Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:39 PM GMT

PDB ID	:	4TW1
Title	:	Crystal structure of the octameric pore complex of the Staphylococcus aureus Bi-component Toxin LukGH
Authors	:	LOGAN, D.T.; HAKANSSON, M.; SALINE, M.; KIMBUNG, R.; BADARAU, A.; ROUHA, H.; NAGY, E.
Deposited on	:	2014-06-29
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

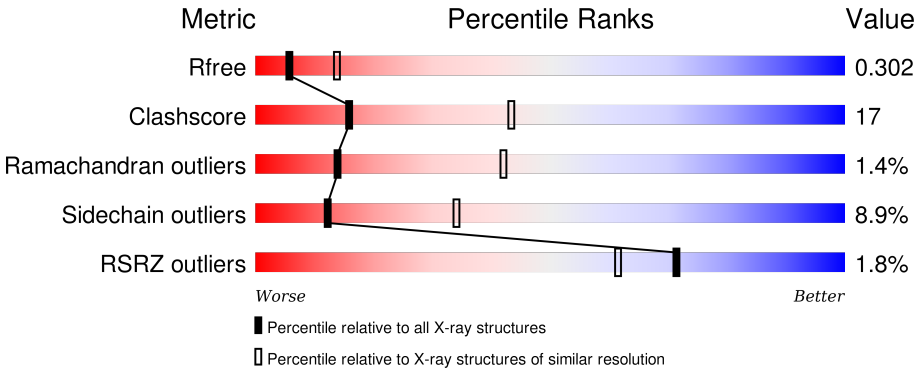
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	311	3% 59% 26% 5% 10%
1	C	311	2% 55% 32% • 10%
1	E	311	2% 57% 32% • 7%
1	G	311	2% 61% 30% • 7%
1	I	311	4% 59% 29% 5% 7%

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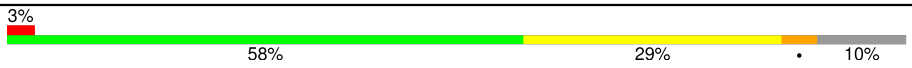
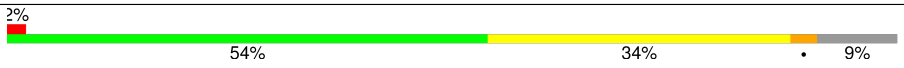
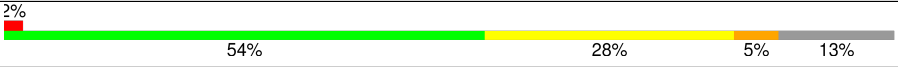
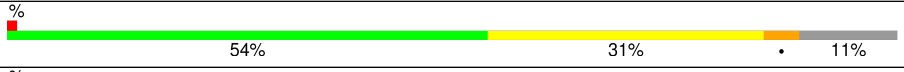
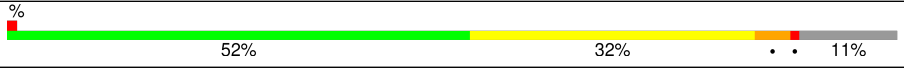
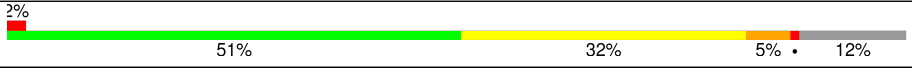
Mol	Chain	Length	Quality of chain
1	K	311	
1	M	311	
1	O	311	
2	B	324	
2	D	324	
2	F	324	
2	H	324	
2	J	324	
2	L	324	
2	N	324	
2	P	324	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37620 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 Possible leukocidin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2289	1433	399	452	5			
1	C	281	Total	C	N	O	S	0	0	0
			2281	1425	398	453	5			
1	E	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	G	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	I	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	K	281	Total	C	N	O	S	0	0	0
			2293	1438	398	452	5			
1	M	287	Total	C	N	O	S	0	0	0
			2332	1460	408	459	5			
1	O	283	Total	C	N	O	S	0	0	0
			2305	1447	400	453	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A8Z4S0
A	0	LEU	-	expression tag	UNP A8Z4S0
C	-1	SER	-	expression tag	UNP A8Z4S0
C	0	LEU	-	expression tag	UNP A8Z4S0
E	-1	SER	-	expression tag	UNP A8Z4S0
E	0	LEU	-	expression tag	UNP A8Z4S0
G	-1	SER	-	expression tag	UNP A8Z4S0
G	0	LEU	-	expression tag	UNP A8Z4S0
I	-1	SER	-	expression tag	UNP A8Z4S0
I	0	LEU	-	expression tag	UNP A8Z4S0
K	-1	SER	-	expression tag	UNP A8Z4S0
K	0	LEU	-	expression tag	UNP A8Z4S0
M	-1	SER	-	expression tag	UNP A8Z4S0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	LEU	-	expression tag	UNP A8Z4S0
O	-1	SER	-	expression tag	UNP A8Z4S0
O	0	LEU	-	expression tag	UNP A8Z4S0

- Molecule 2 is a protein called Possible leukocidin subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	282	Total 2320	C 1462	N 405	O 453	0	0	0
2	D	289	Total 2373	C 1496	N 413	O 464	0	0	0
2	F	284	Total 2340	C 1477	N 407	O 456	0	0	0
2	H	288	Total 2366	C 1492	N 412	O 462	0	0	0
2	J	288	Total 2366	C 1492	N 412	O 462	0	0	0
2	L	288	Total 2366	C 1492	N 412	O 462	0	0	0
2	N	288	Total 2366	C 1492	N 412	O 462	0	0	0
2	P	286	Total 2350	C 1482	N 409	O 459	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	O 9	0	0
3	B	15	Total 15	O 15	0	0
3	C	11	Total 11	O 11	0	0
3	D	8	Total 8	O 8	0	0
3	E	11	Total 11	O 11	0	0
3	F	17	Total 17	O 17	0	0
3	G	13	Total 13	O 13	0	0
3	H	18	Total 18	O 18	0	0

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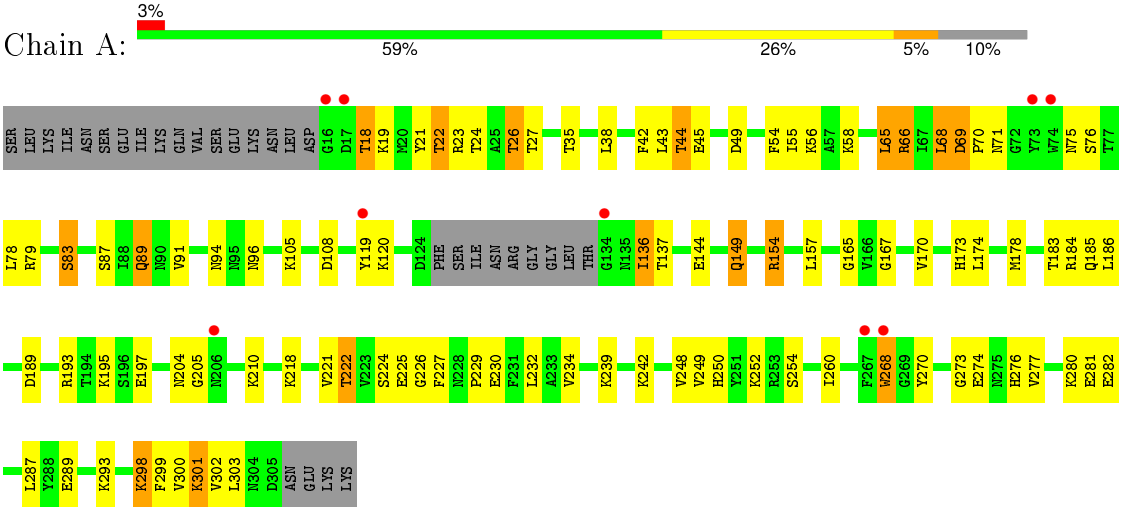
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	10	Total O 10 10	0	0
3	J	17	Total O 17 17	0	0
3	K	12	Total O 12 12	0	0
3	L	16	Total O 16 16	0	0
3	M	11	Total O 11 11	0	0
3	N	9	Total O 9 9	0	0
3	O	11	Total O 11 11	0	0
3	P	17	Total O 17 17	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

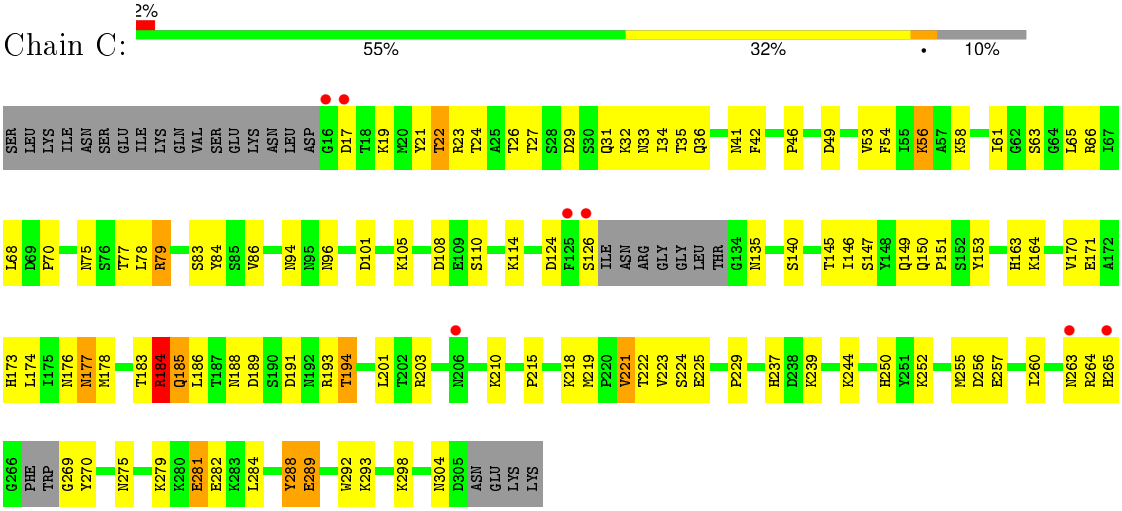
- Molecule 1: Possible leukocidin subunit

Chain A:



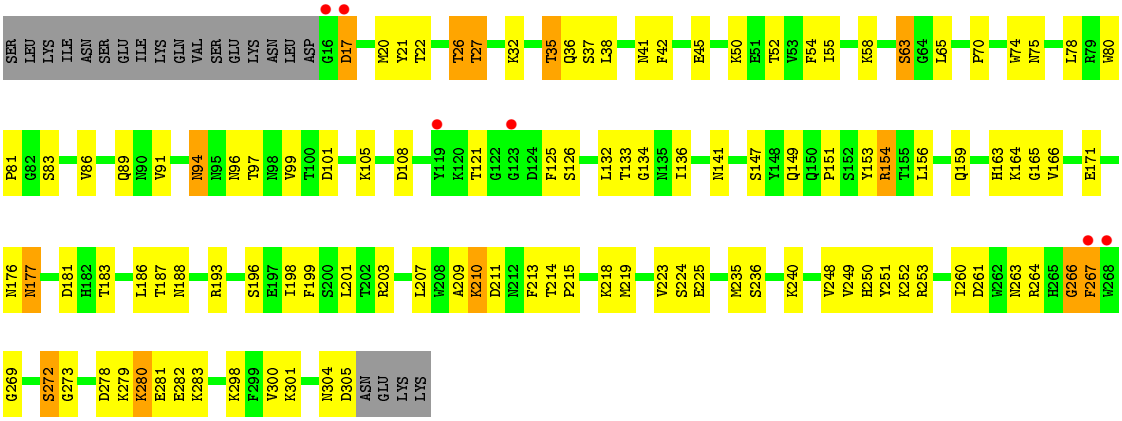
- Molecule 1: Possible leukocidin subunit

Chain C:



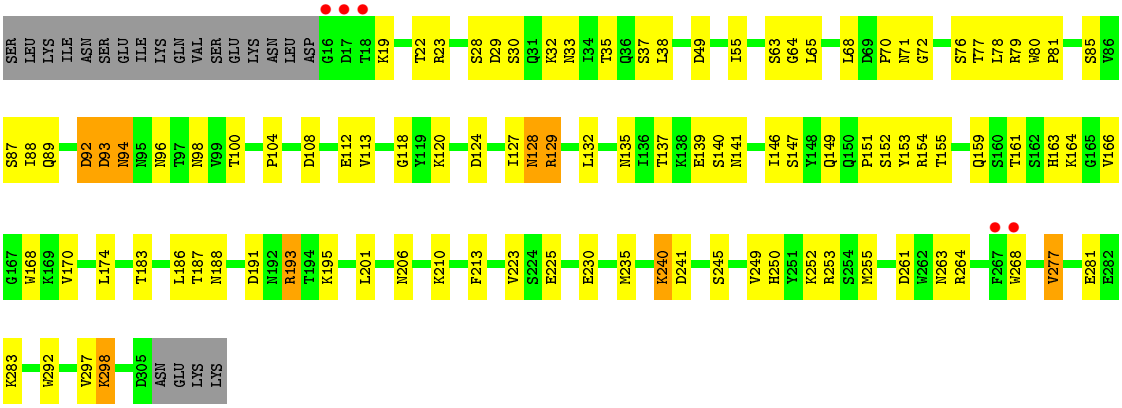
- Molecule 1: Possible leukocidin subunit

Chain E:



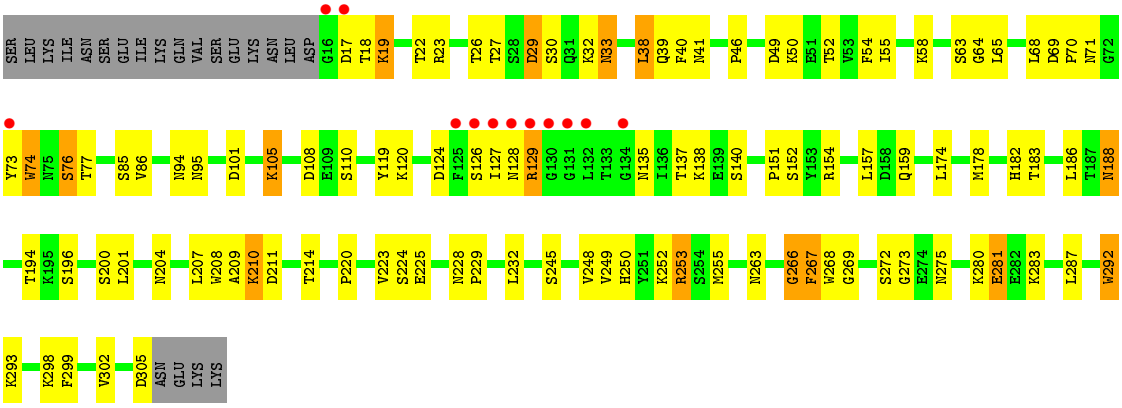
- Molecule 1: Possible leukocidin subunit

Chain G:



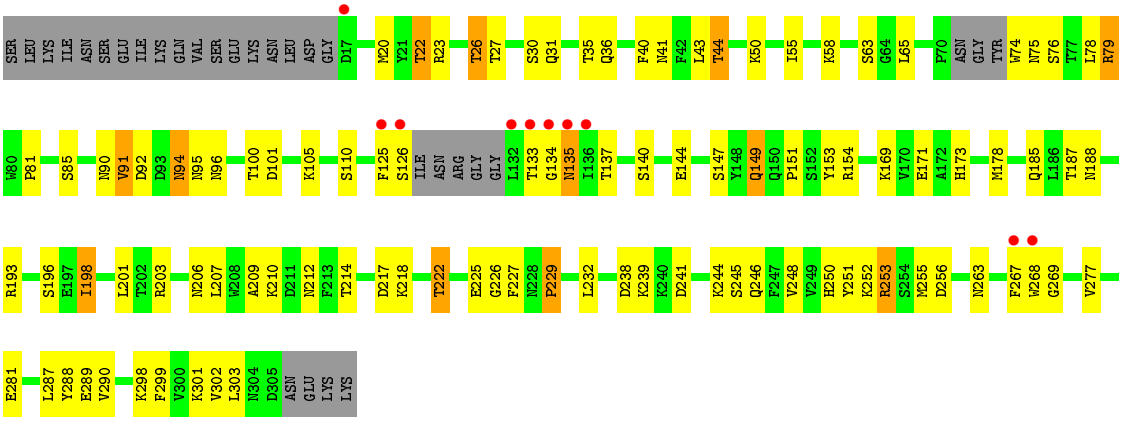
- Molecule 1: Possible leukocidin subunit

Chain I:



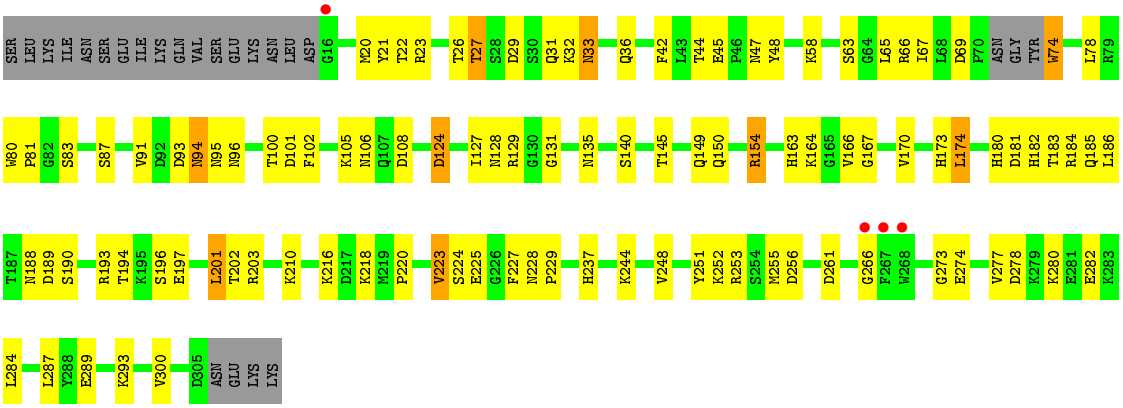
- Molecule 1: Possible leukocidin subunit

Chain K:



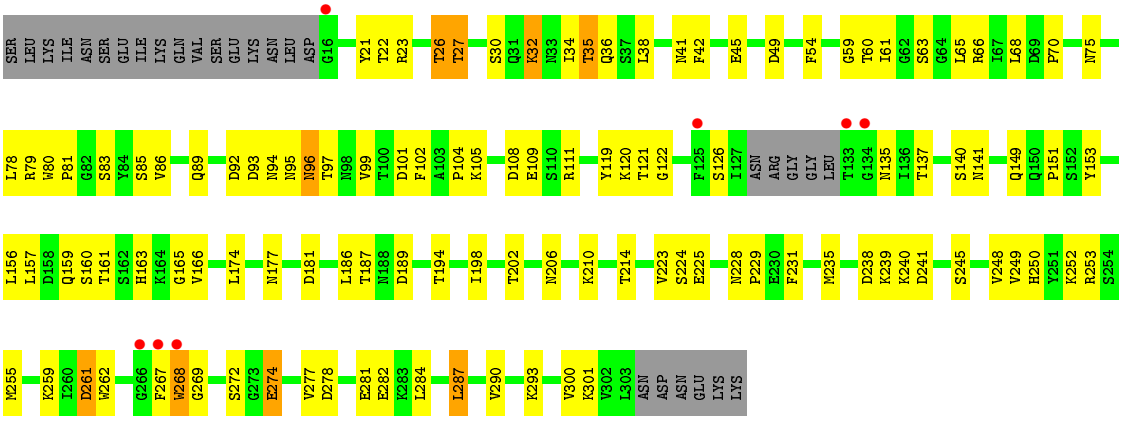
• Molecule 1: Possible leukocidin subunit

Chain M:



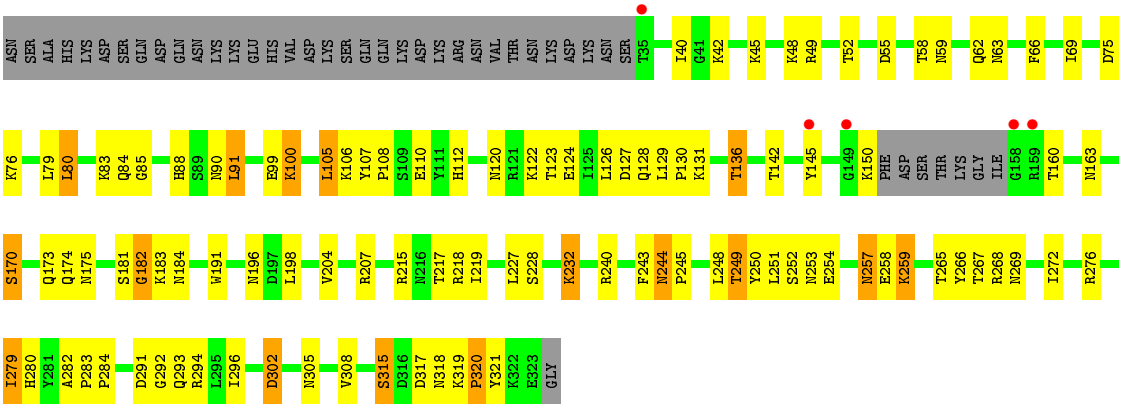
• Molecule 1: Possible leukocidin subunit

Chain O:



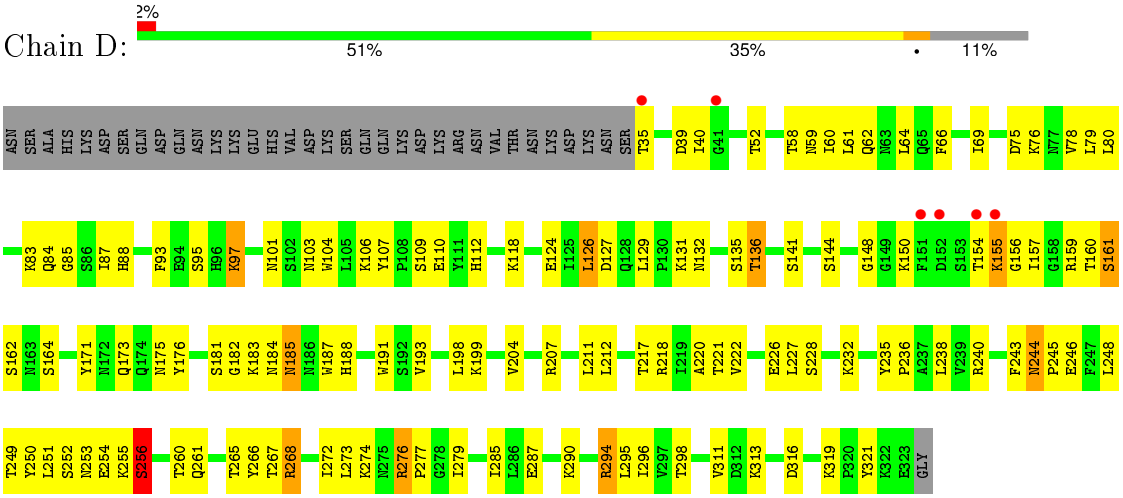
• Molecule 2: Possible leukocidin subunit

Chain B:



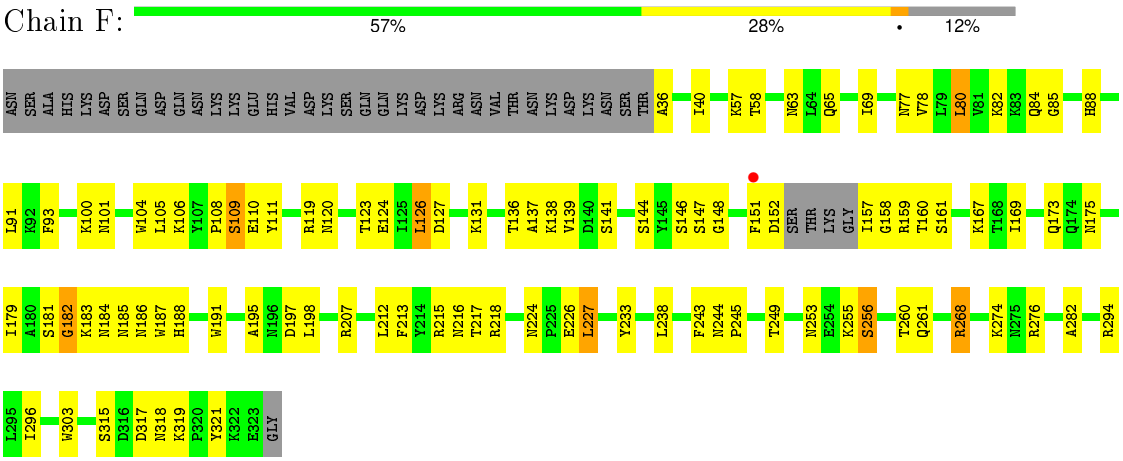
• Molecule 2: Possible leukocidin subunit

Chain D:



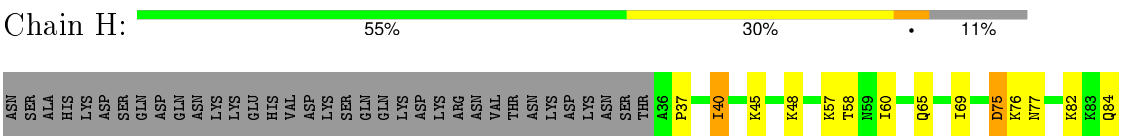
• Molecule 2: Possible leukocidin subunit

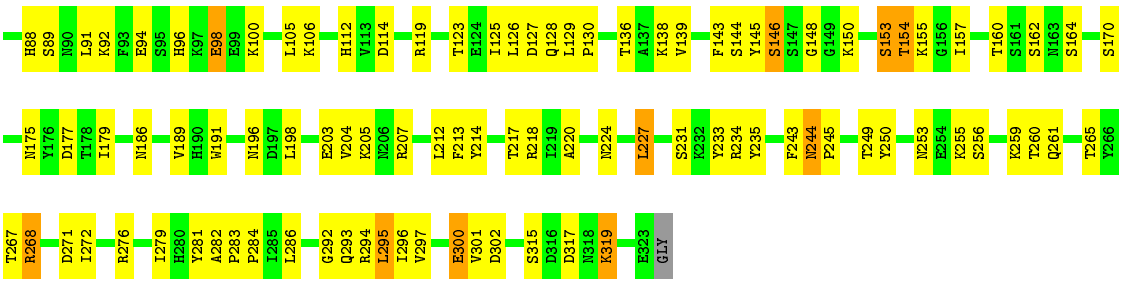
Chain F:



• Molecule 2: Possible leukocidin subunit

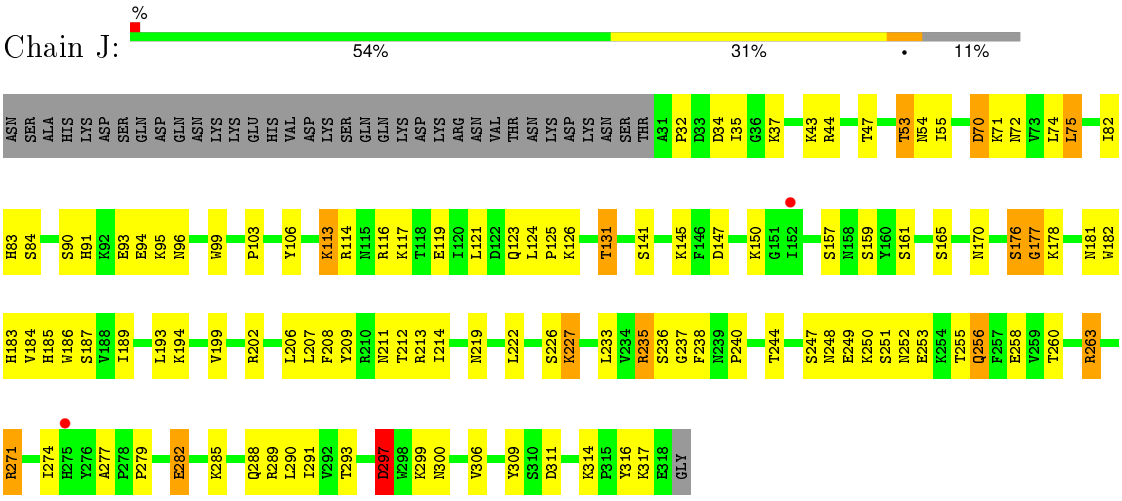
Chain H:





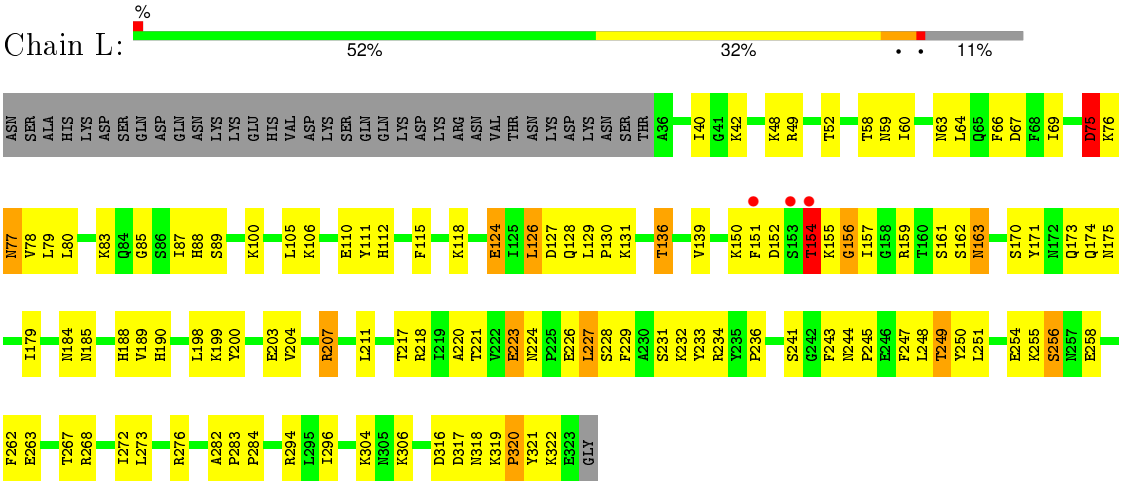
• Molecule 2: Possible leukocidin subunit

Chain J:



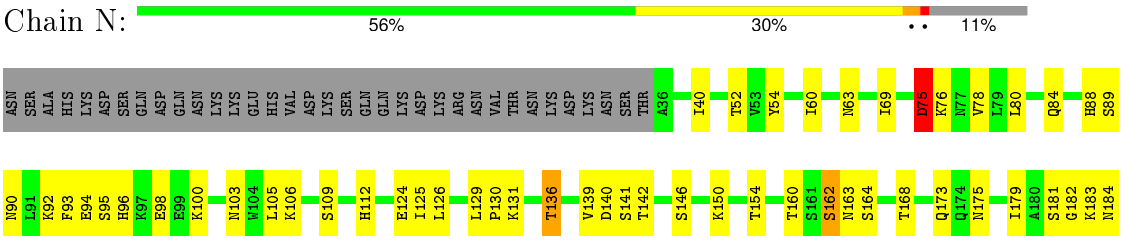
• Molecule 2: Possible leukocidin subunit

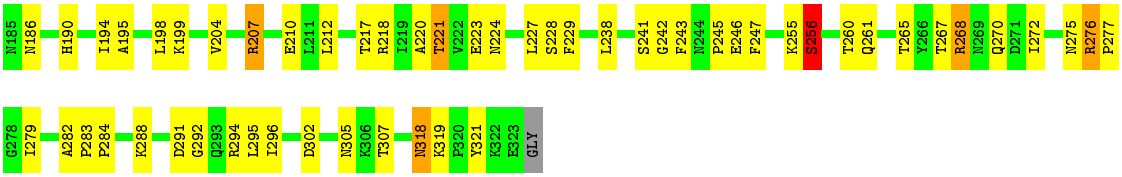
Chain L:



• Molecule 2: Possible leukocidin subunit

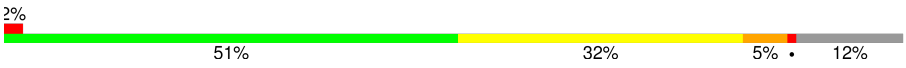
Chain N:

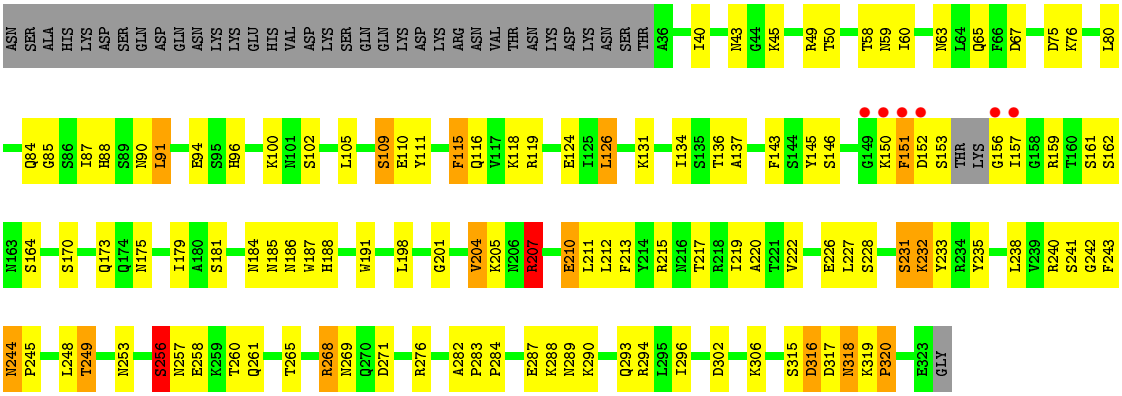




- Molecule 2: Possible leukocidin subunit

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.50Å 198.56Å 179.53Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	48.00 – 2.80 48.19 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.00-2.80) 96.1 (48.19-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.238 , 0.292 0.248 , 0.302	Depositor DCC
R_{free} test set	2205 reflections (1.02%)	DCC
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 218497 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	37620	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.68	0/2345	0.88	1/3170 (0.0%)
1	C	0.67	0/2334	0.82	0/3152
1	E	0.66	0/2414	0.84	1/3264 (0.0%)
1	G	0.68	0/2414	0.86	1/3264 (0.0%)
1	I	0.70	1/2414 (0.0%)	0.88	3/3264 (0.1%)
1	K	0.68	0/2348	0.90	3/3173 (0.1%)
1	M	0.67	0/2388	0.85	0/3227
1	O	0.70	0/2362	0.87	2/3193 (0.1%)
2	B	0.68	0/2371	0.91	2/3202 (0.1%)
2	D	0.71	0/2426	0.88	0/3277
2	F	0.66	0/2392	0.88	1/3230 (0.0%)
2	H	0.68	1/2419 (0.0%)	0.88	2/3267 (0.1%)
2	J	0.69	0/2419	0.91	1/3267 (0.0%)
2	L	0.71	0/2419	0.88	0/3267
2	N	0.68	0/2419	0.86	2/3267 (0.1%)
2	P	0.67	0/2402	0.89	2/3243 (0.1%)
All	All	0.68	2/38286 (0.0%)	0.88	21/51727 (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	E	0	1
1	G	0	2
1	I	0	1
1	K	0	1
2	F	0	1
2	L	0	2
2	N	0	1
2	P	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	292	TRP	CB-CG	-5.77	1.39	1.50
2	H	75	ASP	CB-CG	-5.14	1.41	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	49	ASP	CB-CG-OD1	6.84	124.46	118.30
1	E	253	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	O	287	LEU	CA-CB-CG	6.09	129.31	115.30
2	N	268	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	J	297	ASP	CB-CG-OD1	5.86	123.57	118.30
2	B	302	ASP	CB-CG-OD1	5.71	123.44	118.30
2	H	302	ASP	CB-CG-OD1	5.71	123.44	118.30
2	F	80	LEU	CB-CG-CD1	5.68	120.67	111.00
1	K	253	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	P	49	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	P	207	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	I	253	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	I	253	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	K	217	ASP	CB-CG-OD1	5.25	123.02	118.30
2	B	227	LEU	CA-CB-CG	5.18	127.22	115.30
1	O	32	LYS	CD-CE-NZ	-5.15	99.85	111.70
1	I	29	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	83	SER	CB-CA-C	-5.05	100.51	110.10
2	H	227	LEU	CA-CB-CG	5.01	126.82	115.30
2	N	75	ASP	CB-CA-C	-5.00	100.39	110.40
1	K	74	TRP	CA-CB-CG	5.00	123.20	113.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	94	ASN	Peptide
2	F	36	ALA	Peptide
1	G	128	ASN	Peptide
1	G	93	ASP	Peptide
1	I	94	ASN	Peptide
1	K	229	PRO	Peptide
2	L	156	GLY	Peptide
2	L	75	ASP	Peptide
2	N	75	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	P	256	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2289	0	2171	70	0
1	C	2281	0	2165	80	0
1	E	2356	0	2240	75	0
1	G	2356	0	2240	65	0
1	I	2356	0	2240	84	0
1	K	2293	0	2181	66	0
1	M	2332	0	2221	87	0
1	O	2305	0	2193	77	0
2	B	2320	0	2268	102	0
2	D	2373	0	2321	106	0
2	F	2340	0	2285	93	0
2	H	2366	0	2314	90	0
2	J	2366	0	2314	93	0
2	L	2366	0	2314	102	0
2	N	2366	0	2314	97	0
2	P	2350	0	2293	100	0
3	A	9	0	0	2	0
3	B	15	0	0	4	0
3	C	11	0	0	0	0
3	D	8	0	0	1	0
3	E	11	0	0	2	0
3	F	17	0	0	2	0
3	G	13	0	0	0	0
3	H	18	0	0	1	0
3	I	10	0	0	0	0
3	J	17	0	0	2	0
3	K	12	0	0	1	0
3	L	16	0	0	1	0
3	M	11	0	0	1	0
3	N	9	0	0	1	0
3	O	11	0	0	0	0
3	P	17	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	37620	0	36074	1246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:HD2	2:B:100:LYS:H	1.08	1.16
1:E:183:THR:HG21	3:E:409:HOH:O	1.47	1.13
2:F:88:HIS:HB3	1:G:159:GLN:HG2	1.32	1.12
2:B:170:SER:HB3	3:B:413:HOH:O	1.53	1.09
1:M:26:THR:HG23	2:N:186:ASN:HD22	1.16	1.09
2:L:75:ASP:HB3	2:L:76:LYS:HG3	1.33	1.08
2:H:294:ARG:HH21	2:H:319:LYS:HD3	1.11	1.07
2:D:287:GLU:OE1	2:D:290:LYS:HD3	1.56	1.03
2:B:80:LEU:HD11	2:B:248:LEU:HD23	1.40	1.03
2:N:224:ASN:HB3	2:N:227:LEU:HD12	1.35	1.03
2:B:100:LYS:HB2	2:B:276:ARG:NH2	1.72	1.02
2:P:88:HIS:O	2:P:268:ARG:NH1	1.92	1.02
2:F:100:LYS:HB3	2:F:276:ARG:NH1	1.74	1.02
2:L:80:LEU:HD11	2:L:248:LEU:CD2	1.90	1.01
2:P:207:ARG:HG2	2:P:207:ARG:HH11	1.23	1.00
2:J:70:ASP:HB3	2:J:71:LYS:HG3	1.43	0.97
1:O:177:ASN:HD21	1:O:214:THR:HG21	1.29	0.96
1:A:183:THR:HG21	3:A:409:HOH:O	1.63	0.96
2:L:175:ASN:HB2	1:M:108:ASP:OD1	1.65	0.96
1:K:149:GLN:NE2	1:K:149:GLN:HA	1.80	0.95
1:O:26:THR:HG23	2:P:186:ASN:HD22	1.31	0.95
1:C:101:ASP:OD1	1:C:105:LYS:NZ	1.98	0.95
2:B:58:THR:O	2:B:268:ARG:NH2	1.99	0.94
2:B:294:ARG:HH12	2:B:296:ILE:HD11	1.32	0.94
2:H:294:ARG:HH21	2:H:319:LYS:CD	1.81	0.94
1:M:244:LYS:HD3	1:M:289:GLU:OE2	1.67	0.93
2:J:53:THR:O	2:J:263:ARG:NH2	2.01	0.93
1:M:26:THR:CG2	2:N:186:ASN:HD22	1.80	0.93
2:L:58:THR:O	2:L:268:ARG:NH2	2.01	0.93
1:M:26:THR:HG23	2:N:186:ASN:ND2	1.85	0.92
1:C:83:SER:HB3	1:C:184:ARG:HH21	1.35	0.92
2:B:88:HIS:O	2:B:268:ARG:NH1	2.02	0.92
2:D:316:ASP:OD2	2:D:319:LYS:HG3	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:75:ASP:HB3	2:N:76:LYS:HG3	1.51	0.92
2:H:58:THR:O	2:H:268:ARG:NH2	2.02	0.92
2:B:276:ARG:HH11	2:B:282:ALA:HB3	1.35	0.92
1:C:65:LEU:HD11	1:C:78:LEU:HD11	1.52	0.91
2:B:83:LYS:NZ	2:B:249:THR:HG23	1.83	0.91
2:L:106:LYS:HG2	2:L:272:ILE:HG12	1.49	0.91
2:B:100:LYS:CD	2:B:100:LYS:H	1.79	0.91
2:P:75:ASP:HB3	2:P:76:LYS:HG3	1.53	0.90
2:J:186:TRP:HH2	2:J:244:THR:CG2	1.85	0.90
2:L:80:LEU:HD11	2:L:248:LEU:HD23	1.52	0.89
1:O:35:THR:HG21	2:P:184:ASN:O	1.72	0.89
2:J:186:TRP:HH2	2:J:244:THR:HG22	1.38	0.88
1:K:44:THR:O	1:K:44:THR:HG22	1.71	0.88
2:F:294:ARG:HH11	2:F:296:ILE:HD11	1.36	0.88
2:H:88:HIS:O	2:H:268:ARG:NH1	2.06	0.88
1:K:94:ASN:HD21	1:K:96:ASN:CG	1.75	0.88
2:B:75:ASP:HB3	2:B:76:LYS:HG3	1.56	0.88
2:D:260:THR:HG22	2:D:261:GLN:H	1.40	0.87
2:L:40:ILE:HG21	2:L:126:LEU:HD23	1.54	0.87
1:I:68:LEU:HD12	1:I:77:THR:CG2	2.05	0.87
2:B:294:ARG:HE	2:B:319:LYS:HE3	1.41	0.86
1:K:22:THR:O	1:K:23:ARG:HD3	1.75	0.86
1:C:68:LEU:HD12	1:C:77:THR:HG22	1.56	0.86
2:L:294:ARG:NH1	2:L:296:ILE:HD11	1.90	0.85
1:I:22:THR:O	1:I:23:ARG:HD3	1.77	0.85
1:K:253:ARG:HE	1:K:255:MET:HE2	1.42	0.85
2:L:319:LYS:O	2:L:320:PRO:O	1.93	0.84
2:H:92:LYS:HE3	2:H:94:GLU:OE2	1.77	0.84
1:C:70:PRO:O	1:C:210:LYS:HG3	1.77	0.84
1:G:70:PRO:O	1:G:210:LYS:HE2	1.78	0.84
2:D:58:THR:O	2:D:268:ARG:NH2	2.10	0.84
1:C:22:THR:O	1:C:23:ARG:HD3	1.77	0.84
2:B:122:LYS:HB2	2:B:257:ASN:ND2	1.92	0.84
1:E:26:THR:HG23	2:F:186:ASN:HD22	1.43	0.84
1:I:64:GLY:HA3	1:I:255:MET:HE1	1.59	0.84
2:J:53:THR:HG22	2:J:288:GLN:HB3	1.60	0.83
2:P:40:ILE:HG21	2:P:126:LEU:HD23	1.61	0.83
1:A:18:THR:HG22	1:A:45:GLU:HA	1.60	0.83
2:F:58:THR:O	2:F:268:ARG:NH2	2.12	0.83
1:E:65:LEU:HD11	1:E:78:LEU:HD11	1.58	0.83
1:I:70:PRO:O	1:I:210:LYS:HB2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:294:ARG:HH11	2:P:296:ILE:HD11	1.43	0.82
1:G:253:ARG:HE	1:G:255:MET:HE1	1.45	0.82
1:O:228:ASN:OD1	2:P:131:LYS:HB3	1.79	0.82
2:L:80:LEU:HD11	2:L:248:LEU:HD22	1.61	0.81
2:B:100:LYS:HD2	2:B:100:LYS:N	1.93	0.81
2:D:80:LEU:HD11	2:D:248:LEU:HD22	1.63	0.81
1:A:26:THR:OG1	2:B:124:GLU:OE1	1.98	0.81
2:D:260:THR:HG22	2:D:261:GLN:N	1.97	0.80
1:M:22:THR:O	1:M:23:ARG:HD3	1.80	0.80
1:I:18:THR:HG22	1:I:19:LYS:N	1.97	0.80
2:F:127:ASP:OD1	2:F:131:LYS:HE3	1.81	0.80
2:P:191:TRP:HH2	2:P:249:THR:HG22	1.47	0.80
2:N:40:ILE:HG21	2:N:126:LEU:HD23	1.64	0.80
2:B:259:LYS:HE2	2:B:302:ASP:HB2	1.64	0.80
2:D:144:SER:HB2	2:D:164:SER:HB2	1.64	0.80
2:L:294:ARG:HH12	2:L:296:ILE:HD11	1.46	0.79
2:F:255:LYS:O	2:F:256:SER:HB3	1.82	0.79
2:H:96:HIS:HB3	2:H:98:GLU:OE2	1.82	0.79
2:B:100:LYS:CB	2:B:276:ARG:HH21	1.96	0.79
1:C:65:LEU:CD1	1:C:78:LEU:HD11	2.13	0.79
2:F:40:ILE:HG21	2:F:126:LEU:HD23	1.63	0.79
2:H:294:ARG:NH2	2:H:319:LYS:HD3	1.95	0.78
2:F:294:ARG:NH1	2:F:296:ILE:HD11	1.98	0.78
2:D:106:LYS:HG2	2:D:272:ILE:HG12	1.66	0.78
2:D:211:LEU:HD12	2:D:211:LEU:N	1.98	0.77
1:C:263:ASN:HD22	1:C:270:TYR:HE1	1.33	0.77
2:B:276:ARG:HH11	2:B:282:ALA:CB	1.96	0.77
1:A:19:LYS:HE2	1:A:21:TYR:CZ	2.20	0.77
1:O:149:GLN:HG3	2:P:136:THR:HG21	1.67	0.77
2:D:154:THR:HG22	2:D:155:LYS:HG2	1.67	0.77
2:P:58:THR:O	2:P:268:ARG:NH2	2.19	0.76
1:K:126:SER:OG	1:K:133:THR:HB	1.86	0.76
2:N:294:ARG:CZ	2:N:319:LYS:HD3	2.15	0.76
1:A:35:THR:HB	3:B:414:HOH:O	1.85	0.76
2:L:75:ASP:CB	2:L:76:LYS:HG3	2.15	0.76
2:H:217:THR:HG21	2:H:220:ALA:HB2	1.68	0.76
1:E:38:LEU:HD21	1:E:249:VAL:HG21	1.68	0.76
2:F:157:ILE:HG22	2:F:158:GLY:H	1.49	0.76
1:A:298:LYS:HG2	1:A:299:PHE:O	1.86	0.75
2:F:294:ARG:HH21	2:F:319:LYS:HG2	1.51	0.75
1:M:173:HIS:CE1	1:M:174:LEU:HD12	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:HB2	2:B:276:ARG:HH21	1.48	0.75
2:F:175:ASN:HB2	1:G:108:ASP:OD1	1.86	0.75
2:B:83:LYS:HZ2	2:B:249:THR:HG23	1.52	0.75
2:F:77:ASN:HB2	2:F:253:ASN:HB3	1.68	0.75
1:C:68:LEU:HD12	1:C:77:THR:CG2	2.17	0.74
1:A:38:LEU:HD21	1:A:249:VAL:HG21	1.67	0.74
2:B:83:LYS:HZ1	2:B:249:THR:HG23	1.49	0.74
2:N:276:ARG:HH11	2:N:276:ARG:HB2	1.51	0.74
1:K:253:ARG:HE	1:K:255:MET:CE	2.01	0.74
2:N:243:PHE:CE2	2:N:245:PRO:HB3	2.22	0.74
2:L:87:ILE:HG21	2:L:111:TYR:HD1	1.53	0.74
1:I:266:GLY:O	1:I:267:PHE:HB2	1.88	0.74
2:N:75:ASP:CB	2:N:76:LYS:HG3	2.18	0.74
2:H:144:SER:HB2	2:H:164:SER:OG	1.87	0.74
1:O:177:ASN:HD21	1:O:214:THR:CG2	2.01	0.73
2:J:147:ASP:HB3	2:J:150:LYS:HB2	1.70	0.73
1:K:149:GLN:NE2	1:K:149:GLN:CA	2.50	0.73
1:I:101:ASP:OD1	1:I:105:LYS:NZ	2.20	0.73
1:A:49:ASP:O	1:A:239:LYS:HD2	1.87	0.73
2:H:128:GLN:OE1	2:H:128:GLN:N	2.22	0.73
1:I:68:LEU:HD12	1:I:77:THR:HG21	1.70	0.73
1:I:68:LEU:HD12	1:I:77:THR:HG22	1.71	0.73
1:O:177:ASN:ND2	1:O:214:THR:HG21	2.04	0.73
1:O:65:LEU:HD22	1:O:224:SER:HA	1.71	0.72
2:D:191:TRP:HH2	2:D:249:THR:HG22	1.54	0.72
1:M:65:LEU:HD22	1:M:224:SER:HA	1.70	0.72
1:G:240:LYS:HG3	1:G:241:ASP:N	2.03	0.72
2:L:221:THR:HG22	2:L:227:LEU:HD13	1.71	0.72
1:A:183:THR:CG2	3:A:409:HOH:O	2.29	0.72
1:I:74:TRP:CE3	1:I:74:TRP:HA	2.25	0.72
1:G:22:THR:O	1:G:23:ARG:HD3	1.89	0.72
2:L:75:ASP:HB3	2:L:76:LYS:CG	2.18	0.72
1:A:21:TYR:HB2	1:A:42:PHE:HB2	1.72	0.72
1:O:49:ASP:O	1:O:239:LYS:HD2	1.89	0.72
1:O:66:ARG:NH1	1:O:68:LEU:HD23	2.04	0.72
1:C:83:SER:HB3	1:C:184:ARG:NH2	2.05	0.71
1:I:151:PRO:HB3	2:J:131:THR:HG23	1.70	0.71
1:K:301:LYS:HG2	1:K:302:VAL:O	1.89	0.71
2:P:243:PHE:CE2	2:P:245:PRO:HB3	2.25	0.71
1:M:74:TRP:CE3	1:M:74:TRP:HA	2.23	0.71
1:K:154:ARG:HD3	1:K:173:HIS:CD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ASP:CB	2:H:76:LYS:HG3	2.20	0.71
1:C:24:THR:HG21	2:D:126:LEU:HD11	1.71	0.71
1:A:280:LYS:NZ	1:A:282:GLU:HG2	2.06	0.71
1:A:94:ASN:ND2	1:A:96:ASN:OD1	2.23	0.70
2:P:294:ARG:NH1	2:P:296:ILE:HD11	2.06	0.70
2:F:159:ARG:HD2	1:M:127:ILE:HG12	1.72	0.70
2:B:319:LYS:O	2:B:320:PRO:O	2.09	0.70
1:C:281:GLU:CG	1:C:281:GLU:O	2.38	0.70
2:B:276:ARG:NH1	2:B:282:ALA:CB	2.54	0.70
2:F:100:LYS:HB3	2:F:276:ARG:HH12	1.52	0.70
1:I:65:LEU:HD22	1:I:224:SER:HA	1.73	0.70
2:F:88:HIS:CB	1:G:159:GLN:HG2	2.18	0.70
2:D:212:LEU:HD23	2:D:273:LEU:HD11	1.73	0.70
2:H:260:THR:HG22	2:H:261:GLN:H	1.56	0.70
2:D:101:ASN:OD1	2:D:276:ARG:HB2	1.92	0.69
1:O:151:PRO:HB2	1:O:153:TYR:O	1.92	0.69
1:I:55:ILE:O	1:I:232:LEU:HD12	1.92	0.69
1:M:101:ASP:OD1	1:M:105:LYS:NZ	2.21	0.69
1:K:101:ASP:OD1	1:K:105:LYS:NZ	2.21	0.69
2:L:162:SER:C	2:L:163:ASN:HD22	1.95	0.69
1:E:32:LYS:HE2	1:E:282:GLU:OE1	1.92	0.69
2:B:100:LYS:CB	2:B:276:ARG:NH2	2.50	0.68
2:H:75:ASP:HB3	2:H:76:LYS:HG3	1.72	0.68
1:A:22:THR:O	1:A:23:ARG:HD3	1.93	0.68
1:G:29:ASP:CG	1:G:32:LYS:HG2	2.13	0.68
1:M:33:ASN:HD21	2:N:183:LYS:HE3	1.55	0.68
2:B:294:ARG:NH1	2:B:296:ILE:HD11	2.08	0.68
2:P:232:LYS:O	2:P:240:ARG:HD3	1.94	0.68
1:E:26:THR:CG2	2:F:186:ASN:HD22	2.06	0.68
1:A:56:LYS:HE2	1:A:230:GLU:OE2	1.94	0.68
2:J:186:TRP:CH2	2:J:244:THR:HG22	2.26	0.67
1:M:183:THR:HG22	1:M:188:ASN:OD1	1.95	0.67
2:B:112:HIS:HB2	2:B:267:THR:HB	1.75	0.67
1:C:185:GLN:HG2	1:C:189:ASP:H	1.59	0.67
1:K:92:ASP:OD2	1:K:245:SER:HB3	1.94	0.67
1:C:281:GLU:O	1:C:281:GLU:HG3	1.92	0.67
1:G:80:TRP:HB2	1:G:81:PRO:HD2	1.75	0.67
1:I:18:THR:HG22	1:I:19:LYS:H	1.60	0.67
2:B:80:LEU:HD22	2:B:250:TYR:CE1	2.30	0.67
2:J:219:ASN:HB3	2:J:222:LEU:HD12	1.76	0.67
2:P:243:PHE:C	2:P:244:ASN:HD22	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:GLY:N	2:F:160:THR:O	2.24	0.67
1:I:74:TRP:HE3	1:I:74:TRP:HA	1.60	0.67
2:J:117:LYS:HE3	2:J:252:ASN:HB2	1.76	0.67
2:N:88:HIS:HB3	1:O:159:GLN:HG2	1.76	0.66
2:L:224:ASN:ND2	2:L:227:LEU:HD12	2.10	0.66
1:M:22:THR:HG21	2:N:40:ILE:CD1	2.25	0.66
1:K:44:THR:O	1:K:44:THR:CG2	2.41	0.66
2:F:181:SER:O	2:F:184:ASN:ND2	2.28	0.66
1:I:182:HIS:HA	1:I:188:ASN:OD1	1.95	0.66
1:E:65:LEU:CD1	1:E:78:LEU:HD11	2.26	0.66
2:L:221:THR:OG1	2:L:223:GLU:HG2	1.96	0.66
2:D:75:ASP:HB3	2:D:76:LYS:HG3	1.77	0.66
1:M:32:LYS:O	1:M:33:ASN:HB2	1.94	0.66
1:C:244:LYS:HE3	1:C:289:GLU:OE2	1.95	0.66
2:D:80:LEU:CD1	2:D:248:LEU:HD22	2.26	0.66
2:N:243:PHE:HE2	2:N:245:PRO:HB3	1.61	0.66
2:J:186:TRP:CH2	2:J:244:THR:CG2	2.75	0.65
1:E:300:VAL:HG12	1:E:301:LYS:HG2	1.76	0.65
2:B:45:LYS:O	2:B:69:ILE:HA	1.97	0.65
1:O:41:ASN:HB2	1:O:54:PHE:HB2	1.78	0.65
1:O:66:ARG:HH12	1:O:68:LEU:HD23	1.60	0.65
2:P:100:LYS:CB	2:P:276:ARG:HH21	2.09	0.65
1:M:26:THR:HG21	2:N:124:GLU:HB3	1.78	0.65
2:F:136:THR:HG22	2:F:137:ALA:H	1.62	0.65
1:K:193:ARG:NH2	3:K:407:HOH:O	2.29	0.65
1:K:94:ASN:ND2	1:K:96:ASN:H	1.94	0.65
2:P:84:GLN:HA	2:P:245:PRO:O	1.96	0.65
2:F:233:TYR:OH	1:G:277:VAL:HG11	1.96	0.65
2:H:203:GLU:OE1	2:H:234:ARG:NH2	2.29	0.65
2:P:143:PHE:HE2	2:P:145:TYR:HD2	1.45	0.65
1:M:74:TRP:HE3	1:M:74:TRP:HA	1.60	0.65
1:E:63:SER:HB3	1:E:225:GLU:C	2.18	0.64
1:K:94:ASN:ND2	1:K:96:ASN:CG	2.49	0.64
2:D:260:THR:CG2	2:D:261:GLN:H	2.09	0.64
1:K:92:ASP:HB3	1:K:94:ASN:HB2	1.79	0.64
1:E:263:ASN:O	1:E:269:GLY:HA3	1.97	0.64
2:D:175:ASN:HB2	1:E:108:ASP:OD1	1.97	0.64
1:C:150:GLN:O	1:C:150:GLN:HG2	1.95	0.64
1:K:94:ASN:HD22	1:K:96:ASN:H	1.44	0.64
1:E:37:SER:HB3	1:E:58:LYS:HB3	1.79	0.64
2:B:48:LYS:O	2:B:49:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:LEU:HD11	1:K:78:LEU:HD11	1.79	0.64
1:O:27:THR:HG22	1:O:36:GLN:HB2	1.79	0.64
2:J:293:THR:HG22	2:J:306:VAL:HG23	1.78	0.63
1:O:63:SER:HB3	1:O:225:GLU:C	2.17	0.63
2:F:88:HIS:O	2:F:268:ARG:NH1	2.30	0.63
1:M:96:ASN:O	1:M:237:HIS:HA	1.98	0.63
2:B:302:ASP:OD2	2:B:305:ASN:HB2	1.97	0.63
1:C:34:ILE:HG21	1:C:284:LEU:HB3	1.81	0.63
1:O:26:THR:HG23	2:P:186:ASN:ND2	2.11	0.63
2:D:316:ASP:OD2	2:D:319:LYS:CG	2.44	0.63
1:G:70:PRO:HA	1:G:210:LYS:HG3	1.79	0.63
2:L:63:ASN:OD1	2:L:85:GLY:HA2	1.98	0.63
1:I:225:GLU:HG3	2:J:177:GLY:H	1.63	0.63
2:B:59:ASN:HB3	2:B:90:ASN:HD21	1.62	0.63
1:O:259:LYS:HE2	1:O:261:ASP:OD2	1.99	0.63
1:M:220:PRO:HG2	1:M:223:VAL:HG12	1.80	0.63
1:E:248:VAL:HG12	1:E:250:HIS:NE2	2.13	0.63
1:G:94:ASN:OD1	1:G:96:ASN:N	2.30	0.63
1:O:122:GLY:HA3	1:O:137:THR:OG1	1.99	0.62
2:L:87:ILE:HG21	2:L:111:TYR:CD1	2.34	0.62
2:D:154:THR:HG22	2:D:155:LYS:CG	2.28	0.62
2:H:244:ASN:HD22	2:H:244:ASN:N	1.98	0.62
2:H:255:LYS:O	2:H:256:SER:CB	2.48	0.62
2:H:243:PHE:CE2	2:H:245:PRO:HB3	2.35	0.62
1:E:22:THR:HG23	1:E:41:ASN:OD1	2.00	0.62
2:F:217:THR:HB	1:G:191:ASP:OD1	1.99	0.62
2:N:198:LEU:O	2:N:204:VAL:HA	1.98	0.62
1:I:18:THR:CG2	1:I:19:LYS:N	2.63	0.61
1:O:99:VAL:HA	1:O:235:MET:HG2	1.82	0.61
1:O:38:LEU:HD21	1:O:249:VAL:HG21	1.81	0.61
1:C:184:ARG:HD3	1:C:256:ASP:OD2	1.99	0.61
1:E:225:GLU:HG2	2:F:179:ILE:CG2	2.30	0.61
1:O:137:THR:HG22	2:P:150:LYS:CG	2.30	0.61
2:F:215:ARG:HE	2:F:217:THR:CG2	2.14	0.61
2:P:80:LEU:HD11	2:P:248:LEU:HD23	1.82	0.61
2:J:83:HIS:O	2:J:263:ARG:NH1	2.33	0.61
1:G:225:GLU:HG3	2:H:179:ILE:CG2	2.31	0.61
1:E:186:LEU:HD23	1:E:187:THR:HG23	1.81	0.61
2:L:258:GLU:OE1	2:L:304:LYS:HG3	2.00	0.61
1:K:35:THR:HG21	2:L:184:ASN:O	2.01	0.61
2:D:298:THR:HG22	2:D:311:VAL:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:263:ASN:O	1:K:269:GLY:HA3	2.01	0.61
1:E:183:THR:HG22	1:E:188:ASN:OD1	1.99	0.61
2:L:276:ARG:HH11	2:L:282:ALA:CB	2.14	0.61
1:O:32:LYS:HG2	1:O:282:GLU:OE1	2.00	0.61
2:J:297:ASP:OD2	2:J:300:ASN:ND2	2.34	0.61
2:D:127:ASP:OD1	2:D:131:LYS:HE3	2.01	0.61
1:O:35:THR:CG2	2:P:184:ASN:O	2.48	0.60
2:D:255:LYS:O	2:D:256:SER:HB3	2.00	0.60
1:A:83:SER:HB2	1:A:254:SER:HB3	1.83	0.60
2:N:276:ARG:CB	2:N:276:ARG:HH11	2.14	0.60
2:D:255:LYS:O	2:D:256:SER:CB	2.49	0.60
2:H:191:TRP:HH2	2:H:249:THR:HG23	1.66	0.60
1:O:174:LEU:HD22	1:O:181:ASP:HB3	1.84	0.60
2:D:287:GLU:OE1	2:D:290:LYS:CD	2.42	0.60
1:C:149:GLN:HG3	2:D:136:THR:HG21	1.83	0.60
2:P:75:ASP:CB	2:P:76:LYS:HG3	2.30	0.60
1:I:86:VAL:HA	1:I:250:HIS:O	2.02	0.60
2:L:87:ILE:CG2	2:L:111:TYR:CD1	2.84	0.60
1:M:33:ASN:ND2	2:N:183:LYS:HE3	2.17	0.60
2:P:100:LYS:HB3	2:P:276:ARG:NH2	2.17	0.60
1:O:300:VAL:HG12	1:O:301:LYS:HB3	1.82	0.60
2:H:231:SER:OG	2:H:233:TYR:CD2	2.55	0.60
1:A:173:HIS:ND1	1:A:174:LEU:HG	2.17	0.60
2:L:127:ASP:OD1	2:L:131:LYS:NZ	2.34	0.60
1:E:201:LEU:HD13	1:E:215:PRO:HD3	1.83	0.60
2:N:103:ASN:ND2	2:N:277:PRO:HG3	2.17	0.60
2:F:317:ASP:CG	2:F:318:ASN:H	2.04	0.60
1:M:23:ARG:HD2	2:N:75:ASP:OD2	2.01	0.60
1:O:149:GLN:HG3	2:P:136:THR:CG2	2.30	0.60
1:A:55:ILE:O	1:A:232:LEU:HD12	2.02	0.60
2:F:40:ILE:CG2	2:F:126:LEU:HD23	2.32	0.60
2:P:243:PHE:HE2	2:P:245:PRO:HB3	1.66	0.60
2:D:112:HIS:HB2	2:D:267:THR:HB	1.84	0.60
2:J:271:ARG:NH1	2:J:277:ALA:CB	2.65	0.60
1:A:70:PRO:O	1:A:210:LYS:HD2	2.02	0.60
2:J:271:ARG:HH11	2:J:271:ARG:HB2	1.68	0.59
1:C:185:GLN:HG3	1:C:188:ASN:N	2.17	0.59
2:J:43:LYS:O	2:J:44:ARG:NH1	2.34	0.59
1:O:96:ASN:HB3	1:O:238:ASP:HB2	1.83	0.59
2:N:318:ASN:ND2	3:N:408:HOH:O	2.34	0.59
2:P:91:LEU:CD1	2:P:105:LEU:HD21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:174:LEU:CD2	1:M:181:ASP:HB3	2.32	0.59
3:D:406:HOH:O	1:E:50:LYS:HE3	2.02	0.59
1:M:32:LYS:HG2	1:M:282:GLU:OE2	2.02	0.59
1:M:196:SER:O	1:M:273:GLY:HA3	2.02	0.59
2:J:32:PRO:HD2	3:J:412:HOH:O	2.03	0.59
1:I:64:GLY:HA3	1:I:255:MET:CE	2.32	0.58
1:K:206:ASN:HB2	1:K:268:TRP:CH2	2.38	0.58
2:H:243:PHE:C	2:H:244:ASN:HD22	2.07	0.58
2:B:175:ASN:HB3	2:B:198:LEU:HD23	1.84	0.58
2:H:191:TRP:HH2	2:H:249:THR:CG2	2.17	0.58
2:J:251:SER:H	2:J:299:LYS:HZ1	1.50	0.58
2:L:128:GLN:OE1	2:L:128:GLN:N	2.36	0.58
1:M:174:LEU:HD22	1:M:181:ASP:HB3	1.85	0.58
1:I:50:LYS:HE2	3:P:402:HOH:O	2.04	0.58
2:B:294:ARG:NE	2:B:319:LYS:HE3	2.15	0.58
2:H:153:SER:O	2:H:154:THR:C	2.42	0.58
2:D:83:LYS:HZ1	2:D:249:THR:HG23	1.68	0.58
2:D:198:LEU:O	2:D:204:VAL:HA	2.03	0.58
2:D:232:LYS:HD2	2:D:240:ARG:NH1	2.18	0.58
2:H:260:THR:HG22	2:H:261:GLN:N	2.19	0.58
2:H:231:SER:OG	2:H:233:TYR:HD2	1.87	0.58
1:A:44:THR:O	1:A:44:THR:HG22	2.04	0.58
2:H:84:GLN:HA	2:H:245:PRO:O	2.04	0.58
1:K:196:SER:OG	1:K:198:ILE:HG22	2.03	0.58
1:C:21:TYR:HB2	1:C:42:PHE:HB2	1.86	0.58
2:B:294:ARG:HH21	2:B:319:LYS:CE	2.16	0.58
1:A:280:LYS:HZ3	1:A:282:GLU:HG2	1.67	0.58
1:M:280:LYS:NZ	1:M:282:GLU:OE1	2.36	0.58
2:H:198:LEU:O	2:H:204:VAL:HA	2.04	0.58
2:N:224:ASN:HB3	2:N:227:LEU:CD1	2.23	0.57
2:F:157:ILE:HG22	2:F:158:GLY:N	2.16	0.57
2:P:116:GLN:HG2	2:P:188:HIS:HD2	1.68	0.57
1:K:90:ASN:OD1	1:K:91:VAL:N	2.37	0.57
2:L:87:ILE:CG2	2:L:111:TYR:HD1	2.15	0.57
1:E:151:PRO:HB2	1:E:153:TYR:O	2.03	0.57
1:K:151:PRO:HB3	2:L:136:THR:HG23	1.85	0.57
2:B:122:LYS:HB2	2:B:257:ASN:HD22	1.68	0.57
2:F:181:SER:C	2:F:183:LYS:H	2.07	0.57
2:F:104:TRP:CD1	2:F:274:LYS:HG2	2.40	0.57
1:M:58:LYS:HA	1:M:229:PRO:O	2.04	0.57
1:A:287:LEU:HD23	1:A:300:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:161:THR:HG23	1:O:166:VAL:HA	1.87	0.57
1:C:27:THR:HG22	1:C:36:GLN:HB2	1.87	0.57
1:I:18:THR:CG2	1:I:19:LYS:H	2.16	0.57
2:P:143:PHE:CE2	2:P:145:TYR:HD2	2.23	0.57
1:C:151:PRO:HB2	1:C:153:TYR:O	2.04	0.57
1:K:63:SER:HB2	1:K:81:PRO:HG3	1.87	0.57
1:G:206:ASN:HB2	1:G:268:TRP:CH2	2.40	0.57
1:C:26:THR:HG22	2:D:124:GLU:OE1	2.05	0.57
1:O:135:ASN:HB2	2:P:151:PHE:O	2.03	0.57
2:D:62:GLN:HG2	2:D:266:TYR:CZ	2.39	0.57
2:P:63:ASN:OD1	2:P:85:GLY:HA2	2.05	0.57
1:G:64:GLY:HA3	1:G:255:MET:CE	2.35	0.57
1:G:137:THR:HG22	2:H:150:LYS:HG3	1.86	0.56
2:F:276:ARG:HE	2:F:282:ALA:CB	2.18	0.56
2:B:191:TRP:HH2	2:B:249:THR:HG22	1.71	0.56
2:L:64:LEU:HB3	2:L:66:PHE:CE2	2.40	0.56
2:N:198:LEU:HD12	2:N:212:LEU:HD11	1.87	0.56
1:G:128:ASN:HB3	1:G:129:ARG:O	2.05	0.56
2:H:276:ARG:HE	2:H:282:ALA:HB2	1.70	0.56
2:D:183:LYS:O	2:D:185:ASN:ND2	2.37	0.56
2:P:207:ARG:CG	2:P:207:ARG:HH11	2.07	0.56
1:M:65:LEU:CD1	1:M:78:LEU:HD11	2.35	0.56
2:L:224:ASN:HD22	2:L:227:LEU:HD12	1.69	0.56
1:I:201:LEU:HD13	1:I:214:THR:HA	1.86	0.56
1:E:89:GLN:HG3	1:E:165:GLY:HA3	1.86	0.56
1:G:65:LEU:HD11	1:G:78:LEU:HD11	1.87	0.56
2:J:176:SER:HB2	2:J:185:HIS:HB3	1.87	0.56
1:C:29:ASP:OD1	1:C:31:GLN:N	2.37	0.56
2:F:276:ARG:HE	2:F:282:ALA:HB2	1.70	0.56
1:G:245:SER:HG	1:G:292:TRP:HE1	1.51	0.56
1:I:26:THR:HG21	2:J:119:GLU:HB3	1.86	0.56
1:K:151:PRO:HB2	1:K:153:TYR:O	2.06	0.56
2:P:260:THR:HG22	2:P:261:GLN:N	2.21	0.56
1:G:63:SER:HB3	1:G:225:GLU:C	2.25	0.56
1:I:32:LYS:O	1:I:33:ASN:HB2	2.05	0.56
1:E:26:THR:HG23	2:F:186:ASN:ND2	2.16	0.56
2:H:276:ARG:HE	2:H:282:ALA:CB	2.19	0.56
2:B:215:ARG:CZ	2:B:217:THR:HG21	2.36	0.56
1:M:135:ASN:ND2	2:N:150:LYS:HE2	2.20	0.56
2:P:207:ARG:NH1	2:P:207:ARG:HG2	2.03	0.56
1:I:253:ARG:HE	1:I:255:MET:CE	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:182:HIS:HA	1:M:188:ASN:ND2	2.21	0.56
2:P:100:LYS:HB3	2:P:276:ARG:HH21	1.70	0.56
1:A:248:VAL:HG12	1:A:250:HIS:CD2	2.40	0.56
2:J:93:GLU:HG2	2:J:94:GLU:N	2.21	0.56
1:I:299:PHE:HZ	1:I:302:VAL:HG23	1.71	0.56
2:F:255:LYS:O	2:F:256:SER:CB	2.54	0.56
1:G:29:ASP:OD1	1:G:32:LYS:HG2	2.06	0.56
2:D:127:ASP:OD1	2:D:131:LYS:CE	2.53	0.56
2:J:233:LEU:HA	2:J:237:GLY:O	2.04	0.56
1:K:134:GLY:O	1:K:135:ASN:HB3	2.05	0.56
1:M:22:THR:HG21	2:N:40:ILE:HD12	1.88	0.56
2:N:255:LYS:O	2:N:256:SER:CB	2.54	0.56
1:M:182:HIS:HA	1:M:188:ASN:HD21	1.71	0.55
2:F:233:TYR:O	1:G:154:ARG:NH2	2.38	0.55
2:P:110:GLU:OE2	2:P:207:ARG:NH2	2.39	0.55
2:D:265:THR:HG22	2:D:265:THR:O	2.06	0.55
1:A:44:THR:O	1:A:44:THR:CG2	2.54	0.55
2:P:287:GLU:OE1	2:P:290:LYS:HD3	2.06	0.55
2:P:205:LYS:HE3	2:P:211:LEU:HB3	1.88	0.55
2:B:106:LYS:HE2	2:B:272:ILE:HD11	1.87	0.55
2:F:57:LYS:NZ	2:F:315:SER:HB2	2.20	0.55
1:M:63:SER:HB3	1:M:225:GLU:C	2.26	0.55
1:C:22:THR:HG21	2:D:40:ILE:CD1	2.36	0.55
1:C:185:GLN:CG	1:C:189:ASP:H	2.20	0.55
2:L:184:ASN:OD1	2:L:189:VAL:HA	2.06	0.55
1:A:225:GLU:CG	2:B:182:GLY:H	2.19	0.55
1:G:132:LEU:HB2	2:L:161:SER:HB3	1.88	0.55
2:P:91:LEU:HD12	2:P:105:LEU:HD21	1.89	0.55
2:P:181:SER:O	2:P:184:ASN:ND2	2.40	0.55
1:I:248:VAL:HG23	1:I:287:LEU:HD12	1.88	0.55
1:E:27:THR:HG22	1:E:36:GLN:HB2	1.89	0.55
1:E:132:LEU:HD12	1:I:268:TRP:CD1	2.42	0.55
1:K:149:GLN:HE21	1:K:149:GLN:CA	2.18	0.55
2:F:123:THR:OG1	2:F:253:ASN:OD1	2.23	0.55
1:I:183:THR:HG22	1:I:188:ASN:ND2	2.22	0.55
2:P:100:LYS:HB2	2:P:276:ARG:HH21	1.71	0.55
2:P:319:LYS:O	2:P:320:PRO:O	2.24	0.55
2:D:211:LEU:N	2:D:211:LEU:CD1	2.69	0.55
1:E:225:GLU:HG2	2:F:179:ILE:HG23	1.88	0.55
2:N:291:ASP:OD1	2:N:318:ASN:ND2	2.39	0.55
2:F:88:HIS:HB3	1:G:159:GLN:CG	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:233:TYR:HE2	3:F:410:HOH:O	1.89	0.55
1:M:194:THR:HG21	1:M:203:ARG:HE	1.71	0.55
2:D:83:LYS:NZ	2:D:249:THR:HG23	2.22	0.54
2:F:136:THR:HG22	2:F:137:ALA:N	2.22	0.54
1:E:225:GLU:OE2	2:F:182:GLY:N	2.25	0.54
1:O:137:THR:HG22	2:P:150:LYS:HG2	1.87	0.54
1:G:225:GLU:HG3	2:H:179:ILE:HG22	1.87	0.54
2:L:276:ARG:HH11	2:L:282:ALA:HB3	1.71	0.54
1:A:105:LYS:NZ	2:H:84:GLN:OE1	2.40	0.54
2:F:215:ARG:NE	2:F:217:THR:HG21	2.23	0.54
2:B:207:ARG:HG2	2:B:207:ARG:O	1.98	0.54
2:J:184:VAL:HG21	2:J:244:THR:HG21	1.90	0.54
2:F:215:ARG:NE	2:F:217:THR:CG2	2.71	0.54
2:L:231:SER:OG	2:L:233:TYR:CD2	2.61	0.54
2:N:60:ILE:HG22	2:N:295:LEU:HD23	1.88	0.54
1:M:27:THR:HG23	1:M:284:LEU:HD21	1.89	0.54
2:N:106:LYS:HG2	2:N:272:ILE:HG12	1.88	0.54
2:J:193:LEU:O	2:J:199:VAL:HA	2.07	0.54
1:I:129:ARG:NH1	1:I:129:ARG:HA	2.22	0.54
1:E:252:LYS:HG3	1:E:283:LYS:HB2	1.88	0.54
1:I:196:SER:O	1:I:273:GLY:HA3	2.07	0.54
1:I:120:LYS:HG2	2:P:164:SER:HB3	1.89	0.54
1:A:89:GLN:HG3	1:A:165:GLY:HA3	1.90	0.54
1:C:22:THR:HG23	1:C:41:ASN:OD1	2.07	0.54
2:P:100:LYS:CB	2:P:276:ARG:NH2	2.71	0.54
1:I:26:THR:HG21	2:J:119:GLU:CG	2.38	0.54
2:F:84:GLN:HA	2:F:245:PRO:O	2.07	0.54
1:M:26:THR:HG22	2:N:124:GLU:OE1	2.08	0.54
2:D:88:HIS:O	2:D:268:ARG:NH1	2.40	0.54
2:D:76:LYS:HB3	2:D:253:ASN:O	2.08	0.54
1:I:225:GLU:CG	2:J:177:GLY:H	2.20	0.54
1:A:154:ARG:HD3	1:A:173:HIS:CD2	2.43	0.54
1:O:101:ASP:O	1:O:102:PHE:HB3	2.06	0.54
1:C:22:THR:C	1:C:23:ARG:HD3	2.28	0.54
2:L:87:ILE:HG22	2:L:111:TYR:CE1	2.43	0.54
2:H:123:THR:HG23	2:H:253:ASN:HB2	1.88	0.54
2:B:126:LEU:HD11	2:B:252:SER:HB3	1.90	0.54
2:J:289:ARG:NH2	2:J:314:LYS:HE2	2.22	0.54
2:F:100:LYS:HB3	2:F:276:ARG:HH11	1.66	0.54
2:B:175:ASN:HB2	1:C:108:ASP:OD1	2.08	0.53
2:D:64:LEU:HB3	2:D:66:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ASP:OD1	2:F:131:LYS:CE	2.56	0.53
1:A:19:LYS:HE2	1:A:21:TYR:CE1	2.43	0.53
1:E:248:VAL:HG12	1:E:250:HIS:HE2	1.73	0.53
1:M:154:ARG:HD3	1:M:173:HIS:CD2	2.43	0.53
2:L:221:THR:CG2	2:L:227:LEU:HD13	2.38	0.53
1:G:63:SER:HB3	1:G:225:GLU:O	2.08	0.53
2:N:90:ASN:ND2	2:N:268:ARG:NH2	2.56	0.53
2:N:90:ASN:HD22	2:N:268:ARG:NH2	2.06	0.53
1:E:35:THR:HG21	2:F:184:ASN:O	2.08	0.53
1:I:108:ASP:OD1	2:P:175:ASN:HB2	2.08	0.53
1:E:154:ARG:HG2	1:E:156:LEU:HD21	1.91	0.53
1:A:189:ASP:OD2	2:H:234:ARG:NH1	2.41	0.53
1:M:45:GLU:HB3	1:M:47:ASN:OD1	2.08	0.53
1:M:201:LEU:HD23	1:M:202:THR:HG23	1.89	0.53
2:D:298:THR:HG22	2:D:311:VAL:HG23	1.90	0.53
1:C:150:GLN:O	1:C:150:GLN:CG	2.56	0.53
2:J:293:THR:HG22	2:J:306:VAL:CG2	2.39	0.53
2:B:218:ARG:HD2	2:B:279:ILE:O	2.09	0.53
2:N:95:SER:O	2:N:96:HIS:CD2	2.62	0.53
1:G:124:ASP:HB3	1:G:135:ASN:HB3	1.90	0.53
1:M:93:ASP:OD1	1:M:94:ASN:N	2.42	0.53
2:B:100:LYS:HB3	2:B:276:ARG:HH21	1.73	0.53
2:H:153:SER:OG	2:H:154:THR:N	2.37	0.53
2:L:83:LYS:NZ	2:L:249:THR:CG2	2.72	0.53
2:P:136:THR:HG22	2:P:137:ALA:N	2.24	0.53
2:N:238:LEU:HA	2:N:242:GLY:O	2.09	0.53
2:H:268:ARG:O	2:H:292:GLY:HA2	2.09	0.52
2:H:76:LYS:HB3	2:H:253:ASN:O	2.09	0.52
2:D:60:ILE:HG22	2:D:295:LEU:HD23	1.90	0.52
1:O:186:LEU:HG	1:O:274:GLU:HG3	1.91	0.52
1:C:185:GLN:HG2	1:C:189:ASP:N	2.24	0.52
2:B:279:ILE:HG13	2:B:280:HIS:N	2.24	0.52
2:F:260:THR:HG22	2:F:261:GLN:N	2.24	0.52
2:B:181:SER:O	2:B:184:ASN:ND2	2.42	0.52
1:A:69:ASP:C	1:A:71:ASN:H	2.11	0.52
2:P:50:THR:HG22	2:P:65:GLN:HG3	1.91	0.52
1:O:59:GLY:O	1:O:229:PRO:HD2	2.09	0.52
2:J:235:ARG:NH2	1:K:171:GLU:OE2	2.41	0.52
1:E:80:TRP:HB2	1:E:81:PRO:HD2	1.92	0.52
1:I:39:GLN:HE22	2:J:34:ASP:HA	1.74	0.52
2:F:212:LEU:HG	2:F:213:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:O	1:A:229:PRO:HG2	2.09	0.52
2:D:40:ILE:HG21	2:D:126:LEU:HD23	1.91	0.52
1:M:80:TRP:HB2	1:M:81:PRO:HD2	1.90	0.52
1:E:99:VAL:HA	1:E:235:MET:HG2	1.91	0.52
2:B:120:ASN:ND2	2:B:257:ASN:OD1	2.31	0.52
2:F:40:ILE:HG21	2:F:126:LEU:CD2	2.38	0.52
2:P:67:ASP:HB2	2:P:80:LEU:HB3	1.92	0.52
1:G:118:GLY:HA3	1:G:141:ASN:OD1	2.09	0.52
1:E:147:SER:HA	2:F:139:VAL:O	2.09	0.52
3:J:414:HOH:O	1:K:105:LYS:HE2	2.09	0.52
2:H:294:ARG:HE	2:H:319:LYS:HB3	1.75	0.52
2:F:157:ILE:HG13	1:G:127:ILE:O	2.10	0.52
2:F:109:SER:HB2	2:F:110:GLU:HG3	1.91	0.52
2:J:71:LYS:HB3	2:J:248:ASN:O	2.10	0.52
2:H:75:ASP:HB2	2:H:76:LYS:HG3	1.90	0.52
2:H:153:SER:O	2:H:155:LYS:N	2.43	0.52
2:D:235:TYR:HB2	2:D:240:ARG:HB2	1.92	0.52
1:C:257:GLU:HG3	1:C:279:LYS:HB2	1.91	0.52
1:A:225:GLU:HG3	2:B:182:GLY:H	1.74	0.51
1:K:147:SER:HA	2:L:139:VAL:O	2.09	0.51
1:K:248:VAL:CG1	1:K:250:HIS:NE2	2.73	0.51
1:O:241:ASP:C	1:O:241:ASP:OD1	2.47	0.51
1:K:253:ARG:NE	1:K:255:MET:CE	2.73	0.51
1:G:92:ASP:HB2	1:G:94:ASN:HB3	1.92	0.51
2:J:91:HIS:CD2	2:J:99:TRP:CE3	2.98	0.51
2:F:69:ILE:O	2:F:78:VAL:HB	2.10	0.51
2:J:206:LEU:HD12	2:J:279:PRO:HG2	1.92	0.51
2:J:187:SER:CB	2:J:189:ILE:HD11	2.41	0.51
2:B:215:ARG:NE	2:B:217:THR:CG2	2.74	0.51
1:O:101:ASP:OD1	1:O:105:LYS:NZ	2.43	0.51
2:L:83:LYS:NZ	2:L:249:THR:HG23	2.25	0.51
2:D:243:PHE:HE2	2:D:245:PRO:HB3	1.73	0.51
2:D:161:SER:O	2:D:162:SER:HB3	2.11	0.51
1:C:65:LEU:HD22	1:C:224:SER:HA	1.92	0.51
1:K:96:ASN:HB3	1:K:238:ASP:HB3	1.91	0.51
2:P:265:THR:HG23	2:P:296:ILE:HG12	1.92	0.51
1:I:29:ASP:OD2	1:I:32:LYS:HB2	2.11	0.51
2:F:187:TRP:CE3	2:F:188:HIS:HB2	2.45	0.51
1:A:94:ASN:C	1:A:94:ASN:OD1	2.48	0.51
1:O:137:THR:HG22	2:P:150:LYS:HG3	1.92	0.51
2:N:221:THR:OG1	2:N:223:GLU:OE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:LEU:HD11	2:H:105:LEU:HD21	1.91	0.51
2:J:121:LEU:HD21	2:J:247:SER:HB3	1.93	0.51
1:G:113:VAL:HG22	1:G:146:ILE:HG22	1.93	0.51
1:E:78:LEU:HB2	1:E:213:PHE:CE1	2.46	0.51
1:G:65:LEU:CD1	1:G:78:LEU:HD11	2.41	0.51
2:H:148:GLY:O	2:H:160:THR:HG22	2.11	0.51
2:P:238:LEU:HA	2:P:242:GLY:O	2.09	0.51
2:D:103:ASN:ND2	2:D:277:PRO:HG3	2.26	0.51
2:P:204:VAL:O	2:P:205:LYS:HG3	2.11	0.51
2:J:170:ASN:HB3	2:J:193:LEU:HD23	1.91	0.51
2:D:64:LEU:HB3	2:D:66:PHE:HE2	1.76	0.51
2:D:243:PHE:CE2	2:D:245:PRO:HB3	2.45	0.51
1:A:18:THR:CG2	1:A:45:GLU:HA	2.36	0.51
2:D:176:TYR:CD2	2:D:193:VAL:HG12	2.45	0.51
2:H:125:ILE:HB	2:H:186:ASN:HA	1.92	0.51
2:L:77:ASN:HD21	2:L:255:LYS:HG2	1.76	0.51
1:K:36:GLN:OE1	1:K:288:TYR:OH	2.21	0.51
2:F:215:ARG:HE	2:F:217:THR:HG21	1.77	0.50
2:P:185:ASN:HB2	2:P:187:TRP:H	1.76	0.50
2:H:60:ILE:HG22	2:H:295:LEU:HD23	1.94	0.50
1:K:206:ASN:HB2	1:K:268:TRP:HH2	1.75	0.50
2:L:77:ASN:ND2	2:L:255:LYS:HG2	2.26	0.50
1:K:248:VAL:HG12	1:K:250:HIS:CD2	2.47	0.50
1:K:36:GLN:HG2	1:K:251:TYR:CD1	2.46	0.50
1:M:184:ARG:HD3	1:M:256:ASP:OD2	2.11	0.50
1:A:75:ASN:HA	1:A:260:ILE:O	2.10	0.50
2:H:259:LYS:HD3	2:H:300:GLU:OE2	2.12	0.50
1:G:28:SER:OG	1:G:35:THR:HG23	2.12	0.50
1:G:22:THR:HG21	2:H:40:ILE:HD13	1.93	0.50
2:B:160:THR:HG22	1:C:124:ASP:OD1	2.11	0.50
2:J:74:LEU:HG	2:J:75:LEU:N	2.25	0.50
2:B:84:GLN:HA	2:B:245:PRO:O	2.10	0.50
2:L:198:LEU:O	2:L:204:VAL:HA	2.11	0.50
2:F:100:LYS:CB	2:F:276:ARG:HH12	2.23	0.50
1:I:137:THR:HG22	2:J:145:LYS:HG2	1.93	0.50
1:M:287:LEU:HD23	1:M:300:VAL:HB	1.92	0.50
1:M:67:ILE:HG22	1:M:69:ASP:H	1.77	0.50
2:L:319:LYS:C	2:L:320:PRO:O	2.50	0.50
2:N:229:PHE:CE1	2:N:275:ASN:ND2	2.75	0.50
1:E:196:SER:O	1:E:273:GLY:HA3	2.11	0.50
1:C:219:MET:HB3	1:C:223:VAL:HG13	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:21:TYR:HB2	1:M:42:PHE:HB2	1.94	0.50
2:D:181:SER:HB3	2:D:184:ASN:OD1	2.12	0.50
1:A:221:VAL:HG13	1:A:222:THR:N	2.26	0.50
1:C:201:LEU:HD13	1:C:215:PRO:HD3	1.93	0.50
1:M:277:VAL:HG12	1:M:278:ASP:OD2	2.11	0.50
1:C:265:HIS:O	1:C:269:GLY:N	2.45	0.50
1:C:66:ARG:HH21	1:C:68:LEU:HD23	1.77	0.50
2:B:62:GLN:HG2	2:B:266:TYR:CE2	2.47	0.50
2:B:80:LEU:HD22	2:B:250:TYR:HE1	1.75	0.50
1:E:252:LYS:NZ	1:E:281:GLU:OE1	2.36	0.50
2:N:217:THR:HG21	2:N:220:ALA:HB2	1.93	0.50
2:L:199:LYS:O	2:L:236:PRO:HD3	2.12	0.50
1:O:92:ASP:OD1	1:O:245:SER:HA	2.12	0.50
1:A:170:VAL:HG21	1:A:227:PHE:CZ	2.47	0.50
2:L:59:ASN:C	2:L:60:ILE:HG13	2.32	0.50
1:K:137:THR:HG22	2:L:150:LYS:HG3	1.94	0.50
1:E:176:ASN:O	1:E:177:ASN:HB2	2.12	0.49
2:B:232:LYS:HG3	2:B:240:ARG:NH1	2.27	0.49
1:M:44:THR:HG22	1:M:44:THR:O	2.12	0.49
1:E:183:THR:CG2	3:E:409:HOH:O	2.23	0.49
1:M:186:LEU:CD1	1:M:274:GLU:HG2	2.42	0.49
2:L:64:LEU:HB3	2:L:66:PHE:HE2	1.75	0.49
1:G:92:ASP:CB	1:G:94:ASN:HB3	2.42	0.49
1:C:35:THR:HG21	2:D:184:ASN:O	2.12	0.49
2:B:215:ARG:HG2	2:B:217:THR:HG23	1.94	0.49
2:J:187:SER:HB3	2:J:189:ILE:HD11	1.93	0.49
2:F:173:GLN:HE22	2:F:197:ASP:HB2	1.78	0.49
2:L:48:LYS:HE3	1:M:48:TYR:CD2	2.48	0.49
1:K:225:GLU:HG2	2:L:179:ILE:CG2	2.43	0.49
2:B:66:PHE:CD2	2:B:308:VAL:HG21	2.48	0.49
2:F:216:ASN:OD1	2:F:218:ARG:NH2	2.42	0.49
2:F:159:ARG:HH11	1:M:127:ILE:HD13	1.77	0.49
2:N:255:LYS:O	2:N:256:SER:HB3	2.13	0.49
2:N:218:ARG:HD2	2:N:279:ILE:O	2.12	0.49
1:A:149:GLN:HG3	2:B:136:THR:HG21	1.94	0.49
1:I:186:LEU:HA	1:I:275:ASN:O	2.12	0.49
2:P:269:ASN:HD22	2:P:289:ASN:CG	2.15	0.49
2:B:122:LYS:HB2	2:B:257:ASN:HD21	1.75	0.49
2:P:191:TRP:HH2	2:P:249:THR:CG2	2.22	0.49
2:H:105:LEU:HD23	2:H:106:LYS:N	2.28	0.49
2:F:238:LEU:HD21	2:F:243:PHE:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:252:LYS:HG2	1:O:253:ARG:N	2.27	0.49
2:D:222:VAL:HG22	2:D:277:PRO:HG2	1.94	0.49
2:L:255:LYS:O	2:L:256:SER:CB	2.60	0.49
1:I:49:ASP:OD1	1:I:50:LYS:HG3	2.12	0.49
2:H:127:ASP:O	2:H:250:TYR:N	2.38	0.49
2:N:112:HIS:HB2	2:N:267:THR:HB	1.95	0.49
2:H:281:TYR:CD2	2:H:281:TYR:C	2.86	0.49
2:L:87:ILE:HG22	2:L:111:TYR:HE1	1.77	0.49
2:J:212:THR:HG21	2:J:222:LEU:O	2.12	0.49
2:N:181:SER:HB2	2:N:190:HIS:HB3	1.95	0.48
2:H:57:LYS:NZ	2:H:315:SER:HB2	2.28	0.48
2:H:112:HIS:HB2	2:H:267:THR:HB	1.95	0.48
2:D:129:LEU:HD12	2:D:250:TYR:HE2	1.78	0.48
2:F:215:ARG:HE	2:F:217:THR:HG23	1.77	0.48
1:E:201:LEU:HD13	1:E:214:THR:HA	1.95	0.48
1:A:70:PRO:O	1:A:210:LYS:CD	2.61	0.48
1:O:206:ASN:HB2	1:O:268:TRP:CH2	2.48	0.48
2:B:110:GLU:HB2	2:B:269:ASN:HB2	1.95	0.48
2:D:148:GLY:O	2:D:159:ARG:HG3	2.13	0.48
1:M:228:ASN:HB3	2:N:131:LYS:HD3	1.94	0.48
2:D:191:TRP:HH2	2:D:249:THR:CG2	2.25	0.48
2:B:40:ILE:HG21	2:B:126:LEU:CD1	2.44	0.48
2:P:115:PHE:CD2	2:P:115:PHE:C	2.85	0.48
1:M:127:ILE:HD12	1:M:127:ILE:N	2.28	0.48
2:D:240:ARG:NH2	1:E:171:GLU:OE2	2.45	0.48
2:P:185:ASN:HB2	2:P:188:HIS:H	1.78	0.48
2:N:95:SER:O	2:N:96:HIS:HD2	1.94	0.48
2:L:118:LYS:HE3	2:L:263:GLU:OE2	2.12	0.48
1:E:209:ALA:O	1:E:211:ASP:N	2.46	0.48
2:J:72:ASN:HB2	2:J:248:ASN:HB3	1.94	0.48
2:D:97:LYS:HG2	2:D:97:LYS:H	1.40	0.48
2:B:215:ARG:NE	2:B:217:THR:HG23	2.29	0.48
2:J:289:ARG:HG2	2:J:311:ASP:HB3	1.96	0.48
2:D:52:THR:HG23	2:D:61:LEU:HD11	1.95	0.48
2:F:157:ILE:CG2	2:F:158:GLY:N	2.77	0.48
2:J:289:ARG:NH1	2:J:291:ILE:HD11	2.28	0.48
2:B:99:GLU:HB2	2:B:100:LYS:HD2	1.95	0.48
2:L:88:HIS:O	2:L:268:ARG:NH1	2.46	0.48
2:F:294:ARG:NH2	2:F:319:LYS:HG2	2.25	0.48
2:L:200:TYR:HE1	2:L:203:GLU:OE1	1.95	0.48
1:C:163:HIS:NE2	1:C:164:LYS:HG3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:207:ARG:NH2	2:N:288:LYS:HG3	2.27	0.48
1:E:21:TYR:HB2	1:E:42:PHE:HB2	1.96	0.48
2:L:129:LEU:HA	2:L:130:PRO:C	2.35	0.48
2:J:84:SER:O	2:J:263:ARG:HD3	2.14	0.47
2:P:226:GLU:OE1	2:P:232:LYS:HE2	2.14	0.47
2:D:267:THR:HG21	2:D:321:TYR:HB2	1.96	0.47
2:J:250:LYS:O	2:J:251:SER:OG	2.22	0.47
2:P:198:LEU:O	2:P:204:VAL:HA	2.13	0.47
2:H:82:LYS:HB2	3:H:418:HOH:O	2.13	0.47
1:I:71:ASN:HD22	1:I:208:TRP:HZ3	1.59	0.47
2:D:171:TYR:CD2	2:D:171:TYR:N	2.81	0.47
2:N:181:SER:HB3	2:N:184:ASN:OD1	2.14	0.47
2:J:260:THR:HG23	2:J:291:ILE:HG12	1.96	0.47
2:D:243:PHE:C	2:D:244:ASN:HD22	2.18	0.47
2:D:244:ASN:N	2:D:244:ASN:HD22	2.12	0.47
1:I:186:LEU:HD12	1:I:275:ASN:O	2.15	0.47
2:L:156:GLY:O	2:L:157:ILE:HD13	2.14	0.47
1:I:253:ARG:HE	1:I:255:MET:HE2	1.79	0.47
2:P:276:ARG:HD2	2:P:282:ALA:HB2	1.95	0.47
1:O:34:ILE:HG21	1:O:284:LEU:HB3	1.96	0.47
2:N:270:GLN:OE1	2:N:291:ASP:HB3	2.14	0.47
1:C:32:LYS:HG2	1:C:282:GLU:OE1	2.15	0.47
1:I:76:SER:HB2	1:I:209:ALA:CB	2.44	0.47
1:M:166:VAL:HG22	1:M:167:GLY:N	2.30	0.47
2:P:215:ARG:HB3	2:P:228:SER:O	2.14	0.47
2:J:141:SER:HB3	2:J:157:SER:OG	2.13	0.47
2:H:58:THR:HG22	2:H:293:GLN:HB3	1.97	0.47
1:E:149:GLN:HG3	2:F:136:THR:HG21	1.96	0.47
2:D:232:LYS:O	2:D:240:ARG:HD3	2.14	0.47
2:H:295:LEU:HD11	2:H:297:VAL:CG2	2.44	0.47
1:O:141:ASN:HB3	2:P:146:SER:CB	2.44	0.47
1:K:246:GLN:HB3	1:K:287:LEU:HD11	1.96	0.47
2:N:321:TYR:CD2	2:N:321:TYR:C	2.87	0.47
1:M:65:LEU:HD11	1:M:78:LEU:HD11	1.96	0.47
2:N:88:HIS:ND1	1:O:159:GLN:HA	2.30	0.47
2:N:195:ALA:HB1	2:N:198:LEU:HD21	1.96	0.47
1:G:149:GLN:HE22	2:H:138:LYS:HB2	1.80	0.47
1:I:280:LYS:HG3	1:I:281:GLU:N	2.30	0.47
2:N:305:ASN:O	2:N:307:THR:HG23	2.14	0.47
1:I:22:THR:HG21	2:J:35:ILE:HD12	1.96	0.47
2:P:319:LYS:C	2:P:320:PRO:O	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:ASN:HB3	2:F:303:TRP:CE3	2.49	0.47
2:L:231:SER:OG	2:L:233:TYR:HD2	1.96	0.47
2:N:173:GLN:HG2	1:O:111:ARG:NH2	2.30	0.47
2:P:59:ASN:C	2:P:60:ILE:HG13	2.34	0.47
2:P:294:ARG:HH21	2:P:319:LYS:HG3	1.80	0.47
1:A:280:LYS:HG3	1:A:281:GLU:N	2.29	0.47
1:M:220:PRO:HG2	1:M:223:VAL:CG1	2.44	0.47
2:H:204:VAL:O	2:H:205:LYS:HG3	2.15	0.47
1:A:248:VAL:HG22	1:A:287:LEU:HD12	1.97	0.47
1:C:33:ASN:ND2	2:D:183:LYS:HG2	2.30	0.47
2:L:78:VAL:HG12	2:L:79:LEU:N	2.29	0.47
2:H:283:PRO:HA	2:H:284:PRO:HD3	1.74	0.47
1:E:17:ASP:OD1	1:E:17:ASP:N	2.47	0.47
2:N:175:ASN:ND2	1:O:109:GLU:OE1	2.47	0.47
1:I:252:LYS:HG3	1:I:283:LYS:HB2	1.95	0.47
1:C:221:VAL:HG11	2:D:132:ASN:OD1	2.15	0.47
2:B:244:ASN:HB3	3:B:412:HOH:O	2.13	0.47
2:D:93:PHE:HA	2:D:104:TRP:O	2.14	0.47
1:K:227:PHE:CE2	1:K:229:PRO:HA	2.50	0.47
2:F:181:SER:C	2:F:183:LYS:N	2.68	0.47
1:G:163:HIS:CD2	1:G:164:LYS:HG3	2.50	0.47
2:B:128:GLN:HA	2:B:248:LEU:O	2.15	0.47
1:C:219:MET:HB3	1:C:223:VAL:CG1	2.45	0.47
2:L:115:PHE:CZ	2:L:262:PHE:CD1	3.03	0.47
1:I:17:ASP:OD2	1:I:46:PRO:HB3	2.14	0.47
1:K:26:THR:CG2	2:L:124:GLU:OE1	2.62	0.47
1:C:176:ASN:O	1:C:177:ASN:HB2	2.15	0.47
1:I:225:GLU:HG3	2:J:177:GLY:N	2.29	0.46
1:I:26:THR:HG21	2:J:119:GLU:CB	2.44	0.46
2:B:129:LEU:HA	2:B:130:PRO:C	2.34	0.46
2:J:255:THR:HG22	2:J:256:GLN:N	2.30	0.46
1:O:186:LEU:HD23	1:O:187:THR:HG23	1.98	0.46
1:I:154:ARG:NH1	2:P:235:TYR:O	2.47	0.46
1:C:26:THR:HG21	2:D:124:GLU:HB3	1.97	0.46
2:N:69:ILE:HB	2:N:78:VAL:HB	1.97	0.46
1:C:75:ASN:HA	1:C:260:ILE:O	2.14	0.46
2:L:59:ASN:O	2:L:60:ILE:HG13	2.16	0.46
2:L:154:THR:C	2:L:156:GLY:H	2.19	0.46
1:G:297:VAL:HG12	1:G:298:LYS:N	2.30	0.46
1:G:55:ILE:HG21	1:G:88:ILE:HG21	1.97	0.46
2:L:244:ASN:HA	2:L:245:PRO:HD2	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:O	1:A:71:ASN:N	2.49	0.46
1:A:274:GLU:HG2	1:A:276:HIS:CE1	2.51	0.46
2:N:265:THR:HG23	2:N:296:ILE:HG12	1.97	0.46
2:H:294:ARG:HH11	2:H:296:ILE:HD11	1.80	0.46
2:D:260:THR:CG2	2:D:261:GLN:N	2.65	0.46
2:N:163:ASN:O	1:O:120:LYS:HA	2.15	0.46
2:L:267:THR:HG23	2:L:294:ARG:HB3	1.98	0.46
1:I:41:ASN:HB2	1:I:54:PHE:HB2	1.97	0.46
1:A:120:LYS:HG3	2:H:164:SER:HB3	1.97	0.46
2:L:276:ARG:NH1	2:L:282:ALA:CB	2.78	0.46
1:K:268:TRP:HA	1:K:268:TRP:CE3	2.49	0.46
1:M:135:ASN:HD22	2:N:150:LYS:HE2	1.81	0.46
1:E:36:GLN:HG2	1:E:251:TYR:CD1	2.49	0.46
1:G:147:SER:HA	2:H:139:VAL:O	2.16	0.46
2:P:317:ASP:CG	2:P:318:ASN:H	2.19	0.46
1:C:79:ARG:HG3	1:C:79:ARG:O	2.15	0.46
1:G:250:HIS:CD2	1:G:250:HIS:N	2.83	0.46
2:L:100:LYS:HB3	2:L:276:ARG:NH2	2.31	0.46
2:P:211:LEU:HD23	2:P:211:LEU:HA	1.68	0.46
2:L:69:ILE:HB	2:L:78:VAL:HB	1.97	0.46
1:G:161:THR:HG23	1:G:166:VAL:HA	1.98	0.46
1:I:58:LYS:HA	1:I:229:PRO:O	2.16	0.46
1:A:119:TYR:O	2:H:164:SER:HA	2.16	0.46
1:E:63:SER:HB2	1:E:223:VAL:O	2.16	0.46
1:G:206:ASN:HB2	1:G:268:TRP:HH2	1.80	0.46
1:C:29:ASP:OD1	1:C:29:ASP:C	2.53	0.46
2:L:231:SER:HG	2:L:233:TYR:HD2	1.63	0.46
2:L:185:ASN:HB2	2:L:188:HIS:H	1.79	0.46
1:G:37:SER:O	1:G:38:LEU:HD12	2.16	0.46
1:C:17:ASP:HB3	1:C:46:PRO:HG3	1.98	0.46
2:F:101:ASN:HB3	2:F:274:LYS:HB3	1.97	0.46
2:J:291:ILE:HD12	2:J:309:TYR:CD2	2.51	0.46
2:N:268:ARG:O	2:N:292:GLY:HA2	2.16	0.46
2:J:121:LEU:HD13	2:J:247:SER:H	1.81	0.46
2:L:159:ARG:HH11	2:L:159:ARG:HG3	1.81	0.46
1:I:22:THR:C	1:I:23:ARG:HD3	2.36	0.45
2:P:244:ASN:N	2:P:244:ASN:HD22	2.14	0.45
1:K:169:LYS:NZ	1:K:171:GLU:OE2	2.49	0.45
2:L:173:GLN:HG3	2:L:174:GLN:N	2.31	0.45
1:O:94:ASN:OD1	1:O:95:ASN:N	2.49	0.45
2:L:317:ASP:OD1	2:L:318:ASN:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:HB2	1:C:56:LYS:HE3	1.37	0.45
2:N:98:GLU:HG2	2:N:98:GLU:O	2.16	0.45
2:J:316:TYR:CD2	2:J:316:TYR:C	2.89	0.45
1:M:26:THR:CG2	2:N:124:GLU:OE1	2.63	0.45
2:D:80:LEU:HD13	2:D:250:TYR:CE1	2.52	0.45
2:H:40:ILE:HG21	2:H:126:LEU:HD23	1.98	0.45
1:M:145:THR:OG1	2:N:142:THR:HG23	2.15	0.45
1:K:55:ILE:O	1:K:232:LEU:HD12	2.16	0.45
1:A:108:ASP:OD1	2:H:175:ASN:HB2	2.15	0.45
2:J:123:GLN:OE1	2:J:123:GLN:N	2.50	0.45
2:J:249:GLU:C	2:J:250:LYS:O	2.51	0.45
2:N:179:ILE:HD12	2:N:194:ILE:HD12	1.98	0.45
1:M:197:GLU:OE2	1:M:203:ARG:NH2	2.49	0.45
1:C:163:HIS:CD2	1:C:164:LYS:HG3	2.52	0.45
1:K:20:MET:CE	1:K:41:ASN:HB3	2.47	0.45
2:J:124:LEU:HA	2:J:125:PRO:C	2.37	0.45
2:B:321:TYR:C	2:B:321:TYR:CD2	2.90	0.45
1:C:58:LYS:HA	1:C:229:PRO:O	2.15	0.45
2:B:265:THR:HG23	2:B:296:ILE:HG12	1.98	0.45
1:M:150:GLN:HE21	1:M:174:LEU:HB3	1.81	0.45
1:A:301:LYS:HG3	1:A:302:VAL:O	2.17	0.45
2:L:321:TYR:C	2:L:321:TYR:CD2	2.89	0.45
2:B:276:ARG:NH1	2:B:282:ALA:HB1	2.30	0.45
2:N:40:ILE:HG21	2:N:126:LEU:CD2	2.43	0.45
1:C:263:ASN:ND2	1:C:270:TYR:HE1	2.08	0.45
1:A:70:PRO:O	1:A:210:LYS:HG3	2.17	0.45
1:M:166:VAL:CG2	1:M:167:GLY:N	2.79	0.45
1:C:194:THR:HG21	1:C:203:ARG:HE	1.82	0.45
2:N:246:GLU:O	2:N:247:PHE:CD1	2.70	0.45
2:L:110:GLU:OE1	2:L:112:HIS:NE2	2.46	0.45
1:C:288:TYR:CD2	1:C:288:TYR:N	2.85	0.45
1:O:240:LYS:HB2	1:O:240:LYS:NZ	2.32	0.45
1:E:266:GLY:O	1:E:267:PHE:HB2	2.16	0.45
2:L:40:ILE:HA	2:L:40:ILE:HD12	1.81	0.45
1:I:105:LYS:HE2	3:P:417:HOH:O	2.17	0.45
2:L:163:ASN:HD22	2:L:163:ASN:N	2.15	0.45
2:B:91:LEU:HD11	2:B:105:LEU:HD21	1.98	0.45
2:B:145:TYR:HB2	2:B:163:ASN:HB3	1.99	0.45
1:K:50:LYS:HA	1:K:239:LYS:HG3	1.98	0.45
1:I:266:GLY:O	1:I:267:PHE:CB	2.63	0.45
1:M:188:ASN:O	1:M:190:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:VAL:HG21	2:H:249:THR:CG2	2.47	0.45
1:A:185:GLN:HG3	2:H:231:SER:HB2	1.99	0.45
2:J:291:ILE:HD12	2:J:309:TYR:HD2	1.82	0.45
1:M:20:MET:HG3	1:M:21:TYR:N	2.32	0.45
2:F:173:GLN:NE2	2:F:197:ASP:HB2	2.32	0.45
2:L:226:GLU:OE2	2:L:232:LYS:HD3	2.17	0.45
1:A:195:LYS:HB2	1:A:273:GLY:O	2.17	0.45
2:P:231:SER:C	2:P:233:TYR:H	2.20	0.45
1:G:252:LYS:HB2	1:G:283:LYS:HB2	1.98	0.45
1:E:218:LYS:HD3	1:E:218:LYS:HA	1.79	0.45
2:J:212:THR:O	2:J:213:ARG:NH1	2.50	0.45
2:F:217:THR:CG2	1:G:191:ASP:OD1	2.65	0.45
1:A:69:ASP:C	1:A:71:ASN:N	2.71	0.45
2:L:48:LYS:HB3	1:M:48:TYR:HB2	1.97	0.45
2:B:127:ASP:OD1	2:B:131:LYS:HE3	2.17	0.45
2:H:146:SER:HB3	2:H:162:SER:OG	2.17	0.45
2:H:114:ASP:HB3	2:H:265:THR:HB	1.99	0.45
1:A:268:TRP:CE3	1:A:268:TRP:HA	2.51	0.45
2:H:294:ARG:NH1	2:H:296:ILE:HD11	2.32	0.44
2:D:294:ARG:NH1	2:D:296:ILE:HD11	2.32	0.44
2:N:276:ARG:HB2	2:N:276:ARG:NH1	2.25	0.44
2:J:250:LYS:O	2:J:251:SER:CB	2.63	0.44
2:D:238:LEU:HD21	2:D:243:PHE:HD1	1.81	0.44
2:N:217:THR:CG2	2:N:220:ALA:HB2	2.46	0.44
1:G:183:THR:HG22	1:G:188:ASN:OD1	2.17	0.44
1:E:70:PRO:O	1:E:210:LYS:HG3	2.18	0.44
1:I:128:ASN:HA	2:P:156:GLY:HA3	1.98	0.44
2:L:283:PRO:HA	2:L:284:PRO:HD3	1.74	0.44
2:D:187:TRP:CE3	2:D:188:HIS:HB2	2.52	0.44
1:G:210:LYS:HB3	1:G:210:LYS:HE3	1.81	0.44
2:H:143:PHE:CZ	2:H:145:TYR:HD2	2.35	0.44
1:M:163:HIS:CD2	1:M:164:LYS:HG3	2.52	0.44
1:E:101:ASP:OD1	1:E:105:LYS:NZ	2.35	0.44
1:O:225:GLU:HG2	2:P:179:ILE:CG2	2.46	0.44
2:J:96:ASN:OD1	2:J:271:ARG:NH1	2.50	0.44
2:D:162:SER:HA	1:E:121:THR:O	2.17	0.44
2:H:57:LYS:HZ2	2:H:315:SER:HB2	1.82	0.44
1:O:194:THR:O	1:O:272:SER:HA	2.17	0.44
2:B:173:GLN:HG2	2:B:174:GLN:N	2.33	0.44
2:H:144:SER:HB2	2:H:164:SER:HG	1.83	0.44
2:B:66:PHE:CE2	2:B:308:VAL:HG11	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:149:GLN:HG3	2:N:136:THR:HG21	1.99	0.44
1:G:104:PRO:HD2	1:G:168:TRP:NE1	2.31	0.44
1:O:104:PRO:HD2	1:O:231:PHE:HD1	1.82	0.44
2:P:253:ASN:HD21	2:P:257:ASN:HB3	1.82	0.44
2:H:48:LYS:HG3	2:H:65:GLN:NE2	2.33	0.44
1:O:157:LEU:HD12	1:O:157:LEU:HA	1.83	0.44
2:F:151:PHE:CG	2:F:152:ASP:N	2.86	0.44
1:K:154:ARG:CD	1:K:173:HIS:CD2	2.99	0.44
1:O:153:TYR:HB2	2:P:134:ILE:HD13	1.99	0.44
2:F:181:SER:O	2:F:183:LYS:N	2.50	0.44
2:H:129:LEU:HA	2:H:130:PRO:C	2.38	0.44
2:D:84:GLN:HG2	2:D:246:GLU:HG3	2.00	0.44
2:B:291:ASP:OD1	2:B:292:GLY:N	2.45	0.44
2:L:171:TYR:N	2:L:171:TYR:CD2	2.85	0.44
2:L:105:LEU:HD23	2:L:106:LYS:N	2.32	0.44
1:O:68:LEU:O	1:O:70:PRO:HD3	2.18	0.44
2:B:40:ILE:HG21	2:B:126:LEU:HD12	2.00	0.44
2:J:314:LYS:HE3	2:J:314:LYS:HB3	1.72	0.44
2:B:91:LEU:CD1	2:B:105:LEU:HD21	2.48	0.44
1:M:124:ASP:OD1	1:M:124:ASP:N	2.50	0.44
2:N:84:GLN:HA	2:N:245:PRO:O	2.18	0.44
2:D:103:ASN:HD21	2:D:277:PRO:HG3	1.82	0.44
2:H:189:VAL:HG21	2:H:249:THR:HG21	1.99	0.44
1:C:19:LYS:HE3	1:C:21:TYR:CE1	2.53	0.44
2:D:62:GLN:HG2	2:D:266:TYR:CE1	2.52	0.44
1:I:26:THR:HG21	2:J:119:GLU:HG2	1.99	0.44
2:J:91:HIS:CD2	2:J:99:TRP:CD2	3.06	0.44
2:N:93:PHE:O	2:N:94:GLU:HG3	2.18	0.44
2:P:109:SER:OG	2:P:271:ASP:OD1	2.35	0.44
2:N:54:TYR:HB3	1:O:163:HIS:ND1	2.33	0.44
2:F:224:ASN:HB3	2:F:227:LEU:HD12	1.99	0.44
1:A:222:THR:HA	1:A:226:GLY:O	2.18	0.44
2:H:212:LEU:C	2:H:214:TYR:H	2.21	0.44
2:P:217:THR:HG21	2:P:220:ALA:HB2	1.99	0.44
1:C:145:THR:HA	2:D:141:SER:O	2.18	0.44
2:N:282:ALA:O	2:N:283:PRO:C	2.55	0.44
2:H:157:ILE:HG23	2:H:157:ILE:O	2.18	0.44
1:E:74:TRP:CE3	1:E:74:TRP:HA	2.53	0.44
1:C:41:ASN:HB2	1:C:54:PHE:HB2	2.00	0.44
1:K:302:VAL:O	1:K:303:LEU:HD23	2.18	0.44
1:G:80:TRP:HB2	1:G:81:PRO:CD	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:54:ASN:O	2:J:55:ILE:HG13	2.18	0.44
1:K:222:THR:HA	1:K:226:GLY:O	2.18	0.44
2:D:294:ARG:HE	2:D:319:LYS:HB3	1.82	0.43
1:E:248:VAL:CG1	1:E:250:HIS:NE2	2.81	0.43
1:M:65:LEU:HD12	1:M:78:LEU:HD11	1.98	0.43
1:M:36:GLN:HG2	1:M:251:TYR:CD1	2.53	0.43
2:J:238:PHE:CE2	2:J:240:PRO:HB3	2.53	0.43
1:M:22:THR:CG2	2:N:40:ILE:CD1	2.94	0.43
1:G:64:GLY:HA3	1:G:255:MET:HE1	1.99	0.43
1:O:65:LEU:CD1	1:O:78:LEU:HD11	2.48	0.43
1:O:65:LEU:HD12	1:O:78:LEU:HD11	2.00	0.43
1:I:26:THR:CG2	2:J:119:GLU:HG2	2.49	0.43
2:N:218:ARG:HA	2:N:218:ARG:HD3	1.56	0.43
1:G:38:LEU:HD21	1:G:249:VAL:HG21	1.99	0.43
2:P:153:SER:HG	2:P:156:GLY:N	2.15	0.43
2:H:218:ARG:HD2	2:H:279:ILE:O	2.19	0.43
1:K:185:GLN:OE1	1:K:188:ASN:N	2.51	0.43
1:E:181:ASP:OD2	2:F:167:LYS:NZ	2.48	0.43
2:B:283:PRO:HA	2:B:284:PRO:HD3	1.82	0.43
1:I:38:LEU:HD21	1:I:249:VAL:HG21	2.00	0.43
1:M:128:ASN:N	1:M:128:ASN:OD1	2.51	0.43
1:M:170:VAL:HG21	1:M:227:PHE:CZ	2.54	0.43
2:P:118:LYS:HE2	2:P:118:LYS:HB3	1.72	0.43
2:D:290:LYS:HG3	2:D:290:LYS:O	2.17	0.43
2:N:40:ILE:CG2	2:N:126:LEU:HD23	2.43	0.43
2:H:100:LYS:HG2	2:H:276:ARG:HH12	1.83	0.43
2:F:224:ASN:HD22	2:F:227:LEU:HD12	1.83	0.43
2:F:195:ALA:HB1	2:F:198:LEU:HD21	2.00	0.43
1:I:159:GLN:HE21	2:P:241:SER:HA	1.82	0.43
2:H:45:LYS:O	2:H:69:ILE:HA	2.17	0.43
1:O:262:TRP:CZ2	1:O:269:GLY:HA3	2.53	0.43
1:A:270:TYR:C	1:A:270:TYR:CD1	2.91	0.43
1:K:63:SER:O	1:K:255:MET:HE1	2.18	0.43
1:C:185:GLN:HG3	1:C:188:ASN:H	1.82	0.43
2:N:92:LYS:NZ	2:N:94:GLU:OE2	2.42	0.43
2:F:93:PHE:CG	2:F:226:GLU:HG2	2.53	0.43
1:I:220:PRO:HG2	1:I:223:VAL:HG23	2.00	0.43
1:C:63:SER:HB3	1:C:225:GLU:C	2.38	0.43
1:A:218:LYS:NZ	2:B:196:ASN:OD1	2.52	0.43
2:L:217:THR:CG2	2:L:220:ALA:HB2	2.48	0.43
2:N:181:SER:C	2:N:183:LYS:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ILE:HG23	1:E:199:PHE:N	2.34	0.43
2:L:294:ARG:NH2	2:L:319:LYS:HD3	2.33	0.43
2:P:191:TRP:CH2	2:P:249:THR:HG22	2.39	0.43
2:D:176:TYR:HD2	2:D:193:VAL:HG12	1.83	0.43
2:L:211:LEU:HD23	2:L:211:LEU:HA	1.86	0.43
2:F:191:TRP:HH2	2:F:249:THR:CG2	2.32	0.43
1:M:29:ASP:C	1:M:29:ASP:OD1	2.56	0.43
1:G:193:ARG:H	1:G:193:ARG:HG3	1.30	0.43
2:P:256:SER:OG	2:P:256:SER:O	2.36	0.43
2:B:83:LYS:HZ2	2:B:249:THR:CG2	2.28	0.43
2:P:293:GLN:HA	2:P:316:ASP:O	2.19	0.43
2:J:95:LYS:O	2:J:271:ARG:HG3	2.19	0.43
2:L:83:LYS:HB2	2:L:83:LYS:HE2	1.53	0.43
2:H:106:LYS:HG2	2:H:272:ILE:HG12	2.00	0.43
2:F:238:LEU:HD21	2:F:243:PHE:CD1	2.53	0.43
2:P:231:SER:HG	2:P:233:TYR:HD2	1.65	0.43
2:F:321:TYR:C	2:F:321:TYR:CD2	2.92	0.43
1:I:152:SER:HA	1:I:174:LEU:O	2.19	0.43
1:C:173:HIS:CD2	1:C:174:LEU:HD12	2.53	0.43
1:A:66:ARG:HH11	1:A:68:LEU:HA	1.83	0.43
1:C:218:LYS:HD2	1:C:218:LYS:HA	1.89	0.43
1:E:249:VAL:HG12	1:E:250:HIS:N	2.34	0.43
2:J:271:ARG:HH11	2:J:277:ALA:HB3	1.83	0.43
1:M:58:LYS:O	1:M:229:PRO:HG2	2.19	0.43
2:J:176:SER:C	2:J:178:LYS:H	2.22	0.43
1:I:29:ASP:CG	1:I:32:LYS:HB2	2.39	0.43
2:J:309:TYR:OH	2:J:311:ASP:OD1	2.22	0.43
2:P:59:ASN:O	2:P:60:ILE:HG13	2.19	0.43
2:F:93:PHE:CD1	2:F:226:GLU:HG2	2.54	0.43
1:E:260:ILE:HA	1:E:272:SER:O	2.18	0.43
2:D:107:TYR:CE1	2:D:109:SER:HA	2.54	0.43
1:O:248:VAL:HG12	1:O:250:HIS:CD2	2.54	0.43
1:O:89:GLN:OE1	1:O:165:GLY:HA3	2.19	0.43
1:A:79:ARG:HE	1:A:79:ARG:HB2	1.57	0.43
2:J:282:GLU:OE1	2:J:285:LYS:HD2	2.19	0.43
1:E:219:MET:HB2	1:E:224:SER:HB3	2.01	0.43
1:O:153:TYR:HE1	1:O:223:VAL:HG23	1.84	0.43
1:C:26:THR:CG2	2:D:124:GLU:OE1	2.66	0.43
1:I:298:LYS:HG2	1:I:299:PHE:O	2.19	0.43
2:B:243:PHE:CE2	2:B:245:PRO:HB3	2.54	0.43
2:B:130:PRO:HA	3:B:403:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:LEU:HD23	2:F:106:LYS:N	2.33	0.43
1:E:304:ASN:O	1:E:305:ASP:HB2	2.18	0.43
2:B:55:ASP:OD1	2:B:315:SER:OG	2.36	0.43
1:M:218:LYS:HD3	1:M:218:LYS:HA	1.74	0.43
1:E:248:VAL:CG1	1:E:250:HIS:HE2	2.31	0.43
2:H:255:LYS:O	2:H:256:SER:HB3	2.19	0.43
2:P:260:THR:CG2	2:P:261:GLN:N	2.82	0.43
1:M:184:ARG:CD	1:M:256:ASP:OD2	2.67	0.43
2:B:317:ASP:OD1	2:B:318:ASN:N	2.40	0.43
2:N:52:THR:HG23	2:N:63:ASN:HD22	1.83	0.43
1:O:79:ARG:HG2	1:O:255:MET:CE	2.48	0.43
1:E:163:HIS:CD2	1:E:164:LYS:HG3	2.54	0.43
2:J:37:LYS:HD3	2:J:37:LYS:HA	1.65	0.43
2:L:105:LEU:HB2	2:L:229:PHE:CZ	2.53	0.42
1:E:65:LEU:HD22	1:E:224:SER:HA	2.00	0.42
1:G:64:GLY:HA3	1:G:255:MET:HE3	2.00	0.42
2:P:116:GLN:HG2	2:P:188:HIS:CD2	2.51	0.42
2:F:57:LYS:HZ1	2:F:315:SER:HB2	1.82	0.42
2:D:85:GLY:O	2:D:245:PRO:HD2	2.19	0.42
3:M:409:HOH:O	2:N:131:LYS:HE2	2.19	0.42
2:N:92:LYS:HZ2	2:N:94:GLU:CG	2.32	0.42
1:E:75:ASN:HB2	1:E:260:ILE:O	2.19	0.42
2:D:199:LYS:O	2:D:236:PRO:HG3	2.19	0.42
2:P:94:GLU:OE2	2:P:96:HIS:NE2	2.51	0.42
1:G:201:LEU:HB2	1:G:213:PHE:O	2.19	0.42
2:H:293:GLN:NE2	2:H:317:ASP:OD1	2.47	0.42
1:E:20:MET:SD	1:E:41:ASN:HB3	2.59	0.42
2:J:311:ASP:OD2	2:J:314:LYS:HB2	2.18	0.42
1:M:253:ARG:HG3	1:M:255:MET:SD	2.59	0.42
1:G:155:THR:OG1	1:G:170:VAL:HG22	2.19	0.42
1:I:245:SER:HG	1:I:292:TRP:HE1	1.68	0.42
1:C:252:LYS:HE3	1:C:281:GLU:OE1	2.20	0.42
2:D:75:ASP:CB	2:D:76:LYS:HG3	2.48	0.42
2:N:217:THR:O	2:N:218:ARG:NH1	2.52	0.42
1:C:86:VAL:HA	1:C:250:HIS:O	2.19	0.42
2:D:218:ARG:HD2	2:D:279:ILE:O	2.19	0.42
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.66	0.42
1:E:86:VAL:HA	1:E:250:HIS:O	2.20	0.42
1:M:101:ASP:O	1:M:102:PHE:HB3	2.20	0.42
1:C:153:TYR:HD2	1:C:170:VAL:HG12	1.84	0.42
2:F:84:GLN:HB3	2:F:85:GLY:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:GLN:HE21	2:D:246:GLU:HG3	1.85	0.42
1:E:97:THR:HA	1:E:236:SER:O	2.19	0.42
1:A:65:LEU:HD12	1:A:78:LEU:HD11	2.00	0.42
2:L:218:ARG:HA	2:L:218:ARG:HD3	1.60	0.42
1:M:26:THR:HG21	2:N:124:GLU:CB	2.47	0.42
2:D:106:LYS:HE3	2:D:272:ILE:HD11	2.01	0.42
1:I:38:LEU:HA	1:I:38:LEU:HD12	1.85	0.42
1:E:54:PHE:C	1:E:55:ILE:HG13	2.39	0.42
1:K:178:MET:HB3	1:K:178:MET:HE2	1.95	0.42
1:M:293:LYS:HE2	1:M:293:LYS:HB3	1.86	0.42
2:H:294:ARG:NH2	2:H:319:LYS:CD	2.65	0.42
2:P:316:ASP:OD2	2:P:319:LYS:HG3	2.19	0.42
1:A:154:ARG:NH1	2:H:235:TYR:O	2.44	0.42
2:J:209:TYR:CE2	2:J:211:ASN:HA	2.54	0.42
2:P:302:ASP:OD1	2:P:302:ASP:C	2.58	0.42
2:P:283:PRO:HA	2:P:284:PRO:HD3	1.88	0.42
2:B:294:ARG:HH21	2:B:319:LYS:HE3	1.84	0.42
2:F:294:ARG:HE	2:F:319:LYS:HB3	1.84	0.42
2:P:40:ILE:HA	2:P:40:ILE:HD12	1.86	0.42
2:N:199:LYS:HD3	1:O:111:ARG:HD3	2.02	0.42
1:O:94:ASN:O	1:O:95:ASN:CB	2.68	0.42
2:L:211:LEU:HD23	2:L:284:PRO:HG2	2.02	0.42
1:A:65:LEU:CD1	1:A:78:LEU:HD11	2.49	0.42
1:I:178:MET:HE3	1:I:200:SER:O	2.19	0.42
1:G:120:LYS:HE3	1:G:139:GLU:OE1	2.20	0.42
1:C:96:ASN:O	1:C:237:HIS:HA	2.20	0.42
1:I:194:THR:O	1:I:272:SER:HA	2.20	0.42
1:I:157:LEU:HD12	1:I:157:LEU:HA	1.84	0.42
2:D:321:TYR:CD2	2:D:321:TYR:C	2.93	0.42
1:K:187:THR:HA	1:K:196:SER:HB2	2.02	0.42
1:C:29:ASP:OD2	1:C:32:LYS:HE2	2.19	0.42
2:L:48:LYS:O	2:L:49:ARG:HD3	2.18	0.42
2:L:67:ASP:O	2:L:79:LEU:HD12	2.20	0.42
2:N:130:PRO:HD2	2:N:247:PHE:CD1	2.55	0.42
2:F:321:TYR:HB2	3:F:414:HOH:O	2.20	0.42
2:N:164:SER:HA	1:O:119:TYR:O	2.19	0.42
1:O:80:TRP:CE3	1:O:81:PRO:O	2.72	0.42
1:G:152:SER:HA	1:G:174:LEU:O	2.19	0.42
1:I:263:ASN:O	1:I:269:GLY:HA3	2.19	0.42
1:I:40:PHE:HA	1:I:54:PHE:O	2.20	0.42
1:I:50:LYS:HE3	3:P:416:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:HG12	1:A:301:LYS:HB3	2.01	0.42
2:J:113:LYS:HD3	2:J:113:LYS:HA	1.40	0.42
2:H:231:SER:HG	2:H:233:TYR:HD2	1.68	0.42
2:F:63:ASN:OD1	2:F:85:GLY:HA2	2.20	0.42
2:F:260:THR:CG2	2:F:261:GLN:N	2.83	0.42
2:J:182:TRP:CE3	2:J:183:HIS:HB2	2.54	0.42
1:K:218:LYS:HA	1:K:218:LYS:HD3	1.60	0.42
2:L:151:PHE:CD2	2:L:152:ASP:N	2.88	0.42
1:M:22:THR:CG2	2:N:40:ILE:HD13	2.50	0.41
1:K:22:THR:C	1:K:23:ARG:HD3	2.38	0.41
2:L:87:ILE:CG2	2:L:111:TYR:CE1	3.03	0.41
1:I:49:ASP:OD1	1:I:50:LYS:N	2.53	0.41
2:J:227:LYS:HD2	2:J:235:ARG:NH1	2.35	0.41
2:N:241:SER:HB2	1:O:156:LEU:HB3	2.01	0.41
2:N:162:SER:HA	1:O:121:THR:O	2.20	0.41
2:H:271:ASP:OD2	2:H:286:LEU:HD11	2.20	0.41
1:K:43:LEU:HD12	1:K:44:THR:N	2.35	0.41
1:I:22:THR:HG23	1:I:41:ASN:OD1	2.20	0.41
2:L:221:THR:HG23	2:L:224:ASN:H	1.85	0.41
2:N:198:LEU:HD12	2:N:212:LEU:CD1	2.48	0.41
2:J:271:ARG:HH11	2:J:277:ALA:CB	2.32	0.41
1:M:225:GLU:HG2	2:N:179:ILE:CG2	2.50	0.41
2:B:63:ASN:HB2	2:B:85:GLY:N	2.35	0.41
2:D:218:ARG:HA	2:D:218:ARG:HD3	1.74	0.41
1:A:144:GLU:O	2:B:142:THR:HA	2.21	0.41
1:K:298:LYS:HG2	1:K:299:PHE:O	2.19	0.41
1:M:183:THR:HG23	1:M:185:GLN:H	1.85	0.41
2:P:143:PHE:HE2	2:P:145:TYR:CD2	2.30	0.41
1:I:129:ARG:CZ	1:I:129:ARG:HA	2.50	0.41
2:N:175:ASN:HB2	1:O:108:ASP:OD1	2.20	0.41
1:K:40:PHE:CD1	1:K:55:ILE:HG12	2.55	0.41
1:O:60:THR:HG22	1:O:61:ILE:N	2.36	0.41
2:B:170:SER:HB2	1:C:114:LYS:HG2	2.01	0.41
2:D:298:THR:CG2	2:D:311:VAL:HG23	2.50	0.41
2:P:63:ASN:HB2	2:P:85:GLY:N	2.35	0.41
2:H:177:ASP:OD2	2:H:196:ASN:ND2	2.47	0.41
1:A:178:MET:CE	1:A:197:GLU:OE1	2.68	0.41
1:O:21:TYR:HB2	1:O:42:PHE:HB2	2.01	0.41
2:B:58:THR:HB	2:B:293:GLN:HB3	2.01	0.41
2:B:122:LYS:CB	2:B:257:ASN:HD22	2.32	0.41
2:F:159:ARG:NH1	1:M:127:ILE:HD13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:LEU:O	2:B:204:VAL:HA	2.19	0.41
2:B:55:ASP:CG	2:B:315:SER:OG	2.58	0.41
2:B:79:LEU:HD23	2:B:251:LEU:HD13	2.03	0.41
1:G:98:ASN:O	1:G:235:MET:HA	2.20	0.41
2:P:87:ILE:HG21	2:P:111:TYR:HD1	1.86	0.41
2:B:123:THR:OG1	2:B:253:ASN:OD1	2.39	0.41
2:N:302:ASP:OD1	2:N:302:ASP:C	2.59	0.41
1:A:136:ILE:O	2:B:150:LYS:HB2	2.21	0.41
2:D:265:THR:OG1	2:D:296:ILE:HG12	2.21	0.41
1:C:270:TYR:C	1:C:270:TYR:CD1	2.93	0.41
1:I:120:LYS:HG2	2:P:164:SER:CB	2.50	0.41
2:H:145:TYR:HA	2:H:162:SER:O	2.20	0.41
2:D:78:VAL:HG12	2:D:79:LEU:N	2.36	0.41
1:I:228:ASN:OD1	2:J:126:LYS:HB3	2.20	0.41
1:K:201:LEU:HD13	1:K:214:THR:HA	2.02	0.41
1:E:94:ASN:OD1	1:E:96:ASN:CG	2.59	0.41
1:C:186:LEU:HA	1:C:275:ASN:O	2.20	0.41
2:N:125:ILE:HB	2:N:186:ASN:HA	2.03	0.41
2:F:137:ALA:HB1	2:F:169:ILE:HG23	2.01	0.41
2:B:217:THR:HG22	1:C:191:ASP:OD1	2.21	0.41
2:D:59:ASN:O	2:D:60:ILE:HG13	2.21	0.41
2:L:200:TYR:HA	2:L:234:ARG:O	2.20	0.41
2:D:69:ILE:HB	2:D:78:VAL:HB	2.02	0.41
1:G:187:THR:HG22	1:G:195:LYS:HB3	2.02	0.41
2:F:108:PRO:HG2	2:F:111:TYR:OH	2.20	0.41
1:C:49:ASP:O	1:C:239:LYS:HE3	2.20	0.41
2:D:150:LYS:O	2:D:157:ILE:HA	2.20	0.41
1:G:68:LEU:HB2	1:G:77:THR:O	2.20	0.41
2:J:116:ARG:HA	2:J:116:ARG:HD2	1.93	0.41
2:B:258:GLU:HA	2:B:258:GLU:OE1	2.19	0.41
1:O:27:THR:HG23	1:O:284:LEU:HD21	2.03	0.41
2:L:256:SER:H	2:L:304:LYS:HZ3	1.69	0.41
1:G:128:ASN:HB3	1:G:129:ARG:C	2.40	0.41
1:I:26:THR:CG2	2:J:119:GLU:CG	2.99	0.41
2:J:207:LEU:HG	2:J:208:PHE:CD2	2.56	0.41
1:K:207:LEU:HD12	1:K:212:ASN:HA	2.02	0.41
1:K:79:ARG:HA	1:K:256:ASP:O	2.21	0.41
2:L:80:LEU:HD13	2:L:250:TYR:CE1	2.56	0.41
2:J:84:SER:HA	2:J:103:PRO:HG3	2.02	0.41
2:H:217:THR:CG2	2:H:220:ALA:HB2	2.43	0.41
2:D:276:ARG:HA	2:D:277:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:GLU:OE1	2:D:112:HIS:NE2	2.54	0.41
2:D:87:ILE:HD11	2:D:266:TYR:HB3	2.02	0.41
1:A:225:GLU:HG3	2:B:182:GLY:N	2.36	0.41
2:B:181:SER:C	2:B:183:LYS:H	2.24	0.41
1:C:124:ASP:H	1:C:135:ASN:HB3	1.85	0.41
2:B:85:GLY:O	2:B:245:PRO:HD2	2.21	0.41
1:E:209:ALA:C	1:E:211:ASP:N	2.74	0.41
1:A:268:TRP:HA	1:A:268:TRP:HE3	1.85	0.41
2:N:283:PRO:HA	2:N:284:PRO:HD3	1.82	0.41
1:O:79:ARG:HG2	1:O:255:MET:HE3	2.03	0.41
1:G:151:PRO:HB2	1:G:153:TYR:O	2.21	0.41
2:N:140:ASP:HB2	2:N:168:THR:HB	2.03	0.41
1:C:53:VAL:HG21	1:C:292:TRP:HH2	1.84	0.41
2:H:224:ASN:ND2	2:H:227:LEU:HG	2.36	0.41
2:B:107:TYR:HB2	2:B:108:PRO:HD2	2.02	0.41
2:J:82:ILE:CG2	2:J:106:TYR:HD1	2.34	0.41
2:B:128:GLN:OE1	2:B:128:GLN:N	2.54	0.41
1:O:23:ARG:HD2	2:P:75:ASP:CG	2.42	0.41
1:A:154:ARG:HD3	1:A:173:HIS:HD2	1.84	0.41
2:B:217:THR:O	2:B:218:ARG:HD3	2.21	0.41
1:E:80:TRP:CE2	1:E:199:PHE:HE2	2.39	0.41
2:J:91:HIS:HD2	2:J:99:TRP:CD2	2.38	0.41
2:F:185:ASN:HB2	2:F:188:HIS:H	1.85	0.41
2:P:59:ASN:HB3	2:P:90:ASN:HD21	1.86	0.41
1:I:220:PRO:HG2	1:I:223:VAL:CG2	2.51	0.41
2:D:217:THR:HG23	2:D:220:ALA:HB2	2.03	0.41
1:K:76:SER:N	1:K:209:ALA:HB1	2.36	0.41
1:C:293:LYS:HB3	1:C:293:LYS:HE2	1.77	0.41
2:J:123:GLN:HB2	2:J:244:THR:HG22	2.03	0.40
1:I:248:VAL:CG1	1:I:250:HIS:NE2	2.84	0.40
1:G:118:GLY:CA	1:G:141:ASN:OD1	2.68	0.40
2:N:139:VAL:HA	2:N:168:THR:O	2.22	0.40
2:N:260:THR:HG22	2:N:261:GLN:N	2.36	0.40
1:E:125:PHE:HA	1:E:134:GLY:HA2	2.03	0.40
1:I:69:ASP:OD1	1:I:69:ASP:N	2.50	0.40
2:J:213:ARG:HA	2:J:213:ARG:HD3	1.96	0.40
2:L:63:ASN:O	2:L:64:LEU:HD12	2.21	0.40
1:O:93:ASP:O	1:O:94:ASN:C	2.59	0.40
1:C:63:SER:O	1:C:255:MET:HE1	2.21	0.40
1:C:61:ILE:HG21	1:C:84:TYR:HD1	1.86	0.40
2:D:118:LYS:HA	2:D:118:LYS:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:210:GLU:H	2:P:210:GLU:HG3	1.58	0.40
2:L:207:ARG:HD3	2:L:207:ARG:C	2.41	0.40
1:I:26:THR:HG22	2:J:119:GLU:CD	2.41	0.40
2:D:217:THR:HG21	2:D:227:LEU:O	2.22	0.40
1:E:279:LYS:O	1:E:280:LYS:HB2	2.21	0.40
1:A:87:SER:HA	1:A:167:GLY:HA2	2.04	0.40
2:D:88:HIS:CE1	1:E:159:GLN:HA	2.56	0.40
1:M:180:HIS:HB2	1:M:182:HIS:CE1	2.56	0.40
2:L:130:PRO:HD2	2:L:247:PHE:HD1	1.86	0.40
2:L:243:PHE:CZ	2:L:245:PRO:HA	2.57	0.40
1:E:94:ASN:OD1	1:E:96:ASN:ND2	2.54	0.40
2:D:274:LYS:N	2:D:285:ILE:O	2.51	0.40
2:P:212:LEU:O	2:P:213:PHE:HB2	2.20	0.40
2:J:253:GLU:HA	2:J:253:GLU:OE1	2.21	0.40
1:E:240:LYS:HE3	1:E:240:LYS:HB2	1.87	0.40
1:K:149:GLN:HG3	2:L:136:THR:HG21	2.03	0.40
3:L:415:HOH:O	1:M:105:LYS:HE2	2.21	0.40
2:J:289:ARG:HH11	2:J:291:ILE:HD11	1.85	0.40
2:N:105:LEU:HB2	2:N:229:PHE:CE2	2.57	0.40
2:L:112:HIS:HB3	2:L:190:HIS:CE1	2.56	0.40
2:N:92:LYS:HZ2	2:N:94:GLU:CD	2.24	0.40
1:O:86:VAL:HA	1:O:250:HIS:O	2.22	0.40
1:M:91:VAL:HG21	1:M:248:VAL:HG23	2.02	0.40
1:A:43:LEU:HD23	1:A:54:PHE:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	277/311 (89%)	248 (90%)	28 (10%)	1 (0%)	39 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	275/311 (88%)	247 (90%)	25 (9%)	3 (1%)	17	50
1	E	288/311 (93%)	260 (90%)	22 (8%)	6 (2%)	9	29
1	G	288/311 (93%)	251 (87%)	33 (12%)	4 (1%)	14	42
1	I	288/311 (93%)	262 (91%)	21 (7%)	5 (2%)	11	36
1	K	275/311 (88%)	241 (88%)	29 (10%)	5 (2%)	11	34
1	M	283/311 (91%)	245 (87%)	31 (11%)	7 (2%)	7	24
1	O	279/311 (90%)	249 (89%)	25 (9%)	5 (2%)	11	34
2	B	278/324 (86%)	257 (92%)	19 (7%)	2 (1%)	26	62
2	D	287/324 (89%)	258 (90%)	25 (9%)	4 (1%)	14	42
2	F	280/324 (86%)	261 (93%)	17 (6%)	2 (1%)	26	62
2	H	286/324 (88%)	261 (91%)	20 (7%)	5 (2%)	11	36
2	J	286/324 (88%)	263 (92%)	20 (7%)	3 (1%)	19	52
2	L	286/324 (88%)	259 (91%)	24 (8%)	3 (1%)	19	52
2	N	286/324 (88%)	266 (93%)	17 (6%)	3 (1%)	19	52
2	P	282/324 (87%)	259 (92%)	17 (6%)	6 (2%)	9	29
All	All	4524/5080 (89%)	4087 (90%)	373 (8%)	64 (1%)	14	42

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	320	PRO
1	E	210	LYS
1	E	267	PHE
1	G	94	ASN
2	H	37	PRO
2	H	153	SER
2	H	154	THR
1	I	95	ASN
1	I	210	LYS
1	I	267	PHE
1	K	94	ASN
2	L	154	THR
2	L	320	PRO
1	M	131	GLY
2	P	318	ASN
2	P	320	PRO
1	C	94	ASN

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Mol	Chain	Res	Type
1	C	184	ARG
2	D	256	SER
1	E	177	ASN
1	E	278	ASP
2	F	256	SER
2	J	70	ASP
2	J	227	LYS
1	K	135	ASN
1	K	210	LYS
1	M	33	ASN
1	M	94	ASN
1	M	189	ASP
1	M	210	LYS
2	N	256	SER
1	O	267	PHE
1	O	278	ASP
2	B	182	GLY
1	C	177	ASN
2	D	156	GLY
2	D	226	GLU
1	E	280	LYS
2	F	182	GLY
1	G	72	GLY
1	I	266	GLY
1	K	241	ASP
1	M	266	GLY
1	O	189	ASP
1	E	266	GLY
2	H	213	PHE
1	I	33	ASN
2	J	177	GLY
2	P	119	ARG
2	P	152	ASP
2	D	182	GLY
1	G	33	ASN
1	G	186	LEU
2	H	119	ARG
2	L	316	ASP
1	M	216	LYS
2	N	182	GLY
2	N	318	ASN
2	P	232	LYS

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Mol	Chain	Res	Type
1	A	205	GLY
1	K	267	PHE
1	O	277	VAL
2	P	201	GLY
1	O	198	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	255/283 (90%)	222 (87%)	33 (13%)	5	16
1	C	255/283 (90%)	232 (91%)	23 (9%)	12	34
1	E	262/283 (93%)	240 (92%)	22 (8%)	14	37
1	G	262/283 (93%)	238 (91%)	24 (9%)	11	32
1	I	262/283 (93%)	235 (90%)	27 (10%)	9	26
1	K	257/283 (91%)	230 (90%)	27 (10%)	8	24
1	M	260/283 (92%)	241 (93%)	19 (7%)	17	44
1	O	257/283 (91%)	234 (91%)	23 (9%)	12	34
2	B	261/301 (87%)	243 (93%)	18 (7%)	19	48
2	D	267/301 (89%)	243 (91%)	24 (9%)	12	34
2	F	263/301 (87%)	244 (93%)	19 (7%)	18	45
2	H	266/301 (88%)	252 (95%)	14 (5%)	28	61
2	J	266/301 (88%)	239 (90%)	27 (10%)	9	26
2	L	266/301 (88%)	242 (91%)	24 (9%)	12	34
2	N	266/301 (88%)	249 (94%)	17 (6%)	22	52
2	P	264/301 (88%)	233 (88%)	31 (12%)	7	20
All	All	4189/4672 (90%)	3817 (91%)	372 (9%)	12	34

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	22	THR
1	A	24	THR
1	A	26	THR
1	A	27	THR
1	A	44	THR
1	A	65	LEU
1	A	66	ARG
1	A	68	LEU
1	A	69	ASP
1	A	76	SER
1	A	89	GLN
1	A	91	VAL
1	A	136	ILE
1	A	137	THR
1	A	149	GLN
1	A	154	ARG
1	A	184	ARG
1	A	186	LEU
1	A	193	ARG
1	A	204	ASN
1	A	222	THR
1	A	224	SER
1	A	234	VAL
1	A	242	LYS
1	A	252	LYS
1	A	268	TRP
1	A	277	VAL
1	A	289	GLU
1	A	293	LYS
1	A	298	LYS
1	A	301	LYS
1	A	303	LEU
2	B	42	LYS
2	B	52	THR
2	B	80	LEU
2	B	91	LEU
2	B	100	LYS
2	B	105	LEU
2	B	136	THR
2	B	170	SER
2	B	219	ILE
2	B	228	SER

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Mol	Chain	Res	Type
2	B	232	LYS
2	B	244	ASN
2	B	249	THR
2	B	254	GLU
2	B	257	ASN
2	B	259	LYS
2	B	279	ILE
2	B	315	SER
1	C	22	THR
1	C	56	LYS
1	C	79	ARG
1	C	110	SER
1	C	126	SER
1	C	140	SER
1	C	146	ILE
1	C	147	SER
1	C	171	GLU
1	C	178	MET
1	C	183	THR
1	C	184	ARG
1	C	185	GLN
1	C	193	ARG
1	C	194	THR
1	C	221	VAL
1	C	222	THR
1	C	264	ARG
1	C	281	GLU
1	C	288	TYR
1	C	289	GLU
1	C	298	LYS
1	C	304	ASN
2	D	35	THR
2	D	39	ASP
2	D	95	SER
2	D	97	LYS
2	D	126	LEU
2	D	135	SER
2	D	136	THR
2	D	155	LYS
2	D	160	THR
2	D	161	SER
2	D	173	GLN

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Mol	Chain	Res	Type
2	D	185	ASN
2	D	207	ARG
2	D	221	THR
2	D	228	SER
2	D	244	ASN
2	D	251	LEU
2	D	252	SER
2	D	254	GLU
2	D	256	SER
2	D	268	ARG
2	D	276	ARG
2	D	294	ARG
2	D	313	LYS
1	E	17	ASP
1	E	26	THR
1	E	27	THR
1	E	35	THR
1	E	45	GLU
1	E	52	THR
1	E	63	SER
1	E	83	SER
1	E	91	VAL
1	E	126	SER
1	E	133	THR
1	E	136	ILE
1	E	141	ASN
1	E	154	ARG
1	E	166	VAL
1	E	193	ARG
1	E	203	ARG
1	E	207	LEU
1	E	261	ASP
1	E	264	ARG
1	E	272	SER
1	E	298	LYS
2	F	65	GLN
2	F	80	LEU
2	F	82	LYS
2	F	91	LEU
2	F	109	SER
2	F	119	ARG
2	F	120	ASN

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Mol	Chain	Res	Type
2	F	124	GLU
2	F	126	LEU
2	F	138	LYS
2	F	141	SER
2	F	144	SER
2	F	146	SER
2	F	147	SER
2	F	161	SER
2	F	207	ARG
2	F	227	LEU
2	F	244	ASN
2	F	268	ARG
1	G	19	LYS
1	G	30	SER
1	G	71	ASN
1	G	76	SER
1	G	79	ARG
1	G	85	SER
1	G	87	SER
1	G	89	GLN
1	G	92	ASP
1	G	93	ASP
1	G	100	THR
1	G	112	GLU
1	G	129	ARG
1	G	140	SER
1	G	193	ARG
1	G	223	VAL
1	G	230	GLU
1	G	240	LYS
1	G	261	ASP
1	G	263	ASN
1	G	264	ARG
1	G	277	VAL
1	G	281	GLU
1	G	298	LYS
2	H	40	ILE
2	H	77	ASN
2	H	89	SER
2	H	98	GLU
2	H	136	THR
2	H	146	SER

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Mol	Chain	Res	Type
2	H	170	SER
2	H	207	ARG
2	H	244	ASN
2	H	268	ARG
2	H	295	LEU
2	H	300	GLU
2	H	301	VAL
2	H	319	LYS
1	I	19	LYS
1	I	27	THR
1	I	30	SER
1	I	38	LEU
1	I	52	THR
1	I	63	SER
1	I	73	TYR
1	I	74	TRP
1	I	76	SER
1	I	85	SER
1	I	105	LYS
1	I	110	SER
1	I	119	TYR
1	I	124	ASP
1	I	126	SER
1	I	127	ILE
1	I	129	ARG
1	I	135	ASN
1	I	138	LYS
1	I	140	SER
1	I	188	ASN
1	I	204	ASN
1	I	207	LEU
1	I	211	ASP
1	I	281	GLU
1	I	293	LYS
1	I	305	ASP
2	J	47	THR
2	J	53	THR
2	J	75	LEU
2	J	90	SER
2	J	113	LYS
2	J	114	ARG
2	J	131	THR

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Mol	Chain	Res	Type
2	J	159	SER
2	J	161	SER
2	J	165	SER
2	J	176	SER
2	J	181	ASN
2	J	194	LYS
2	J	202	ARG
2	J	214	ILE
2	J	226	SER
2	J	235	ARG
2	J	236	SER
2	J	256	GLN
2	J	258	GLU
2	J	263	ARG
2	J	271	ARG
2	J	274	ILE
2	J	282	GLU
2	J	290	LEU
2	J	297	ASP
2	J	317	LYS
1	K	22	THR
1	K	26	THR
1	K	27	THR
1	K	30	SER
1	K	31	GLN
1	K	44	THR
1	K	58	LYS
1	K	75	ASN
1	K	79	ARG
1	K	85	SER
1	K	91	VAL
1	K	95	ASN
1	K	100	THR
1	K	110	SER
1	K	125	PHE
1	K	140	SER
1	K	144	GLU
1	K	149	GLN
1	K	198	ILE
1	K	203	ARG
1	K	222	THR
1	K	244	LYS

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Mol	Chain	Res	Type
1	K	252	LYS
1	K	277	VAL
1	K	281	GLU
1	K	289	GLU
1	K	290	VAL
2	L	42	LYS
2	L	52	THR
2	L	75	ASP
2	L	77	ASN
2	L	89	SER
2	L	124	GLU
2	L	126	LEU
2	L	136	THR
2	L	154	THR
2	L	155	LYS
2	L	163	ASN
2	L	170	SER
2	L	207	ARG
2	L	223	GLU
2	L	227	LEU
2	L	228	SER
2	L	241	SER
2	L	249	THR
2	L	251	LEU
2	L	254	GLU
2	L	256	SER
2	L	273	LEU
2	L	306	LYS
2	L	322	LYS
1	M	27	THR
1	M	31	GLN
1	M	66	ARG
1	M	74	TRP
1	M	83	SER
1	M	87	SER
1	M	95	ASN
1	M	100	THR
1	M	106	ASN
1	M	124	ASP
1	M	129	ARG
1	M	140	SER
1	M	154	ARG

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Mol	Chain	Res	Type
1	M	174	LEU
1	M	193	ARG
1	M	201	LEU
1	M	223	VAL
1	M	252	LYS
1	M	261	ASP
2	N	80	LEU
2	N	89	SER
2	N	100	LYS
2	N	109	SER
2	N	129	LEU
2	N	136	THR
2	N	141	SER
2	N	146	SER
2	N	154	THR
2	N	160	THR
2	N	162	SER
2	N	207	ARG
2	N	210	GLU
2	N	221	THR
2	N	228	SER
2	N	256	SER
2	N	276	ARG
1	O	22	THR
1	O	26	THR
1	O	27	THR
1	O	30	SER
1	O	35	THR
1	O	45	GLU
1	O	75	ASN
1	O	83	SER
1	O	85	SER
1	O	96	ASN
1	O	97	THR
1	O	126	SER
1	O	140	SER
1	O	160	SER
1	O	202	THR
1	O	210	LYS
1	O	261	ASP
1	O	268	TRP
1	O	274	GLU

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Mol	Chain	Res	Type
1	O	281	GLU
1	O	287	LEU
1	O	290	VAL
1	O	293	LYS
2	P	43	ASN
2	P	45	LYS
2	P	91	LEU
2	P	102	SER
2	P	109	SER
2	P	115	PHE
2	P	124	GLU
2	P	126	LEU
2	P	151	PHE
2	P	157	ILE
2	P	159	ARG
2	P	161	SER
2	P	162	SER
2	P	170	SER
2	P	173	GLN
2	P	204	VAL
2	P	207	ARG
2	P	210	GLU
2	P	219	ILE
2	P	222	VAL
2	P	227	LEU
2	P	231	SER
2	P	244	ASN
2	P	249	THR
2	P	256	SER
2	P	258	GLU
2	P	268	ARG
2	P	288	LYS
2	P	306	LYS
2	P	315	SER
2	P	316	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	263	ASN
2	B	63	ASN

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Mol	Chain	Res	Type
2	B	103	ASN
2	B	253	ASN
1	C	39	GLN
1	C	96	ASN
1	C	159	GLN
1	C	182	HIS
1	C	204	ASN
1	C	295	HIS
2	D	84	GLN
2	D	185	ASN
2	D	244	ASN
1	E	75	ASN
1	E	96	ASN
1	E	141	ASN
1	E	246	GLN
2	F	65	GLN
2	F	173	GLN
2	F	224	ASN
1	G	75	ASN
1	G	149	GLN
1	G	180	HIS
2	H	103	ASN
2	H	208	ASN
2	H	224	ASN
2	H	244	ASN
1	I	71	ASN
1	I	135	ASN
1	I	188	ASN
1	I	263	ASN
2	J	180	ASN
1	K	94	ASN
1	K	149	GLN
1	K	173	HIS
1	K	296	ASN
2	L	103	ASN
2	L	163	ASN
2	L	244	ASN
1	M	33	ASN
1	M	39	GLN
1	M	41	ASN
1	M	96	ASN
1	M	173	HIS

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Mol	Chain	Res	Type
2	N	63	ASN
2	N	116	GLN
2	N	173	GLN
2	N	318	ASN
1	O	159	GLN
1	O	177	ASN
2	P	173	GLN
2	P	186	ASN
2	P	188	HIS
2	P	244	ASN
2	P	269	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	281/311 (90%)	-0.18	9 (3%) 51 39	17, 32, 79, 101	0
1	C	281/311 (90%)	-0.09	7 (2%) 61 48	16, 37, 77, 101	0
1	E	290/311 (93%)	-0.13	6 (2%) 67 56	17, 37, 72, 100	0
1	G	290/311 (93%)	-0.24	5 (1%) 73 63	13, 34, 75, 101	0
1	I	290/311 (93%)	-0.23	12 (4%) 41 29	13, 30, 81, 123	0
1	K	281/311 (90%)	-0.21	10 (3%) 46 34	17, 33, 70, 98	0
1	M	287/311 (92%)	-0.27	4 (1%) 78 69	13, 31, 67, 98	0
1	O	283/311 (90%)	-0.26	7 (2%) 61 48	17, 32, 77, 98	0
2	B	282/324 (87%)	-0.27	5 (1%) 71 61	16, 31, 58, 95	0
2	D	289/324 (89%)	-0.29	6 (2%) 67 56	18, 33, 61, 97	0
2	F	284/324 (87%)	-0.38	1 (0%) 93 90	14, 31, 57, 104	0
2	H	288/324 (88%)	-0.39	0 100 100	15, 28, 62, 86	0
2	J	288/324 (88%)	-0.34	2 (0%) 89 84	16, 29, 58, 98	0
2	L	288/324 (88%)	-0.34	3 (1%) 84 77	14, 27, 52, 110	0
2	N	288/324 (88%)	-0.38	0 100 100	15, 29, 55, 76	0
2	P	286/324 (88%)	-0.34	6 (2%) 67 56	16, 29, 62, 108	0
All	All	4576/5080 (90%)	-0.27	83 (1%) 71 61	13, 31, 69, 123	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	16	GLY	5.5
1	M	267	PHE	4.8
1	C	126	SER	4.8
2	L	154	THR	4.6
1	I	134	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	P	150	LYS	4.1
1	C	16	GLY	4.0
1	A	134	GLY	4.0
1	I	132	LEU	3.8
1	K	133	THR	3.6
2	D	35	THR	3.6
1	K	132	LEU	3.6
1	I	130	GLY	3.6
1	A	267	PHE	3.6
1	E	268	TRP	3.5
1	G	268	TRP	3.5
1	A	74	TRP	3.5
2	P	151	PHE	3.5
1	K	125	PHE	3.4
1	E	267	PHE	3.4
2	P	149	GLY	3.3
1	I	127	ILE	3.3
1	K	267	PHE	3.3
2	P	157	ILE	3.2
1	C	125	PHE	3.2
1	O	133	THR	3.2
1	A	206	ASN	3.2
1	M	268	TRP	3.2
2	J	152	ILE	3.1
1	G	267	PHE	3.1
1	O	134	GLY	3.1
1	E	17	ASP	3.1
1	K	135	ASN	3.0
1	I	16	GLY	3.0
2	B	35	THR	2.9
1	A	73	TYR	2.9
1	A	16	GLY	2.9
2	L	153	SER	2.9
1	C	206	ASN	2.9
1	K	134	GLY	2.9
1	A	17	ASP	2.9
1	C	263	ASN	2.9
1	I	128	ASN	2.9
1	K	126	SER	2.8
1	K	268	TRP	2.8
1	G	18	THR	2.8
1	O	125	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	17	ASP	2.8
1	O	267	PHE	2.7
2	L	151	PHE	2.7
1	I	125	PHE	2.7
1	A	268	TRP	2.7
2	F	151	PHE	2.7
1	I	131	GLY	2.7
2	D	154	THR	2.6
1	M	16	GLY	2.6
2	B	149	GLY	2.5
1	I	129	ARG	2.5
1	C	17	ASP	2.5
1	K	17	ASP	2.5
1	I	17	ASP	2.5
2	B	159	ARG	2.4
2	B	158	GLY	2.4
1	K	136	ILE	2.4
1	A	119	TYR	2.3
1	C	265	HIS	2.3
1	O	266	GLY	2.3
1	O	16	GLY	2.2
2	P	156	GLY	2.2
1	I	126	SER	2.2
2	P	152	ASP	2.2
1	E	16	GLY	2.2
2	D	151	PHE	2.1
2	J	275	HIS	2.1
2	D	41	GLY	2.1
1	I	73	TYR	2.1
2	D	152	ASP	2.1
1	E	123	GLY	2.1
1	E	119	TYR	2.0
2	B	145	TYR	2.0
2	D	155	LYS	2.0
1	M	266	GLY	2.0
1	O	268	TRP	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.