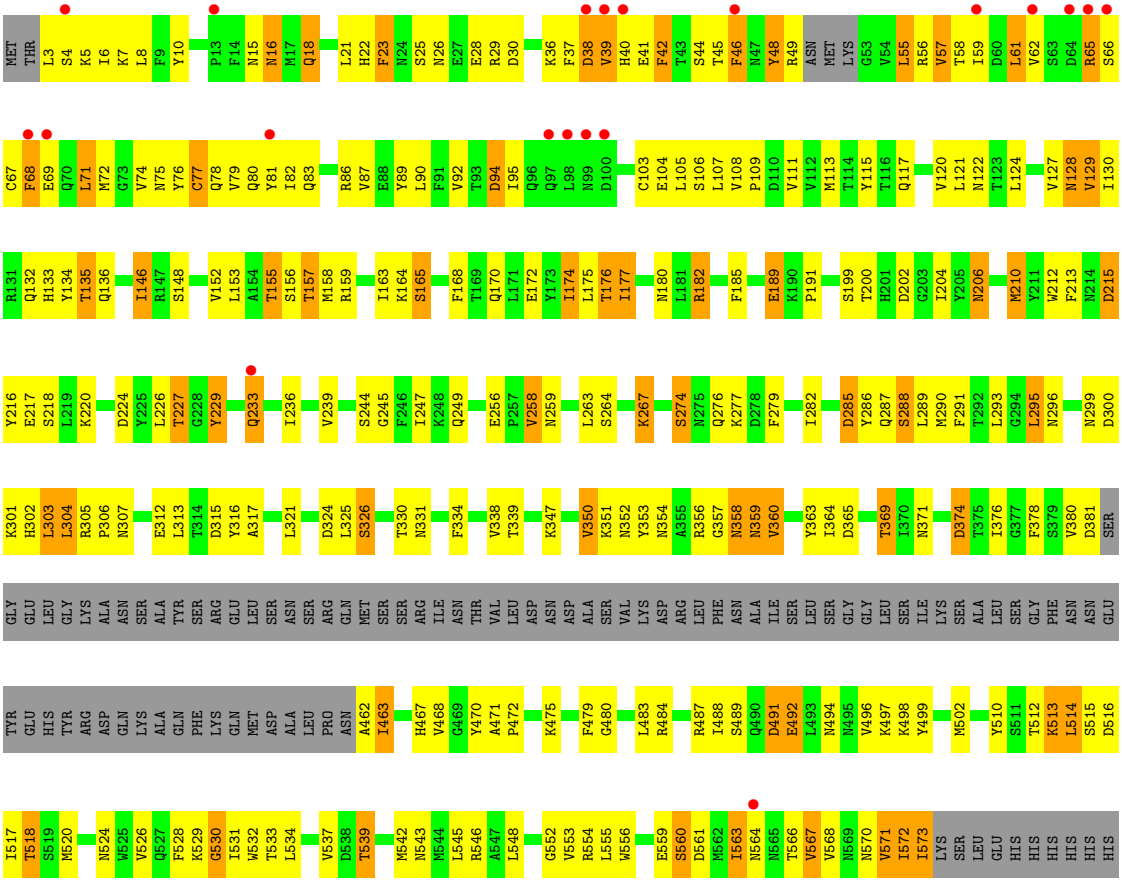
Chain E:







• Molecule 1: Major tail protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	205.61Å 209.64Å 102.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.01 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.01) 98.1 (50.00-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.21 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.282 0.235 , 0.279	Depositor DCC
R_{free} test set	4390 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	75.3	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 98.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23688	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.90	0/4030	0.97	4/5464 (0.1%)
1	B	0.89	3/4030 (0.1%)	0.94	3/5464 (0.1%)
1	C	0.80	1/4030 (0.0%)	0.89	2/5464 (0.0%)
1	D	0.77	0/4030	0.88	1/5464 (0.0%)
1	E	0.81	2/4030 (0.0%)	0.90	1/5464 (0.0%)
1	F	0.87	1/4030 (0.0%)	0.94	1/5464 (0.0%)
All	All	0.84	7/24180 (0.0%)	0.92	12/32784 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	3
1	E	0	3
1	F	0	2
All	All	0	15

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ASN	CG-ND2	-9.03	1.10	1.32
1	B	299	ASN	CG-OD1	-7.23	1.08	1.24
1	C	299	ASN	CG-ND2	-6.63	1.16	1.32
1	F	492	GLU	CG-CD	5.74	1.60	1.51
1	E	551	ALA	CA-CB	-5.69	1.40	1.52
1	B	492	GLU	CB-CG	5.43	1.62	1.52
1	E	492	GLU	CB-CG	5.26	1.62	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	304	LEU	CB-CG-CD1	-8.30	96.89	111.00
1	B	374	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	C	304	LEU	CB-CG-CD1	-5.99	100.81	111.00
1	B	304	LEU	CB-CG-CD1	-5.98	100.83	111.00
1	D	365	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	304	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	B	554	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	356	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	304	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	A	278	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	C	159	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	241	ILE	CB-CA-C	-5.10	101.41	111.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	ARG	Peptide
1	A	71	LEU	Peptide
1	B	183	LYS	Peptide
1	B	356	ARG	Peptide
1	B	71	LEU	Peptide
1	C	356	ARG	Peptide
1	C	71	LEU	Peptide
1	D	183	LYS	Peptide
1	D	356	ARG	Peptide
1	D	71	LEU	Peptide
1	E	183	LYS	Peptide
1	E	356	ARG	Peptide
1	E	71	LEU	Peptide
1	F	356	ARG	Peptide
1	F	71	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3832	264	3
1	B	3948	0	3832	264	3
1	C	3948	0	3832	282	1
1	D	3948	0	3832	284	0
1	E	3948	0	3832	271	0
1	F	3948	0	3832	279	1
All	All	23688	0	22992	1585	4

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 34.

All (1585) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ILE:O	1:A:573:ILE:HG22	1.66	0.93
1:F:573:ILE:O	1:F:573:ILE:HG22	1.70	0.91
1:D:158:MET:O	1:D:159:ARG:HD3	1.70	0.91
1:E:573:ILE:HG22	1:E:573:ILE:O	1.71	0.91
1:C:299:ASN:N	1:C:299:ASN:HD22	1.63	0.89
1:B:573:ILE:HG22	1:B:573:ILE:O	1.72	0.88
1:E:285:ASP:OD1	1:E:288:SER:OG	1.90	0.88
1:D:573:ILE:HG22	1:D:573:ILE:O	1.73	0.87
1:A:573:ILE:O	1:A:573:ILE:CG2	2.23	0.86
1:C:285:ASP:OD1	1:C:288:SER:OG	1.93	0.86
1:C:542:MET:HE1	1:C:545:LEU:HD23	1.58	0.86
1:C:573:ILE:HG22	1:C:573:ILE:O	1.75	0.85
1:D:285:ASP:OD1	1:D:288:SER:OG	1.92	0.85
1:F:215:ASP:OD1	1:F:216:TYR:N	2.10	0.85
1:C:542:MET:CE	1:C:545:LEU:HD23	2.08	0.83
1:B:215:ASP:OD1	1:B:216:TYR:N	2.12	0.82
1:F:285:ASP:OD1	1:F:288:SER:OG	1.97	0.82
1:D:157:THR:HG23	1:D:157:THR:O	1.79	0.81
1:F:573:ILE:O	1:F:573:ILE:CG2	2.27	0.81
1:B:572:ILE:O	1:B:572:ILE:HG22	1.81	0.81
1:D:572:ILE:HG22	1:D:572:ILE:O	1.81	0.81
1:B:26:ASN:OD1	1:B:29:ARG:NH2	2.15	0.80
1:D:215:ASP:OD1	1:D:216:TYR:N	2.13	0.80
1:C:158:MET:O	1:C:159:ARG:HD3	1.82	0.80
1:D:573:ILE:O	1:D:573:ILE:CG2	2.31	0.79
1:A:3:LEU:HD21	1:B:68:PHE:CE2	2.18	0.79
1:C:572:ILE:HG22	1:C:572:ILE:O	1.83	0.79
1:F:26:ASN:OD1	1:F:29:ARG:NH2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ILE:HG22	1:A:572:ILE:O	1.81	0.78
1:E:26:ASN:OD1	1:E:29:ARG:NH2	2.16	0.78
1:A:285:ASP:OD1	1:A:288:SER:OG	2.02	0.78
1:E:572:ILE:O	1:E:572:ILE:HG22	1.84	0.77
1:C:215:ASP:OD1	1:C:216:TYR:N	2.16	0.77
1:C:299:ASN:N	1:C:299:ASN:ND2	2.26	0.77
1:E:215:ASP:OD1	1:E:216:TYR:N	2.17	0.77
1:A:3:LEU:N	1:A:44:SER:O	2.18	0.77
1:A:37:PHE:CZ	1:A:40:HIS:O	2.39	0.76
1:B:573:ILE:O	1:B:573:ILE:CG2	2.33	0.76
1:A:313:LEU:HB2	1:A:321:LEU:HB3	1.68	0.76
1:F:572:ILE:HG22	1:F:572:ILE:O	1.86	0.76
1:C:573:ILE:O	1:C:573:ILE:CG2	2.34	0.76
1:B:75:ASN:O	1:B:92:VAL:N	2.18	0.76
1:E:516:ASP:OD2	1:E:518:THR:N	2.19	0.76
1:F:78:GLN:HG2	1:F:79:VAL:N	2.00	0.76
1:E:37:PHE:CZ	1:E:40:HIS:O	2.39	0.75
1:C:312:GLU:OE2	1:C:484:ARG:NH1	2.19	0.75
1:D:516:ASP:OD2	1:D:518:THR:N	2.19	0.75
1:F:542:MET:CE	1:F:545:LEU:HD23	2.17	0.75
1:F:158:MET:O	1:F:159:ARG:HD3	1.87	0.75
1:A:233:GLN:NE2	1:A:380:VAL:HG13	2.02	0.75
1:B:164:LYS:O	1:B:282:ILE:HD11	1.87	0.74
1:A:215:ASP:OD1	1:A:216:TYR:N	2.21	0.74
1:A:158:MET:O	1:A:159:ARG:HD3	1.88	0.74
1:E:158:MET:O	1:E:159:ARG:HD3	1.87	0.73
1:B:115:TYR:CE1	1:B:537:VAL:HG13	2.24	0.73
1:A:26:ASN:OD1	1:A:29:ARG:NH2	2.22	0.73
1:A:157:THR:CG2	1:A:489:SER:H	2.01	0.73
1:D:26:ASN:OD1	1:D:29:ARG:NH2	2.21	0.73
1:B:285:ASP:OD1	1:B:288:SER:OG	2.06	0.73
1:D:157:THR:CG2	1:D:489:SER:H	2.01	0.73
1:B:59:ILE:O	1:B:59:ILE:HG23	1.87	0.73
1:B:157:THR:O	1:B:157:THR:HG23	1.88	0.73
1:D:542:MET:O	1:D:545:LEU:N	2.22	0.73
1:A:164:LYS:O	1:A:282:ILE:HD11	1.89	0.72
1:A:290:MET:HE3	1:A:295:LEU:HB3	1.71	0.72
1:A:75:ASN:O	1:A:92:VAL:N	2.23	0.72
1:F:529:LYS:O	1:F:530:GLY:O	2.08	0.72
1:C:164:LYS:O	1:C:282:ILE:HD11	1.89	0.72
1:F:46:PHE:CB	1:F:57:VAL:HG23	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ILE:HD12	1:F:146:ILE:O	1.90	0.72
1:E:573:ILE:O	1:E:573:ILE:CG2	2.38	0.72
1:F:516:ASP:OD2	1:F:518:THR:N	2.20	0.72
1:D:127:VAL:HG21	1:D:528:PHE:CD1	2.24	0.71
1:D:233:GLN:NE2	1:D:380:VAL:HG13	2.06	0.71
1:B:37:PHE:CZ	1:B:40:HIS:O	2.42	0.71
1:C:146:ILE:HD12	1:C:146:ILE:O	1.89	0.71
1:A:542:MET:O	1:A:545:LEU:N	2.23	0.71
1:D:37:PHE:CZ	1:D:40:HIS:O	2.43	0.71
1:F:127:VAL:HG21	1:F:528:PHE:CD1	2.26	0.71
1:B:502:MET:HG2	1:B:567:VAL:HG11	1.72	0.71
1:E:233:GLN:NE2	1:E:380:VAL:HG13	2.06	0.71
1:B:516:ASP:OD2	1:B:518:THR:N	2.18	0.71
1:C:26:ASN:OD1	1:C:29:ARG:NH2	2.24	0.71
1:C:516:ASP:OD2	1:C:518:THR:N	2.20	0.70
1:E:157:THR:HG23	1:E:157:THR:O	1.90	0.70
1:A:59:ILE:HG23	1:A:59:ILE:O	1.91	0.70
1:A:127:VAL:HG21	1:A:528:PHE:CD1	2.25	0.70
1:B:233:GLN:NE2	1:B:380:VAL:HG13	2.07	0.70
1:A:516:ASP:OD2	1:A:518:THR:N	2.20	0.70
1:B:29:ARG:HD3	1:B:89:TYR:CE2	2.27	0.70
1:C:3:LEU:N	1:C:44:SER:O	2.24	0.70
1:F:157:THR:HG23	1:F:157:THR:O	1.90	0.70
1:C:298:ILE:C	1:C:299:ASN:HD22	1.94	0.70
1:A:542:MET:CE	1:A:545:LEU:HD23	2.22	0.70
1:D:124:LEU:HD22	1:D:532:TRP:HB2	1.73	0.70
1:E:347:LYS:HE2	1:E:369:THR:CG2	2.22	0.69
1:E:189:GLU:C	1:E:191:PRO:HD3	2.13	0.69
1:E:164:LYS:O	1:E:282:ILE:HD11	1.92	0.69
1:E:189:GLU:O	1:E:191:PRO:HD3	1.92	0.69
1:C:189:GLU:O	1:C:191:PRO:HD3	1.91	0.69
1:D:164:LYS:O	1:D:282:ILE:HD11	1.93	0.69
1:A:78:GLN:HG2	1:A:79:VAL:N	2.07	0.69
1:A:542:MET:HA	1:A:542:MET:HE2	1.74	0.69
1:F:542:MET:HE1	1:F:545:LEU:HD23	1.74	0.69
1:A:146:ILE:HD12	1:A:146:ILE:O	1.92	0.69
1:B:146:ILE:HD12	1:B:146:ILE:O	1.92	0.69
1:E:542:MET:CE	1:E:545:LEU:HD23	2.23	0.69
1:F:37:PHE:CZ	1:F:40:HIS:O	2.46	0.69
1:F:157:THR:CG2	1:F:489:SER:H	2.06	0.69
1:D:224:ASP:O	1:D:227:THR:OG1	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:THR:CG2	1:E:489:SER:H	2.06	0.68
1:B:26:ASN:HB3	1:B:29:ARG:CZ	2.24	0.68
1:E:127:VAL:HG21	1:E:528:PHE:CD1	2.28	0.68
1:B:42:PHE:CE1	1:B:59:ILE:HD12	2.27	0.68
1:C:42:PHE:CE1	1:C:59:ILE:HD12	2.28	0.68
1:C:233:GLN:NE2	1:C:380:VAL:HG13	2.09	0.68
1:F:542:MET:O	1:F:545:LEU:N	2.27	0.68
1:C:347:LYS:HE2	1:C:369:THR:HG22	1.73	0.68
1:F:542:MET:HA	1:F:542:MET:HE2	1.75	0.68
1:C:189:GLU:C	1:C:191:PRO:HD3	2.14	0.68
1:B:542:MET:HE2	1:B:542:MET:HA	1.76	0.68
1:C:374:ASP:OD1	1:C:374:ASP:N	2.25	0.68
1:A:563:ILE:N	1:A:563:ILE:HD13	2.09	0.68
1:B:127:VAL:HG21	1:B:528:PHE:CD1	2.28	0.67
1:F:124:LEU:HD22	1:F:532:TRP:HB2	1.76	0.67
1:E:347:LYS:HE2	1:E:369:THR:HG22	1.77	0.67
1:A:470:TYR:CG	1:A:479:PHE:CE1	2.82	0.67
1:B:158:MET:O	1:B:159:ARG:HD3	1.94	0.67
1:D:120:VAL:HG23	1:D:121:LEU:N	2.08	0.67
1:D:180:ASN:OD1	1:D:182:ARG:HG2	1.95	0.67
1:D:290:MET:HE3	1:D:295:LEU:CB	2.25	0.67
1:A:180:ASN:OD1	1:A:182:ARG:HG2	1.94	0.67
1:B:111:VAL:HB	1:B:545:LEU:HD13	1.77	0.67
1:C:127:VAL:HG21	1:C:528:PHE:CD1	2.30	0.67
1:D:312:GLU:OE2	1:D:484:ARG:NH1	2.28	0.67
1:F:92:VAL:HG23	1:F:92:VAL:O	1.94	0.67
1:A:177:ILE:HD13	1:A:177:ILE:O	1.95	0.66
1:A:286:TYR:N	1:A:331:ASN:OD1	2.28	0.66
1:B:177:ILE:HG22	1:B:236:ILE:HG23	1.78	0.66
1:C:30:ASP:OD2	1:C:89:TYR:OH	2.11	0.66
1:B:189:GLU:O	1:B:191:PRO:HD3	1.95	0.66
1:E:312:GLU:OE2	1:E:484:ARG:NH1	2.29	0.66
1:B:258:VAL:HG13	1:B:259:ASN:H	1.59	0.66
1:B:164:LYS:C	1:B:282:ILE:CD1	2.64	0.66
1:C:180:ASN:OD1	1:C:182:ARG:HG2	1.96	0.66
1:B:470:TYR:CG	1:B:479:PHE:CE1	2.83	0.66
1:C:37:PHE:CZ	1:C:40:HIS:O	2.49	0.66
1:D:78:GLN:HG2	1:D:79:VAL:N	2.11	0.66
1:E:146:ILE:O	1:E:146:ILE:HD12	1.96	0.66
1:B:312:GLU:OE2	1:B:484:ARG:NH1	2.28	0.66
1:F:189:GLU:C	1:F:191:PRO:HD3	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASP:N	1:A:374:ASP:OD1	2.29	0.66
1:C:347:LYS:HE2	1:C:369:THR:CG2	2.25	0.66
1:B:133:HIS:HB3	1:B:520:MET:HE3	1.77	0.65
1:E:470:TYR:CG	1:E:479:PHE:CE1	2.83	0.65
1:C:124:LEU:HD22	1:C:532:TRP:HB2	1.78	0.65
1:C:542:MET:HE2	1:C:542:MET:HA	1.76	0.65
1:A:42:PHE:CE1	1:A:59:ILE:HD12	2.32	0.65
1:D:542:MET:CE	1:D:545:LEU:HD23	2.27	0.65
1:A:174:ILE:HG12	1:A:176:THR:HG22	1.77	0.65
1:C:29:ARG:HD3	1:C:89:TYR:CE2	2.32	0.65
1:E:75:ASN:O	1:E:92:VAL:N	2.30	0.65
1:B:542:MET:O	1:B:545:LEU:N	2.29	0.65
1:E:542:MET:HE2	1:E:542:MET:HA	1.77	0.65
1:A:258:VAL:HG13	1:A:259:ASN:H	1.62	0.65
1:B:133:HIS:HB3	1:B:520:MET:CE	2.27	0.65
1:D:146:ILE:HD12	1:D:146:ILE:O	1.97	0.65
1:F:180:ASN:OD1	1:F:182:ARG:HG2	1.96	0.65
1:C:463:ILE:O	1:C:463:ILE:CD1	2.45	0.64
1:A:133:HIS:HB3	1:A:520:MET:HE3	1.79	0.64
1:C:224:ASP:O	1:C:227:THR:OG1	2.14	0.64
1:E:59:ILE:HG23	1:E:59:ILE:O	1.98	0.64
1:F:233:GLN:NE2	1:F:380:VAL:HG13	2.13	0.64
1:A:57:VAL:CG1	1:A:57:VAL:O	2.45	0.64
1:A:124:LEU:HD22	1:A:532:TRP:HB2	1.79	0.64
1:E:78:GLN:HG2	1:E:79:VAL:N	2.13	0.64
1:B:463:ILE:O	1:B:463:ILE:CD1	2.46	0.64
1:E:172:GLU:OE1	1:E:212:TRP:HH2	1.80	0.64
1:A:157:THR:HG23	1:A:157:THR:O	1.98	0.64
1:C:40:HIS:CE1	1:C:42:PHE:HB3	2.33	0.64
1:D:563:ILE:HD13	1:D:563:ILE:N	2.13	0.64
1:C:563:ILE:N	1:C:563:ILE:HD13	2.13	0.64
1:B:78:GLN:HG2	1:B:79:VAL:N	2.12	0.64
1:C:542:MET:O	1:C:545:LEU:N	2.31	0.64
1:F:206:ASN:OD1	1:F:210:MET:CE	2.46	0.64
1:C:172:GLU:OE1	1:C:212:TRP:HH2	1.80	0.63
1:C:164:LYS:C	1:C:282:ILE:CD1	2.67	0.63
1:E:124:LEU:HD22	1:E:532:TRP:HB2	1.79	0.63
1:F:290:MET:HE3	1:F:295:LEU:HB2	1.80	0.63
1:B:120:VAL:HG23	1:B:121:LEU:N	2.13	0.63
1:F:172:GLU:OE1	1:F:212:TRP:HH2	1.80	0.63
1:E:29:ARG:HD2	1:E:30:ASP:OD2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PHE:CD1	1:B:38:ASP:N	2.65	0.63
1:D:172:GLU:OE1	1:D:212:TRP:HH2	1.80	0.63
1:B:174:ILE:HG12	1:B:176:THR:HG22	1.78	0.63
1:C:78:GLN:HG2	1:C:79:VAL:N	2.14	0.63
1:F:120:VAL:HG23	1:F:121:LEU:N	2.13	0.63
1:A:106:SER:O	1:A:107:LEU:HD12	1.99	0.63
1:B:172:GLU:OE1	1:B:212:TRP:HH2	1.82	0.63
1:D:42:PHE:CE1	1:D:59:ILE:HD12	2.33	0.63
1:F:312:GLU:OE2	1:F:484:ARG:NH1	2.32	0.63
1:B:189:GLU:C	1:B:191:PRO:HD3	2.18	0.63
1:D:157:THR:O	1:D:157:THR:CG2	2.47	0.63
1:D:380:VAL:HG12	1:D:381:ASP:N	2.14	0.63
1:D:46:PHE:CB	1:D:57:VAL:HG23	2.29	0.62
1:B:18:GLN:NE2	1:B:552:GLY:O	2.32	0.62
1:F:258:VAL:HG13	1:F:259:ASN:H	1.64	0.62
1:F:233:GLN:O	1:F:236:ILE:HG13	2.00	0.62
1:A:135:THR:O	1:A:136:GLN:C	2.38	0.62
1:E:563:ILE:HD13	1:E:563:ILE:N	2.14	0.62
1:E:534:LEU:HB2	1:E:542:MET:CE	2.30	0.62
1:E:542:MET:HE2	1:E:545:LEU:HD23	1.79	0.62
1:B:46:PHE:CD2	1:B:46:PHE:O	2.53	0.62
1:B:224:ASP:O	1:B:227:THR:OG1	2.17	0.62
1:F:313:LEU:HB2	1:F:321:LEU:HB3	1.82	0.62
1:B:347:LYS:HE2	1:B:369:THR:CG2	2.29	0.62
1:C:157:THR:CG2	1:C:489:SER:H	2.12	0.62
1:F:189:GLU:O	1:F:191:PRO:HD3	2.00	0.62
1:C:286:TYR:N	1:C:331:ASN:OD1	2.33	0.62
1:D:75:ASN:O	1:D:92:VAL:N	2.31	0.62
1:E:356:ARG:NH2	1:F:487:ARG:O	2.32	0.62
1:F:46:PHE:HB3	1:F:57:VAL:HG23	1.82	0.62
1:B:40:HIS:CE1	1:B:42:PHE:HB3	2.35	0.62
1:F:75:ASN:O	1:F:92:VAL:N	2.33	0.62
1:A:120:VAL:HG23	1:A:121:LEU:N	2.15	0.62
1:E:380:VAL:HG12	1:E:381:ASP:N	2.15	0.62
1:F:177:ILE:HD13	1:F:177:ILE:O	1.99	0.62
1:F:351:LYS:O	1:F:352:ASN:HB2	1.99	0.62
1:E:40:HIS:CE1	1:E:42:PHE:HB3	2.34	0.61
1:E:29:ARG:HD3	1:E:89:TYR:CE2	2.34	0.61
1:D:134:TYR:O	1:D:572:ILE:HD13	1.99	0.61
1:C:5:LYS:NZ	1:C:41:GLU:OE2	2.33	0.61
1:A:312:GLU:OE2	1:A:484:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ASN:HB3	1:B:29:ARG:NH2	2.14	0.61
1:B:182:ARG:CZ	1:B:267:LYS:HE2	2.30	0.61
1:E:42:PHE:CE1	1:E:59:ILE:HD12	2.36	0.61
1:A:29:ARG:HD3	1:A:89:TYR:CE2	2.36	0.61
1:A:40:HIS:CE1	1:A:42:PHE:HB3	2.35	0.61
1:A:224:ASP:O	1:A:227:THR:OG1	2.18	0.61
1:B:124:LEU:HD22	1:B:532:TRP:HB2	1.81	0.61
1:F:290:MET:HE3	1:F:295:LEU:CB	2.30	0.61
1:B:37:PHE:HZ	1:B:40:HIS:O	1.82	0.61
1:B:180:ASN:OD1	1:B:182:ARG:HG2	2.00	0.61
1:E:8:LEU:O	1:E:37:PHE:CZ	2.54	0.61
1:E:164:LYS:C	1:E:282:ILE:CD1	2.69	0.61
1:E:463:ILE:O	1:E:463:ILE:CD1	2.49	0.61
1:F:3:LEU:N	1:F:44:SER:O	2.33	0.61
1:F:164:LYS:O	1:F:282:ILE:HD11	2.01	0.61
1:A:174:ILE:HD13	1:A:174:ILE:O	2.01	0.61
1:E:120:VAL:HG23	1:E:121:LEU:N	2.15	0.61
1:F:217:GLU:O	1:F:220:LYS:N	2.33	0.61
1:F:224:ASP:O	1:F:227:THR:OG1	2.19	0.61
1:A:542:MET:HE1	1:A:545:LEU:HD23	1.83	0.60
1:D:566:THR:O	1:D:567:VAL:C	2.39	0.60
1:D:542:MET:HA	1:D:542:MET:HE2	1.83	0.60
1:F:135:THR:O	1:F:136:GLN:C	2.39	0.60
1:A:182:ARG:CZ	1:A:267:LYS:HE2	2.31	0.60
1:B:75:ASN:N	1:B:75:ASN:OD1	2.34	0.60
1:B:313:LEU:HB2	1:B:321:LEU:HB3	1.82	0.60
1:A:164:LYS:C	1:A:282:ILE:CD1	2.70	0.60
1:B:380:VAL:HG12	1:B:381:ASP:N	2.16	0.60
1:C:470:TYR:CG	1:C:479:PHE:CE1	2.89	0.60
1:C:37:PHE:CD1	1:C:38:ASP:N	2.68	0.60
1:C:566:THR:O	1:C:567:VAL:C	2.40	0.60
1:D:542:MET:HE2	1:D:545:LEU:HD23	1.81	0.60
1:E:46:PHE:CB	1:E:57:VAL:HG23	2.31	0.60
1:E:206:ASN:OD1	1:E:210:MET:CE	2.48	0.60
1:B:290:MET:HE3	1:B:295:LEU:CB	2.31	0.60
1:D:374:ASP:OD1	1:D:374:ASP:N	2.35	0.60
1:F:90:LEU:HD22	1:F:107:LEU:HD23	1.83	0.60
1:A:8:LEU:O	1:A:37:PHE:CZ	2.54	0.60
1:B:157:THR:CG2	1:B:489:SER:H	2.13	0.60
1:D:174:ILE:HG12	1:D:176:THR:HG22	1.82	0.60
1:B:128:ASN:C	1:B:128:ASN:ND2	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:MET:CE	1:B:545:LEU:HD23	2.32	0.60
1:A:15:ASN:CG	1:F:546:ARG:NH2	2.56	0.60
1:A:463:ILE:CD1	1:A:463:ILE:O	2.50	0.60
1:F:347:LYS:HE2	1:F:369:THR:CG2	2.32	0.60
1:A:111:VAL:HB	1:A:545:LEU:HD13	1.83	0.59
1:D:40:HIS:CE1	1:D:42:PHE:HB3	2.37	0.59
1:D:233:GLN:O	1:D:236:ILE:HG13	2.02	0.59
1:D:560:SER:O	1:D:564:ASN:ND2	2.34	0.59
1:C:546:ARG:NH2	1:D:15:ASN:OD1	2.35	0.59
1:E:174:ILE:HG12	1:E:176:THR:HG22	1.83	0.59
1:E:182:ARG:NH2	1:E:267:LYS:HE2	2.17	0.59
1:F:563:ILE:HD13	1:F:563:ILE:N	2.17	0.59
1:B:79:VAL:HG11	1:B:81:TYR:CE2	2.37	0.59
1:E:79:VAL:HG11	1:E:81:TYR:CE2	2.37	0.59
1:F:470:TYR:CG	1:F:479:PHE:CE1	2.91	0.59
1:D:133:HIS:HB3	1:D:520:MET:HE3	1.84	0.59
1:F:347:LYS:HE2	1:F:369:THR:HG22	1.85	0.59
1:B:563:ILE:HD13	1:B:563:ILE:N	2.17	0.59
1:D:189:GLU:O	1:D:191:PRO:HD3	2.03	0.59
1:E:182:ARG:CZ	1:E:267:LYS:HE2	2.31	0.59
1:F:463:ILE:CD1	1:F:463:ILE:O	2.51	0.59
1:F:566:THR:O	1:F:567:VAL:C	2.41	0.59
1:A:128:ASN:C	1:A:128:ASN:ND2	2.55	0.59
1:C:206:ASN:OD1	1:C:210:MET:CE	2.50	0.59
1:D:215:ASP:OD1	1:D:215:ASP:C	2.41	0.59
1:A:359:ASN:O	1:A:360:VAL:C	2.41	0.59
1:B:6:ILE:CG2	1:B:7:LYS:N	2.65	0.59
1:A:177:ILE:CG2	1:A:236:ILE:HG12	2.32	0.59
1:B:566:THR:O	1:B:567:VAL:C	2.39	0.59
1:E:502:MET:HG2	1:E:567:VAL:HG11	1.84	0.59
1:C:135:THR:O	1:C:136:GLN:C	2.38	0.59
1:D:3:LEU:N	1:D:44:SER:O	2.36	0.59
1:D:258:VAL:HG13	1:D:259:ASN:H	1.68	0.59
1:D:470:TYR:CG	1:D:479:PHE:CE1	2.91	0.59
1:E:282:ILE:HG23	1:E:334:PHE:CD2	2.37	0.59
1:F:164:LYS:C	1:F:282:ILE:CD1	2.71	0.59
1:B:174:ILE:HD13	1:B:174:ILE:O	2.02	0.59
1:B:347:LYS:HE2	1:B:369:THR:HG22	1.84	0.59
1:C:18:GLN:NE2	1:C:552:GLY:O	2.34	0.59
1:C:258:VAL:HG13	1:C:259:ASN:H	1.68	0.59
1:E:5:LYS:NZ	1:E:41:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:OG	1:B:45:THR:N	2.36	0.58
1:B:67:CYS:O	1:B:68:PHE:HB2	2.03	0.58
1:F:380:VAL:HG12	1:F:381:ASP:N	2.18	0.58
1:F:563:ILE:O	1:F:564:ASN:ND2	2.36	0.58
1:A:18:GLN:NE2	1:A:552:GLY:O	2.34	0.58
1:C:120:VAL:HG23	1:C:121:LEU:N	2.17	0.58
1:D:256:GLU:O	1:D:264:SER:HA	2.04	0.58
1:D:290:MET:HE3	1:D:295:LEU:HB2	1.85	0.58
1:E:75:ASN:HA	1:E:92:VAL:HG22	1.85	0.58
1:E:290:MET:HE3	1:E:295:LEU:CB	2.33	0.58
1:D:59:ILE:HG23	1:D:59:ILE:O	2.03	0.58
1:D:164:LYS:C	1:D:282:ILE:CD1	2.72	0.58
1:F:40:HIS:CE1	1:F:42:PHE:HB3	2.38	0.58
1:F:566:THR:O	1:F:568:VAL:N	2.35	0.58
1:C:29:ARG:HD2	1:C:30:ASP:OD2	2.03	0.58
1:C:380:VAL:HG12	1:C:381:ASP:N	2.19	0.58
1:E:258:VAL:HG13	1:E:259:ASN:H	1.67	0.58
1:F:41:GLU:HG2	1:F:41:GLU:O	2.03	0.58
1:F:286:TYR:N	1:F:331:ASN:OD1	2.36	0.58
1:F:302:HIS:CD2	1:F:303:LEU:HD13	2.38	0.58
1:C:174:ILE:HG12	1:C:176:THR:HG22	1.85	0.58
1:F:215:ASP:OD1	1:F:215:ASP:C	2.42	0.58
1:C:67:CYS:O	1:C:68:PHE:HB2	2.04	0.58
1:D:5:LYS:NZ	1:D:41:GLU:OE2	2.36	0.58
1:D:299:ASN:N	1:D:299:ASN:ND2	2.51	0.58
1:D:546:ARG:NH2	1:E:15:ASN:CG	2.57	0.58
1:E:172:GLU:HB3	1:E:212:TRP:CH2	2.38	0.58
1:B:5:LYS:NZ	1:B:41:GLU:OE2	2.37	0.58
1:D:174:ILE:HD13	1:D:174:ILE:O	2.04	0.58
1:E:529:LYS:O	1:E:530:GLY:O	2.22	0.58
1:F:29:ARG:HD3	1:F:89:TYR:CE2	2.39	0.58
1:C:313:LEU:HB2	1:C:321:LEU:HB3	1.86	0.58
1:D:57:VAL:CG1	1:D:57:VAL:O	2.51	0.58
1:E:229:TYR:N	1:E:229:TYR:CD2	2.71	0.58
1:B:529:LYS:O	1:B:530:GLY:O	2.21	0.58
1:F:30:ASP:OD2	1:F:89:TYR:OH	2.20	0.58
1:F:516:ASP:OD2	1:F:518:THR:HG22	2.03	0.58
1:D:90:LEU:HA	1:D:109:PRO:HA	1.84	0.57
1:F:306:PRO:HD3	1:F:326:SER:HB3	1.85	0.57
1:B:563:ILE:O	1:B:564:ASN:ND2	2.37	0.57
1:C:157:THR:HG23	1:C:157:THR:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:HIS:HB3	1:F:520:MET:HE3	1.86	0.57
1:A:177:ILE:HG22	1:A:236:ILE:HG23	1.86	0.57
1:E:258:VAL:HG22	1:E:259:ASN:N	2.18	0.57
1:D:463:ILE:O	1:D:463:ILE:CD1	2.53	0.57
1:E:286:TYR:N	1:E:331:ASN:OD1	2.37	0.57
1:C:298:ILE:HB	1:C:299:ASN:ND2	2.19	0.57
1:D:8:LEU:O	1:D:37:PHE:CZ	2.58	0.57
1:A:67:CYS:O	1:A:68:PHE:HB2	2.05	0.57
1:A:380:VAL:HG12	1:A:381:ASP:N	2.19	0.57
1:E:542:MET:O	1:E:545:LEU:N	2.35	0.57
1:F:42:PHE:CE1	1:F:59:ILE:HD12	2.40	0.57
1:F:59:ILE:HG23	1:F:59:ILE:O	2.05	0.57
1:F:177:ILE:HG22	1:F:236:ILE:HG23	1.87	0.57
1:A:215:ASP:OD1	1:A:215:ASP:C	2.43	0.57
1:B:491:ASP:O	1:B:492:GLU:C	2.39	0.57
1:F:182:ARG:CZ	1:F:267:LYS:HE2	2.35	0.57
1:C:215:ASP:OD1	1:C:215:ASP:C	2.44	0.57
1:C:305:ARG:HB2	1:C:306:PRO:HD2	1.86	0.57
1:D:502:MET:HG2	1:D:567:VAL:HG11	1.87	0.57
1:B:374:ASP:OD1	1:B:374:ASP:N	2.38	0.57
1:D:46:PHE:HB3	1:D:57:VAL:HG23	1.87	0.57
1:D:67:CYS:O	1:D:68:PHE:HB2	2.05	0.57
1:E:233:GLN:O	1:E:236:ILE:HG13	2.05	0.57
1:E:539:THR:CG2	1:F:94:ASP:HA	2.34	0.57
1:F:67:CYS:O	1:F:68:PHE:HB2	2.04	0.57
1:A:37:PHE:HZ	1:A:40:HIS:O	1.88	0.57
1:C:152:VAL:HG21	1:C:307:ASN:HD21	1.70	0.57
1:D:37:PHE:CD1	1:D:38:ASP:N	2.73	0.57
1:A:290:MET:CE	1:A:295:LEU:HB3	2.34	0.56
1:B:59:ILE:O	1:B:59:ILE:CG2	2.51	0.56
1:B:356:ARG:NH2	1:C:487:ARG:O	2.38	0.56
1:D:135:THR:O	1:D:136:GLN:C	2.42	0.56
1:D:339:THR:HG21	1:E:472:PRO:HB3	1.87	0.56
1:E:553:VAL:HG12	1:E:555:LEU:HD12	1.87	0.56
1:A:46:PHE:CB	1:A:57:VAL:HG23	2.36	0.56
1:D:18:GLN:NE2	1:D:552:GLY:O	2.39	0.56
1:D:471:ALA:HB3	1:D:472:PRO:HD3	1.86	0.56
1:E:111:VAL:HB	1:E:545:LEU:HD13	1.87	0.56
1:E:224:ASP:O	1:E:227:THR:OG1	2.21	0.56
1:B:134:TYR:O	1:B:572:ILE:HD13	2.05	0.56
1:B:229:TYR:CD2	1:B:229:TYR:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:LEU:HB2	1:D:321:LEU:HB3	1.87	0.56
1:E:46:PHE:O	1:E:46:PHE:CD2	2.58	0.56
1:F:18:GLN:NE2	1:F:552:GLY:O	2.38	0.56
1:F:133:HIS:HB3	1:F:520:MET:CE	2.35	0.56
1:C:148:SER:CB	1:D:156:SER:O	2.54	0.56
1:D:286:TYR:N	1:D:331:ASN:OD1	2.38	0.56
1:A:133:HIS:HB3	1:A:520:MET:CE	2.35	0.56
1:E:305:ARG:HB2	1:E:306:PRO:HD2	1.86	0.56
1:D:148:SER:CB	1:E:156:SER:O	2.53	0.56
1:F:44:SER:OG	1:F:45:THR:N	2.37	0.56
1:A:90:LEU:HD22	1:A:107:LEU:HD23	1.88	0.56
1:B:233:GLN:O	1:B:236:ILE:HG13	2.06	0.56
1:D:90:LEU:HD22	1:D:107:LEU:HD23	1.86	0.56
1:B:286:TYR:CE1	1:B:301:LYS:HE3	2.41	0.56
1:E:46:PHE:HB3	1:E:57:VAL:HG23	1.87	0.56
1:E:180:ASN:OD1	1:E:182:ARG:HG2	2.06	0.56
1:F:502:MET:HG2	1:F:567:VAL:HG11	1.88	0.56
1:A:79:VAL:HG11	1:A:81:TYR:CE2	2.41	0.56
1:B:502:MET:O	1:B:554:ARG:NH1	2.36	0.56
1:C:6:ILE:CG2	1:C:7:LYS:N	2.69	0.56
1:D:175:LEU:CD1	1:D:177:ILE:HG23	2.36	0.56
1:D:351:LYS:HG2	1:D:352:ASN:OD1	2.06	0.56
1:E:37:PHE:HZ	1:E:40:HIS:O	1.87	0.56
1:E:290:MET:HE3	1:E:295:LEU:HB2	1.88	0.56
1:F:5:LYS:NZ	1:F:41:GLU:OE2	2.38	0.56
1:F:134:TYR:O	1:F:572:ILE:HD13	2.05	0.56
1:A:172:GLU:OE1	1:A:212:TRP:HH2	1.89	0.56
1:B:45:THR:HG23	1:B:45:THR:O	2.05	0.56
1:C:8:LEU:O	1:C:37:PHE:CZ	2.59	0.56
1:C:42:PHE:CE1	1:C:59:ILE:CD1	2.89	0.56
1:E:3:LEU:N	1:E:44:SER:O	2.39	0.56
1:E:67:CYS:SG	1:E:68:PHE:N	2.79	0.56
1:F:305:ARG:HB2	1:F:306:PRO:HD2	1.87	0.56
1:A:134:TYR:O	1:A:572:ILE:HD13	2.06	0.55
1:A:177:ILE:HG21	1:A:236:ILE:HG12	1.87	0.55
1:A:290:MET:HE3	1:A:295:LEU:CB	2.35	0.55
1:B:46:PHE:CB	1:B:57:VAL:HG23	2.36	0.55
1:C:59:ILE:HG23	1:C:59:ILE:O	2.05	0.55
1:C:258:VAL:HG22	1:C:259:ASN:N	2.20	0.55
1:A:502:MET:HG2	1:A:567:VAL:HG11	1.87	0.55
1:D:189:GLU:C	1:D:191:PRO:HD3	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:566:THR:O	1:D:568:VAL:N	2.40	0.55
1:C:133:HIS:HB3	1:C:520:MET:CE	2.36	0.55
1:E:566:THR:O	1:E:567:VAL:C	2.43	0.55
1:F:175:LEU:CD1	1:F:177:ILE:HG23	2.36	0.55
1:E:174:ILE:HD13	1:E:174:ILE:O	2.05	0.55
1:F:374:ASP:N	1:F:374:ASP:OD1	2.32	0.55
1:A:206:ASN:OD1	1:A:210:MET:CE	2.55	0.55
1:B:8:LEU:O	1:B:37:PHE:CZ	2.60	0.55
1:B:57:VAL:O	1:B:57:VAL:CG1	2.55	0.55
1:C:174:ILE:O	1:C:174:ILE:HD13	2.06	0.55
1:D:534:LEU:HB2	1:D:542:MET:CE	2.36	0.55
1:E:471:ALA:HB3	1:E:472:PRO:HD3	1.89	0.55
1:F:75:ASN:HA	1:F:92:VAL:HG22	1.89	0.55
1:A:359:ASN:C	1:A:360:VAL:O	2.41	0.55
1:E:128:ASN:C	1:E:128:ASN:ND2	2.58	0.55
1:F:157:THR:O	1:F:157:THR:CG2	2.54	0.55
1:F:177:ILE:CG2	1:F:236:ILE:HG12	2.36	0.55
1:A:156:SER:O	1:F:148:SER:CB	2.55	0.55
1:C:566:THR:O	1:C:568:VAL:N	2.40	0.55
1:D:12:THR:HG21	1:D:76:TYR:HB2	1.89	0.55
1:B:566:THR:O	1:B:568:VAL:N	2.39	0.55
1:D:79:VAL:HG11	1:D:81:TYR:CE2	2.42	0.55
1:E:563:ILE:O	1:E:564:ASN:ND2	2.40	0.55
1:A:175:LEU:CD1	1:A:177:ILE:HG23	2.37	0.55
1:C:471:ALA:HB3	1:C:472:PRO:HD3	1.89	0.55
1:F:534:LEU:HB2	1:F:542:MET:CE	2.37	0.55
1:A:15:ASN:OD1	1:F:546:ARG:NH2	2.40	0.54
1:A:305:ARG:HB2	1:A:306:PRO:HD2	1.88	0.54
1:B:90:LEU:HA	1:B:109:PRO:HA	1.88	0.54
1:E:296:ASN:O	1:E:300:ASP:HB2	2.06	0.54
1:A:189:GLU:O	1:A:191:PRO:HD3	2.08	0.54
1:A:256:GLU:O	1:A:264:SER:HA	2.07	0.54
1:A:566:THR:O	1:A:567:VAL:C	2.46	0.54
1:C:134:TYR:O	1:C:572:ILE:HD13	2.07	0.54
1:C:518:THR:HG23	1:C:518:THR:O	2.06	0.54
1:C:534:LEU:HB2	1:C:542:MET:SD	2.47	0.54
1:C:546:ARG:NH2	1:D:15:ASN:CG	2.60	0.54
1:E:256:GLU:O	1:E:264:SER:HA	2.07	0.54
1:F:26:ASN:O	1:F:29:ARG:HB3	2.06	0.54
1:A:41:GLU:HG2	1:A:41:GLU:O	2.07	0.54
1:B:175:LEU:CD1	1:B:177:ILE:HG23	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:VAL:HG11	1:C:81:TYR:CE2	2.42	0.54
1:C:177:ILE:HD13	1:C:177:ILE:O	2.08	0.54
1:E:374:ASP:OD1	1:E:374:ASP:N	2.36	0.54
1:B:546:ARG:NH2	1:C:15:ASN:OD1	2.41	0.54
1:D:229:TYR:N	1:D:229:TYR:CD2	2.75	0.54
1:E:67:CYS:O	1:E:68:PHE:HB2	2.07	0.54
1:B:30:ASP:OD2	1:B:89:TYR:OH	2.21	0.54
1:C:175:LEU:CD1	1:C:177:ILE:HG23	2.37	0.54
1:C:190:LYS:O	1:C:190:LYS:HG2	2.06	0.54
1:D:172:GLU:HB3	1:D:212:TRP:CH2	2.43	0.54
1:D:206:ASN:OD1	1:D:210:MET:CE	2.56	0.54
1:A:471:ALA:HB3	1:A:472:PRO:HD3	1.90	0.54
1:C:182:ARG:CZ	1:C:267:LYS:HE2	2.37	0.54
1:E:135:THR:O	1:E:136:GLN:C	2.46	0.54
1:E:204:ILE:HD13	1:F:468:VAL:HG23	1.90	0.54
1:F:174:ILE:HG12	1:F:176:THR:HG22	1.88	0.54
1:A:57:VAL:O	1:A:57:VAL:HG12	2.07	0.54
1:A:189:GLU:C	1:A:191:PRO:HD3	2.27	0.54
1:D:3:LEU:HD21	1:E:68:PHE:CE2	2.43	0.54
1:F:8:LEU:O	1:F:37:PHE:CZ	2.61	0.54
1:B:291:PHE:C	1:B:291:PHE:CD2	2.80	0.54
1:B:360:VAL:HG23	1:B:363:TYR:HB2	1.88	0.54
1:C:128:ASN:C	1:C:128:ASN:ND2	2.62	0.54
1:D:44:SER:OG	1:D:45:THR:N	2.41	0.54
1:E:44:SER:OG	1:E:45:THR:N	2.40	0.54
1:F:46:PHE:HB2	1:F:57:VAL:HG23	1.88	0.54
1:F:46:PHE:O	1:F:46:PHE:CD2	2.61	0.54
1:A:59:ILE:O	1:A:59:ILE:CG2	2.56	0.54
1:C:279:PHE:HB3	1:C:282:ILE:HG22	1.89	0.54
1:D:204:ILE:HD13	1:E:468:VAL:HG23	1.90	0.54
1:D:305:ARG:HB2	1:D:306:PRO:HD2	1.90	0.54
1:E:152:VAL:HG22	1:E:153:LEU:N	2.23	0.54
1:C:46:PHE:CB	1:C:57:VAL:HG23	2.37	0.54
1:D:46:PHE:CE1	1:D:55:LEU:CD1	2.91	0.54
1:E:532:TRP:CZ2	1:E:546:ARG:HA	2.43	0.53
1:F:174:ILE:HD13	1:F:174:ILE:O	2.08	0.53
1:A:229:TYR:N	1:A:229:TYR:CD2	2.75	0.53
1:B:23:PHE:N	1:B:23:PHE:CD2	2.75	0.53
1:B:182:ARG:NH2	1:B:267:LYS:HE2	2.24	0.53
1:D:158:MET:O	1:D:159:ARG:CD	2.50	0.53
1:F:229:TYR:N	1:F:229:TYR:CD2	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:HG21	1:B:76:TYR:HB2	1.90	0.53
1:B:534:LEU:HB2	1:B:542:MET:CE	2.37	0.53
1:B:542:MET:HE2	1:B:545:LEU:HD23	1.90	0.53
1:F:212:TRP:CZ3	1:F:247:ILE:HG13	2.43	0.53
1:A:172:GLU:HB3	1:A:212:TRP:CH2	2.44	0.53
1:C:463:ILE:O	1:C:463:ILE:HD12	2.09	0.53
1:D:182:ARG:CZ	1:D:267:LYS:HE2	2.38	0.53
1:A:470:TYR:HB3	1:A:479:PHE:CD1	2.44	0.53
1:B:286:TYR:N	1:B:331:ASN:OD1	2.41	0.53
1:C:302:HIS:CD2	1:C:303:LEU:HD13	2.43	0.53
1:E:18:GLN:NE2	1:E:552:GLY:O	2.39	0.53
1:E:37:PHE:CD1	1:E:38:ASP:N	2.77	0.53
1:E:470:TYR:HB3	1:E:479:PHE:CD1	2.44	0.53
1:A:44:SER:OG	1:A:45:THR:N	2.40	0.53
1:A:185:PHE:CE2	1:A:259:ASN:HB2	2.43	0.53
1:B:339:THR:HG21	1:C:472:PRO:HB3	1.91	0.53
1:B:463:ILE:O	1:B:463:ILE:HD13	2.09	0.53
1:E:46:PHE:CE1	1:E:55:LEU:CD1	2.91	0.53
1:F:152:VAL:HG21	1:F:307:ASN:HD21	1.73	0.53
1:F:534:LEU:HB2	1:F:542:MET:HE3	1.91	0.53
1:E:133:HIS:HB3	1:E:520:MET:HE3	1.91	0.53
1:E:175:LEU:CD1	1:E:177:ILE:HG23	2.39	0.53
1:A:37:PHE:CD1	1:A:38:ASP:N	2.75	0.53
1:A:233:GLN:O	1:A:236:ILE:HG13	2.09	0.53
1:C:46:PHE:HB3	1:C:57:VAL:HG23	1.90	0.53
1:C:60:ASP:HA	1:C:102:VAL:HG22	1.91	0.53
1:D:148:SER:HB3	1:E:156:SER:O	2.09	0.53
1:E:157:THR:O	1:E:157:THR:CG2	2.55	0.53
1:E:491:ASP:O	1:E:492:GLU:C	2.47	0.53
1:F:182:ARG:NH2	1:F:267:LYS:HE2	2.24	0.53
1:D:152:VAL:HG22	1:D:153:LEU:N	2.23	0.53
1:D:152:VAL:HG21	1:D:307:ASN:HD21	1.74	0.53
1:F:177:ILE:HG21	1:F:236:ILE:HG12	1.90	0.53
1:F:471:ALA:HB3	1:F:472:PRO:HD3	1.90	0.53
1:A:358:ASN:CG	1:A:358:ASN:O	2.47	0.52
1:B:259:ASN:O	1:B:260:GLY:C	2.46	0.52
1:D:46:PHE:CD2	1:D:46:PHE:O	2.62	0.52
1:D:302:HIS:CD2	1:D:303:LEU:HD13	2.44	0.52
1:D:572:ILE:O	1:D:572:ILE:CG2	2.50	0.52
1:E:26:ASN:HB3	1:E:29:ARG:CZ	2.39	0.52
1:E:90:LEU:HA	1:E:109:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:VAL:HG13	1:F:163:ILE:HD12	1.89	0.52
1:F:286:TYR:CE1	1:F:301:LYS:HE3	2.44	0.52
1:B:90:LEU:HD22	1:B:107:LEU:HD23	1.90	0.52
1:E:134:TYR:O	1:E:572:ILE:HD13	2.09	0.52
1:F:124:LEU:HD21	1:F:532:TRP:HE3	1.73	0.52
1:F:172:GLU:HB3	1:F:212:TRP:CH2	2.44	0.52
1:C:46:PHE:O	1:C:46:PHE:CD2	2.63	0.52
1:E:215:ASP:OD1	1:E:215:ASP:C	2.46	0.52
1:E:313:LEU:HB2	1:E:321:LEU:HB3	1.90	0.52
1:F:359:ASN:O	1:F:360:VAL:C	2.45	0.52
1:A:491:ASP:O	1:A:494:ASN:N	2.41	0.52
1:A:529:LYS:O	1:A:530:GLY:O	2.28	0.52
1:A:542:MET:O	1:A:543:ASN:C	2.48	0.52
1:B:157:THR:O	1:B:157:THR:CG2	2.56	0.52
1:B:572:ILE:O	1:B:572:ILE:CG2	2.49	0.52
1:C:148:SER:HB3	1:D:156:SER:O	2.09	0.52
1:C:256:GLU:O	1:C:264:SER:HA	2.08	0.52
1:C:516:ASP:OD2	1:C:517:ILE:N	2.42	0.52
1:D:26:ASN:O	1:D:29:ARG:HB3	2.09	0.52
1:D:30:ASP:OD2	1:D:89:TYR:OH	2.21	0.52
1:D:177:ILE:HG22	1:D:236:ILE:HG23	1.92	0.52
1:D:358:ASN:CG	1:D:358:ASN:O	2.48	0.52
1:A:217:GLU:O	1:A:220:LYS:N	2.42	0.52
1:B:164:LYS:C	1:B:282:ILE:HD11	2.29	0.52
1:C:75:ASN:O	1:C:92:VAL:N	2.40	0.52
1:C:502:MET:HG2	1:C:567:VAL:HG11	1.91	0.52
1:C:539:THR:CG2	1:D:94:ASP:HA	2.39	0.52
1:F:359:ASN:C	1:F:360:VAL:O	2.48	0.52
1:A:470:TYR:CB	1:A:479:PHE:CE1	2.93	0.52
1:B:42:PHE:CE2	1:B:44:SER:HB2	2.44	0.52
1:B:470:TYR:HB3	1:B:479:PHE:CD1	2.44	0.52
1:E:363:TYR:HD2	1:F:316:TYR:CE1	2.28	0.52
1:F:256:GLU:O	1:F:264:SER:HA	2.09	0.52
1:B:217:GLU:O	1:B:220:LYS:N	2.42	0.52
1:B:286:TYR:HE1	1:B:301:LYS:HE3	1.74	0.52
1:C:45:THR:HG23	1:C:45:THR:O	2.10	0.52
1:A:157:THR:HG22	1:A:488:ILE:HB	1.91	0.52
1:A:520:MET:SD	1:A:572:ILE:HG12	2.50	0.52
1:B:135:THR:O	1:B:136:GLN:C	2.44	0.52
1:B:285:ASP:HA	1:B:331:ASN:OD1	2.10	0.52
1:C:111:VAL:HB	1:C:545:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLU:CD	1:C:212:TRP:CZ2	2.83	0.52
1:D:111:VAL:HB	1:D:545:LEU:HD13	1.91	0.52
1:D:516:ASP:OD2	1:D:518:THR:HG22	2.09	0.52
1:D:546:ARG:NH2	1:E:15:ASN:OD1	2.43	0.52
1:E:177:ILE:HG22	1:E:236:ILE:HG23	1.91	0.52
1:B:3:LEU:N	1:B:44:SER:O	2.43	0.52
1:C:175:LEU:HD11	1:C:177:ILE:HG23	1.92	0.52
1:F:37:PHE:CD1	1:F:38:ASP:N	2.78	0.52
1:F:37:PHE:HZ	1:F:40:HIS:O	1.92	0.52
1:A:563:ILE:O	1:A:564:ASN:ND2	2.42	0.52
1:B:560:SER:O	1:B:564:ASN:ND2	2.41	0.52
1:E:175:LEU:HD23	1:E:239:VAL:HB	1.92	0.52
1:E:285:ASP:OD2	1:E:287:GLN:N	2.42	0.52
1:A:5:LYS:NZ	1:A:41:GLU:OE2	2.43	0.51
1:A:472:PRO:HB3	1:F:339:THR:HG21	1.92	0.51
1:C:48:TYR:OH	1:C:109:PRO:HG3	2.11	0.51
1:C:539:THR:HG23	1:D:93:THR:O	2.10	0.51
1:D:128:ASN:C	1:D:128:ASN:ND2	2.64	0.51
1:A:46:PHE:HB3	1:A:57:VAL:HG23	1.91	0.51
1:B:324:ASP:OD1	1:B:324:ASP:C	2.48	0.51
1:D:306:PRO:HD3	1:D:326:SER:HB3	1.92	0.51
1:F:90:LEU:HA	1:F:109:PRO:HA	1.93	0.51
1:B:148:SER:CB	1:C:156:SER:O	2.58	0.51
1:C:41:GLU:O	1:C:41:GLU:HG2	2.11	0.51
1:C:164:LYS:CB	1:C:282:ILE:HD12	2.40	0.51
1:D:356:ARG:NH2	1:E:487:ARG:O	2.42	0.51
1:C:534:LEU:HB2	1:C:542:MET:CE	2.41	0.51
1:D:347:LYS:HE2	1:D:369:THR:CG2	2.41	0.51
1:A:182:ARG:NH2	1:A:267:LYS:HE2	2.25	0.51
1:C:206:ASN:OD1	1:C:210:MET:HE1	2.09	0.51
1:C:356:ARG:NH2	1:D:487:ARG:O	2.38	0.51
1:D:542:MET:O	1:D:543:ASN:C	2.48	0.51
1:E:351:LYS:O	1:E:352:ASN:HB2	2.10	0.51
1:F:6:ILE:CG2	1:F:7:LYS:N	2.73	0.51
1:A:157:THR:HG23	1:A:489:SER:H	1.75	0.51
1:B:75:ASN:HA	1:B:92:VAL:HG22	1.91	0.51
1:D:175:LEU:HD11	1:D:177:ILE:HG23	1.91	0.51
1:A:48:TYR:OH	1:A:109:PRO:HG3	2.11	0.51
1:A:534:LEU:HB2	1:A:542:MET:CE	2.41	0.51
1:C:46:PHE:CE1	1:C:55:LEU:CD1	2.94	0.51
1:C:351:LYS:HG2	1:C:352:ASN:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:ASN:OD1	1:D:571:VAL:HG22	2.11	0.51
1:F:206:ASN:OD1	1:F:210:MET:HE1	2.11	0.51
1:B:164:LYS:CB	1:B:282:ILE:HD12	2.41	0.51
1:C:133:HIS:CD2	1:C:525:TRP:H	2.29	0.51
1:C:290:MET:HE3	1:C:295:LEU:HD23	1.93	0.51
1:E:6:ILE:CG2	1:E:7:LYS:N	2.74	0.51
1:E:566:THR:O	1:E:568:VAL:N	2.44	0.51
1:B:148:SER:HB3	1:C:156:SER:O	2.10	0.51
1:C:177:ILE:HG22	1:C:236:ILE:HG23	1.93	0.51
1:C:185:PHE:CE2	1:C:259:ASN:HB2	2.46	0.51
1:D:45:THR:HG23	1:D:45:THR:O	2.11	0.51
1:D:563:ILE:O	1:D:564:ASN:ND2	2.44	0.51
1:E:285:ASP:HA	1:E:331:ASN:OD1	2.11	0.51
1:F:111:VAL:HB	1:F:545:LEU:HD13	1.93	0.51
1:A:45:THR:O	1:A:45:THR:HG23	2.10	0.51
1:A:537:VAL:O	1:A:538:ASP:C	2.48	0.51
1:B:215:ASP:OD1	1:B:215:ASP:C	2.48	0.51
1:D:553:VAL:HG12	1:D:555:LEU:HD12	1.91	0.51
1:E:79:VAL:CG1	1:E:81:TYR:CE2	2.93	0.51
1:E:324:ASP:OD1	1:E:324:ASP:C	2.49	0.51
1:F:491:ASP:O	1:F:492:GLU:C	2.47	0.51
1:F:572:ILE:O	1:F:572:ILE:CG2	2.54	0.51
1:C:172:GLU:HB3	1:C:212:TRP:CH2	2.46	0.50
1:C:233:GLN:O	1:C:236:ILE:HG13	2.11	0.50
1:D:133:HIS:HB3	1:D:520:MET:CE	2.40	0.50
1:E:57:VAL:O	1:E:57:VAL:CG1	2.58	0.50
1:F:157:THR:HG22	1:F:488:ILE:HB	1.93	0.50
1:B:42:PHE:CE1	1:B:59:ILE:CD1	2.93	0.50
1:D:360:VAL:HG13	1:E:163:ILE:HD12	1.93	0.50
1:E:185:PHE:CE2	1:E:259:ASN:HB2	2.46	0.50
1:E:208:TYR:CZ	1:F:463:ILE:HG12	2.45	0.50
1:E:286:TYR:HE1	1:E:301:LYS:HG3	1.75	0.50
1:F:175:LEU:HD11	1:F:177:ILE:HG23	1.93	0.50
1:F:217:GLU:O	1:F:218:SER:C	2.48	0.50
1:F:358:ASN:CG	1:F:358:ASN:O	2.50	0.50
1:A:177:ILE:CB	1:A:236:ILE:HA	2.42	0.50
1:B:46:PHE:CE1	1:B:55:LEU:CD1	2.94	0.50
1:C:44:SER:OG	1:C:45:THR:N	2.42	0.50
1:D:152:VAL:O	1:D:152:VAL:HG13	2.09	0.50
1:F:502:MET:O	1:F:554:ARG:NH1	2.41	0.50
1:A:12:THR:HG21	1:A:76:TYR:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:O	1:A:46:PHE:CD2	2.64	0.50
1:C:360:VAL:HG13	1:D:163:ILE:HD12	1.92	0.50
1:C:553:VAL:HG12	1:C:555:LEU:HD12	1.92	0.50
1:E:359:ASN:O	1:E:360:VAL:C	2.50	0.50
1:F:46:PHE:CE1	1:F:55:LEU:CD1	2.94	0.50
1:F:172:GLU:CD	1:F:212:TRP:CH2	2.85	0.50
1:B:79:VAL:CG1	1:B:81:TYR:CE2	2.94	0.50
1:C:164:LYS:HB2	1:C:282:ILE:HD12	1.94	0.50
1:C:212:TRP:O	1:C:213:PHE:CD2	2.65	0.50
1:C:229:TYR:N	1:C:229:TYR:CD2	2.79	0.50
1:C:559:GLU:O	1:C:560:SER:C	2.50	0.50
1:D:120:VAL:CG2	1:D:121:LEU:N	2.73	0.50
1:D:491:ASP:O	1:D:494:ASN:N	2.44	0.50
1:F:164:LYS:CB	1:F:282:ILE:HD12	2.42	0.50
1:A:46:PHE:CE1	1:A:55:LEU:CD1	2.94	0.50
1:C:212:TRP:CZ3	1:C:247:ILE:HG13	2.47	0.50
1:C:545:LEU:O	1:C:546:ARG:C	2.50	0.50
1:E:59:ILE:O	1:E:59:ILE:CG2	2.59	0.50
1:E:164:LYS:C	1:E:282:ILE:HD11	2.31	0.50
1:A:90:LEU:HA	1:A:109:PRO:HA	1.93	0.50
1:B:175:LEU:HD11	1:B:177:ILE:HG23	1.93	0.50
1:B:306:PRO:HD3	1:B:326:SER:HB3	1.92	0.50
1:E:95:ILE:HG12	1:E:105:LEU:HD22	1.94	0.50
1:E:541:HIS:O	1:E:545:LEU:HB2	2.11	0.50
1:F:470:TYR:HB3	1:F:479:PHE:CD1	2.47	0.50
1:A:542:MET:HE2	1:A:545:LEU:HD23	1.93	0.50
1:B:152:VAL:HG22	1:B:153:LEU:N	2.27	0.50
1:E:106:SER:O	1:E:107:LEU:HD12	2.11	0.50
1:F:79:VAL:HG11	1:F:81:TYR:CE2	2.47	0.50
1:F:172:GLU:CD	1:F:212:TRP:CZ2	2.85	0.50
1:F:491:ASP:O	1:F:494:ASN:N	2.44	0.50
1:F:520:MET:HB3	1:F:570:ASN:OD1	2.12	0.50
1:A:226:LEU:HD12	1:A:233:GLN:HB3	1.94	0.50
1:E:90:LEU:HD22	1:E:107:LEU:HD23	1.94	0.50
1:E:133:HIS:HB3	1:E:520:MET:CE	2.42	0.50
1:F:78:GLN:CG	1:F:79:VAL:N	2.73	0.50
1:A:6:ILE:CG2	1:A:7:LYS:N	2.75	0.49
1:B:360:VAL:CG2	1:B:363:TYR:HB2	2.42	0.49
1:C:90:LEU:HD22	1:C:107:LEU:HD23	1.94	0.49
1:C:285:ASP:HA	1:C:331:ASN:OD1	2.12	0.49
1:D:157:THR:HG22	1:D:488:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:LYS:O	1:D:352:ASN:HB2	2.13	0.49
1:E:157:THR:HG22	1:E:488:ILE:HB	1.93	0.49
1:E:305:ARG:HB2	1:E:306:PRO:CD	2.43	0.49
1:F:185:PHE:CE2	1:F:259:ASN:HB2	2.46	0.49
1:F:202:ASP:OD2	1:F:274:SER:OG	2.30	0.49
1:B:48:TYR:CE1	1:B:55:LEU:HD22	2.48	0.49
1:B:172:GLU:HB3	1:B:212:TRP:CH2	2.47	0.49
1:B:282:ILE:HG23	1:B:334:PHE:CD2	2.47	0.49
1:D:29:ARG:HD2	1:D:30:ASP:OD2	2.11	0.49
1:D:92:VAL:HG23	1:D:92:VAL:O	2.12	0.49
1:E:172:GLU:OE1	1:E:212:TRP:CH2	2.64	0.49
1:E:172:GLU:CD	1:E:212:TRP:CH2	2.85	0.49
1:F:23:PHE:CD2	1:F:23:PHE:N	2.80	0.49
1:F:351:LYS:HG2	1:F:352:ASN:OD1	2.12	0.49
1:A:165:SER:HA	1:A:282:ILE:HD13	1.94	0.49
1:B:26:ASN:O	1:B:29:ARG:HB3	2.12	0.49
1:B:67:CYS:SG	1:B:68:PHE:N	2.85	0.49
1:C:296:ASN:O	1:C:300:ASP:HB2	2.12	0.49
1:C:306:PRO:HD3	1:C:326:SER:HB3	1.94	0.49
1:C:339:THR:HG21	1:D:472:PRO:HB3	1.93	0.49
1:E:130:ILE:CG2	1:E:527:GLN:HG2	2.43	0.49
1:E:172:GLU:CD	1:E:212:TRP:CZ2	2.85	0.49
1:E:532:TRP:HZ2	1:E:546:ARG:HA	1.76	0.49
1:F:152:VAL:HG13	1:F:152:VAL:O	2.11	0.49
1:F:172:GLU:OE1	1:F:212:TRP:CH2	2.64	0.49
1:A:339:THR:HG21	1:B:472:PRO:HB3	1.93	0.49
1:B:202:ASP:OD2	1:B:274:SER:OG	2.30	0.49
1:C:6:ILE:HG23	1:C:7:LYS:N	2.27	0.49
1:F:285:ASP:OD2	1:F:287:GLN:N	2.45	0.49
1:A:156:SER:O	1:F:148:SER:HB3	2.12	0.49
1:B:542:MET:HB3	1:B:546:ARG:NH1	2.27	0.49
1:A:177:ILE:HG22	1:A:236:ILE:HA	1.94	0.49
1:A:360:VAL:HG23	1:A:363:TYR:HB2	1.94	0.49
1:B:307:ASN:OD1	1:B:307:ASN:N	2.36	0.49
1:D:244:SER:O	1:D:245:GLY:C	2.51	0.49
1:E:128:ASN:HB2	1:E:510:TYR:HA	1.94	0.49
1:F:75:ASN:OD1	1:F:75:ASN:N	2.45	0.49
1:A:75:ASN:HA	1:A:92:VAL:HG22	1.95	0.49
1:B:286:TYR:C	1:B:286:TYR:CD2	2.85	0.49
1:C:106:SER:O	1:C:107:LEU:HD12	2.13	0.49
1:C:291:PHE:C	1:C:291:PHE:CD2	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:LEU:HD12	1:D:484:ARG:N	2.28	0.49
1:A:10:TYR:HB2	1:A:38:ASP:HB2	1.94	0.49
1:A:144:GLU:OE1	1:A:356:ARG:NH1	2.46	0.49
1:C:23:PHE:CD2	1:C:23:PHE:N	2.80	0.49
1:C:290:MET:HE2	1:C:295:LEU:HB3	1.94	0.49
1:F:566:THR:C	1:F:568:VAL:N	2.64	0.49
1:B:6:ILE:HG23	1:B:7:LYS:N	2.27	0.49
1:C:324:ASP:OD1	1:C:324:ASP:C	2.51	0.49
1:D:206:ASN:OD1	1:D:210:MET:HE1	2.13	0.49
1:E:122:ASN:OD1	1:E:517:ILE:HG12	2.13	0.49
1:B:61:LEU:HD12	1:B:61:LEU:N	2.28	0.49
1:B:516:ASP:OD2	1:B:518:THR:HG22	2.13	0.49
1:C:360:VAL:HG23	1:C:363:TYR:HB2	1.95	0.49
1:E:129:VAL:CG2	1:E:130:ILE:N	2.76	0.49
1:A:124:LEU:HD21	1:A:532:TRP:HE3	1.78	0.48
1:A:239:VAL:HG22	1:A:376:ILE:HG13	1.95	0.48
1:A:282:ILE:HD11	1:A:483:LEU:HB3	1.95	0.48
1:B:177:ILE:CG2	1:B:236:ILE:HG12	2.43	0.48
1:B:299:ASN:ND2	1:B:571:VAL:HG22	2.27	0.48
1:B:360:VAL:HG13	1:C:163:ILE:HD12	1.95	0.48
1:D:276:GLN:O	1:D:277:LYS:C	2.50	0.48
1:E:26:ASN:HB3	1:E:29:ARG:NH2	2.28	0.48
1:F:45:THR:HG23	1:F:45:THR:O	2.12	0.48
1:F:177:ILE:HD13	1:F:177:ILE:C	2.34	0.48
1:A:572:ILE:O	1:A:573:ILE:HB	2.12	0.48
1:B:185:PHE:CE2	1:B:259:ASN:HB2	2.48	0.48
1:B:276:GLN:O	1:B:277:LYS:C	2.51	0.48
1:D:285:ASP:O	1:D:286:TYR:C	2.50	0.48
1:E:470:TYR:CB	1:E:479:PHE:CE1	2.95	0.48
1:F:128:ASN:HB2	1:F:510:TYR:HA	1.94	0.48
1:F:516:ASP:CG	1:F:518:THR:HG22	2.34	0.48
1:F:572:ILE:O	1:F:573:ILE:HB	2.12	0.48
1:A:37:PHE:CE1	1:A:40:HIS:O	2.66	0.48
1:A:148:SER:CB	1:B:156:SER:O	2.62	0.48
1:A:305:ARG:HB2	1:A:306:PRO:CD	2.42	0.48
1:A:307:ASN:OD1	1:A:307:ASN:N	2.44	0.48
1:A:351:LYS:O	1:A:352:ASN:HB2	2.13	0.48
1:A:502:MET:O	1:A:554:ARG:NH1	2.41	0.48
1:B:256:GLU:O	1:B:264:SER:HA	2.13	0.48
1:B:542:MET:O	1:B:543:ASN:C	2.51	0.48
1:C:157:THR:HG22	1:C:488:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LYS:C	1:C:282:ILE:HD11	2.32	0.48
1:C:177:ILE:HG22	1:C:236:ILE:HA	1.95	0.48
1:C:177:ILE:CG2	1:C:236:ILE:HG12	2.43	0.48
1:D:172:GLU:CD	1:D:212:TRP:CH2	2.86	0.48
1:E:463:ILE:O	1:E:463:ILE:HD13	2.13	0.48
1:E:559:GLU:O	1:E:560:SER:C	2.50	0.48
1:F:120:VAL:CG2	1:F:121:LEU:N	2.76	0.48
1:A:121:LEU:O	1:A:124:LEU:HD12	2.13	0.48
1:A:470:TYR:CG	1:A:479:PHE:HE1	2.30	0.48
1:C:12:THR:HG21	1:C:76:TYR:HB2	1.95	0.48
1:C:172:GLU:CD	1:C:212:TRP:CH2	2.87	0.48
1:E:164:LYS:CB	1:E:282:ILE:HD12	2.43	0.48
1:E:544:MET:O	1:E:548:LEU:HB2	2.13	0.48
1:F:553:VAL:HG12	1:F:555:LEU:HD12	1.94	0.48
1:B:129:VAL:CG2	1:B:130:ILE:N	2.77	0.48
1:C:8:LEU:CD2	1:C:77:CYS:HB2	2.44	0.48
1:C:90:LEU:HA	1:C:109:PRO:HA	1.95	0.48
1:E:23:PHE:N	1:E:23:PHE:CD2	2.80	0.48
1:E:339:THR:HG21	1:F:472:PRO:HB3	1.93	0.48
1:F:463:ILE:O	1:F:463:ILE:HD12	2.14	0.48
1:A:516:ASP:OD2	1:A:518:THR:HG22	2.14	0.48
1:B:158:MET:C	1:B:159:ARG:HG2	2.33	0.48
1:B:177:ILE:HD13	1:B:177:ILE:O	2.13	0.48
1:B:282:ILE:HD11	1:B:483:LEU:HB3	1.95	0.48
1:D:212:TRP:O	1:D:213:PHE:CD2	2.66	0.48
1:D:363:TYR:HD2	1:E:316:TYR:CE1	2.30	0.48
1:D:559:GLU:O	1:D:560:SER:C	2.51	0.48
1:E:48:TYR:OH	1:E:109:PRO:HG3	2.14	0.48
1:E:206:ASN:OD1	1:E:210:MET:HE1	2.12	0.48
1:F:26:ASN:HB3	1:F:29:ARG:CZ	2.42	0.48
1:F:496:VAL:O	1:F:497:LYS:C	2.52	0.48
1:A:42:PHE:CE2	1:A:44:SER:HB2	2.49	0.48
1:A:61:LEU:N	1:A:61:LEU:HD12	2.29	0.48
1:C:511:SER:O	1:C:511:SER:OG	2.30	0.48
1:D:158:MET:C	1:D:159:ARG:HG2	2.34	0.48
1:E:380:VAL:O	1:E:462:ALA:N	2.47	0.48
1:E:498:LYS:O	1:E:499:TYR:C	2.52	0.48
1:E:516:ASP:OD2	1:E:518:THR:HG22	2.14	0.48
1:E:554:ARG:HG2	1:E:556:TRP:NE1	2.28	0.48
1:F:282:ILE:HD12	1:F:282:ILE:HA	1.71	0.48
1:F:512:THR:HG23	1:F:513:LYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:C	1:A:282:ILE:HD11	2.34	0.48
1:B:55:LEU:N	1:B:55:LEU:HD23	2.29	0.48
1:B:285:ASP:OD2	1:B:287:GLN:N	2.46	0.48
1:C:470:TYR:HB3	1:C:479:PHE:CD1	2.49	0.48
1:D:115:TYR:CE1	1:D:537:VAL:HG13	2.49	0.48
1:E:175:LEU:HD11	1:E:177:ILE:HG23	1.95	0.48
1:E:560:SER:O	1:E:564:ASN:ND2	2.44	0.48
1:F:78:GLN:HG2	1:F:79:VAL:H	1.79	0.48
1:F:92:VAL:O	1:F:92:VAL:CG2	2.59	0.48
1:F:95:ILE:HG12	1:F:105:LEU:HD22	1.96	0.48
1:A:3:LEU:HD11	1:B:68:PHE:CZ	2.49	0.48
1:A:177:ILE:HD13	1:A:177:ILE:C	2.32	0.48
1:A:212:TRP:CZ3	1:A:247:ILE:HG13	2.49	0.48
1:B:172:GLU:OE2	1:B:245:GLY:N	2.45	0.48
1:B:511:SER:O	1:B:511:SER:OG	2.28	0.48
1:B:559:GLU:O	1:B:560:SER:C	2.53	0.48
1:E:12:THR:HG21	1:E:76:TYR:HB2	1.95	0.48
1:B:212:TRP:HA	1:B:212:TRP:CE3	2.49	0.48
1:B:290:MET:HE3	1:B:295:LEU:HB3	1.96	0.48
1:B:296:ASN:O	1:B:300:ASP:HB2	2.14	0.48
1:C:258:VAL:HG12	1:C:263:LEU:O	2.12	0.48
1:D:285:ASP:OD2	1:D:287:GLN:N	2.46	0.48
1:E:249:GLN:OE1	1:E:249:GLN:HA	2.13	0.48
1:F:177:ILE:HG22	1:F:236:ILE:HA	1.96	0.48
1:B:172:GLU:OE1	1:B:212:TRP:CH2	2.65	0.47
1:C:534:LEU:HB2	1:C:542:MET:HE3	1.94	0.47
1:D:172:GLU:OE1	1:D:212:TRP:CH2	2.65	0.47
1:D:172:GLU:CD	1:D:212:TRP:CZ2	2.87	0.47
1:E:45:THR:HG23	1:E:45:THR:O	2.13	0.47
1:E:212:TRP:O	1:E:213:PHE:CD2	2.67	0.47
1:F:258:VAL:HG22	1:F:259:ASN:N	2.28	0.47
1:A:172:GLU:CD	1:A:212:TRP:CZ2	2.87	0.47
1:B:463:ILE:O	1:B:463:ILE:HD12	2.15	0.47
1:C:157:THR:HG23	1:C:489:SER:H	1.79	0.47
1:D:48:TYR:OH	1:D:109:PRO:HG3	2.13	0.47
1:B:563:ILE:C	1:B:564:ASN:ND2	2.68	0.47
1:D:29:ARG:HD3	1:D:89:TYR:CE2	2.49	0.47
1:D:258:VAL:HG22	1:D:259:ASN:N	2.30	0.47
1:D:516:ASP:OD1	1:D:518:THR:HG22	2.14	0.47
1:D:549:PHE:O	1:D:552:GLY:N	2.47	0.47
1:A:380:VAL:O	1:A:462:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ARG:HB2	1:B:306:PRO:HD2	1.95	0.47
1:B:470:TYR:CB	1:B:479:PHE:CE1	2.98	0.47
1:C:463:ILE:O	1:C:463:ILE:HD13	2.13	0.47
1:C:498:LYS:O	1:C:499:TYR:C	2.52	0.47
1:C:571:VAL:HG13	1:C:572:ILE:N	2.30	0.47
1:D:177:ILE:HD13	1:D:177:ILE:O	2.14	0.47
1:D:470:TYR:HB3	1:D:479:PHE:CD1	2.50	0.47
1:E:61:LEU:CD2	1:E:67:CYS:SG	3.02	0.47
1:E:463:ILE:O	1:E:463:ILE:HD12	2.14	0.47
1:E:470:TYR:CG	1:E:479:PHE:HE1	2.28	0.47
1:F:177:ILE:CB	1:F:236:ILE:HA	2.44	0.47
1:F:353:TYR:O	1:F:354:ASN:HB3	2.15	0.47
1:B:3:LEU:CB	1:B:45:THR:HB	2.44	0.47
1:B:3:LEU:HB3	1:B:45:THR:HB	1.96	0.47
1:B:572:ILE:O	1:B:573:ILE:HB	2.14	0.47
1:D:129:VAL:CG2	1:D:130:ILE:N	2.78	0.47
1:D:233:GLN:HG3	1:D:380:VAL:HG22	1.97	0.47
1:F:164:LYS:C	1:F:282:ILE:HD11	2.35	0.47
1:B:177:ILE:HG21	1:B:236:ILE:HG12	1.96	0.47
1:D:37:PHE:HZ	1:D:40:HIS:O	1.94	0.47
1:F:8:LEU:CD2	1:F:77:CYS:HB2	2.45	0.47
1:A:157:THR:HB	1:A:492:GLU:OE1	2.14	0.47
1:A:217:GLU:O	1:A:218:SER:C	2.52	0.47
1:B:274:SER:HB2	1:B:338:VAL:CG2	2.45	0.47
1:B:335:ASP:OD2	1:B:351:LYS:HD2	2.15	0.47
1:C:10:TYR:HB2	1:C:38:ASP:HB2	1.96	0.47
1:C:48:TYR:CE1	1:C:55:LEU:HD22	2.49	0.47
1:D:124:LEU:HD21	1:D:532:TRP:HE3	1.80	0.47
1:D:155:THR:HG21	1:D:307:ASN:O	2.15	0.47
1:D:177:ILE:CB	1:D:236:ILE:HA	2.45	0.47
1:E:42:PHE:CE2	1:E:44:SER:HB2	2.49	0.47
1:E:48:TYR:CE1	1:E:55:LEU:HD22	2.50	0.47
1:E:357:GLY:HA2	1:E:358:ASN:HA	1.69	0.47
1:F:212:TRP:O	1:F:213:PHE:CD2	2.67	0.47
1:F:542:MET:O	1:F:543:ASN:C	2.52	0.47
1:A:173:TYR:CD2	1:A:173:TYR:N	2.83	0.47
1:A:175:LEU:HD13	1:A:177:ILE:HG23	1.96	0.47
1:B:128:ASN:HB2	1:B:510:TYR:HA	1.97	0.47
1:B:470:TYR:CG	1:B:479:PHE:HE1	2.33	0.47
1:C:26:ASN:O	1:C:29:ARG:HB3	2.13	0.47
1:C:172:GLU:OE1	1:C:212:TRP:CH2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:ILE:O	1:C:564:ASN:ND2	2.48	0.47
1:D:286:TYR:CE1	1:D:301:LYS:HE3	2.50	0.47
1:E:212:TRP:O	1:E:213:PHE:CG	2.68	0.47
1:E:572:ILE:O	1:E:572:ILE:CG2	2.51	0.47
1:F:206:ASN:OD1	1:F:210:MET:HE3	2.15	0.47
1:F:516:ASP:OD1	1:F:518:THR:HG22	2.14	0.47
1:B:177:ILE:HG22	1:B:236:ILE:HA	1.96	0.47
1:B:177:ILE:CB	1:B:236:ILE:HA	2.45	0.47
1:C:155:THR:HG21	1:C:307:ASN:O	2.15	0.47
1:E:21:LEU:HD12	1:E:556:TRP:O	2.15	0.47
1:E:537:VAL:O	1:E:539:THR:N	2.48	0.47
1:A:23:PHE:N	1:A:23:PHE:CD2	2.82	0.47
1:B:212:TRP:O	1:B:213:PHE:CD2	2.68	0.47
1:C:285:ASP:O	1:C:286:TYR:C	2.53	0.47
1:E:177:ILE:HD13	1:E:177:ILE:O	2.15	0.47
1:F:128:ASN:C	1:F:128:ASN:ND2	2.67	0.47
1:F:571:VAL:HG13	1:F:572:ILE:N	2.30	0.47
1:A:164:LYS:CB	1:A:282:ILE:HD12	2.45	0.46
1:A:276:GLN:O	1:A:277:LYS:C	2.52	0.46
1:A:487:ARG:HG2	1:A:488:ILE:N	2.30	0.46
1:B:120:VAL:CG2	1:B:121:LEU:N	2.77	0.46
1:C:282:ILE:HD11	1:C:483:LEU:HB3	1.95	0.46
1:D:164:LYS:C	1:D:282:ILE:HD11	2.35	0.46
1:D:185:PHE:CE2	1:D:259:ASN:HB2	2.49	0.46
1:E:37:PHE:CE1	1:E:40:HIS:O	2.68	0.46
1:F:48:TYR:CE1	1:F:55:LEU:HD22	2.50	0.46
1:F:324:ASP:C	1:F:324:ASP:OD1	2.52	0.46
1:A:12:THR:HG22	1:A:75:ASN:OD1	2.15	0.46
1:A:286:TYR:C	1:A:286:TYR:CD2	2.88	0.46
1:A:491:ASP:O	1:A:492:GLU:C	2.51	0.46
1:C:37:PHE:HZ	1:C:40:HIS:O	1.96	0.46
1:D:571:VAL:HG13	1:D:572:ILE:N	2.31	0.46
1:D:572:ILE:O	1:D:573:ILE:HB	2.14	0.46
1:E:311:ALA:HB2	1:E:325:LEU:HD22	1.97	0.46
1:A:120:VAL:CG2	1:A:121:LEU:N	2.77	0.46
1:C:133:HIS:HB3	1:C:520:MET:HE2	1.97	0.46
1:C:323:ILE:HG23	1:C:353:TYR:CE1	2.49	0.46
1:D:12:THR:HG21	1:D:76:TYR:CB	2.45	0.46
1:D:463:ILE:O	1:D:463:ILE:HD12	2.14	0.46
1:D:529:LYS:O	1:D:530:GLY:O	2.33	0.46
1:F:155:THR:HG21	1:F:307:ASN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:PHE:C	1:F:291:PHE:CD2	2.89	0.46
1:A:29:ARG:HD2	1:A:30:ASP:OD2	2.16	0.46
1:A:68:PHE:CE2	1:F:3:LEU:HD21	2.51	0.46
1:A:172:GLU:CD	1:A:212:TRP:CH2	2.88	0.46
1:A:285:ASP:HA	1:A:331:ASN:OD1	2.15	0.46
1:A:285:ASP:O	1:A:286:TYR:C	2.53	0.46
1:B:516:ASP:OD2	1:B:517:ILE:N	2.47	0.46
1:D:75:ASN:HA	1:D:92:VAL:HG22	1.98	0.46
1:E:10:TYR:HB2	1:E:38:ASP:HB2	1.97	0.46
1:E:41:GLU:O	1:E:41:GLU:HG2	2.15	0.46
1:F:315:ASP:C	1:F:317:ALA:H	2.18	0.46
1:A:152:VAL:HG22	1:A:153:LEU:N	2.31	0.46
1:B:164:LYS:O	1:B:282:ILE:CD1	2.59	0.46
1:C:26:ASN:HB3	1:C:29:ARG:CZ	2.45	0.46
1:C:286:TYR:C	1:C:286:TYR:CD2	2.89	0.46
1:D:541:HIS:O	1:D:545:LEU:HB2	2.16	0.46
1:E:120:VAL:CG2	1:E:121:LEU:N	2.78	0.46
1:E:177:ILE:HG22	1:E:236:ILE:HA	1.96	0.46
1:E:291:PHE:C	1:E:291:PHE:CD2	2.89	0.46
1:E:542:MET:O	1:E:543:ASN:C	2.54	0.46
1:A:520:MET:HE1	1:A:572:ILE:HG12	1.98	0.46
1:B:152:VAL:HG21	1:B:307:ASN:HD21	1.81	0.46
1:B:172:GLU:CD	1:B:212:TRP:CZ2	2.88	0.46
1:E:212:TRP:HA	1:E:212:TRP:CE3	2.50	0.46
1:F:10:TYR:HB2	1:F:38:ASP:HB2	1.97	0.46
1:F:285:ASP:O	1:F:286:TYR:C	2.54	0.46
1:A:95:ILE:HG12	1:A:105:LEU:HD22	1.98	0.46
1:A:177:ILE:HB	1:A:236:ILE:HA	1.97	0.46
1:A:463:ILE:O	1:A:463:ILE:HD13	2.15	0.46
1:C:79:VAL:CG1	1:C:81:TYR:CE2	2.99	0.46
1:F:38:ASP:O	1:F:39:VAL:HG23	2.16	0.46
1:B:165:SER:HA	1:B:282:ILE:HD13	1.98	0.46
1:B:212:TRP:CZ3	1:B:247:ILE:HG13	2.51	0.46
1:C:57:VAL:O	1:C:57:VAL:CG1	2.63	0.46
1:C:177:ILE:CB	1:C:236:ILE:HA	2.45	0.46
1:C:290:MET:HE2	1:C:290:MET:HB3	1.89	0.46
1:C:348:VAL:CG2	1:C:349:TYR:N	2.77	0.46
1:D:217:GLU:O	1:D:220:LYS:N	2.49	0.46
1:D:249:GLN:HA	1:D:249:GLN:OE1	2.16	0.46
1:D:307:ASN:OD1	1:D:307:ASN:N	2.45	0.46
1:E:310:THR:HG22	1:E:486:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:ASN:O	1:E:358:ASN:CG	2.53	0.46
1:F:177:ILE:HB	1:F:236:ILE:HA	1.97	0.46
1:A:546:ARG:NH2	1:B:15:ASN:CG	2.69	0.46
1:B:276:GLN:O	1:B:277:LYS:O	2.33	0.46
1:C:380:VAL:O	1:C:462:ALA:N	2.48	0.46
1:D:233:GLN:HG3	1:D:380:VAL:CG2	2.46	0.46
1:D:548:LEU:HD23	1:D:548:LEU:HA	1.84	0.46
1:E:152:VAL:HG21	1:E:307:ASN:HD21	1.81	0.46
1:E:571:VAL:HG13	1:E:572:ILE:N	2.31	0.46
1:F:48:TYR:OH	1:F:109:PRO:HG3	2.16	0.46
1:B:351:LYS:O	1:B:352:ASN:HB2	2.14	0.46
1:C:371:ASN:C	1:C:371:ASN:OD1	2.55	0.46
1:D:42:PHE:CE2	1:D:44:SER:HB2	2.51	0.46
1:D:259:ASN:O	1:D:260:GLY:C	2.55	0.46
1:D:491:ASP:O	1:D:492:GLU:C	2.54	0.46
1:D:498:LYS:O	1:D:499:TYR:C	2.54	0.46
1:E:306:PRO:HD3	1:E:326:SER:HB3	1.98	0.46
1:A:463:ILE:O	1:A:463:ILE:HD12	2.15	0.45
1:A:563:ILE:N	1:A:563:ILE:CD1	2.78	0.45
1:B:549:PHE:O	1:B:552:GLY:N	2.49	0.45
1:C:541:HIS:O	1:C:545:LEU:HB2	2.17	0.45
1:D:157:THR:HB	1:D:492:GLU:OE1	2.17	0.45
1:D:299:ASN:ND2	1:D:299:ASN:H	2.15	0.45
1:E:319:ASN:C	1:E:320:ARG:HG2	2.36	0.45
1:F:6:ILE:HG23	1:F:7:LYS:N	2.31	0.45
1:F:25:SER:OG	1:F:28:GLU:HG3	2.16	0.45
1:F:380:VAL:O	1:F:462:ALA:N	2.49	0.45
1:A:148:SER:HB3	1:B:156:SER:O	2.16	0.45
1:A:259:ASN:O	1:A:260:GLY:C	2.51	0.45
1:B:165:SER:CA	1:B:282:ILE:HD13	2.46	0.45
1:C:95:ILE:HG12	1:C:105:LEU:HD22	1.99	0.45
1:C:120:VAL:CG2	1:C:121:LEU:N	2.79	0.45
1:C:133:HIS:HB3	1:C:520:MET:HE3	1.97	0.45
1:E:8:LEU:CD2	1:E:77:CYS:HB2	2.46	0.45
1:E:92:VAL:HG23	1:E:92:VAL:O	2.16	0.45
1:E:302:HIS:CD2	1:E:303:LEU:HD13	2.51	0.45
1:F:82:ILE:HA	1:F:83:GLN:HA	1.74	0.45
1:F:520:MET:HE1	1:F:572:ILE:HG12	1.98	0.45
1:A:38:ASP:O	1:A:39:VAL:HG23	2.16	0.45
1:A:42:PHE:CE1	1:A:59:ILE:CD1	2.99	0.45
1:A:290:MET:CE	1:A:295:LEU:CB	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ASP:O	1:B:541:HIS:N	2.40	0.45
1:C:285:ASP:OD2	1:C:285:ASP:C	2.55	0.45
1:D:177:ILE:HB	1:D:236:ILE:HA	1.98	0.45
1:D:212:TRP:CZ3	1:D:247:ILE:HG13	2.51	0.45
1:D:511:SER:O	1:D:511:SER:OG	2.28	0.45
1:E:129:VAL:HG23	1:E:130:ILE:H	1.81	0.45
1:E:177:ILE:CG2	1:E:236:ILE:HG12	2.46	0.45
1:E:217:GLU:O	1:E:220:LYS:N	2.49	0.45
1:C:177:ILE:HG21	1:C:236:ILE:HG12	1.98	0.45
1:C:351:LYS:O	1:C:352:ASN:HB2	2.17	0.45
1:D:122:ASN:OD1	1:D:517:ILE:HG12	2.16	0.45
1:E:244:SER:O	1:E:245:GLY:C	2.55	0.45
1:F:516:ASP:OD2	1:F:517:ILE:N	2.49	0.45
1:F:559:GLU:O	1:F:560:SER:C	2.55	0.45
1:A:79:VAL:CG1	1:A:81:TYR:CE2	3.00	0.45
1:A:172:GLU:CD	1:A:245:GLY:H	2.20	0.45
1:B:8:LEU:CD2	1:B:77:CYS:HB2	2.46	0.45
1:C:286:TYR:CE1	1:C:301:LYS:HE3	2.51	0.45
1:C:305:ARG:HB2	1:C:306:PRO:CD	2.46	0.45
1:E:38:ASP:O	1:E:39:VAL:HG23	2.16	0.45
1:F:59:ILE:O	1:F:59:ILE:CG2	2.64	0.45
1:A:559:GLU:O	1:A:560:SER:C	2.55	0.45
1:B:41:GLU:O	1:B:41:GLU:HG2	2.16	0.45
1:C:75:ASN:OD1	1:C:75:ASN:N	2.50	0.45
1:C:175:LEU:HD23	1:C:239:VAL:HB	1.99	0.45
1:C:282:ILE:HD12	1:C:282:ILE:HA	1.75	0.45
1:F:26:ASN:HB3	1:F:29:ARG:NH2	2.31	0.45
1:F:463:ILE:O	1:F:463:ILE:HD13	2.16	0.45
1:A:174:ILE:CG1	1:A:176:THR:HG22	2.44	0.45
1:A:324:ASP:C	1:A:324:ASP:OD1	2.54	0.45
1:B:46:PHE:HB3	1:B:57:VAL:HG23	1.98	0.45
1:B:498:LYS:O	1:B:499:TYR:C	2.54	0.45
1:B:525:TRP:CZ3	1:B:554:ARG:NH1	2.84	0.45
1:C:75:ASN:HA	1:C:92:VAL:HG22	1.99	0.45
1:C:129:VAL:CG2	1:C:130:ILE:N	2.79	0.45
1:C:212:TRP:HA	1:C:212:TRP:CE3	2.51	0.45
1:C:358:ASN:O	1:C:358:ASN:CG	2.54	0.45
1:C:560:SER:O	1:C:564:ASN:ND2	2.43	0.45
1:D:305:ARG:HB2	1:D:306:PRO:CD	2.47	0.45
1:E:286:TYR:C	1:E:286:TYR:CD2	2.89	0.45
1:F:172:GLU:CD	1:F:245:GLY:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:CE1	1:A:55:LEU:HD22	2.51	0.45
1:A:175:LEU:HD11	1:A:177:ILE:HG23	1.99	0.45
1:A:306:PRO:HD3	1:A:326:SER:HB3	1.98	0.45
1:B:95:ILE:HG12	1:B:105:LEU:HD22	1.97	0.45
1:B:290:MET:HE3	1:B:295:LEU:HB2	1.98	0.45
1:C:82:ILE:HA	1:C:83:GLN:HA	1.70	0.45
1:C:276:GLN:O	1:C:277:LYS:C	2.53	0.45
1:C:483:LEU:HD12	1:C:484:ARG:N	2.32	0.45
1:D:371:ASN:OD1	1:D:371:ASN:C	2.55	0.45
1:E:212:TRP:CZ3	1:E:247:ILE:HG13	2.52	0.45
1:E:351:LYS:HG2	1:E:352:ASN:OD1	2.17	0.45
1:F:3:LEU:O	1:F:82:ILE:HG13	2.17	0.45
1:F:23:PHE:HD2	1:F:117:GLN:OE1	2.00	0.45
1:A:106:SER:C	1:A:107:LEU:HD12	2.36	0.45
1:A:155:THR:HG21	1:A:307:ASN:O	2.16	0.45
1:B:129:VAL:HG23	1:B:130:ILE:H	1.82	0.45
1:B:206:ASN:OD1	1:B:210:MET:CE	2.65	0.45
1:C:71:LEU:HD12	1:C:71:LEU:O	2.16	0.45
1:C:531:ILE:HD12	1:C:531:ILE:HA	1.87	0.45
1:D:148:SER:HB2	1:E:156:SER:O	2.16	0.45
1:E:282:ILE:HD11	1:E:483:LEU:HB3	1.99	0.45
1:E:371:ASN:C	1:E:371:ASN:OD1	2.55	0.45
1:A:156:SER:O	1:F:148:SER:HB2	2.17	0.45
1:B:124:LEU:HD21	1:B:532:TRP:HE3	1.81	0.45
1:B:157:THR:HB	1:B:492:GLU:OE1	2.17	0.45
1:B:358:ASN:O	1:B:358:ASN:CG	2.55	0.45
1:B:544:MET:O	1:B:548:LEU:HB2	2.17	0.45
1:B:546:ARG:NH2	1:C:15:ASN:CG	2.70	0.45
1:C:319:ASN:C	1:C:320:ARG:HG2	2.37	0.45
1:D:182:ARG:NH2	1:D:267:LYS:HE2	2.32	0.45
1:D:212:TRP:O	1:D:213:PHE:CG	2.70	0.45
1:E:274:SER:HB2	1:E:338:VAL:CG2	2.47	0.45
1:E:359:ASN:C	1:E:360:VAL:O	2.52	0.45
1:B:566:THR:C	1:B:568:VAL:N	2.67	0.44
1:D:133:HIS:CD2	1:D:525:TRP:H	2.36	0.44
1:D:202:ASP:OD2	1:D:274:SER:OG	2.35	0.44
1:E:158:MET:C	1:E:159:ARG:HG2	2.37	0.44
1:E:572:ILE:O	1:E:573:ILE:HB	2.17	0.44
1:F:124:LEU:CD2	1:F:532:TRP:HB2	2.45	0.44
1:F:531:ILE:HD12	1:F:531:ILE:HA	1.78	0.44
1:A:96:GLN:OE1	1:F:49:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:OD1	1:B:517:ILE:HG12	2.17	0.44
1:B:525:TRP:CE3	1:B:554:ARG:NH1	2.85	0.44
1:C:190:LYS:O	1:C:190:LYS:CG	2.62	0.44
1:C:542:MET:O	1:C:543:ASN:C	2.56	0.44
1:C:566:THR:C	1:C:568:VAL:N	2.68	0.44
1:D:128:ASN:HB2	1:D:510:TYR:HA	1.99	0.44
1:D:286:TYR:C	1:D:286:TYR:CD2	2.90	0.44
1:E:276:GLN:O	1:E:277:LYS:C	2.56	0.44
1:F:115:TYR:CE1	1:F:537:VAL:HG13	2.52	0.44
1:F:164:LYS:HB2	1:F:282:ILE:HD12	1.99	0.44
1:F:360:VAL:HG23	1:F:363:TYR:HB2	2.00	0.44
1:A:152:VAL:HG21	1:A:307:ASN:HD21	1.81	0.44
1:A:177:ILE:HD13	1:A:177:ILE:H	1.82	0.44
1:A:293:LEU:HD22	1:A:309:VAL:HG11	2.00	0.44
1:A:347:LYS:HE2	1:A:369:THR:CG2	2.47	0.44
1:A:566:THR:O	1:A:568:VAL:N	2.49	0.44
1:B:65:ARG:HG2	1:B:66:SER:N	2.32	0.44
1:B:164:LYS:HB2	1:B:282:ILE:HD12	2.00	0.44
1:B:172:GLU:CD	1:B:212:TRP:CH2	2.90	0.44
1:C:8:LEU:HD22	1:C:77:CYS:HB2	1.98	0.44
1:C:166:GLU:OE1	1:C:279:PHE:HA	2.17	0.44
1:C:529:LYS:O	1:C:530:GLY:O	2.35	0.44
1:C:572:ILE:O	1:C:573:ILE:HB	2.18	0.44
1:D:82:ILE:HA	1:D:83:GLN:HA	1.75	0.44
1:E:220:LYS:O	1:E:221:GLU:C	2.54	0.44
1:E:360:VAL:HG23	1:E:363:TYR:HB2	1.97	0.44
1:F:529:LYS:O	1:F:530:GLY:C	2.55	0.44
1:B:302:HIS:CD2	1:B:303:LEU:HD13	2.52	0.44
1:C:274:SER:HB2	1:C:338:VAL:CG2	2.48	0.44
1:D:157:THR:HG23	1:D:489:SER:H	1.81	0.44
1:D:534:LEU:HB2	1:D:542:MET:HE1	1.98	0.44
1:E:61:LEU:HD12	1:E:61:LEU:N	2.33	0.44
1:E:65:ARG:HG2	1:E:66:SER:N	2.32	0.44
1:E:75:ASN:OD1	1:E:75:ASN:N	2.48	0.44
1:F:81:TYR:HE1	1:F:86:ARG:NH2	2.15	0.44
1:F:127:VAL:CG2	1:F:528:PHE:CD1	2.99	0.44
1:B:23:PHE:HD2	1:B:117:GLN:OE1	2.01	0.44
1:C:38:ASP:O	1:C:39:VAL:HG23	2.17	0.44
1:C:172:GLU:OE2	1:C:245:GLY:N	2.47	0.44
1:D:177:ILE:HG22	1:D:236:ILE:HA	1.98	0.44
1:D:502:MET:O	1:D:554:ARG:NH1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TRP:CE3	1:A:212:TRP:HA	2.53	0.44
1:B:177:ILE:HB	1:B:236:ILE:HA	2.00	0.44
1:C:502:MET:O	1:C:554:ARG:NH1	2.44	0.44
1:D:79:VAL:CG1	1:D:81:TYR:CE2	3.00	0.44
1:D:532:TRP:CZ2	1:D:546:ARG:HA	2.53	0.44
1:A:299:ASN:ND2	1:A:299:ASN:N	2.65	0.44
1:C:124:LEU:HD21	1:C:532:TRP:HE3	1.82	0.44
1:C:152:VAL:HG22	1:C:153:LEU:N	2.33	0.44
1:D:38:ASP:O	1:D:39:VAL:HG23	2.17	0.44
1:E:133:HIS:CD2	1:E:525:TRP:H	2.36	0.44
1:F:175:LEU:HD13	1:F:177:ILE:HG23	2.00	0.44
1:F:313:LEU:HD23	1:F:313:LEU:HA	1.79	0.44
1:A:75:ASN:OD1	1:A:75:ASN:N	2.50	0.44
1:A:82:ILE:HA	1:A:83:GLN:HA	1.70	0.44
1:A:516:ASP:OD2	1:A:517:ILE:N	2.50	0.44
1:A:560:SER:O	1:A:564:ASN:ND2	2.44	0.44
1:B:487:ARG:HG2	1:B:488:ILE:N	2.33	0.44
1:C:164:LYS:O	1:C:282:ILE:CD1	2.60	0.44
1:D:359:ASN:O	1:D:360:VAL:C	2.56	0.44
1:D:509:ASP:O	1:D:510:TYR:C	2.56	0.44
1:F:106:SER:O	1:F:107:LEU:HD12	2.17	0.44
1:A:164:LYS:HB2	1:A:282:ILE:HD12	1.99	0.44
1:A:206:ASN:OD1	1:A:210:MET:HE3	2.17	0.44
1:A:285:ASP:OD2	1:A:287:GLN:N	2.50	0.44
1:B:38:ASP:O	1:B:39:VAL:HG23	2.18	0.44
1:C:491:ASP:O	1:C:494:ASN:N	2.51	0.44
1:C:520:MET:SD	1:C:572:ILE:HG12	2.58	0.44
1:E:177:ILE:HG21	1:E:236:ILE:HG12	1.99	0.44
1:F:152:VAL:HG22	1:F:153:LEU:N	2.32	0.44
1:F:279:PHE:HB3	1:F:282:ILE:HG22	2.00	0.44
1:C:533:THR:HG23	1:D:15:ASN:ND2	2.33	0.43
1:D:37:PHE:CE1	1:D:40:HIS:O	2.71	0.43
1:D:566:THR:C	1:D:568:VAL:N	2.70	0.43
1:F:42:PHE:CE2	1:F:44:SER:HB2	2.53	0.43
1:F:542:MET:HE2	1:F:545:LEU:HD23	1.96	0.43
1:B:285:ASP:OD2	1:B:285:ASP:C	2.56	0.43
1:C:165:SER:HA	1:C:282:ILE:HD13	1.99	0.43
1:C:516:ASP:OD2	1:C:518:THR:HG22	2.18	0.43
1:D:6:ILE:CG2	1:D:7:LYS:N	2.80	0.43
1:D:48:TYR:CE1	1:D:55:LEU:HD22	2.53	0.43
1:D:291:PHE:C	1:D:291:PHE:CD2	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:LEU:HD12	1:E:233:GLN:HB3	2.00	0.43
1:E:537:VAL:O	1:E:538:ASP:C	2.55	0.43
1:F:5:LYS:HB3	1:F:80:GLN:HG3	2.00	0.43
1:A:68:PHE:CZ	1:F:3:LEU:HD11	2.53	0.43
1:C:359:ASN:O	1:C:360:VAL:C	2.55	0.43
1:E:175:LEU:HA	1:E:239:VAL:HB	2.00	0.43
1:E:217:GLU:O	1:E:218:SER:C	2.54	0.43
1:A:206:ASN:OD1	1:A:210:MET:HE1	2.19	0.43
1:B:258:VAL:HG22	1:B:259:ASN:N	2.33	0.43
1:D:57:VAL:O	1:D:57:VAL:HG12	2.18	0.43
1:D:124:LEU:CD2	1:D:532:TRP:HB2	2.46	0.43
1:D:347:LYS:HE2	1:D:369:THR:HG22	1.99	0.43
1:E:165:SER:CA	1:E:282:ILE:HD13	2.48	0.43
1:E:573:ILE:HD13	1:E:573:ILE:N	2.33	0.43
1:F:363:TYR:CD1	1:F:364:ILE:HG23	2.53	0.43
1:F:514:LEU:HD12	1:F:514:LEU:HA	1.78	0.43
1:A:321:LEU:HA	1:A:321:LEU:HD12	1.77	0.43
1:B:282:ILE:HD12	1:B:282:ILE:HA	1.79	0.43
1:B:299:ASN:OD1	1:B:299:ASN:N	2.48	0.43
1:D:12:THR:HG22	1:D:75:ASN:OD1	2.18	0.43
1:D:110:ASP:OD1	1:D:113:MET:HB2	2.18	0.43
1:E:75:ASN:CA	1:E:92:VAL:HG22	2.48	0.43
1:F:21:LEU:HG	1:F:22:HIS:N	2.34	0.43
1:F:249:GLN:OE1	1:F:249:GLN:HA	2.19	0.43
1:A:215:ASP:OD1	1:A:217:GLU:N	2.51	0.43
1:C:212:TRP:O	1:C:213:PHE:CG	2.71	0.43
1:C:357:GLY:HA2	1:C:358:ASN:HA	1.68	0.43
1:C:542:MET:CE	1:C:542:MET:HA	2.48	0.43
1:D:360:VAL:HG23	1:D:363:TYR:HB2	2.00	0.43
1:D:520:MET:HB3	1:D:570:ASN:OD1	2.19	0.43
1:E:12:THR:HG21	1:E:76:TYR:CB	2.47	0.43
1:E:115:TYR:CE1	1:E:537:VAL:HG13	2.53	0.43
1:E:124:LEU:HD21	1:E:532:TRP:HE3	1.83	0.43
1:E:169:THR:HG23	1:E:170:GLN:HG3	2.00	0.43
1:E:512:THR:HG23	1:E:513:LYS:N	2.34	0.43
1:F:122:ASN:OD1	1:F:517:ILE:HG12	2.18	0.43
1:A:157:THR:CG2	1:A:157:THR:O	2.64	0.43
1:B:3:LEU:HB3	1:B:45:THR:CB	2.48	0.43
1:B:520:MET:HB3	1:B:570:ASN:OD1	2.18	0.43
1:D:23:PHE:CD2	1:D:23:PHE:N	2.86	0.43
1:D:59:ILE:O	1:D:59:ILE:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:MET:HE3	1:D:295:LEU:HB3	1.99	0.43
1:E:152:VAL:O	1:E:152:VAL:HG13	2.16	0.43
1:F:55:LEU:N	1:F:55:LEU:HD23	2.33	0.43
1:F:498:LYS:O	1:F:499:TYR:C	2.55	0.43
1:A:27:GLU:HG2	1:A:28:GLU:N	2.34	0.43
1:C:152:VAL:O	1:C:152:VAL:HG13	2.19	0.43
1:D:129:VAL:HG23	1:D:130:ILE:H	1.84	0.43
1:D:220:LYS:O	1:D:221:GLU:C	2.57	0.43
1:D:310:THR:HG22	1:D:486:GLY:HA3	2.01	0.43
1:E:293:LEU:HD22	1:E:309:VAL:HG11	2.00	0.43
1:E:491:ASP:O	1:E:494:ASN:N	2.51	0.43
1:F:42:PHE:CE1	1:F:59:ILE:CD1	3.02	0.43
1:F:357:GLY:HA2	1:F:358:ASN:HA	1.77	0.43
1:A:3:LEU:HD11	1:B:68:PHE:HZ	1.84	0.43
1:A:496:VAL:O	1:A:497:LYS:C	2.56	0.43
1:B:48:TYR:OH	1:B:109:PRO:HG3	2.19	0.43
1:C:282:ILE:HG23	1:C:334:PHE:CD2	2.54	0.43
1:D:212:TRP:HA	1:D:212:TRP:CE3	2.54	0.43
1:E:23:PHE:HD2	1:E:117:GLN:OE1	2.01	0.43
1:E:177:ILE:CB	1:E:236:ILE:HA	2.49	0.43
1:F:168:PHE:CD2	1:F:480:GLY:HA2	2.54	0.43
1:A:371:ASN:OD1	1:A:371:ASN:C	2.54	0.43
1:A:534:LEU:HD23	1:A:534:LEU:HA	1.83	0.43
1:B:175:LEU:HD13	1:B:177:ILE:HG23	2.00	0.43
1:B:249:GLN:HA	1:B:249:GLN:OE1	2.18	0.43
1:C:12:THR:HG22	1:C:75:ASN:OD1	2.19	0.43
1:C:157:THR:HB	1:C:492:GLU:OE1	2.19	0.43
1:C:534:LEU:HD23	1:C:534:LEU:HA	1.90	0.43
1:E:12:THR:HA	1:E:13:PRO:HD3	1.87	0.43
1:E:374:ASP:HB3	1:E:467:HIS:O	2.19	0.43
1:F:8:LEU:HD22	1:F:77:CYS:HB2	2.01	0.43
1:F:29:ARG:HD2	1:F:30:ASP:OD2	2.18	0.43
1:A:282:ILE:HD12	1:A:282:ILE:HA	1.73	0.42
1:A:291:PHE:CD2	1:A:291:PHE:C	2.92	0.42
1:A:572:ILE:O	1:A:572:ILE:CG2	2.50	0.42
1:B:189:GLU:CD	1:B:189:GLU:N	2.73	0.42
1:D:10:TYR:HB2	1:D:38:ASP:HB2	2.00	0.42
1:D:95:ILE:HG12	1:D:105:LEU:HD22	2.01	0.42
1:D:177:ILE:CG2	1:D:236:ILE:HG12	2.48	0.42
1:E:71:LEU:HD12	1:E:71:LEU:O	2.18	0.42
1:F:3:LEU:HB3	1:F:45:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:TYR:C	1:F:286:TYR:CD2	2.92	0.42
1:A:112:VAL:CG2	1:A:548:LEU:CD1	2.97	0.42
1:A:274:SER:HB2	1:A:338:VAL:CG2	2.49	0.42
1:A:563:ILE:HD13	1:A:563:ILE:H	1.80	0.42
1:C:363:TYR:CD1	1:C:364:ILE:HG23	2.54	0.42
1:C:363:TYR:HD2	1:D:316:TYR:CE1	2.37	0.42
1:D:130:ILE:CG2	1:D:527:GLN:HG2	2.49	0.42
1:D:164:LYS:CB	1:D:282:ILE:HD12	2.49	0.42
1:D:516:ASP:CG	1:D:518:THR:HG22	2.38	0.42
1:E:282:ILE:HD12	1:E:282:ILE:HA	1.67	0.42
1:A:16:ASN:HB3	1:F:531:ILE:CD1	2.49	0.42
1:A:65:ARG:HG2	1:A:66:SER:N	2.34	0.42
1:A:277:LYS:O	1:A:336:SER:OG	2.37	0.42
1:A:537:VAL:O	1:A:539:THR:N	2.52	0.42
1:B:112:VAL:CG2	1:B:548:LEU:CD1	2.97	0.42
1:B:491:ASP:O	1:B:494:ASN:N	2.52	0.42
1:C:470:TYR:CB	1:C:479:PHE:CE1	3.02	0.42
1:C:514:LEU:HD12	1:C:514:LEU:HA	1.90	0.42
1:C:516:ASP:OD1	1:C:518:THR:HG22	2.19	0.42
1:A:531:ILE:HD12	1:A:531:ILE:HA	1.84	0.42
1:B:111:VAL:CB	1:B:545:LEU:HD13	2.47	0.42
1:B:133:HIS:HB3	1:B:520:MET:HE2	2.00	0.42
1:C:165:SER:CA	1:C:282:ILE:HD13	2.49	0.42
1:D:112:VAL:CG2	1:D:548:LEU:CD1	2.97	0.42
1:E:134:TYR:HH	1:E:507:CYS:HG	1.63	0.42
1:E:157:THR:HB	1:E:492:GLU:OE1	2.19	0.42
1:A:553:VAL:HG12	1:A:555:LEU:HD12	2.00	0.42
1:B:174:ILE:CG1	1:B:176:THR:HG22	2.48	0.42
1:B:571:VAL:HG13	1:B:572:ILE:N	2.34	0.42
1:C:92:VAL:HG23	1:C:92:VAL:O	2.20	0.42
1:D:172:GLU:OE2	1:D:245:GLY:N	2.49	0.42
1:D:542:MET:HB3	1:D:546:ARG:NH1	2.34	0.42
1:E:542:MET:HB3	1:E:546:ARG:NH1	2.34	0.42
1:A:55:LEU:N	1:A:55:LEU:HD23	2.34	0.42
1:C:42:PHE:CE2	1:C:44:SER:HB2	2.54	0.42
1:C:48:TYR:CD2	1:C:55:LEU:HD13	2.55	0.42
1:C:226:LEU:HD12	1:C:233:GLN:HB3	2.01	0.42
1:C:249:GLN:OE1	1:C:249:GLN:HA	2.19	0.42
1:C:491:ASP:O	1:C:492:GLU:C	2.58	0.42
1:D:41:GLU:O	1:D:41:GLU:HG2	2.20	0.42
1:D:258:VAL:HG12	1:D:263:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:PHE:HB3	1:D:282:ILE:HG22	2.02	0.42
1:D:315:ASP:HB3	1:D:370:ILE:HD11	2.01	0.42
1:E:516:ASP:OD1	1:E:518:THR:HG22	2.20	0.42
1:A:254:ASP:O	1:A:255:HIS:C	2.57	0.42
1:B:42:PHE:CG	1:B:43:THR:N	2.85	0.42
1:B:244:SER:O	1:B:245:GLY:C	2.58	0.42
1:B:539:THR:CG2	1:B:540:GLY:N	2.82	0.42
1:C:177:ILE:HB	1:C:236:ILE:HA	2.01	0.42
1:C:263:LEU:HD12	1:C:263:LEU:HA	1.90	0.42
1:D:120:VAL:HG23	1:D:121:LEU:H	1.81	0.42
1:D:124:LEU:HD22	1:D:532:TRP:CB	2.47	0.42
1:D:323:ILE:HG23	1:D:353:TYR:CE1	2.55	0.42
1:D:470:TYR:CB	1:D:479:PHE:CE1	3.02	0.42
1:E:534:LEU:HB2	1:E:542:MET:HE1	2.01	0.42
1:F:65:ARG:HG2	1:F:66:SER:N	2.35	0.42
1:F:104:GLU:O	1:F:105:LEU:HD23	2.19	0.42
1:F:165:SER:HA	1:F:282:ILE:HD13	2.01	0.42
1:F:571:VAL:CG1	1:F:572:ILE:N	2.79	0.42
1:B:359:ASN:O	1:B:360:VAL:C	2.58	0.42
1:C:531:ILE:CD1	1:D:16:ASN:HB3	2.49	0.42
1:D:359:ASN:C	1:D:360:VAL:O	2.58	0.42
1:F:236:ILE:HG21	1:F:378:PHE:CE2	2.55	0.42
1:F:289:LEU:HD11	1:F:293:LEU:HD11	2.01	0.42
1:F:542:MET:O	1:F:545:LEU:CB	2.68	0.42
1:C:124:LEU:HD22	1:C:532:TRP:CB	2.46	0.42
1:C:124:LEU:CD2	1:C:532:TRP:HB2	2.46	0.42
1:C:182:ARG:NH2	1:C:267:LYS:HE2	2.35	0.42
1:C:285:ASP:OD2	1:C:287:GLN:N	2.53	0.42
1:C:549:PHE:O	1:C:552:GLY:N	2.53	0.42
1:D:25:SER:OG	1:D:28:GLU:HG3	2.19	0.42
1:D:89:TYR:N	1:D:89:TYR:CD2	2.88	0.42
1:D:476:GLN:O	1:D:478:LYS:HG2	2.20	0.42
1:F:4:SER:HA	1:F:82:ILE:HG12	2.01	0.42
1:F:132:GLN:OE1	1:F:515:SER:HB3	2.20	0.42
1:F:285:ASP:HA	1:F:331:ASN:OD1	2.19	0.42
1:A:48:TYR:CD2	1:A:55:LEU:HD13	2.55	0.42
1:A:132:GLN:OE1	1:A:515:SER:HB3	2.19	0.42
1:A:164:LYS:O	1:A:282:ILE:CD1	2.60	0.42
1:A:165:SER:CA	1:A:282:ILE:HD13	2.49	0.42
1:A:356:ARG:NH2	1:B:487:ARG:O	2.52	0.42
1:B:57:VAL:O	1:B:57:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:THR:HG23	1:B:546:ARG:NH2	2.35	0.42
1:C:290:MET:CE	1:C:295:LEU:HB3	2.50	0.42
1:D:177:ILE:HG21	1:D:236:ILE:HG12	2.01	0.42
1:D:299:ASN:H	1:D:299:ASN:HD22	1.68	0.42
1:D:380:VAL:O	1:D:462:ALA:N	2.53	0.42
1:E:106:SER:C	1:E:107:LEU:HD12	2.41	0.42
1:F:534:LEU:HD23	1:F:534:LEU:HA	1.84	0.42
1:A:12:THR:OG1	1:A:13:PRO:HD2	2.19	0.41
1:A:255:HIS:O	1:A:256:GLU:HG3	2.20	0.41
1:A:350:VAL:HG22	1:A:353:TYR:HB2	2.01	0.41
1:B:348:VAL:CG2	1:B:349:TYR:N	2.81	0.41
1:C:61:LEU:N	1:C:61:LEU:HD12	2.34	0.41
1:C:325:LEU:HD12	1:C:325:LEU:HA	1.90	0.41
1:D:46:PHE:CE1	1:D:55:LEU:HD12	2.55	0.41
1:F:56:ARG:HD3	1:F:104:GLU:OE1	2.20	0.41
1:F:561:ASP:OD2	1:F:566:THR:HG21	2.19	0.41
1:A:5:LYS:HB3	1:A:80:GLN:HG3	2.02	0.41
1:C:332:LEU:HA	1:C:332:LEU:HD12	1.84	0.41
1:D:61:LEU:N	1:D:61:LEU:HD12	2.35	0.41
1:D:282:ILE:HD12	1:D:282:ILE:HA	1.67	0.41
1:D:285:ASP:HA	1:D:331:ASN:OD1	2.19	0.41
1:D:544:MET:O	1:D:548:LEU:HB2	2.21	0.41
1:D:561:ASP:O	1:D:563:ILE:N	2.53	0.41
1:F:350:VAL:HG22	1:F:353:TYR:HB2	2.02	0.41
1:A:130:ILE:O	1:A:131:ARG:CG	2.69	0.41
1:A:347:LYS:HE2	1:A:369:THR:HG22	2.01	0.41
1:A:542:MET:O	1:A:546:ARG:N	2.53	0.41
1:A:563:ILE:C	1:A:564:ASN:ND2	2.74	0.41
1:B:189:GLU:CD	1:B:189:GLU:H	2.24	0.41
1:C:81:TYR:HE1	1:C:86:ARG:NH2	2.18	0.41
1:D:304:LEU:HD23	1:D:304:LEU:HA	1.83	0.41
1:D:532:TRP:HZ2	1:D:546:ARG:HA	1.86	0.41
1:E:531:ILE:O	1:E:531:ILE:CG2	2.68	0.41
1:E:566:THR:C	1:E:568:VAL:N	2.70	0.41
1:F:165:SER:CA	1:F:282:ILE:HD13	2.50	0.41
1:F:212:TRP:CE3	1:F:212:TRP:HA	2.55	0.41
1:A:299:ASN:ND2	1:A:299:ASN:H	2.18	0.41
1:A:514:LEU:HD21	1:A:528:PHE:CE2	2.55	0.41
1:B:37:PHE:C	1:B:38:ASP:CG	2.79	0.41
1:B:168:PHE:CD2	1:B:480:GLY:HA2	2.55	0.41
1:B:531:ILE:HD12	1:B:531:ILE:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ASN:HB3	1:C:29:ARG:NH2	2.36	0.41
1:C:166:GLU:OE1	1:C:279:PHE:CA	2.68	0.41
1:C:542:MET:O	1:C:545:LEU:CB	2.69	0.41
1:E:46:PHE:CE1	1:E:55:LEU:HD12	2.54	0.41
1:E:258:VAL:HG12	1:E:263:LEU:O	2.19	0.41
1:E:487:ARG:HG2	1:E:488:ILE:N	2.35	0.41
1:E:531:ILE:HD12	1:E:531:ILE:HA	1.82	0.41
1:F:76:TYR:OH	1:F:113:MET:HG2	2.20	0.41
1:F:282:ILE:HG23	1:F:334:PHE:CD2	2.55	0.41
1:F:371:ASN:OD1	1:F:371:ASN:C	2.57	0.41
1:F:470:TYR:CB	1:F:479:PHE:CE1	3.03	0.41
1:A:541:HIS:O	1:A:545:LEU:HB2	2.19	0.41
1:B:12:THR:HG21	1:B:76:TYR:CB	2.51	0.41
1:B:48:TYR:CD2	1:B:55:LEU:HD13	2.55	0.41
1:B:133:HIS:CD2	1:B:525:TRP:H	2.39	0.41
1:C:112:VAL:CG2	1:C:548:LEU:CD1	2.99	0.41
1:D:81:TYR:HE1	1:D:86:ARG:NH2	2.19	0.41
1:D:293:LEU:HD22	1:D:309:VAL:HG11	2.02	0.41
1:E:360:VAL:CG2	1:E:363:TYR:HB2	2.51	0.41
1:F:121:LEU:O	1:F:124:LEU:HD12	2.19	0.41
1:F:129:VAL:CG2	1:F:130:ILE:N	2.83	0.41
1:A:95:ILE:CD1	1:A:105:LEU:HD22	2.50	0.41
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.83	0.41
1:A:533:THR:HG23	1:A:546:ARG:NH2	2.36	0.41
1:D:165:SER:CA	1:D:282:ILE:HD13	2.51	0.41
1:D:286:TYR:HE1	1:D:301:LYS:HE3	1.85	0.41
1:F:79:VAL:CG1	1:F:81:TYR:CE2	3.03	0.41
1:A:158:MET:C	1:A:159:ARG:HG2	2.41	0.41
1:A:311:ALA:HB2	1:A:325:LEU:HD22	2.03	0.41
1:B:291:PHE:C	1:B:291:PHE:HD2	2.24	0.41
1:B:548:LEU:HD23	1:B:548:LEU:HA	1.81	0.41
1:C:55:LEU:HD23	1:C:55:LEU:N	2.36	0.41
1:C:177:ILE:HD13	1:C:177:ILE:C	2.41	0.41
1:D:348:VAL:HG13	1:D:368:LEU:HB3	2.03	0.41
1:E:483:LEU:HD12	1:E:484:ARG:N	2.36	0.41
1:F:276:GLN:O	1:F:277:LYS:C	2.59	0.41
1:B:82:ILE:HA	1:B:83:GLN:HA	1.72	0.41
1:B:138:GLU:OE2	1:B:515:SER:HB2	2.21	0.41
1:C:12:THR:HG21	1:C:76:TYR:CB	2.50	0.41
1:C:487:ARG:HG2	1:C:488:ILE:N	2.35	0.41
1:D:127:VAL:CG2	1:D:528:PHE:CD1	3.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:ASP:OD1	1:D:324:ASP:C	2.59	0.41
1:E:42:PHE:CE1	1:E:59:ILE:CD1	3.03	0.41
1:E:55:LEU:HD23	1:E:55:LEU:N	2.36	0.41
1:E:164:LYS:HB2	1:E:282:ILE:HD12	2.03	0.41
1:F:3:LEU:CB	1:F:45:THR:HB	2.50	0.41
1:A:360:VAL:CG2	1:A:363:TYR:HB2	2.50	0.41
1:A:572:ILE:O	1:A:573:ILE:CB	2.67	0.41
1:B:338:VAL:CG2	1:B:338:VAL:O	2.67	0.41
1:B:371:ASN:OD1	1:B:371:ASN:C	2.59	0.41
1:B:542:MET:HE1	1:B:545:LEU:HD23	2.02	0.41
1:C:189:GLU:N	1:C:189:GLU:CD	2.74	0.41
1:C:220:LYS:O	1:C:221:GLU:C	2.59	0.41
1:C:520:MET:HB3	1:C:570:ASN:OD1	2.21	0.41
1:D:27:GLU:HG2	1:D:28:GLU:N	2.36	0.41
1:D:164:LYS:O	1:D:282:ILE:CD1	2.66	0.41
1:D:164:LYS:HB2	1:D:282:ILE:HD12	2.03	0.41
1:D:487:ARG:HG2	1:D:488:ILE:N	2.35	0.41
1:D:516:ASP:OD2	1:D:517:ILE:N	2.54	0.41
1:E:130:ILE:HB	1:E:527:GLN:HG2	2.03	0.41
1:E:157:THR:HG23	1:E:489:SER:H	1.82	0.41
1:E:210:MET:HE2	1:E:210:MET:HB3	1.99	0.41
1:E:224:ASP:C	1:E:226:LEU:N	2.73	0.41
1:E:519:SER:O	1:E:573:ILE:HG12	2.21	0.41
1:E:531:ILE:HG13	1:F:15:ASN:OD1	2.21	0.41
1:E:533:THR:HG23	1:E:546:ARG:NH2	2.35	0.41
1:F:282:ILE:HD11	1:F:483:LEU:HB3	2.02	0.41
1:F:305:ARG:HB2	1:F:306:PRO:CD	2.50	0.41
1:F:572:ILE:O	1:F:573:ILE:C	2.59	0.41
1:A:249:GLN:OE1	1:A:249:GLN:HA	2.21	0.41
1:A:316:TYR:CE2	1:A:482:HIS:CD2	3.09	0.41
1:B:357:GLY:HA2	1:B:358:ASN:HA	1.67	0.41
1:B:516:ASP:OD1	1:B:518:THR:HG22	2.21	0.41
1:B:545:LEU:O	1:B:546:ARG:C	2.57	0.41
1:C:42:PHE:CD1	1:C:59:ILE:HD11	2.56	0.41
1:C:512:THR:HG23	1:C:513:LYS:N	2.34	0.41
1:C:563:ILE:HD13	1:C:563:ILE:H	1.85	0.41
1:C:571:VAL:CG1	1:C:572:ILE:N	2.81	0.41
1:D:463:ILE:O	1:D:463:ILE:HD13	2.20	0.41
1:E:8:LEU:CD1	1:E:105:LEU:HD11	2.51	0.41
1:E:124:LEU:CD2	1:E:532:TRP:HB2	2.47	0.41
1:E:177:ILE:HB	1:E:236:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:LEU:HD12	1:F:556:TRP:O	2.21	0.41
1:F:353:TYR:O	1:F:354:ASN:CB	2.67	0.41
1:F:374:ASP:HB3	1:F:467:HIS:O	2.20	0.41
1:F:532:TRP:CZ2	1:F:546:ARG:HA	2.56	0.41
1:A:139:TYR:O	1:A:140:GLU:C	2.59	0.40
1:A:220:LYS:O	1:A:221:GLU:C	2.57	0.40
1:B:573:ILE:N	1:B:573:ILE:HD13	2.36	0.40
1:C:76:TYR:OH	1:C:113:MET:HG2	2.22	0.40
1:C:89:TYR:CD2	1:C:89:TYR:N	2.89	0.40
1:C:236:ILE:HG21	1:C:378:PHE:CE2	2.55	0.40
1:C:512:THR:HG23	1:C:513:LYS:O	2.21	0.40
1:C:533:THR:HG23	1:C:546:ARG:NH2	2.36	0.40
1:D:75:ASN:OD1	1:D:75:ASN:N	2.53	0.40
1:D:215:ASP:OD1	1:D:217:GLU:N	2.52	0.40
1:D:282:ILE:HD11	1:D:483:LEU:HB3	2.03	0.40
1:E:148:SER:CB	1:F:156:SER:O	2.69	0.40
1:E:348:VAL:CG2	1:E:349:TYR:N	2.82	0.40
1:F:210:MET:HE2	1:F:210:MET:HB3	2.03	0.40
1:F:296:ASN:O	1:F:300:ASP:HB2	2.21	0.40
1:A:67:CYS:SG	1:A:68:PHE:N	2.94	0.40
1:A:128:ASN:C	1:A:128:ASN:HD22	2.25	0.40
1:A:189:GLU:CD	1:A:189:GLU:N	2.75	0.40
1:A:570:ASN:O	1:A:571:VAL:HG23	2.21	0.40
1:A:571:VAL:HG13	1:A:572:ILE:N	2.36	0.40
1:C:514:LEU:HD21	1:C:528:PHE:CE2	2.56	0.40
1:D:23:PHE:HD2	1:D:117:GLN:OE1	2.04	0.40
1:D:55:LEU:N	1:D:55:LEU:HD23	2.37	0.40
1:D:129:VAL:HG23	1:D:130:ILE:N	2.36	0.40
1:D:514:LEU:HD21	1:D:528:PHE:CE2	2.56	0.40
1:E:6:ILE:HG23	1:E:7:LYS:N	2.37	0.40
1:E:138:GLU:OE2	1:E:515:SER:HB2	2.20	0.40
1:F:16:ASN:HD21	1:F:18:GLN:HG3	1.86	0.40
1:F:37:PHE:CE1	1:F:40:HIS:O	2.74	0.40
1:F:48:TYR:CD2	1:F:55:LEU:HD13	2.56	0.40
1:F:106:SER:C	1:F:107:LEU:HD12	2.42	0.40
1:F:170:GLN:O	1:F:244:SER:CB	2.70	0.40
1:F:560:SER:O	1:F:564:ASN:ND2	2.52	0.40
1:F:570:ASN:O	1:F:571:VAL:HG23	2.22	0.40
1:A:7:LYS:HG3	1:A:37:PHE:CE2	2.57	0.40
1:A:511:SER:HB2	1:B:567:VAL:HG21	2.02	0.40
1:A:542:MET:HB3	1:A:546:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:HA	1:B:13:PRO:HD3	1.89	0.40
1:C:69:GLU:O	1:C:69:GLU:HG2	2.21	0.40
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.93	0.40
1:D:8:LEU:CD2	1:D:77:CYS:HB2	2.51	0.40
1:D:12:THR:HA	1:D:13:PRO:HD3	1.89	0.40
1:D:518:THR:O	1:D:518:THR:HG23	2.21	0.40
1:E:148:SER:HB3	1:F:156:SER:O	2.22	0.40
1:E:202:ASP:OD2	1:E:274:SER:OG	2.40	0.40
1:F:212:TRP:O	1:F:213:PHE:CG	2.74	0.40
1:B:5:LYS:HB3	1:B:80:GLN:HG3	2.03	0.40
1:B:71:LEU:CG	1:B:71:LEU:O	2.69	0.40
1:B:130:ILE:O	1:B:131:ARG:CG	2.69	0.40
1:B:217:GLU:O	1:B:218:SER:C	2.60	0.40
1:B:227:THR:O	1:B:230:PRO:HD3	2.22	0.40
1:C:165:SER:HB3	1:C:482:HIS:ND1	2.35	0.40
1:C:210:MET:HE2	1:C:210:MET:HB3	2.03	0.40
1:C:307:ASN:OD1	1:C:307:ASN:N	2.46	0.40
1:D:46:PHE:CE1	1:D:55:LEU:HD11	2.57	0.40
1:D:177:ILE:HD13	1:D:177:ILE:H	1.85	0.40
1:D:496:VAL:O	1:D:497:LYS:C	2.59	0.40
1:E:48:TYR:CD2	1:E:55:LEU:HD13	2.56	0.40
1:F:61:LEU:HD12	1:F:61:LEU:N	2.36	0.40
1:F:75:ASN:CA	1:F:92:VAL:HG22	2.51	0.40
1:A:71:LEU:CG	1:A:71:LEU:O	2.68	0.40
1:A:239:VAL:O	1:A:375:THR:HA	2.21	0.40
1:B:175:LEU:HD23	1:B:239:VAL:HB	2.04	0.40
1:B:359:ASN:C	1:B:360:VAL:O	2.59	0.40
1:B:538:ASP:O	1:B:540:GLY:N	2.54	0.40
1:C:538:ASP:O	1:C:541:HIS:N	2.52	0.40
1:C:541:HIS:O	1:C:545:LEU:N	2.54	0.40
1:C:572:ILE:O	1:C:573:ILE:C	2.58	0.40
1:D:42:PHE:CE1	1:D:59:ILE:CD1	3.03	0.40
1:D:111:VAL:CG2	1:D:545:LEU:HD13	2.51	0.40
1:D:274:SER:HB2	1:D:338:VAL:CG2	2.52	0.40
1:D:475:LYS:HD2	1:D:475:LYS:HA	1.96	0.40
1:D:561:ASP:C	1:D:563:ILE:N	2.74	0.40
1:E:174:ILE:CG1	1:E:176:THR:HG22	2.50	0.40
1:E:563:ILE:C	1:E:564:ASN:ND2	2.74	0.40
1:F:95:ILE:CD1	1:F:105:LEU:HD22	2.51	0.40
1:F:286:TYR:HE1	1:F:301:LYS:HE3	1.84	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:O	1:B:291:PHE:CZ[2_665]	1.96	0.24
1:C:295:LEU:O	1:F:65:ARG:NH2[1_556]	2.07	0.13
1:A:255:HIS:O	1:B:291:PHE:CE2[2_665]	2.09	0.11
1:A:255:HIS:C	1:B:291:PHE:CZ[2_665]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	482/583 (83%)	386 (80%)	82 (17%)	14 (3%)	4 24
1	B	482/583 (83%)	390 (81%)	82 (17%)	10 (2%)	7 33
1	C	482/583 (83%)	387 (80%)	86 (18%)	9 (2%)	8 36
1	D	482/583 (83%)	388 (80%)	81 (17%)	13 (3%)	5 26
1	E	482/583 (83%)	390 (81%)	85 (18%)	7 (2%)	10 42
1	F	482/583 (83%)	387 (80%)	85 (18%)	10 (2%)	7 33
All	All	2892/3498 (83%)	2328 (80%)	501 (17%)	63 (2%)	6 31

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	VAL
1	A	530	GLY
1	A	539	THR
1	B	258	VAL
1	B	530	GLY
1	C	258	VAL
1	C	530	GLY
1	D	258	VAL
1	D	530	GLY
1	D	539	THR

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Mol	Chain	Res	Type
1	E	258	VAL
1	E	530	GLY
1	E	539	THR
1	F	258	VAL
1	F	530	GLY
1	F	539	THR
1	A	68	PHE
1	A	233	GLN
1	A	255	HIS
1	B	68	PHE
1	B	539	THR
1	C	68	PHE
1	C	539	THR
1	D	68	PHE
1	E	68	PHE
1	F	68	PHE
1	A	36	LYS
1	D	550	GLU
1	F	567	VAL
1	A	546	ARG
1	A	567	VAL
1	B	304	LEU
1	A	39	VAL
1	A	360	VAL
1	A	538	ASP
1	B	39	VAL
1	B	277	LYS
1	B	567	VAL
1	C	567	VAL
1	D	250	GLU
1	D	567	VAL
1	F	233	GLN
1	F	304	LEU
1	A	260	GLY
1	B	36	LYS
1	C	39	VAL
1	D	39	VAL
1	D	371	ASN
1	D	542	MET
1	E	39	VAL
1	F	36	LYS
1	F	39	VAL

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Mol	Chain	Res	Type
1	B	572	ILE
1	D	245	GLY
1	E	567	VAL
1	C	190	LYS
1	D	260	GLY
1	A	572	ILE
1	C	360	VAL
1	C	572	ILE
1	D	572	ILE
1	E	572	ILE
1	F	572	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	446/529 (84%)	368 (82%)	78 (18%)	2 10
1	B	446/529 (84%)	369 (83%)	77 (17%)	2 10
1	C	446/529 (84%)	369 (83%)	77 (17%)	2 10
1	D	446/529 (84%)	367 (82%)	79 (18%)	2 9
1	E	446/529 (84%)	365 (82%)	81 (18%)	1 9
1	F	446/529 (84%)	367 (82%)	79 (18%)	2 9
All	All	2676/3174 (84%)	2205 (82%)	471 (18%)	2 10

All (471) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	18	GLN
1	A	23	PHE
1	A	38	ASP
1	A	46	PHE
1	A	48	TYR
1	A	55	LEU

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Mol	Chain	Res	Type
1	A	57	VAL
1	A	58	THR
1	A	61	LEU
1	A	62	VAL
1	A	65	ARG
1	A	66	SER
1	A	69	GLU
1	A	71	LEU
1	A	72	MET
1	A	74	VAL
1	A	87	VAL
1	A	94	ASP
1	A	103	CYS
1	A	108	VAL
1	A	128	ASN
1	A	129	VAL
1	A	135	THR
1	A	146	ILE
1	A	155	THR
1	A	157	THR
1	A	165	SER
1	A	174	ILE
1	A	176	THR
1	A	177	ILE
1	A	182	ARG
1	A	189	GLU
1	A	199	SER
1	A	200	THR
1	A	204	ILE
1	A	206	ASN
1	A	210	MET
1	A	215	ASP
1	A	226	LEU
1	A	227	THR
1	A	229	TYR
1	A	239	VAL
1	A	249	GLN
1	A	263	LEU
1	A	267	LYS
1	A	274	SER
1	A	285	ASP
1	A	288	SER

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Mol	Chain	Res	Type
1	A	295	LEU
1	A	299	ASN
1	A	303	LEU
1	A	320	ARG
1	A	330	THR
1	A	338	VAL
1	A	350	VAL
1	A	358	ASN
1	A	359	ASN
1	A	360	VAL
1	A	365	ASP
1	A	369	THR
1	A	374	ASP
1	A	376	ILE
1	A	463	ILE
1	A	491	ASP
1	A	513	LYS
1	A	514	LEU
1	A	518	THR
1	A	524	ASN
1	A	526	VAL
1	A	533	THR
1	A	539	THR
1	A	548	LEU
1	A	560	SER
1	A	563	ILE
1	A	568	VAL
1	A	571	VAL
1	A	573	ILE
1	B	16	ASN
1	B	18	GLN
1	B	23	PHE
1	B	26	ASN
1	B	38	ASP
1	B	46	PHE
1	B	48	TYR
1	B	55	LEU
1	B	57	VAL
1	B	58	THR
1	B	61	LEU
1	B	62	VAL
1	B	65	ARG

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Mol	Chain	Res	Type
1	B	69	GLU
1	B	71	LEU
1	B	72	MET
1	B	74	VAL
1	B	94	ASP
1	B	103	CYS
1	B	108	VAL
1	B	128	ASN
1	B	129	VAL
1	B	135	THR
1	B	146	ILE
1	B	155	THR
1	B	157	THR
1	B	165	SER
1	B	174	ILE
1	B	176	THR
1	B	177	ILE
1	B	182	ARG
1	B	189	GLU
1	B	199	SER
1	B	200	THR
1	B	204	ILE
1	B	206	ASN
1	B	208	TYR
1	B	210	MET
1	B	215	ASP
1	B	226	LEU
1	B	227	THR
1	B	229	TYR
1	B	239	VAL
1	B	249	GLN
1	B	263	LEU
1	B	267	LYS
1	B	274	SER
1	B	285	ASP
1	B	288	SER
1	B	295	LEU
1	B	299	ASN
1	B	303	LEU
1	B	320	ARG
1	B	325	LEU
1	B	326	SER

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Mol	Chain	Res	Type
1	B	330	THR
1	B	338	VAL
1	B	350	VAL
1	B	358	ASN
1	B	359	ASN
1	B	360	VAL
1	B	365	ASP
1	B	369	THR
1	B	374	ASP
1	B	376	ILE
1	B	463	ILE
1	B	491	ASP
1	B	513	LYS
1	B	514	LEU
1	B	524	ASN
1	B	526	VAL
1	B	533	THR
1	B	548	LEU
1	B	560	SER
1	B	563	ILE
1	B	571	VAL
1	B	573	ILE
1	C	16	ASN
1	C	18	GLN
1	C	23	PHE
1	C	38	ASP
1	C	46	PHE
1	C	48	TYR
1	C	55	LEU
1	C	57	VAL
1	C	58	THR
1	C	61	LEU
1	C	62	VAL
1	C	65	ARG
1	C	69	GLU
1	C	71	LEU
1	C	74	VAL
1	C	94	ASP
1	C	103	CYS
1	C	108	VAL
1	C	128	ASN
1	C	129	VAL

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Mol	Chain	Res	Type
1	C	135	THR
1	C	146	ILE
1	C	155	THR
1	C	157	THR
1	C	165	SER
1	C	174	ILE
1	C	176	THR
1	C	177	ILE
1	C	182	ARG
1	C	189	GLU
1	C	199	SER
1	C	200	THR
1	C	204	ILE
1	C	206	ASN
1	C	210	MET
1	C	215	ASP
1	C	226	LEU
1	C	227	THR
1	C	229	TYR
1	C	239	VAL
1	C	263	LEU
1	C	267	LYS
1	C	274	SER
1	C	278	ASP
1	C	285	ASP
1	C	288	SER
1	C	295	LEU
1	C	299	ASN
1	C	303	LEU
1	C	320	ARG
1	C	325	LEU
1	C	326	SER
1	C	330	THR
1	C	338	VAL
1	C	348	VAL
1	C	350	VAL
1	C	358	ASN
1	C	359	ASN
1	C	360	VAL
1	C	365	ASP
1	C	369	THR
1	C	374	ASP

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Mol	Chain	Res	Type
1	C	376	ILE
1	C	463	ILE
1	C	491	ASP
1	C	513	LYS
1	C	514	LEU
1	C	518	THR
1	C	524	ASN
1	C	526	VAL
1	C	533	THR
1	C	539	THR
1	C	548	LEU
1	C	560	SER
1	C	563	ILE
1	C	571	VAL
1	C	573	ILE
1	D	16	ASN
1	D	18	GLN
1	D	23	PHE
1	D	38	ASP
1	D	42	PHE
1	D	46	PHE
1	D	48	TYR
1	D	55	LEU
1	D	57	VAL
1	D	58	THR
1	D	61	LEU
1	D	62	VAL
1	D	65	ARG
1	D	69	GLU
1	D	71	LEU
1	D	72	MET
1	D	74	VAL
1	D	87	VAL
1	D	94	ASP
1	D	103	CYS
1	D	108	VAL
1	D	128	ASN
1	D	129	VAL
1	D	135	THR
1	D	146	ILE
1	D	155	THR
1	D	157	THR

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Mol	Chain	Res	Type
1	D	165	SER
1	D	174	ILE
1	D	176	THR
1	D	177	ILE
1	D	182	ARG
1	D	189	GLU
1	D	199	SER
1	D	200	THR
1	D	204	ILE
1	D	206	ASN
1	D	210	MET
1	D	215	ASP
1	D	226	LEU
1	D	227	THR
1	D	229	TYR
1	D	239	VAL
1	D	263	LEU
1	D	267	LYS
1	D	274	SER
1	D	278	ASP
1	D	285	ASP
1	D	288	SER
1	D	295	LEU
1	D	299	ASN
1	D	303	LEU
1	D	320	ARG
1	D	325	LEU
1	D	330	THR
1	D	338	VAL
1	D	350	VAL
1	D	358	ASN
1	D	359	ASN
1	D	360	VAL
1	D	365	ASP
1	D	369	THR
1	D	374	ASP
1	D	376	ILE
1	D	463	ILE
1	D	513	LYS
1	D	514	LEU
1	D	518	THR
1	D	524	ASN

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Mol	Chain	Res	Type
1	D	526	VAL
1	D	533	THR
1	D	539	THR
1	D	548	LEU
1	D	560	SER
1	D	563	ILE
1	D	566	THR
1	D	571	VAL
1	D	572	ILE
1	D	573	ILE
1	E	16	ASN
1	E	18	GLN
1	E	23	PHE
1	E	26	ASN
1	E	38	ASP
1	E	46	PHE
1	E	48	TYR
1	E	55	LEU
1	E	57	VAL
1	E	58	THR
1	E	61	LEU
1	E	62	VAL
1	E	65	ARG
1	E	69	GLU
1	E	71	LEU
1	E	72	MET
1	E	74	VAL
1	E	94	ASP
1	E	103	CYS
1	E	108	VAL
1	E	128	ASN
1	E	129	VAL
1	E	135	THR
1	E	146	ILE
1	E	155	THR
1	E	157	THR
1	E	165	SER
1	E	174	ILE
1	E	176	THR
1	E	177	ILE
1	E	182	ARG
1	E	189	GLU

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Mol	Chain	Res	Type
1	E	199	SER
1	E	200	THR
1	E	204	ILE
1	E	206	ASN
1	E	210	MET
1	E	215	ASP
1	E	226	LEU
1	E	227	THR
1	E	229	TYR
1	E	239	VAL
1	E	249	GLN
1	E	263	LEU
1	E	267	LYS
1	E	274	SER
1	E	278	ASP
1	E	285	ASP
1	E	288	SER
1	E	295	LEU
1	E	299	ASN
1	E	303	LEU
1	E	320	ARG
1	E	325	LEU
1	E	330	THR
1	E	338	VAL
1	E	350	VAL
1	E	358	ASN
1	E	359	ASN
1	E	360	VAL
1	E	365	ASP
1	E	369	THR
1	E	374	ASP
1	E	376	ILE
1	E	463	ILE
1	E	475	LYS
1	E	476	GLN
1	E	513	LYS
1	E	514	LEU
1	E	518	THR
1	E	524	ASN
1	E	526	VAL
1	E	533	THR
1	E	539	THR

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Mol	Chain	Res	Type
1	E	548	LEU
1	E	560	SER
1	E	563	ILE
1	E	568	VAL
1	E	571	VAL
1	E	572	ILE
1	E	573	ILE
1	F	16	ASN
1	F	18	GLN
1	F	23	PHE
1	F	38	ASP
1	F	42	PHE
1	F	46	PHE
1	F	48	TYR
1	F	55	LEU
1	F	57	VAL
1	F	58	THR
1	F	61	LEU
1	F	62	VAL
1	F	65	ARG
1	F	69	GLU
1	F	71	LEU
1	F	72	MET
1	F	74	VAL
1	F	77	CYS
1	F	87	VAL
1	F	94	ASP
1	F	103	CYS
1	F	108	VAL
1	F	128	ASN
1	F	129	VAL
1	F	135	THR
1	F	146	ILE
1	F	155	THR
1	F	157	THR
1	F	165	SER
1	F	174	ILE
1	F	176	THR
1	F	177	ILE
1	F	182	ARG
1	F	189	GLU
1	F	199	SER

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Mol	Chain	Res	Type
1	F	200	THR
1	F	204	ILE
1	F	206	ASN
1	F	210	MET
1	F	215	ASP
1	F	226	LEU
1	F	227	THR
1	F	229	TYR
1	F	239	VAL
1	F	263	LEU
1	F	267	LYS
1	F	274	SER
1	F	285	ASP
1	F	288	SER
1	F	295	LEU
1	F	299	ASN
1	F	303	LEU
1	F	325	LEU
1	F	326	SER
1	F	330	THR
1	F	338	VAL
1	F	350	VAL
1	F	358	ASN
1	F	359	ASN
1	F	360	VAL
1	F	365	ASP
1	F	369	THR
1	F	374	ASP
1	F	376	ILE
1	F	463	ILE
1	F	475	LYS
1	F	491	ASP
1	F	513	LYS
1	F	514	LEU
1	F	518	THR
1	F	524	ASN
1	F	526	VAL
1	F	533	THR
1	F	539	THR
1	F	548	LEU
1	F	560	SER
1	F	563	ILE

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Mol	Chain	Res	Type
1	F	571	VAL
1	F	573	ILE

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

Mol	Chain	Res	Type
1	A	40	HIS
1	A	233	GLN
1	B	40	HIS
1	B	233	GLN
1	B	564	ASN
1	C	40	HIS
1	C	233	GLN
1	C	299	ASN
1	D	40	HIS
1	D	233	GLN
1	E	40	HIS
1	E	233	GLN
1	F	40	HIS
1	F	233	GLN
1	F	564	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	488/583 (83%)	-0.12	11 (2%)	60	31	48, 91, 189, 275	0
1	B	488/583 (83%)	-0.31	4 (0%)	86	65	50, 92, 180, 276	0
1	C	488/583 (83%)	-0.23	15 (3%)	49	21	58, 102, 192, 278	0
1	D	488/583 (83%)	-0.12	25 (5%)	28	10	65, 104, 205, 279	0
1	E	488/583 (83%)	-0.19	15 (3%)	49	21	58, 103, 198, 275	0
1	F	488/583 (83%)	-0.24	20 (4%)	37	14	52, 94, 194, 281	0
All	All	2928/3498 (83%)	-0.20	90 (3%)	49	21	48, 99, 194, 281	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	VAL	9.7
1	F	39	VAL	8.7
1	B	39	VAL	7.5
1	D	40	HIS	7.2
1	A	68	PHE	7.2
1	A	39	VAL	6.9
1	C	40	HIS	6.6
1	D	62	VAL	6.4
1	D	47	ASN	5.7
1	D	58	THR	5.6
1	E	98	LEU	5.3
1	A	62	VAL	5.1
1	A	40	HIS	5.1
1	D	39	VAL	4.9
1	F	98	LEU	4.9
1	D	46	PHE	4.8
1	F	38	ASP	4.6
1	A	69	GLU	4.5
1	E	58	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	93	THR	4.2
1	E	6	ILE	4.0
1	F	40	HIS	3.9
1	E	62	VAL	3.9
1	F	97	GLN	3.9
1	C	53	GLY	3.8
1	F	68	PHE	3.8
1	D	77	CYS	3.7
1	D	6	ILE	3.7
1	A	46	PHE	3.6
1	E	102	VAL	3.4
1	E	46	PHE	3.4
1	D	55	LEU	3.4
1	D	54	VAL	3.4
1	B	68	PHE	3.4
1	B	47	ASN	3.4
1	D	68	PHE	3.4
1	C	66	SER	3.3
1	F	4	SER	3.2
1	C	67	CYS	3.2
1	F	46	PHE	3.1
1	C	64	ASP	3.1
1	D	98	LEU	3.0
1	E	60	ASP	3.0
1	E	54	VAL	3.0
1	D	53	GLY	2.9
1	F	81	TYR	2.9
1	F	62	VAL	2.9
1	E	39	VAL	2.9
1	E	14	PHE	2.9
1	D	79	VAL	2.9
1	F	99	ASN	2.9
1	C	55	LEU	2.7
1	A	98	LEU	2.7
1	C	63	SER	2.7
1	E	53	GLY	2.7
1	D	104	GLU	2.7
1	C	11	ASN	2.6
1	A	188	ALA	2.5
1	D	80	GLN	2.5
1	A	38	ASP	2.5
1	E	97	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	66	SER	2.5
1	D	8	LEU	2.5
1	D	48	TYR	2.4
1	B	65	ARG	2.4
1	D	60	ASP	2.4
1	C	80	GLN	2.4
1	D	225	TYR	2.3
1	F	564	ASN	2.3
1	C	73	GLY	2.3
1	F	65	ARG	2.3
1	C	49	ARG	2.3
1	F	59	ILE	2.3
1	E	42	PHE	2.3
1	C	6	ILE	2.3
1	C	54	VAL	2.2
1	D	530	GLY	2.2
1	F	100	ASP	2.2
1	F	69	GLU	2.2
1	E	59	ILE	2.2
1	F	13	PRO	2.2
1	A	47	ASN	2.2
1	D	57	VAL	2.2
1	D	81	TYR	2.2
1	D	49	ARG	2.1
1	D	56	ARG	2.1
1	A	191	PRO	2.1
1	C	268	LEU	2.1
1	F	233	GLN	2.0
1	F	64	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.