



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 10:37 AM UTC

PDB ID : 5TBK / pdb_00005tbk
Title : Crystal structure of human importin $\alpha 3$ bound to RCC1
Authors : Sankhala, R.S.; Lokareddy, R.K.; Pumroy, R.A.; Cingolani, G.
Deposited on : 2016-09-12
Resolution : 3.45 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

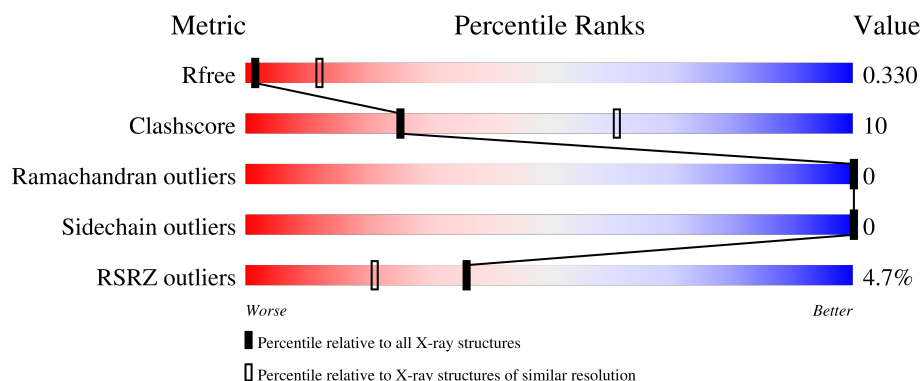
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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 $\leq 5\%$. 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	521	3% 63% 17% 20%
1	B	521	4% 64% 16% 20%
1	C	521	2% 66% 14% 20%
1	D	521	5% 62% 18% 20%
1	E	521	4% 64% 16% 20%

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Mol	Chain	Length	Quality of chain
1	F	521	 3% 64% 16% 20%
1	G	521	 2% 64% 16% 20%
1	H	521	 % 65% 15% 20%
2	I	421	 8% 75% 24%
2	J	421	 % 77% 22% .
2	K	421	 3% 74% 25% .
2	L	421	 7% 73% 26% .
2	M	421	 5% 73% 26%
2	N	421	 5% 78% 22% .
2	O	421	 4% 76% 24% .
2	P	421	 12% 76% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50677 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 Importin subunit alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3219	2043	545	618	13			
1	B	415	Total	C	N	O	S	0	0	0
			3187	2024	541	609	13			
1	C	417	Total	C	N	O	S	0	0	0
			3200	2031	543	613	13			
1	D	415	Total	C	N	O	S	0	0	0
			3206	2036	543	614	13			
1	E	416	Total	C	N	O	S	0	0	0
			3194	2028	542	611	13			
1	F	416	Total	C	N	O	S	0	0	0
			3194	2028	542	611	13			
1	G	417	Total	C	N	O	S	0	0	0
			3200	2031	543	613	13			
1	H	417	Total	C	N	O	S	0	0	0
			3200	2031	543	613	13			

- Molecule 2 is a protein called Regulator of chromosome condensation.

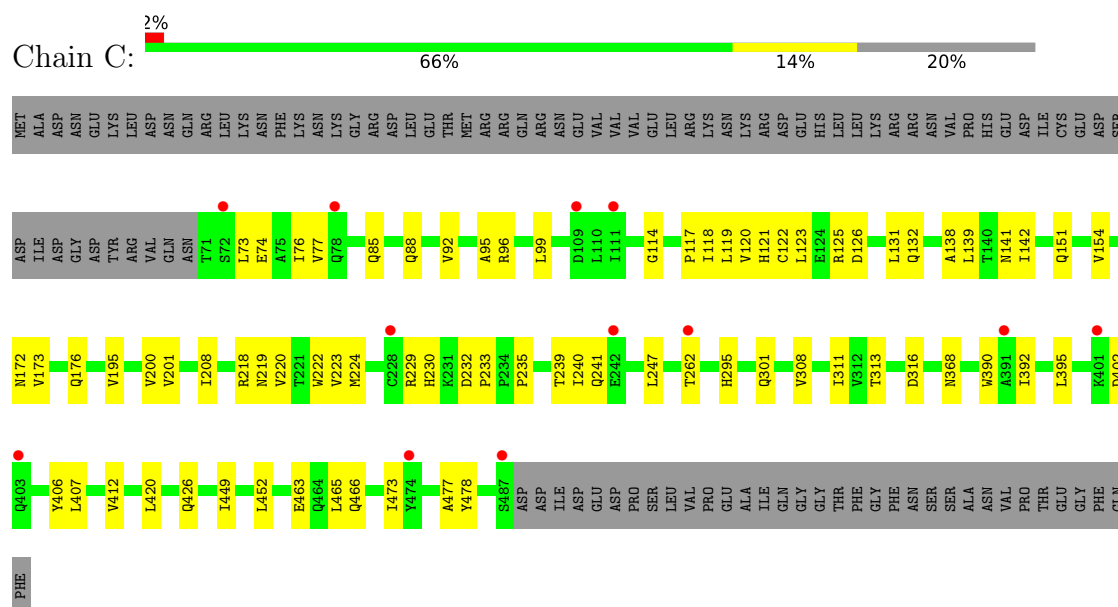
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	419	Total	C	N	O	S	0	0	0
			3139	1954	562	604	19			
2	K	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			
2	L	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			
2	M	419	Total	C	N	O	S	0	0	0
			3139	1954	562	604	19			
2	N	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			
2	O	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			

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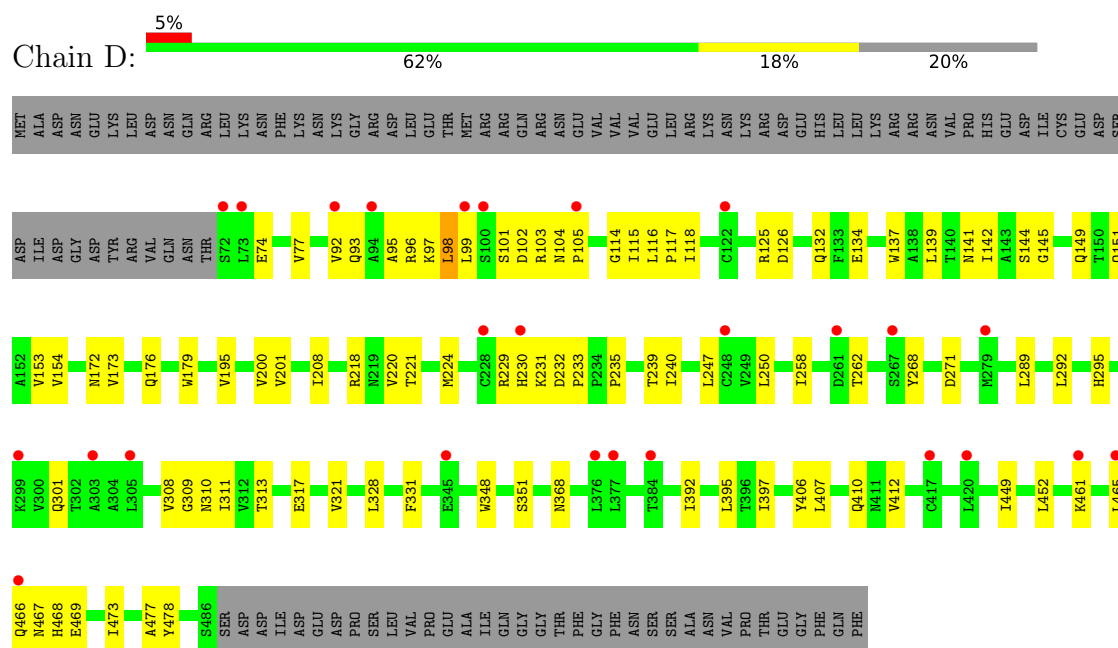
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	419	Total	C	N	O	S	0	0	0
			3139	1954	562	604	19			
2	J	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			

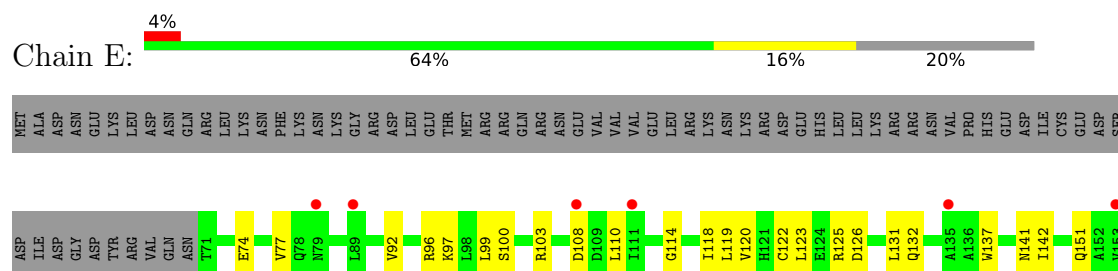
- Molecule 1: Importin subunit alpha-3

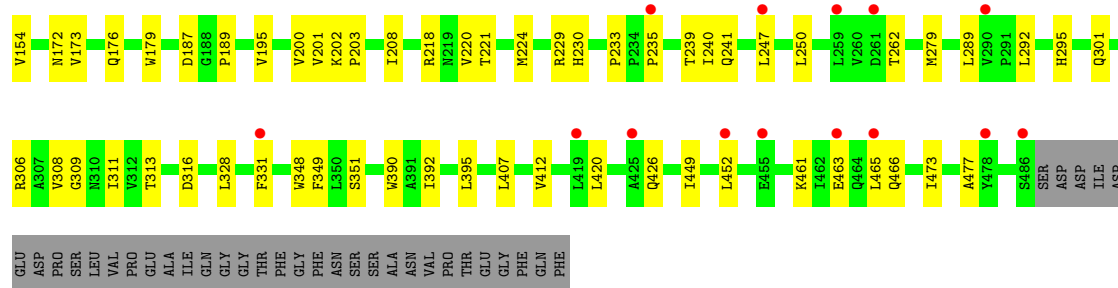


- Molecule 1: Importin subunit alpha-3

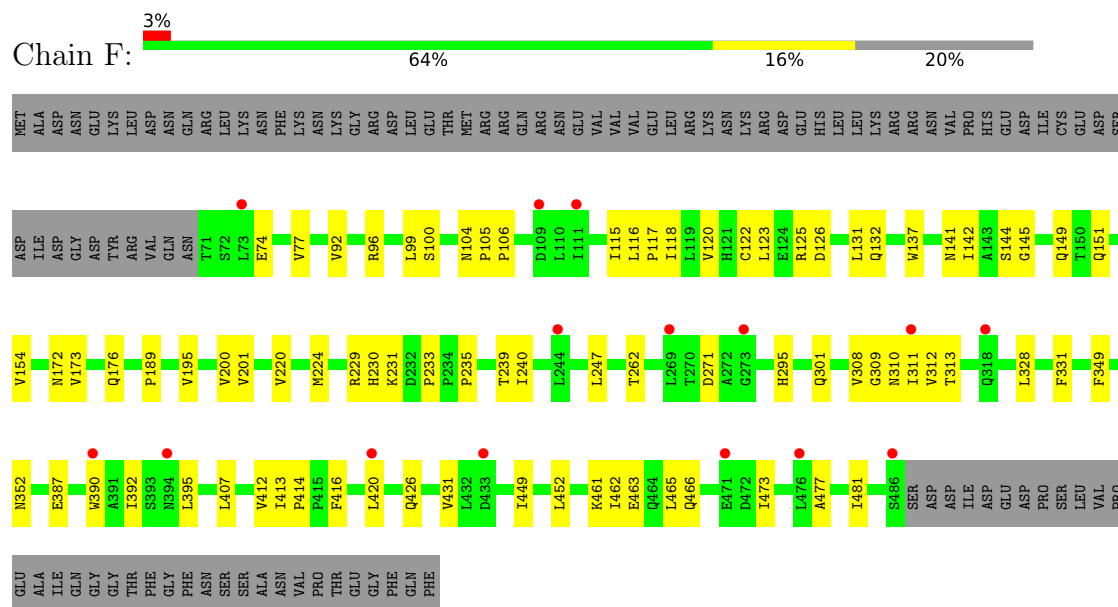


- Molecule 1: Importin subunit alpha-3

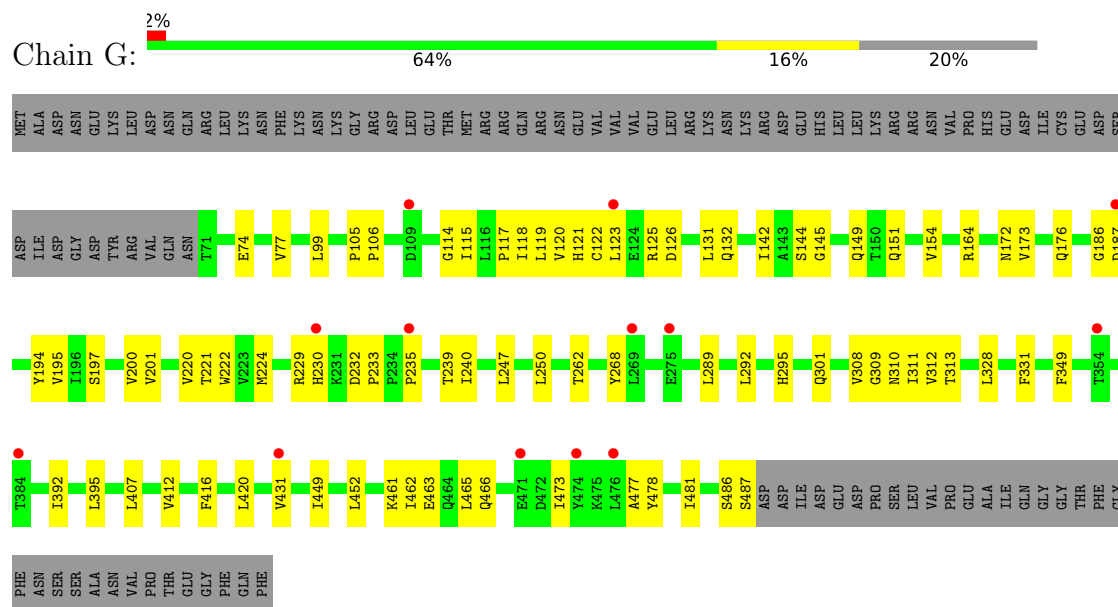




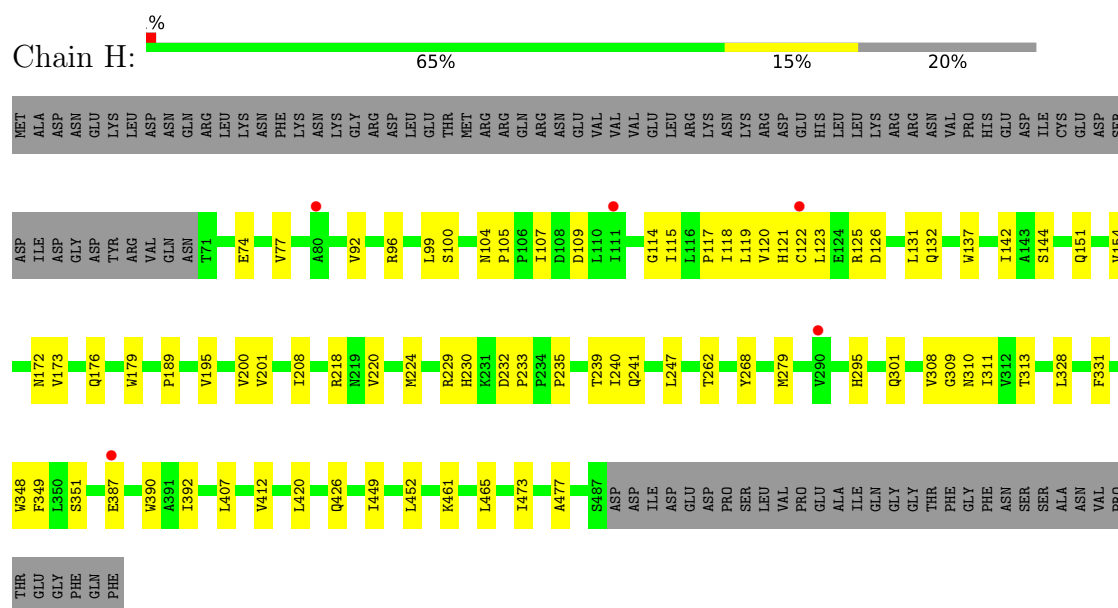
- Molecule 1: Importin subunit alpha-3



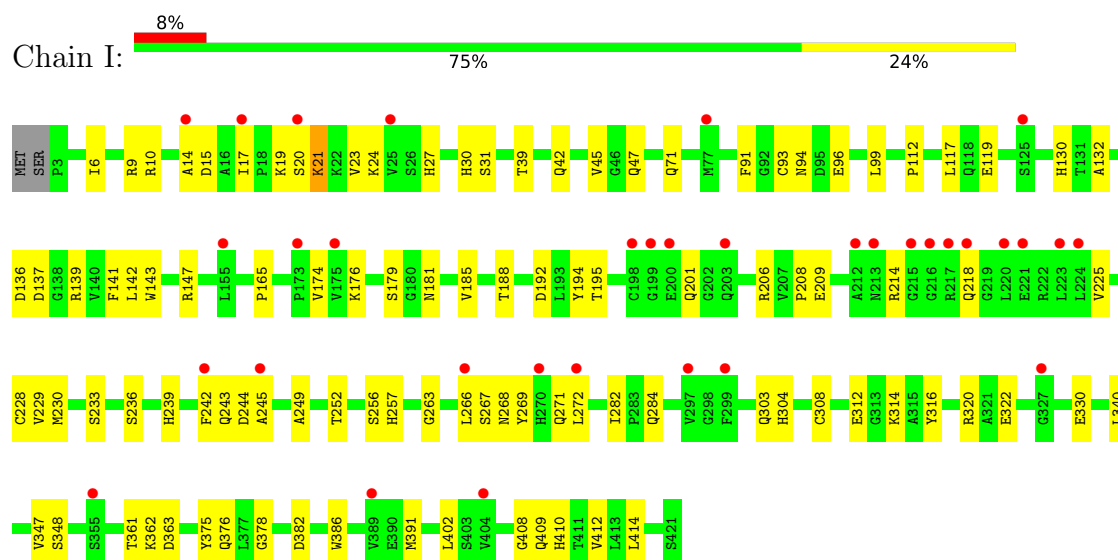
- Molecule 1: Importin subunit alpha-3



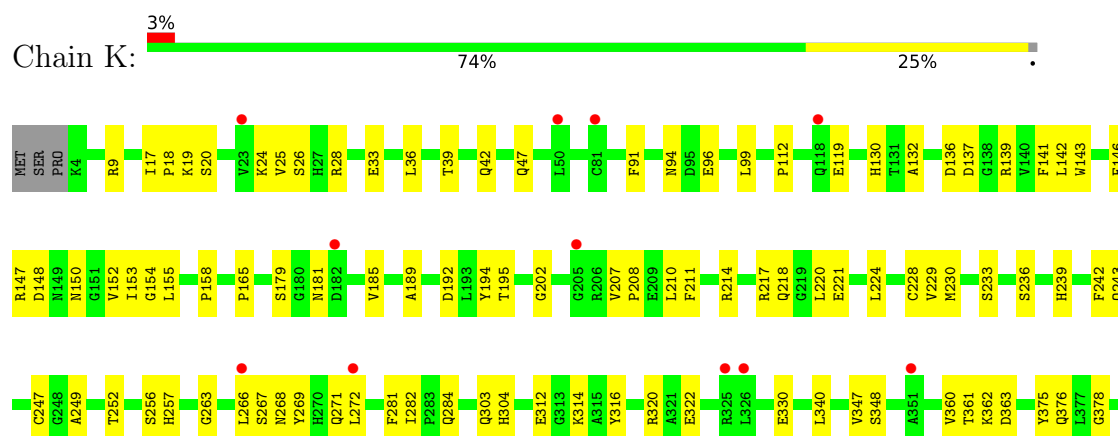
- Molecule 1: Importin subunit alpha-3

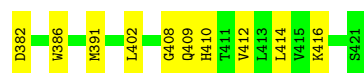


• Molecule 2: Regulator of chromosome condensation

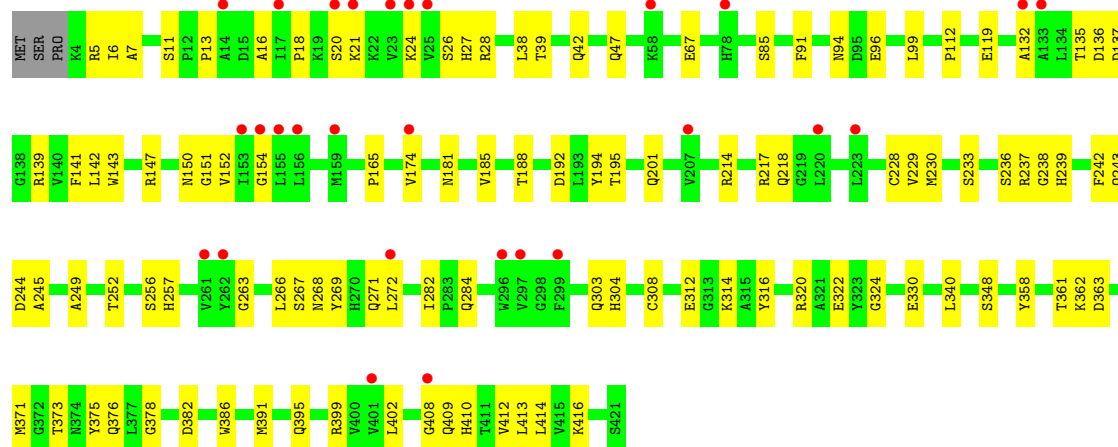
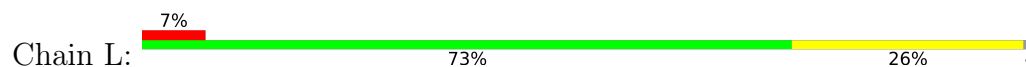


• Molecule 2: Regulator of chromosome condensation

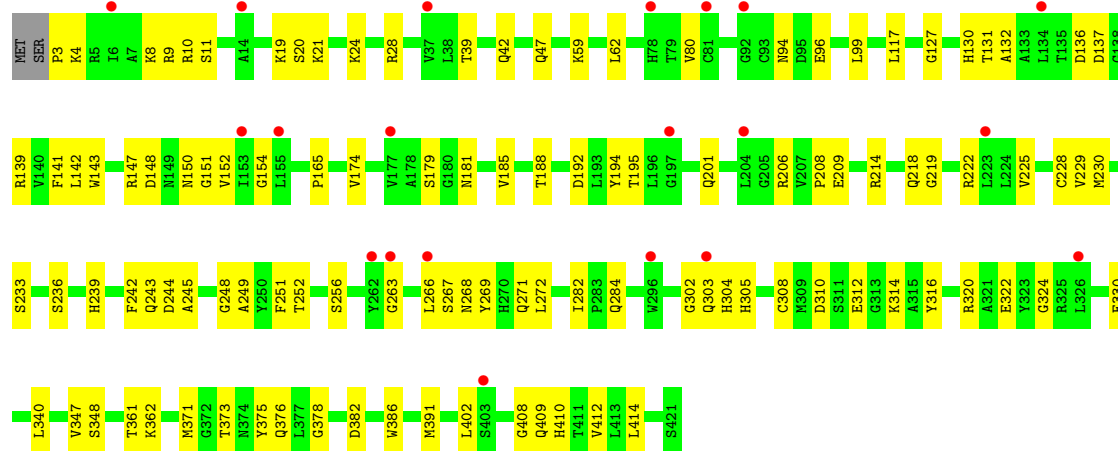
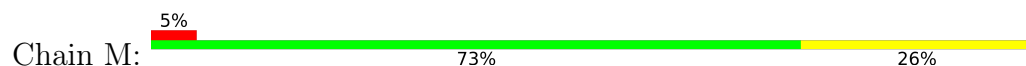




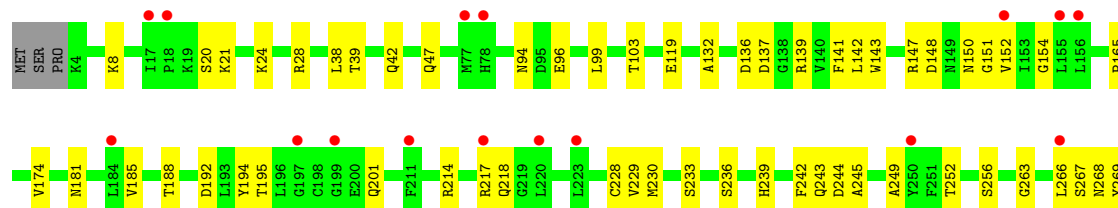
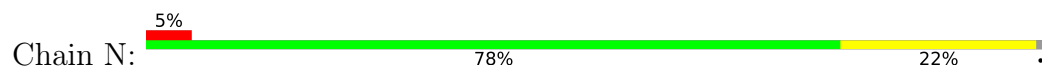
• Molecule 2: Regulator of chromosome condensation

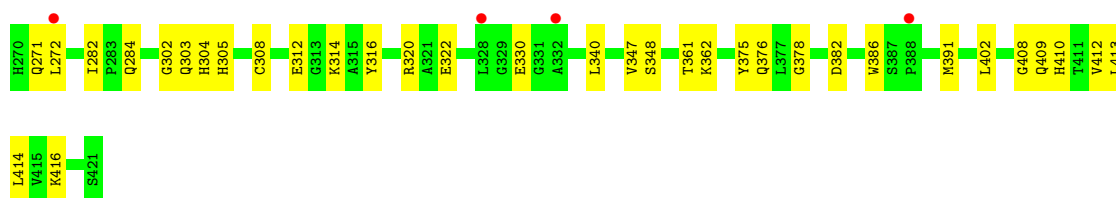


• Molecule 2: Regulator of chromosome condensation

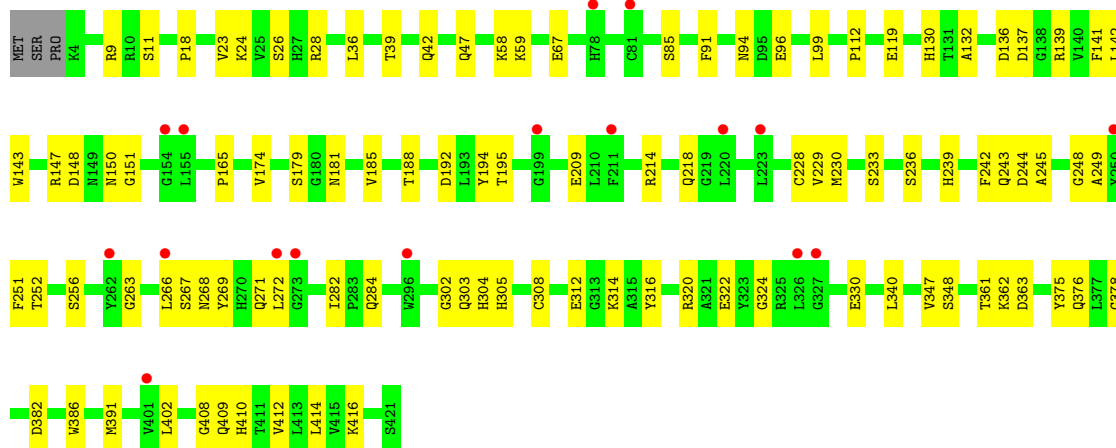
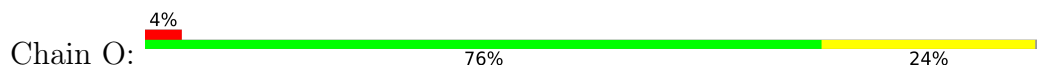


• Molecule 2: Regulator of chromosome condensation

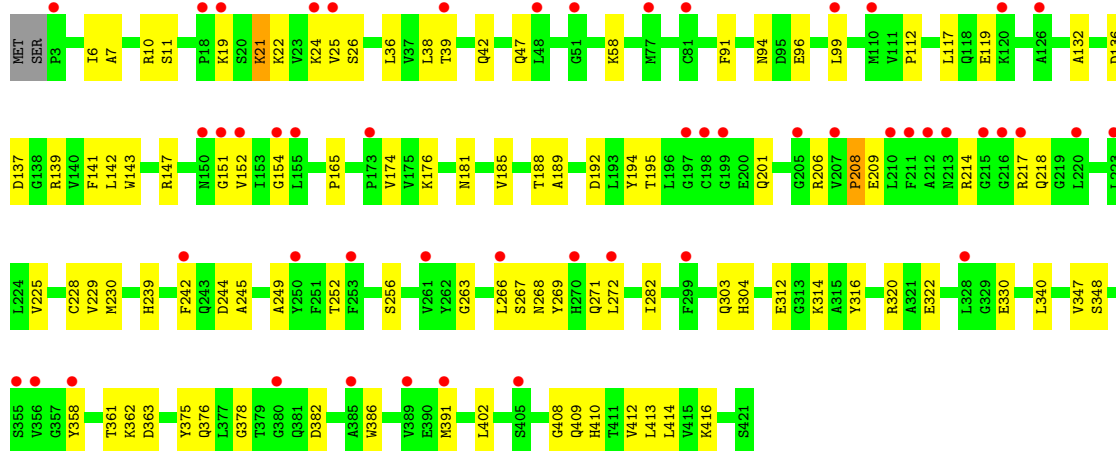
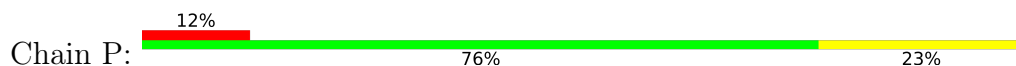




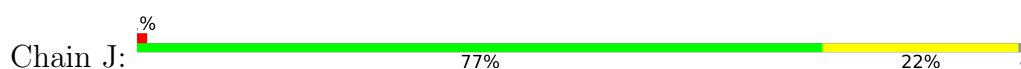
• Molecule 2: Regulator of chromosome condensation

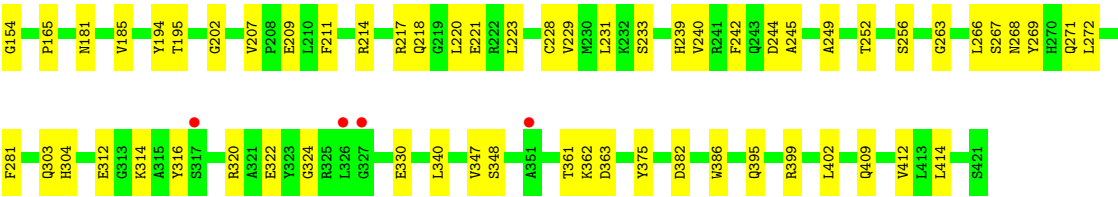


• Molecule 2: Regulator of chromosome condensation



• Molecule 2: Regulator of chromosome condensation





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	127.40Å 162.49Å 161.59Å 75.65° 85.63° 72.17°	Depositor
Resolution (Å)	19.99 – 3.45 19.99 – 3.45	Depositor EDS
% Data completeness (in resolution range)	75.5 (19.99-3.45) 79.8 (19.99-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.278 , 0.296 0.309 , 0.330	Depositor DCC
R_{free} test set	2000 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 16.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	50677	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7376e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/3279	0.49	2/4481 (0.0%)
1	B	0.25	0/3247	0.39	0/4439
1	C	0.30	0/3260	0.43	0/4457
1	D	0.26	0/3266	0.45	1/4463 (0.0%)
1	E	0.20	0/3254	0.37	0/4449
1	F	0.23	0/3254	0.38	0/4449
1	G	0.23	0/3260	0.40	0/4457
1	H	0.20	0/3260	0.37	0/4457
2	I	0.15	0/3198	0.41	2/4313 (0.0%)
2	J	0.22	0/3190	0.46	0/4302
2	K	0.22	0/3190	0.42	0/4302
2	L	0.14	0/3190	0.38	0/4302
2	M	0.17	0/3198	0.37	0/4313
2	N	0.13	0/3190	0.36	0/4302
2	O	0.16	0/3190	0.38	0/4302
2	P	0.16	0/3198	0.43	2/4313 (0.0%)
All	All	0.22	0/51624	0.41	7/70101 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	LEU	N-CA-C	7.07	119.84	111.71
1	D	98	LEU	N-CA-C	7.01	119.78	111.71
2	P	21	LYS	N-CA-C	6.33	119.54	110.24
2	P	208	PRO	N-CA-C	5.72	121.07	113.40
1	A	96	ARG	N-CA-C	-5.45	106.33	112.87
2	I	21	LYS	CA-C-N	-5.13	115.57	122.86
2	I	21	LYS	C-N-CA	-5.13	115.57	122.86

There are no chirality outliers.

There are no planarity outliers.

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	3219	0	3241	84	0
1	B	3187	0	3192	64	0
1	C	3200	0	3204	56	0
1	D	3206	0	3229	83	0
1	E	3194	0	3199	61	0
1	F	3194	0	3199	53	0
1	G	3200	0	3204	57	0
1	H	3200	0	3204	56	0
2	I	3139	0	3110	74	0
2	J	3132	0	3102	72	0
2	K	3132	0	3102	76	0
2	L	3132	0	3102	78	0
2	M	3139	0	3110	71	0
2	N	3132	0	3102	57	0
2	O	3132	0	3102	70	0
2	P	3139	0	3110	81	0
All	All	50677	0	50512	968	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 10.

All (968) 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:80:ALA:CA	1:A:88:GLN:HE22	1.36	1.38
1:A:80:ALA:HA	1:A:88:GLN:NE2	1.38	1.32
1:D:95:ALA:O	1:D:98:LEU:HG	1.38	1.20
1:B:226:ASN:OD1	2:I:20:SER:HB2	1.47	1.14
1:D:99:LEU:HD11	2:P:24:LYS:O	1.50	1.11
2:J:233:SER:HB3	2:J:240:VAL:HG23	1.19	1.09
1:A:95:ALA:O	1:A:98:LEU:HG	1.52	1.08
1:B:229:ARG:HH21	2:I:20:SER:HB3	1.15	1.04
1:B:229:ARG:NH2	2:I:20:SER:HB3	1.71	1.04
2:J:211:PHE:HB3	2:J:214:ARG:HD3	1.36	1.01
2:J:233:SER:CB	2:J:240:VAL:HG23	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD11	2:K:24:LYS:O	1.73	0.89
2:P:6:ILE:HG22	2:P:7:ALA:N	1.88	0.88
2:J:233:SER:HB3	2:J:240:VAL:CG2	2.05	0.86
2:K:137:ASP:OD2	2:K:139:ARG:NH1	2.09	0.84
1:A:82:SER:N	1:A:88:GLN:OE1	2.12	0.82
1:A:80:ALA:HA	1:A:88:GLN:HE22	0.66	0.82
1:A:98:LEU:HA	1:A:101:SER:HB2	1.61	0.81
2:J:137:ASP:OD2	2:J:139:ARG:NH1	2.14	0.81
2:P:6:ILE:HG22	2:P:7:ALA:O	1.80	0.81
2:P:209:GLU:O	2:P:214:ARG:NH2	2.13	0.81
1:D:99:LEU:CD1	2:P:24:LYS:O	2.28	0.80
1:A:80:ALA:C	1:A:88:GLN:HE22	1.89	0.80
1:A:368:ASN:OD1	2:J:217:ARG:NH1	2.15	0.80
2:L:137:ASP:OD2	2:L:139:ARG:NH1	2.16	0.79
1:A:99:LEU:HD21	1:A:141:ASN:CG	2.08	0.78
1:E:137:TRP:HE1	2:L:26:SER:HB2	1.47	0.78
2:M:137:ASP:OD2	2:M:139:ARG:NH1	2.17	0.77
2:N:137:ASP:OD2	2:N:139:ARG:NH1	2.17	0.77
2:M:42:GLN:HB2	2:M:409:GLN:HB3	1.67	0.76
1:B:218:ARG:NH1	2:I:119:GLU:OE2	2.18	0.76
1:D:99:LEU:HD12	2:P:26:SER:N	1.99	0.76
1:E:218:ARG:NH1	2:L:119:GLU:OE2	2.18	0.76
2:O:137:ASP:OD2	2:O:139:ARG:NH1	2.19	0.75
2:J:233:SER:CB	2:J:240:VAL:CG2	2.64	0.74
1:B:226:ASN:OD1	2:I:20:SER:CB	2.33	0.74
1:D:144:SER:O	2:P:21:LYS:HD3	1.88	0.74
1:G:115:ILE:O	1:G:119:LEU:HG	1.87	0.73
1:B:222:TRP:HE1	2:I:20:SER:HA	1.52	0.72
2:I:209:GLU:O	2:I:214:ARG:NH2	2.21	0.72
1:G:144:SER:HA	2:N:21:LYS:HD2	1.72	0.72
2:I:137:ASP:OD2	2:I:139:ARG:NH1	2.23	0.72
1:E:235:PRO:HG2	1:E:240:ILE:HD11	1.72	0.71
1:D:99:LEU:HD21	1:D:141:ASN:HB3	1.72	0.71
2:I:42:GLN:HB2	2:I:409:GLN:HB3	1.73	0.71
2:P:6:ILE:CG2	2:P:7:ALA:N	2.54	0.71
1:A:487:SER:HB3	2:M:62:LEU:HB3	1.73	0.71
1:D:114:GLY:O	1:D:117:PRO:HD2	1.89	0.71
1:G:99:LEU:HD13	1:G:142:ILE:HD11	1.72	0.71
1:H:218:ARG:NH1	2:O:119:GLU:OE2	2.24	0.70
1:G:122:CYS:HB2	1:G:131:LEU:HD21	1.73	0.70
2:M:151:GLY:H	2:O:150:ASN:HA	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD21	1:A:141:ASN:HB3	1.72	0.70
1:A:88:GLN:HE21	1:A:88:GLN:HA	1.57	0.70
1:C:402:ASP:HB3	2:K:214:ARG:HH21	1.57	0.69
1:B:295:HIS:O	1:B:301:GLN:NE2	2.25	0.69
2:P:137:ASP:OD2	2:P:139:ARG:NH1	2.24	0.69
1:F:99:LEU:HD13	1:F:142:ILE:HD11	1.75	0.69
2:O:209:GLU:O	2:O:214:ARG:NH2	2.26	0.69
2:L:237:ARG:HG2	2:L:238:GLY:H	1.56	0.69
1:A:218:ARG:NH1	2:K:119:GLU:OE2	2.25	0.69
1:C:313:THR:HG22	1:C:313:THR:O	1.92	0.69
1:H:117:PRO:O	1:H:121:HIS:ND1	2.24	0.69
1:H:295:HIS:O	1:H:301:GLN:NE2	2.25	0.68
2:L:42:GLN:HB2	2:L:409:GLN:HB3	1.75	0.68
2:P:42:GLN:HB2	2:P:409:GLN:HB3	1.75	0.68
1:C:218:ARG:NH1	2:J:119:GLU:OE2	2.26	0.68
1:D:229:ARG:NH1	2:P:19:LYS:HB3	2.09	0.68
1:F:312:VAL:O	2:M:8:LYS:NZ	2.26	0.68
1:E:295:HIS:O	1:E:301:GLN:NE2	2.25	0.68
2:N:42:GLN:HB2	2:N:409:GLN:HB3	1.74	0.68
1:D:295:HIS:O	1:D:301:GLN:NE2	2.26	0.68
1:C:235:PRO:HG2	1:C:240:ILE:HD11	1.76	0.67
2:O:233:SER:HB3	2:O:236:SER:HA	1.76	0.67
1:H:122:CYS:HB2	1:H:131:LEU:HD21	1.75	0.67
1:E:99:LEU:HD13	1:E:142:ILE:HD11	1.76	0.67
2:O:42:GLN:HB2	2:O:409:GLN:HB3	1.77	0.67
1:G:235:PRO:HG2	1:G:240:ILE:HD11	1.74	0.67
1:H:348:TRP:CZ2	2:O:11:SER:HB3	2.30	0.67
2:J:96:GLU:OE2	2:J:147:ARG:NH2	2.28	0.67
1:D:218:ARG:NH1	2:P:119:GLU:OE2	2.28	0.66
1:H:235:PRO:HG2	1:H:240:ILE:HD11	1.78	0.66
1:A:99:LEU:HD21	1:A:141:ASN:CB	2.25	0.66
1:C:99:LEU:HD13	1:C:142:ILE:HD11	1.76	0.66
2:M:209:GLU:O	2:M:214:ARG:NH2	2.29	0.66
1:A:478:TYR:OH	2:M:59:LYS:N	2.26	0.66
1:A:402:ASP:HB2	2:J:214:ARG:HH22	1.59	0.66
2:K:42:GLN:HB2	2:K:409:GLN:HB3	1.78	0.65
1:D:99:LEU:CD1	2:P:25:VAL:HA	2.27	0.65
1:H:99:LEU:HD13	1:H:142:ILE:HD11	1.76	0.65
2:L:233:SER:HB3	2:L:236:SER:HA	1.79	0.65
1:A:99:LEU:HD12	2:K:26:SER:H	1.62	0.65
1:A:88:GLN:NE2	1:A:88:GLN:HA	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:27:HIS:HB3	2:I:30:HIS:CE1	2.31	0.65
1:B:99:LEU:HD13	1:B:142:ILE:HD11	1.79	0.65
1:F:295:HIS:O	1:F:301:GLN:NE2	2.29	0.65
1:A:80:ALA:C	1:A:88:GLN:NE2	2.53	0.64
1:B:273:GLY:HA2	2:I:10:ARG:HH22	1.62	0.64
1:A:406:TYR:HB2	2:J:218:GLN:HG3	1.79	0.64
1:B:466:GLN:O	1:B:466:GLN:HG3	1.97	0.64
1:A:295:HIS:O	1:A:301:GLN:NE2	2.31	0.64
1:C:478:TYR:HE2	2:O:59:LYS:HB2	1.62	0.64
2:I:42:GLN:O	2:I:47:GLN:NE2	2.31	0.64
1:A:471:GLU:HA	1:A:474:TYR:CE2	2.33	0.63
1:D:93:GLN:HG2	1:D:134:GLU:CD	2.22	0.63
2:M:42:GLN:O	2:M:47:GLN:NE2	2.31	0.63
2:J:42:GLN:HB2	2:J:409:GLN:HB3	1.80	0.63
2:N:312:GLU:OE1	2:N:314:LYS:NZ	2.31	0.63
2:K:39:THR:HG22	2:K:412:VAL:HG22	1.79	0.63
2:K:96:GLU:OE2	2:K:147:ARG:NH2	2.31	0.63
1:A:80:ALA:C	1:A:88:GLN:OE1	2.42	0.62
1:A:99:LEU:HD12	2:K:26:SER:N	2.14	0.62
2:L:39:THR:HG22	2:L:412:VAL:HG22	1.81	0.62
2:J:312:GLU:OE1	2:J:314:LYS:NZ	2.32	0.62
1:B:122:CYS:HB2	1:B:131:LEU:HD21	1.81	0.62
1:F:235:PRO:HG2	1:F:240:ILE:HD11	1.81	0.62
1:B:247:LEU:HD22	1:B:262:THR:HG23	1.79	0.62
2:P:6:ILE:HG22	2:P:7:ALA:H	1.62	0.62
2:O:42:GLN:O	2:O:47:GLN:NE2	2.32	0.62
2:N:42:GLN:O	2:N:47:GLN:NE2	2.32	0.62
2:N:96:GLU:OE2	2:N:147:ARG:NH2	2.32	0.62
1:D:116:LEU:HD21	1:D:142:ILE:HD13	1.81	0.62
2:L:151:GLY:O	2:L:217:ARG:NH2	2.32	0.62
2:M:96:GLU:OE2	2:M:147:ARG:NH2	2.33	0.62
2:P:42:GLN:O	2:P:47:GLN:NE2	2.32	0.62
1:A:116:LEU:HD21	1:A:142:ILE:HD13	1.80	0.62
2:K:312:GLU:OE1	2:K:314:LYS:NZ	2.33	0.62
2:J:153:ILE:HB	2:J:220:LEU:HD21	1.81	0.62
1:D:95:ALA:O	1:D:98:LEU:CG	2.32	0.62
1:D:98:LEU:O	1:D:102:ASP:N	2.31	0.62
2:P:96:GLU:OE2	2:P:147:ARG:NH2	2.33	0.62
2:J:211:PHE:CB	2:J:214:ARG:HD3	2.21	0.62
2:L:312:GLU:OE1	2:L:314:LYS:NZ	2.32	0.61
2:M:233:SER:HB3	2:M:236:SER:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:312:GLU:OE1	2:P:314:LYS:NZ	2.33	0.61
1:B:392:ILE:HG23	1:B:407:LEU:HD21	1.83	0.61
2:O:39:THR:HG22	2:O:412:VAL:HG22	1.81	0.61
1:A:235:PRO:HG2	1:A:240:ILE:HD11	1.81	0.61
1:B:229:ARG:NH2	2:I:20:SER:CB	2.58	0.61
1:D:99:LEU:HD12	2:P:26:SER:H	1.63	0.61
2:N:233:SER:HB3	2:N:236:SER:HA	1.81	0.61
2:J:231:LEU:O	2:J:239:HIS:HB2	2.00	0.61
1:G:312:VAL:O	2:N:8:LYS:NZ	2.27	0.61
1:G:229:ARG:NH1	1:G:268:TYR:OH	2.33	0.61
1:D:98:LEU:HA	1:D:101:SER:HB2	1.82	0.61
2:J:211:PHE:HE1	2:J:223:LEU:HD21	1.65	0.61
1:A:99:LEU:CD2	1:A:141:ASN:HB3	2.31	0.61
1:C:126:ASP:OD1	1:C:132:GLN:NE2	2.27	0.61
2:O:230:MET:HE1	2:O:239:HIS:HB3	1.83	0.61
2:I:96:GLU:OE2	2:I:147:ARG:NH2	2.33	0.60
1:E:316:ASP:OD2	2:L:5:ARG:NH2	2.33	0.60
1:C:295:HIS:O	1:C:301:GLN:NE2	2.32	0.60
1:C:368:ASN:OD1	2:K:217:ARG:NH2	2.33	0.60
2:L:230:MET:HE1	2:L:239:HIS:HB3	1.84	0.60
2:J:217:ARG:O	2:J:221:GLU:HB2	2.02	0.60
1:H:247:LEU:HD22	1:H:262:THR:HG23	1.84	0.60
1:E:122:CYS:HB2	1:E:131:LEU:HD21	1.82	0.60
2:I:192:ASP:OD1	2:I:239:HIS:NE2	2.35	0.60
2:I:312:GLU:OE1	2:I:314:LYS:NZ	2.32	0.60
2:I:19:LYS:HB3	2:I:21:LYS:HE3	1.84	0.60
2:M:214:ARG:NH1	2:M:218:GLN:OE1	2.34	0.60
2:J:42:GLN:O	2:J:47:GLN:NE2	2.35	0.60
2:K:28:ARG:HH22	2:K:243:GLN:HG2	1.66	0.60
2:L:96:GLU:OE2	2:L:147:ARG:NH2	2.35	0.60
1:G:74:GLU:O	1:G:77:VAL:HG22	2.02	0.60
1:B:229:ARG:HH21	2:I:20:SER:CB	2.03	0.59
1:C:117:PRO:O	1:C:121:HIS:ND1	2.29	0.59
1:G:295:HIS:O	1:G:301:GLN:NE2	2.33	0.59
2:N:181:ASN:ND2	2:N:249:ALA:HB1	2.17	0.59
2:P:208:PRO:HB3	2:P:282:ILE:HD11	1.83	0.59
2:I:94:ASN:HB2	2:I:99:LEU:HD12	1.83	0.59
2:I:320:ARG:NH2	2:I:322:GLU:OE1	2.36	0.59
2:P:181:ASN:ND2	2:P:249:ALA:HB1	2.18	0.59
1:D:95:ALA:C	1:D:98:LEU:HG	2.26	0.59
2:N:320:ARG:NH2	2:N:322:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ASP:OD1	1:E:132:GLN:NE2	2.33	0.59
1:F:247:LEU:HD22	1:F:262:THR:HG23	1.84	0.59
2:L:42:GLN:O	2:L:47:GLN:NE2	2.36	0.59
2:N:230:MET:HE1	2:N:239:HIS:HB3	1.85	0.59
2:J:266:LEU:O	2:J:271:GLN:NE2	2.36	0.59
1:D:126:ASP:OD1	1:D:132:GLN:NE2	2.32	0.58
1:E:247:LEU:HD22	1:E:262:THR:HG23	1.85	0.58
2:O:96:GLU:OE2	2:O:147:ARG:NH2	2.36	0.58
1:E:348:TRP:CD2	2:L:11:SER:HB2	2.38	0.58
2:I:181:ASN:ND2	2:I:249:ALA:HB1	2.18	0.58
2:O:320:ARG:NH2	2:O:322:GLU:OE1	2.36	0.58
2:L:267:SER:HB2	2:L:272:LEU:HD12	1.85	0.58
2:J:320:ARG:NH2	2:J:322:GLU:OE1	2.37	0.58
1:C:119:LEU:HD22	1:C:139:LEU:HG	1.86	0.58
2:O:181:ASN:ND2	2:O:249:ALA:HB1	2.19	0.58
1:E:392:ILE:HG23	1:E:407:LEU:HD21	1.85	0.58
1:F:122:CYS:HB2	1:F:131:LEU:HD21	1.85	0.58
2:J:143:TRP:HB3	2:J:165:PRO:HA	1.85	0.58
1:C:96:ARG:NH2	2:J:26:SER:OG	2.37	0.58
1:A:318:GLN:NE2	1:B:275:GLU:OE1	2.37	0.58
1:A:80:ALA:CA	1:A:88:GLN:NE2	2.21	0.57
1:B:126:ASP:OD1	1:B:132:GLN:NE2	2.32	0.57
1:C:201:VAL:HG21	1:C:239:THR:HG23	1.85	0.57
2:M:39:THR:HG22	2:M:412:VAL:HG22	1.86	0.57
2:O:130:HIS:HE1	2:O:179:SER:HB3	1.68	0.57
2:P:6:ILE:CG2	2:P:7:ALA:H	2.14	0.57
1:B:137:TRP:CH2	2:I:24:LYS:HE2	2.39	0.57
1:D:392:ILE:HG23	1:D:407:LEU:HD21	1.86	0.57
2:I:266:LEU:O	2:I:271:GLN:NE2	2.38	0.57
2:K:148:ASP:C	2:K:150:ASN:H	2.12	0.57
2:M:192:ASP:OD1	2:M:239:HIS:NE2	2.37	0.57
1:D:235:PRO:HG2	1:D:240:ILE:HD11	1.86	0.57
2:I:39:THR:HG22	2:I:412:VAL:HG22	1.86	0.57
2:L:181:ASN:ND2	2:L:249:ALA:HB1	2.19	0.57
2:P:375:TYR:CZ	2:P:382:ASP:HB3	2.39	0.57
2:J:39:THR:HG22	2:J:412:VAL:HG22	1.86	0.57
2:J:209:GLU:HG3	2:J:281:PHE:CD2	2.40	0.57
1:G:392:ILE:HG23	1:G:407:LEU:HD21	1.86	0.57
2:I:130:HIS:HE1	2:I:179:SER:HB3	1.68	0.57
2:K:153:ILE:HB	2:K:220:LEU:HD21	1.85	0.57
2:O:267:SER:HB2	2:O:272:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:320:ARG:NH2	2:P:322:GLU:OE1	2.38	0.57
1:D:461:LYS:O	1:D:465:LEU:HB2	2.03	0.57
1:F:392:ILE:HG23	1:F:407:LEU:HD21	1.86	0.57
2:I:242:PHE:HA	2:I:256:SER:HA	1.86	0.57
2:L:192:ASP:OD1	2:L:239:HIS:NE2	2.38	0.57
2:O:94:ASN:HB2	2:O:99:LEU:HD12	1.86	0.57
1:G:395:LEU:HD22	1:G:407:LEU:HD22	1.87	0.57
2:K:217:ARG:O	2:K:221:GLU:HB2	2.04	0.57
2:N:39:THR:HG22	2:N:412:VAL:HG22	1.84	0.57
2:M:130:HIS:HE1	2:M:179:SER:HB3	1.68	0.57
2:P:266:LEU:O	2:P:271:GLN:NE2	2.37	0.57
2:P:94:ASN:HB2	2:P:99:LEU:HD12	1.87	0.57
1:A:126:ASP:OD1	1:A:132:GLN:NE2	2.27	0.57
2:K:192:ASP:OD1	2:K:239:HIS:NE2	2.38	0.57
2:M:267:SER:HB2	2:M:272:LEU:HD12	1.87	0.57
2:P:143:TRP:HB3	2:P:165:PRO:HA	1.87	0.57
2:M:312:GLU:OE1	2:M:314:LYS:NZ	2.34	0.56
2:N:94:ASN:HB2	2:N:99:LEU:HD12	1.87	0.56
1:C:73:LEU:HD12	1:C:74:GLU:HB2	1.87	0.56
2:K:266:LEU:O	2:K:271:GLN:NE2	2.38	0.56
2:O:192:ASP:OD1	2:O:239:HIS:NE2	2.38	0.56
1:A:392:ILE:HG23	1:A:407:LEU:HD21	1.86	0.56
1:D:104:ASN:HB2	1:D:105:PRO:HD3	1.86	0.56
2:M:94:ASN:HB2	2:M:99:LEU:HD12	1.87	0.56
2:M:320:ARG:NH2	2:M:322:GLU:OE1	2.38	0.56
2:K:228:CYS:SG	2:K:229:VAL:N	2.79	0.56
2:L:266:LEU:O	2:L:271:GLN:NE2	2.38	0.56
1:E:108:ASP:O	1:E:110:LEU:N	2.38	0.56
1:H:308:VAL:HA	1:H:311:ILE:HD12	1.87	0.56
1:H:392:ILE:HG23	1:H:407:LEU:HD21	1.87	0.56
2:L:320:ARG:NH2	2:L:322:GLU:OE1	2.38	0.56
2:O:312:GLU:OE1	2:O:314:LYS:NZ	2.34	0.56
1:C:141:ASN:OD1	2:J:23:VAL:HG13	2.05	0.56
2:O:143:TRP:HB3	2:O:165:PRO:HA	1.87	0.56
1:C:122:CYS:HB2	1:C:131:LEU:HD21	1.87	0.56
2:L:143:TRP:HB3	2:L:165:PRO:HA	1.88	0.56
2:P:242:PHE:HA	2:P:256:SER:HA	1.88	0.56
1:A:103:ARG:NH1	2:K:189:ALA:O	2.35	0.56
2:K:33:GLU:OE2	2:K:416:LYS:HE2	2.06	0.56
2:K:181:ASN:ND2	2:K:249:ALA:HB1	2.20	0.56
2:N:266:LEU:O	2:N:271:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:228:CYS:SG	2:L:229:VAL:N	2.79	0.55
2:J:233:SER:HB2	2:J:240:VAL:HG22	1.88	0.55
1:A:310:ASN:O	1:A:313:THR:OG1	2.21	0.55
1:F:387:GLU:OE1	2:M:9:ARG:NH2	2.39	0.55
2:M:266:LEU:O	2:M:271:GLN:NE2	2.39	0.55
1:C:406:TYR:HB2	2:K:218:GLN:HG3	1.86	0.55
1:F:473:ILE:O	1:F:477:ALA:HB2	2.06	0.55
1:G:115:ILE:CG2	1:G:119:LEU:HD11	2.36	0.55
1:G:186:GLY:HA3	2:N:20:SER:OG	2.07	0.55
2:M:143:TRP:HB3	2:M:165:PRO:HA	1.88	0.55
2:P:192:ASP:OD1	2:P:239:HIS:NE2	2.40	0.55
1:C:229:ARG:HG2	1:C:230:HIS:H	1.71	0.55
2:I:267:SER:HB2	2:I:272:LEU:HD12	1.89	0.55
1:E:96:ARG:NH2	2:L:26:SER:OG	2.40	0.55
1:E:137:TRP:NE1	2:L:26:SER:HB2	2.21	0.55
1:G:176:GLN:HE22	2:N:24:LYS:HD3	1.71	0.55
2:I:143:TRP:HB3	2:I:165:PRO:HA	1.87	0.55
2:I:230:MET:HE1	2:I:239:HIS:HB3	1.87	0.55
1:A:122:CYS:HB2	1:A:131:LEU:HD21	1.89	0.55
1:G:117:PRO:O	1:G:121:HIS:ND1	2.25	0.55
2:P:176:LYS:NZ	2:P:244:ASP:OD1	2.40	0.55
1:E:187:ASP:HA	2:L:21:LYS:NZ	2.22	0.55
2:K:94:ASN:HB2	2:K:99:LEU:HD12	1.88	0.55
1:E:308:VAL:HA	1:E:311:ILE:HD12	1.89	0.54
2:I:375:TYR:CZ	2:I:382:ASP:HB3	2.42	0.54
1:A:96:ARG:NH1	2:K:26:SER:OG	2.40	0.54
2:L:28:ARG:HH22	2:L:243:GLN:HG2	1.72	0.54
2:M:181:ASN:ND2	2:M:249:ALA:HB1	2.21	0.54
2:N:143:TRP:HB3	2:N:165:PRO:HA	1.88	0.54
2:J:211:PHE:CE1	2:J:223:LEU:HD21	2.43	0.54
1:A:115:ILE:HA	1:A:118:ILE:HD12	1.90	0.54
1:B:310:ASN:O	1:B:313:THR:OG1	2.23	0.54
1:E:189:PRO:HB2	1:E:233:PRO:HG2	1.90	0.54
1:G:115:ILE:HG22	1:G:119:LEU:CD1	2.38	0.54
1:G:120:VAL:O	1:G:123:LEU:HB3	2.07	0.54
2:I:176:LYS:NZ	2:I:244:ASP:OD1	2.40	0.54
1:C:392:ILE:HG23	1:C:407:LEU:HD21	1.88	0.54
2:N:192:ASP:OD1	2:N:239:HIS:NE2	2.40	0.54
2:P:230:MET:HE1	2:P:239:HIS:HB3	1.89	0.54
2:J:267:SER:HB2	2:J:272:LEU:HD12	1.89	0.54
2:N:267:SER:HB2	2:N:272:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:266:LEU:O	2:O:271:GLN:NE2	2.40	0.54
1:H:126:ASP:OD1	1:H:132:GLN:NE2	2.33	0.54
1:A:195:VAL:HG12	1:A:200:VAL:HG11	1.90	0.54
2:J:233:SER:HB2	2:J:240:VAL:CG2	2.38	0.54
1:A:366:ASP:O	2:J:217:ARG:NH2	2.40	0.54
1:B:144:SER:HB2	2:I:23:VAL:HG22	1.90	0.54
1:B:351:SER:OG	2:I:9:ARG:NH2	2.41	0.54
2:K:42:GLN:O	2:K:47:GLN:NE2	2.40	0.54
2:L:94:ASN:HB2	2:L:99:LEU:HD12	1.89	0.54
2:O:228:CYS:SG	2:O:229:VAL:N	2.81	0.54
1:B:222:TRP:CZ2	2:I:20:SER:O	2.61	0.53
1:B:235:PRO:HG2	1:B:240:ILE:HD11	1.89	0.53
1:D:96:ARG:HG2	1:D:137:TRP:CD1	2.43	0.53
1:H:328:LEU:HA	1:H:331:PHE:HD2	1.72	0.53
1:B:387:GLU:OE1	2:I:9:ARG:NH2	2.37	0.53
2:N:228:CYS:SG	2:N:229:VAL:N	2.82	0.53
2:O:185:VAL:HG12	2:O:195:THR:HG22	1.91	0.53
1:G:420:LEU:HB3	1:G:465:LEU:HD11	1.90	0.53
2:K:267:SER:HB2	2:K:272:LEU:HD12	1.91	0.53
2:P:39:THR:HG22	2:P:412:VAL:HG22	1.89	0.53
1:A:282:ASP:OD1	1:B:241:GLN:NE2	2.42	0.53
1:A:402:ASP:HB2	2:J:214:ARG:NH2	2.24	0.53
2:I:228:CYS:SG	2:I:229:VAL:N	2.82	0.53
1:H:107:ILE:C	1:H:109:ASP:H	2.16	0.53
2:I:15:ASP:O	2:I:17:ILE:N	2.39	0.53
2:M:228:CYS:SG	2:M:229:VAL:N	2.81	0.53
1:F:229:ARG:NH2	2:M:20:SER:OG	2.42	0.53
1:H:348:TRP:CH2	2:O:11:SER:HB3	2.44	0.53
2:I:233:SER:HB3	2:I:236:SER:HA	1.91	0.53
2:I:316:TYR:HE1	2:I:340:LEU:HD13	1.74	0.53
2:K:17:ILE:HB	2:K:18:PRO:HD3	1.90	0.53
2:L:316:TYR:HE1	2:L:340:LEU:HD13	1.74	0.53
2:M:316:TYR:HE1	2:M:340:LEU:HD13	1.74	0.53
2:O:214:ARG:NH1	2:O:218:GLN:OE1	2.42	0.53
2:P:228:CYS:SG	2:P:229:VAL:N	2.81	0.53
2:J:132:ALA:HB2	2:J:142:LEU:HD13	1.91	0.53
1:F:74:GLU:O	1:F:77:VAL:HG22	2.09	0.53
1:H:105:PRO:O	1:H:107:ILE:N	2.41	0.53
2:K:185:VAL:HG12	2:K:195:THR:HG22	1.91	0.53
2:J:228:CYS:SG	2:J:229:VAL:N	2.82	0.52
1:A:201:VAL:HG21	1:A:239:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ARG:CZ	2:P:19:LYS:HB3	2.40	0.52
2:O:316:TYR:HE1	2:O:340:LEU:HD13	1.75	0.52
1:C:218:ARG:NH1	2:J:118:GLN:O	2.42	0.52
1:E:97:LYS:HE3	2:L:28:ARG:HA	1.90	0.52
2:K:143:TRP:HB3	2:K:165:PRO:HA	1.91	0.52
1:B:229:ARG:HG2	1:B:230:HIS:H	1.74	0.52
1:C:313:THR:O	1:C:313:THR:CG2	2.58	0.52
1:H:179:TRP:CE2	2:O:24:LYS:HG3	2.44	0.52
1:C:473:ILE:O	1:C:477:ALA:CB	2.58	0.52
1:D:229:ARG:HG2	1:D:230:HIS:H	1.74	0.52
1:G:247:LEU:HD22	1:G:262:THR:HG23	1.91	0.52
2:N:316:TYR:HE1	2:N:340:LEU:HD13	1.73	0.52
1:D:368:ASN:OD1	2:I:214:ARG:HA	2.09	0.52
1:E:187:ASP:HA	2:L:21:LYS:HZ1	1.74	0.52
1:E:420:LEU:HB3	1:E:465:LEU:HD11	1.92	0.52
2:P:267:SER:HB2	2:P:272:LEU:HD12	1.91	0.52
1:G:473:ILE:O	1:G:477:ALA:HB2	2.09	0.52
2:J:242:PHE:HA	2:J:256:SER:HA	1.92	0.52
1:C:473:ILE:O	1:C:477:ALA:HB2	2.09	0.52
2:K:320:ARG:NH2	2:K:322:GLU:OE1	2.39	0.52
2:J:181:ASN:ND2	2:J:249:ALA:HB1	2.25	0.52
1:B:449:ILE:HA	1:B:452:LEU:HD12	1.90	0.52
2:I:378:GLY:HA3	2:I:391:MET:HE3	1.92	0.52
2:M:185:VAL:HG12	2:M:195:THR:HG22	1.92	0.52
2:O:28:ARG:HH22	2:O:243:GLN:HG2	1.74	0.52
2:M:230:MET:HE1	2:M:239:HIS:HB3	1.90	0.52
2:J:217:ARG:O	2:J:221:GLU:CB	2.58	0.51
2:J:316:TYR:HE1	2:J:340:LEU:HD13	1.75	0.51
1:B:189:PRO:HB2	1:B:233:PRO:HG2	1.92	0.51
1:A:92:VAL:HG11	1:A:131:LEU:HD12	1.93	0.51
1:C:402:ASP:CB	2:K:214:ARG:HH21	2.23	0.51
2:J:252:THR:O	2:J:263:GLY:HA2	2.10	0.51
1:A:99:LEU:CD1	2:K:25:VAL:HA	2.40	0.51
1:D:116:LEU:CD2	1:D:142:ILE:HD13	2.41	0.51
1:A:229:ARG:HG2	1:A:230:HIS:H	1.74	0.51
1:H:229:ARG:HG2	1:H:268:TYR:CE2	2.45	0.51
2:K:316:TYR:HE1	2:K:340:LEU:HD13	1.75	0.51
1:A:96:ARG:HG2	1:A:137:TRP:CD1	2.46	0.51
1:F:420:LEU:HB3	1:F:465:LEU:HD11	1.91	0.51
2:P:151:GLY:O	2:P:217:ARG:NH2	2.44	0.51
2:K:158:PRO:HG3	2:K:224:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:185:VAL:HG12	2:L:195:THR:HG22	1.91	0.51
2:K:230:MET:HE1	2:K:239:HIS:HB3	1.92	0.51
2:K:252:THR:O	2:K:263:GLY:HA2	2.11	0.51
1:D:74:GLU:O	1:D:77:VAL:HG22	2.11	0.51
2:M:148:ASP:C	2:M:150:ASN:H	2.19	0.51
2:P:358:TYR:OH	2:P:376:GLN:O	2.23	0.51
1:B:309:GLY:O	1:B:313:THR:HG23	2.10	0.51
1:C:92:VAL:HG11	1:C:131:LEU:HD12	1.92	0.51
1:C:220:VAL:HG12	1:C:224:MET:HE3	1.93	0.51
1:C:247:LEU:HD22	1:C:262:THR:HG23	1.93	0.50
1:E:328:LEU:HA	1:E:331:PHE:HD2	1.77	0.50
2:P:10:ARG:HG2	2:P:11:SER:H	1.76	0.50
1:C:395:LEU:HD22	1:C:407:LEU:HD22	1.94	0.50
1:E:141:ASN:ND2	2:L:24:LYS:O	2.31	0.50
1:F:229:ARG:HG2	1:F:230:HIS:H	1.76	0.50
1:G:172:ASN:OD1	1:G:173:VAL:N	2.44	0.50
2:P:316:TYR:HE1	2:P:340:LEU:HD13	1.76	0.50
1:C:114:GLY:O	1:C:118:ILE:HG12	2.11	0.50
1:F:104:ASN:N	1:F:105:PRO:HD3	2.25	0.50
2:K:375:TYR:CZ	2:K:382:ASP:HB3	2.46	0.50
1:A:247:LEU:HD22	1:A:262:THR:HG23	1.93	0.50
1:D:179:TRP:CZ2	2:P:22:LYS:HE3	2.47	0.50
1:E:229:ARG:HG2	1:E:230:HIS:H	1.77	0.50
1:E:407:LEU:HG	1:E:412:VAL:HG11	1.93	0.50
1:B:473:ILE:O	1:B:477:ALA:HB2	2.11	0.50
1:E:461:LYS:O	1:E:465:LEU:HG	2.12	0.50
1:F:126:ASP:OD1	1:F:132:GLN:NE2	2.33	0.50
2:L:214:ARG:NH1	2:L:218:GLN:OE1	2.38	0.50
2:M:28:ARG:HH22	2:M:243:GLN:HG2	1.76	0.50
1:A:80:ALA:C	1:A:88:GLN:CD	2.80	0.50
1:B:222:TRP:HZ2	2:I:20:SER:O	1.94	0.50
1:C:466:GLN:HB2	2:O:58:LYS:HZ1	1.76	0.50
2:M:252:THR:O	2:M:263:GLY:HA2	2.12	0.50
1:B:410:GLN:OE1	2:P:214:ARG:NH1	2.44	0.50
1:E:195:VAL:HG12	1:E:200:VAL:HG11	1.93	0.50
1:G:229:ARG:HG2	1:G:230:HIS:H	1.76	0.50
2:N:28:ARG:HH22	2:N:243:GLN:HG2	1.76	0.50
2:P:185:VAL:HG12	2:P:195:THR:HG22	1.94	0.50
1:E:473:ILE:O	1:E:477:ALA:HB2	2.11	0.50
2:N:185:VAL:HG12	2:N:195:THR:HG22	1.94	0.50
1:H:407:LEU:HG	1:H:412:VAL:HG11	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:473:ILE:O	1:H:477:ALA:HB2	2.12	0.49
2:O:148:ASP:C	2:O:150:ASN:H	2.20	0.49
1:A:104:ASN:HB2	1:A:105:PRO:HD3	1.95	0.49
1:H:420:LEU:HB3	1:H:465:LEU:HD11	1.94	0.49
2:P:132:ALA:HB2	2:P:142:LEU:HD13	1.94	0.49
2:J:94:ASN:HB2	2:J:99:LEU:HD12	1.94	0.49
1:G:328:LEU:HA	1:G:331:PHE:HD2	1.78	0.49
1:H:195:VAL:HG12	1:H:200:VAL:HG11	1.94	0.49
2:I:252:THR:O	2:I:263:GLY:HA2	2.12	0.49
1:D:247:LEU:HD22	1:D:262:THR:HG23	1.94	0.49
1:D:397:ILE:HG21	2:P:6:ILE:HD11	1.93	0.49
1:D:449:ILE:HA	1:D:452:LEU:HD12	1.95	0.49
1:G:478:TYR:OH	2:P:58:LYS:N	2.44	0.49
1:B:407:LEU:HG	1:B:412:VAL:HG11	1.94	0.49
1:D:99:LEU:HD21	1:D:141:ASN:CB	2.40	0.49
1:E:108:ASP:C	1:E:110:LEU:N	2.68	0.49
1:E:176:GLN:OE1	2:L:24:LYS:HE2	2.12	0.49
1:F:473:ILE:O	1:F:477:ALA:CB	2.60	0.49
2:I:185:VAL:HG12	2:I:195:THR:HG22	1.94	0.49
2:I:268:ASN:OD1	2:I:269:TYR:N	2.46	0.49
1:A:407:LEU:HG	1:A:412:VAL:HG11	1.94	0.49
1:B:473:ILE:O	1:B:477:ALA:CB	2.60	0.49
1:E:74:GLU:O	1:E:77:VAL:HG22	2.12	0.49
1:A:309:GLY:O	1:A:313:THR:HG23	2.12	0.49
1:D:99:LEU:HD13	2:P:25:VAL:HA	1.93	0.49
1:F:390:TRP:HZ2	1:F:426:GLN:HE21	1.61	0.49
2:L:402:LEU:N	2:L:414:LEU:O	2.45	0.49
2:P:376:GLN:NE2	2:P:408:GLY:O	2.46	0.49
1:A:88:GLN:HE21	1:A:88:GLN:CA	2.18	0.49
1:B:74:GLU:O	1:B:77:VAL:HG22	2.12	0.49
1:E:220:VAL:HG12	1:E:224:MET:HE3	1.94	0.49
1:B:220:VAL:HG12	1:B:224:MET:HE3	1.93	0.49
1:G:126:ASP:OD1	1:G:132:GLN:NE2	2.36	0.49
1:H:172:ASN:OD1	1:H:173:VAL:N	2.45	0.49
1:D:473:ILE:O	1:D:477:ALA:HB2	2.13	0.49
1:G:201:VAL:HG21	1:G:239:THR:HG23	1.95	0.49
1:H:390:TRP:HZ2	1:H:426:GLN:HE21	1.61	0.49
2:I:132:ALA:HB2	2:I:142:LEU:HD13	1.95	0.49
2:P:252:THR:O	2:P:263:GLY:HA2	2.13	0.49
2:J:268:ASN:OD1	2:J:269:TYR:N	2.46	0.49
1:G:195:VAL:HG12	1:G:200:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:151:GLY:O	2:N:217:ARG:NH2	2.44	0.48
1:A:172:ASN:OD1	1:A:173:VAL:N	2.46	0.48
1:H:114:GLY:O	1:H:118:ILE:HG12	2.13	0.48
1:H:449:ILE:HA	1:H:452:LEU:HD12	1.95	0.48
1:H:473:ILE:O	1:H:477:ALA:CB	2.61	0.48
2:L:252:THR:O	2:L:263:GLY:HA2	2.13	0.48
1:A:220:VAL:HG12	1:A:224:MET:HE3	1.95	0.48
1:F:144:SER:HA	2:M:21:LYS:CG	2.43	0.48
1:F:120:VAL:O	1:F:123:LEU:HB3	2.13	0.48
1:G:473:ILE:O	1:G:477:ALA:CB	2.62	0.48
1:H:125:ARG:O	1:H:132:GLN:NE2	2.45	0.48
2:N:252:THR:O	2:N:263:GLY:HA2	2.13	0.48
2:N:402:LEU:N	2:N:414:LEU:O	2.45	0.48
2:P:119:GLU:HG3	2:P:141:PHE:HE2	1.78	0.48
1:C:449:ILE:HA	1:C:452:LEU:HD12	1.96	0.48
1:D:473:ILE:O	1:D:477:ALA:CB	2.62	0.48
1:G:232:ASP:HB3	1:G:233:PRO:HD3	1.95	0.48
2:O:252:THR:O	2:O:263:GLY:HA2	2.13	0.48
2:J:375:TYR:CZ	2:J:382:ASP:HB3	2.48	0.48
1:F:308:VAL:HG12	1:F:349:PHE:HE1	1.79	0.48
1:A:95:ALA:O	1:A:97:LYS:N	2.47	0.48
1:D:328:LEU:HA	1:D:331:PHE:HD2	1.77	0.48
1:C:172:ASN:OD1	1:C:173:VAL:N	2.46	0.48
1:E:241:GLN:NE2	1:E:279:MET:SD	2.84	0.48
2:M:132:ALA:HB2	2:M:142:LEU:HD13	1.95	0.48
1:B:328:LEU:HA	1:B:331:PHE:HD2	1.78	0.48
1:E:92:VAL:HG11	1:E:131:LEU:HD12	1.96	0.48
1:E:151:GLN:HA	1:E:154:VAL:HG22	1.95	0.48
1:H:387:GLU:OE1	2:O:9:ARG:NH2	2.46	0.48
2:M:242:PHE:HA	2:M:256:SER:HA	1.96	0.48
2:M:347:VAL:HA	2:M:361:THR:HA	1.95	0.48
2:N:375:TYR:CZ	2:N:382:ASP:HB3	2.49	0.48
1:B:195:VAL:HG12	1:B:200:VAL:HG11	1.95	0.48
1:E:395:LEU:HD22	1:E:407:LEU:HD22	1.96	0.48
1:H:104:ASN:N	1:H:105:PRO:HD3	2.28	0.48
1:H:232:ASP:HB3	1:H:233:PRO:HD3	1.95	0.48
2:O:347:VAL:HA	2:O:361:THR:HA	1.96	0.48
2:O:402:LEU:N	2:O:414:LEU:O	2.43	0.48
2:J:14:ALA:HB3	2:J:17:ILE:CG1	2.44	0.48
1:A:137:TRP:CZ3	2:K:24:LYS:HE3	2.49	0.47
2:I:214:ARG:HD2	2:I:218:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:ASN:HB2	2:L:217:ARG:HH21	1.79	0.47
2:M:19:LYS:O	2:M:21:LYS:N	2.47	0.47
2:O:47:GLN:HG3	2:O:410:HIS:ND1	2.28	0.47
2:P:402:LEU:N	2:P:414:LEU:O	2.45	0.47
2:J:207:VAL:HB	2:J:211:PHE:CZ	2.49	0.47
1:D:172:ASN:OD1	1:D:173:VAL:N	2.48	0.47
1:F:189:PRO:HB2	1:F:233:PRO:HG2	1.96	0.47
1:H:309:GLY:HA3	1:H:348:TRP:CZ3	2.48	0.47
1:E:308:VAL:HG12	1:E:349:PHE:HE1	1.79	0.47
1:E:390:TRP:HZ2	1:E:426:GLN:HE21	1.63	0.47
2:P:208:PRO:HB3	2:P:282:ILE:CD1	2.44	0.47
1:A:241:GLN:NE2	1:A:279:MET:SD	2.84	0.47
1:B:231:LYS:HD3	1:B:271:ASP:OD2	2.14	0.47
1:E:473:ILE:O	1:E:477:ALA:CB	2.62	0.47
2:K:91:PHE:HB3	2:K:112:PRO:HA	1.96	0.47
2:K:242:PHE:HA	2:K:256:SER:HA	1.96	0.47
2:L:378:GLY:HA3	2:L:391:MET:HE3	1.97	0.47
2:O:361:THR:OG1	2:O:363:ASP:OD1	2.21	0.47
2:P:244:ASP:OD1	2:P:245:ALA:N	2.46	0.47
2:J:244:ASP:OD1	2:J:245:ALA:N	2.46	0.47
2:J:402:LEU:N	2:J:414:LEU:O	2.46	0.47
1:B:172:ASN:OD1	1:B:173:VAL:N	2.47	0.47
1:C:195:VAL:HG12	1:C:200:VAL:HG11	1.95	0.47
1:D:176:GLN:HE22	2:P:24:LYS:HD3	1.80	0.47
1:F:220:VAL:HG12	1:F:224:MET:HE3	1.96	0.47
2:I:402:LEU:N	2:I:414:LEU:O	2.42	0.47
2:M:268:ASN:OD1	2:M:269:TYR:N	2.48	0.47
2:O:132:ALA:HB2	2:O:142:LEU:HD13	1.96	0.47
2:P:268:ASN:OD1	2:P:269:TYR:N	2.46	0.47
1:D:406:TYR:O	1:D:410:GLN:HG2	2.14	0.47
2:N:132:ALA:HB2	2:N:142:LEU:HD13	1.95	0.47
2:O:376:GLN:NE2	2:O:408:GLY:O	2.48	0.47
2:P:119:GLU:HG3	2:P:141:PHE:CE2	2.50	0.47
1:A:449:ILE:HA	1:A:452:LEU:HD12	1.97	0.47
1:B:289:LEU:HD12	1:B:292:LEU:HD12	1.96	0.47
1:E:309:GLY:O	1:E:313:THR:HG23	2.15	0.47
2:I:47:GLN:HG3	2:I:410:HIS:ND1	2.29	0.47
2:K:402:LEU:N	2:K:414:LEU:O	2.45	0.47
2:L:194:TYR:HE1	2:L:228:CYS:HB2	1.79	0.47
2:J:209:GLU:HG3	2:J:281:PHE:HD2	1.76	0.47
1:C:151:GLN:HA	1:C:154:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:PRO:HB3	1:E:230:HIS:HB3	1.97	0.47
1:F:201:VAL:HG21	1:F:239:THR:HG23	1.95	0.47
1:C:316:ASP:OD1	2:J:5:ARG:NH2	2.48	0.47
1:D:231:LYS:HD3	1:D:271:ASP:OD2	2.15	0.47
1:E:201:VAL:HG21	1:E:239:THR:HG23	1.97	0.47
1:G:194:TYR:O	1:G:197:SER:OG	2.31	0.47
1:G:222:TRP:HZ2	2:N:20:SER:O	1.97	0.47
1:H:310:ASN:O	1:H:313:THR:OG1	2.27	0.47
2:N:94:ASN:ND2	2:N:103:THR:OG1	2.42	0.47
1:F:328:LEU:HA	1:F:331:PHE:HD2	1.79	0.47
2:L:132:ALA:HB2	2:L:142:LEU:HD13	1.97	0.47
1:G:125:ARG:O	1:G:132:GLN:NE2	2.48	0.46
2:I:194:TYR:HE1	2:I:228:CYS:HB2	1.80	0.46
2:K:136:ASP:OD1	2:K:137:ASP:N	2.48	0.46
2:K:268:ASN:OD1	2:K:269:TYR:N	2.48	0.46
1:A:332:PRO:HA	1:A:372:MET:HE1	1.98	0.46
1:D:232:ASP:HB3	1:D:233:PRO:HD3	1.96	0.46
1:F:309:GLY:O	1:F:313:THR:HG23	2.14	0.46
1:G:289:LEU:HD12	1:G:292:LEU:HD12	1.97	0.46
1:H:92:VAL:HG11	1:H:131:LEU:HD12	1.97	0.46
2:M:402:LEU:N	2:M:414:LEU:O	2.46	0.46
1:A:74:GLU:O	1:A:77:VAL:HG22	2.14	0.46
1:D:467:ASN:OD1	1:D:468:HIS:N	2.48	0.46
1:E:108:ASP:C	1:E:110:LEU:H	2.22	0.46
2:L:268:ASN:OD1	2:L:269:TYR:N	2.48	0.46
2:M:47:GLN:HG3	2:M:410:HIS:ND1	2.30	0.46
2:N:268:ASN:OD1	2:N:269:TYR:N	2.48	0.46
1:D:220:VAL:HG12	1:D:224:MET:HE3	1.97	0.46
1:H:328:LEU:HA	1:H:331:PHE:CD2	2.50	0.46
2:O:268:ASN:OD1	2:O:269:TYR:N	2.48	0.46
2:J:185:VAL:HG12	2:J:195:THR:HG22	1.97	0.46
1:E:172:ASN:OD1	1:E:173:VAL:N	2.49	0.46
1:H:229:ARG:HH22	2:O:18:PRO:HG2	1.80	0.46
1:H:461:LYS:O	1:H:465:LEU:HG	2.16	0.46
2:I:361:THR:OG1	2:I:363:ASP:OD1	2.21	0.46
2:K:130:HIS:HE1	2:K:179:SER:HB3	1.81	0.46
2:O:242:PHE:HA	2:O:256:SER:HA	1.98	0.46
2:J:119:GLU:HG3	2:J:141:PHE:HE2	1.81	0.46
1:F:463:GLU:O	1:F:466:GLN:HG2	2.15	0.46
2:M:244:ASP:OD1	2:M:245:ALA:N	2.45	0.46
2:O:375:TYR:CZ	2:O:382:ASP:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:378:GLY:HA3	2:O:391:MET:HE3	1.96	0.46
1:A:103:ARG:HD3	2:K:189:ALA:O	2.16	0.46
1:G:105:PRO:N	1:G:106:PRO:CD	2.79	0.46
1:G:308:VAL:HA	1:G:311:ILE:HD12	1.97	0.46
2:K:361:THR:OG1	2:K:363:ASP:OD1	2.22	0.46
2:N:378:GLY:HA3	2:N:391:MET:HE3	1.98	0.46
2:L:242:PHE:HA	2:L:256:SER:HA	1.97	0.46
1:C:74:GLU:O	1:C:77:VAL:HG22	2.16	0.46
2:K:208:PRO:C	2:K:210:LEU:H	2.24	0.46
2:K:233:SER:OG	2:K:236:SER:HB3	2.16	0.46
2:J:91:PHE:HB3	2:J:112:PRO:HA	1.98	0.46
1:A:473:ILE:O	1:A:477:ALA:HB2	2.16	0.46
1:C:229:ARG:HG2	1:C:230:HIS:N	2.31	0.46
1:G:461:LYS:O	1:G:465:LEU:HG	2.16	0.46
2:I:31:SER:HB2	2:I:71:GLN:HB2	1.98	0.46
1:B:92:VAL:HG11	1:B:131:LEU:HD12	1.98	0.45
1:F:151:GLN:HA	1:F:154:VAL:HG22	1.98	0.45
2:L:6:ILE:HG22	2:L:7:ALA:N	2.31	0.45
2:L:375:TYR:CZ	2:L:382:ASP:HB3	2.51	0.45
2:J:136:ASP:OD1	2:J:137:ASP:N	2.49	0.45
1:C:402:ASP:HB3	2:K:214:ARG:NH2	2.27	0.45
1:D:309:GLY:O	1:D:313:THR:HG23	2.17	0.45
1:E:306:ARG:HH12	2:L:13:PRO:HA	1.81	0.45
1:G:308:VAL:HG12	1:G:349:PHE:HE1	1.81	0.45
1:H:96:ARG:NH2	2:O:26:SER:OG	2.50	0.45
1:H:220:VAL:HG12	1:H:224:MET:HE3	1.98	0.45
1:A:232:ASP:HB3	1:A:233:PRO:HD3	1.98	0.45
1:D:139:LEU:HD22	1:D:153:VAL:HG13	1.97	0.45
2:I:376:GLN:NE2	2:I:408:GLY:O	2.50	0.45
2:P:214:ARG:NH1	2:P:218:GLN:OE1	2.50	0.45
1:D:103:ARG:HD3	2:P:189:ALA:O	2.17	0.45
1:D:310:ASN:O	1:D:313:THR:OG1	2.27	0.45
1:E:308:VAL:HG12	1:E:349:PHE:CE1	2.51	0.45
1:H:189:PRO:HB3	1:H:230:HIS:HB3	1.99	0.45
1:H:387:GLU:CD	2:O:9:ARG:HH22	2.25	0.45
2:P:361:THR:OG1	2:P:363:ASP:OD1	2.23	0.45
1:A:116:LEU:HB2	1:A:117:PRO:HD3	1.98	0.45
1:F:125:ARG:O	1:F:132:GLN:NE2	2.47	0.45
1:B:151:GLN:HA	1:B:154:VAL:HG22	1.98	0.45
1:D:99:LEU:CD2	1:D:141:ASN:HB3	2.45	0.45
1:D:407:LEU:HG	1:D:412:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ILE:HD11	1:E:224:MET:HE1	1.99	0.45
1:F:176:GLN:HE22	2:M:24:LYS:HD3	1.80	0.45
1:G:308:VAL:HG12	1:G:349:PHE:CE1	2.51	0.45
2:I:303:GLN:HG3	2:I:304:HIS:ND1	2.32	0.45
2:L:395:GLN:OE1	2:L:399:ARG:NH1	2.50	0.45
2:P:330:GLU:HA	2:P:386:TRP:HB3	1.98	0.45
2:P:347:VAL:HA	2:P:361:THR:HA	1.98	0.45
2:J:361:THR:OG1	2:J:363:ASP:OD1	2.22	0.45
1:D:99:LEU:HD12	2:P:25:VAL:C	2.41	0.45
1:D:99:LEU:HD21	1:D:141:ASN:CG	2.42	0.45
1:F:390:TRP:CD1	2:M:9:ARG:HH12	2.35	0.45
1:F:407:LEU:HG	1:F:412:VAL:HG11	1.98	0.45
1:G:114:GLY:O	1:G:118:ILE:HG12	2.16	0.45
1:G:313:THR:HA	2:N:8:LYS:HE2	1.98	0.45
1:H:151:GLN:HA	1:H:154:VAL:HG22	1.98	0.45
2:K:347:VAL:HA	2:K:361:THR:HA	1.99	0.45
1:D:95:ALA:O	1:D:98:LEU:N	2.49	0.45
1:D:201:VAL:HG21	1:D:239:THR:HG23	1.98	0.45
1:E:119:LEU:HA	1:E:122:CYS:SG	2.57	0.45
2:M:80:VAL:HG21	2:M:131:THR:HG21	1.98	0.45
2:M:136:ASP:OD1	2:M:137:ASP:N	2.50	0.45
2:N:308:CYS:SG	2:N:316:TYR:HB2	2.57	0.45
2:O:244:ASP:OD1	2:O:245:ALA:N	2.46	0.45
1:E:103:ARG:HD3	2:L:257:HIS:ND1	2.32	0.45
1:F:308:VAL:HA	1:F:311:ILE:HD12	1.98	0.45
1:F:462:ILE:HG22	1:F:481:ILE:HD11	1.99	0.45
2:M:194:TYR:HE1	2:M:228:CYS:HB2	1.82	0.45
2:N:214:ARG:NH1	2:N:218:GLN:OE1	2.48	0.45
1:A:208:ILE:HD11	1:A:224:MET:HE1	1.99	0.45
1:B:222:TRP:NE1	2:I:20:SER:HA	2.28	0.45
1:D:96:ARG:HD2	1:D:96:ARG:O	2.17	0.45
1:E:114:GLY:O	1:E:118:ILE:HG12	2.17	0.45
1:F:145:GLY:HA3	1:F:149:GLN:OE1	2.17	0.45
1:H:74:GLU:O	1:H:77:VAL:HG22	2.16	0.45
2:K:36:LEU:O	2:K:414:LEU:HD12	2.17	0.45
2:K:194:TYR:HE1	2:K:228:CYS:HB2	1.81	0.45
2:L:119:GLU:HG3	2:L:141:PHE:HE2	1.82	0.45
2:N:244:ASP:OD1	2:N:245:ALA:N	2.47	0.45
2:P:47:GLN:HG3	2:P:410:HIS:ND1	2.32	0.45
1:B:119:LEU:HA	1:B:122:CYS:SG	2.58	0.44
1:D:308:VAL:HA	1:D:311:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:309:GLY:O	1:H:313:THR:HG23	2.17	0.44
2:I:174:VAL:HA	2:I:188:THR:HA	1.99	0.44
2:L:376:GLN:NE2	2:L:408:GLY:O	2.50	0.44
2:N:347:VAL:HA	2:N:361:THR:HA	1.99	0.44
2:O:136:ASP:OD1	2:O:137:ASP:N	2.50	0.44
1:B:410:GLN:HE22	2:P:214:ARG:NE	2.15	0.44
1:C:119:LEU:HD11	1:C:138:ALA:HB3	1.99	0.44
1:D:144:SER:O	2:P:21:LYS:CD	2.62	0.44
1:D:466:GLN:OE1	1:D:478:TYR:HD1	2.01	0.44
1:F:116:LEU:HB2	1:F:117:PRO:HD3	1.99	0.44
1:F:172:ASN:OD1	1:F:173:VAL:N	2.50	0.44
1:H:119:LEU:HA	1:H:122:CYS:SG	2.58	0.44
2:I:330:GLU:HA	2:I:386:TRP:HB3	1.98	0.44
2:L:119:GLU:HG3	2:L:141:PHE:CE2	2.51	0.44
2:N:242:PHE:HA	2:N:256:SER:HA	1.99	0.44
1:E:120:VAL:O	1:E:123:LEU:HB3	2.17	0.44
1:G:145:GLY:HA3	1:G:149:GLN:OE1	2.16	0.44
2:K:211:PHE:HB2	2:K:214:ARG:HD2	1.99	0.44
2:O:36:LEU:O	2:O:414:LEU:HD12	2.17	0.44
2:P:136:ASP:OD1	2:P:137:ASP:N	2.49	0.44
1:E:100:SER:OG	2:L:26:SER:HB3	2.17	0.44
1:G:478:TYR:CE2	2:P:58:LYS:HB2	2.52	0.44
1:D:289:LEU:HD12	1:D:292:LEU:HD12	1.99	0.44
2:N:330:GLU:HA	2:N:386:TRP:HB3	2.00	0.44
2:N:376:GLN:NE2	2:N:408:GLY:O	2.50	0.44
2:P:194:TYR:HE1	2:P:228:CYS:HB2	1.83	0.44
1:A:95:ALA:C	1:A:97:LYS:N	2.74	0.44
1:B:308:VAL:HA	1:B:311:ILE:HD12	2.00	0.44
1:F:395:LEU:HD22	1:F:407:LEU:HD22	1.99	0.44
2:N:119:GLU:HG3	2:N:141:PHE:HE2	1.83	0.44
1:A:308:VAL:HG12	1:A:349:PHE:HE1	1.82	0.44
1:B:201:VAL:HG21	1:B:239:THR:HG23	1.98	0.44
1:B:306:ARG:NH1	2:I:14:ALA:HB2	2.33	0.44
1:C:222:TRP:CE2	2:J:22:LYS:HD3	2.53	0.44
1:D:95:ALA:C	1:D:97:LYS:H	2.25	0.44
1:D:395:LEU:HD22	1:D:407:LEU:HD22	2.00	0.44
1:G:187:ASP:HA	2:N:21:LYS:NZ	2.33	0.44
2:J:330:GLU:HA	2:J:386:TRP:HB3	1.99	0.44
1:D:151:GLN:HA	1:D:154:VAL:HG22	2.00	0.44
1:D:208:ILE:HD11	1:D:224:MET:HE1	1.99	0.44
1:H:176:GLN:HE22	2:O:24:LYS:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:211:PHE:CB	2:K:214:ARG:HD2	2.47	0.44
2:L:348:SER:HB3	2:L:362:LYS:HA	1.99	0.44
2:N:348:SER:HB3	2:N:362:LYS:HA	2.00	0.44
1:C:308:VAL:HA	1:C:311:ILE:HD12	1.99	0.44
1:G:220:VAL:HG12	1:G:224:MET:HE3	2.00	0.44
1:G:309:GLY:O	1:G:313:THR:HG23	2.17	0.44
1:B:397:ILE:HD13	2:I:6:ILE:HG13	2.00	0.43
1:D:221:THR:HG22	1:D:250:LEU:HD13	2.00	0.43
2:L:27:HIS:ND1	2:L:28:ARG:N	2.66	0.43
2:M:150:ASN:HA	2:O:151:GLY:N	2.33	0.43
2:M:308:CYS:SG	2:M:316:TYR:HB2	2.58	0.43
2:M:375:TYR:CZ	2:M:382:ASP:HB3	2.53	0.43
2:M:378:GLY:HA3	2:M:391:MET:HE3	1.99	0.43
2:N:194:TYR:HE1	2:N:228:CYS:HB2	1.83	0.43
1:E:463:GLU:O	1:E:466:GLN:HG2	2.18	0.43
1:F:308:VAL:HG12	1:F:349:PHE:CE1	2.53	0.43
1:A:321:VAL:HG21	1:B:237:MET:HG2	2.01	0.43
1:F:449:ILE:HA	1:F:452:LEU:HD12	2.00	0.43
2:L:27:HIS:CE1	2:L:28:ARG:HG2	2.53	0.43
2:M:148:ASP:C	2:M:150:ASN:N	2.77	0.43
2:M:376:GLN:NE2	2:M:408:GLY:O	2.52	0.43
1:A:98:LEU:O	1:A:102:ASP:N	2.41	0.43
1:C:463:GLU:O	1:C:466:GLN:HG2	2.19	0.43
1:G:151:GLN:HA	1:G:154:VAL:HG22	2.00	0.43
1:H:348:TRP:O	1:H:351:SER:OG	2.23	0.43
2:K:119:GLU:HG3	2:K:141:PHE:HE2	1.83	0.43
2:K:303:GLN:HG3	2:K:304:HIS:ND1	2.33	0.43
2:L:16:ALA:C	2:L:18:PRO:HD2	2.42	0.43
2:N:150:ASN:HB2	2:N:217:ARG:HH21	1.84	0.43
1:A:176:GLN:OE1	2:K:24:LYS:HE2	2.18	0.43
1:F:189:PRO:HB3	1:F:230:HIS:HB3	2.00	0.43
1:G:486:SER:O	1:G:487:SER:OG	2.31	0.43
2:I:136:ASP:OD1	2:I:137:ASP:N	2.51	0.43
2:I:244:ASP:OD1	2:I:245:ALA:N	2.48	0.43
2:K:348:SER:N	2:K:360:VAL:O	2.50	0.43
2:O:302:GLY:HA3	2:O:305:HIS:CE1	2.53	0.43
1:A:95:ALA:C	1:A:97:LYS:H	2.27	0.43
1:C:219:ASN:O	1:C:223:VAL:HG23	2.18	0.43
1:F:416:PHE:CZ	1:F:431:VAL:HA	2.54	0.43
2:O:194:TYR:HE1	2:O:228:CYS:HB2	1.84	0.43
2:P:206:ARG:HB3	2:P:229:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:119:GLU:HG3	2:J:141:PHE:CE2	2.53	0.43
1:A:328:LEU:HA	1:A:331:PHE:HD2	1.84	0.43
1:B:467:ASN:OD1	1:B:468:HIS:HB2	2.19	0.43
1:C:85:GLN:HA	1:C:88:GLN:HB2	2.00	0.43
1:C:407:LEU:HG	1:C:412:VAL:HG11	2.00	0.43
1:H:120:VAL:O	1:H:123:LEU:HB3	2.19	0.43
1:H:201:VAL:HG21	1:H:239:THR:HG23	2.00	0.43
2:I:91:PHE:HB3	2:I:112:PRO:HA	2.00	0.43
2:N:136:ASP:OD1	2:N:137:ASP:N	2.51	0.43
1:A:96:ARG:HD2	1:A:96:ARG:O	2.19	0.43
1:A:309:GLY:HA3	1:A:348:TRP:CZ3	2.54	0.43
1:D:145:GLY:HA3	1:D:149:GLN:OE1	2.18	0.43
1:D:195:VAL:HG12	1:D:200:VAL:HG11	2.00	0.43
1:E:179:TRP:NE1	2:L:24:LYS:HB2	2.34	0.43
1:E:449:ILE:HA	1:E:452:LEU:HD12	2.01	0.43
2:K:185:VAL:HG22	2:K:247:CYS:SG	2.59	0.43
2:M:219:GLY:O	2:M:222:ARG:N	2.51	0.43
1:D:95:ALA:C	1:D:97:LYS:N	2.74	0.43
1:E:125:ARG:O	1:E:132:GLN:NE2	2.51	0.43
1:G:126:ASP:OD2	1:G:164:ARG:NH2	2.52	0.43
2:M:324:GLY:HA2	2:M:386:TRP:CE3	2.54	0.43
2:J:117:LEU:HD11	2:J:141:PHE:CE2	2.54	0.43
1:D:469:GLU:H	1:D:469:GLU:CD	2.25	0.43
1:H:241:GLN:NE2	1:H:279:MET:SD	2.91	0.43
2:N:303:GLN:HG3	2:N:304:HIS:ND1	2.34	0.43
1:D:92:VAL:O	1:D:95:ALA:HB3	2.19	0.42
1:G:221:THR:HG22	1:G:250:LEU:HD13	2.00	0.42
1:H:309:GLY:HA3	1:H:348:TRP:HZ3	1.84	0.42
2:L:136:ASP:OD1	2:L:137:ASP:N	2.51	0.42
2:M:150:ASN:CG	2:O:150:ASN:HB3	2.44	0.42
2:J:303:GLN:HG3	2:J:304:HIS:ND1	2.34	0.42
1:B:93:GLN:O	1:B:97:LYS:HG2	2.19	0.42
1:C:120:VAL:O	1:C:123:LEU:HB3	2.19	0.42
1:D:317:GLU:O	1:D:321:VAL:HG23	2.19	0.42
1:A:123:LEU:HD11	1:A:165:LEU:HD11	2.02	0.42
1:D:93:GLN:O	1:D:96:ARG:N	2.53	0.42
2:L:308:CYS:SG	2:L:316:TYR:HB2	2.59	0.42
2:L:324:GLY:HA2	2:L:386:TRP:CE3	2.55	0.42
2:M:152:VAL:HG12	2:M:154:GLY:H	1.84	0.42
2:M:348:SER:HB3	2:M:362:LYS:HA	2.00	0.42
2:N:402:LEU:HD11	2:N:416:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:91:PHE:HB3	2:P:112:PRO:HA	2.02	0.42
2:P:174:VAL:HA	2:P:188:THR:HA	2.00	0.42
2:J:152:VAL:HG12	2:J:154:GLY:H	1.84	0.42
1:A:151:GLN:HA	1:A:154:VAL:HG22	2.01	0.42
1:C:232:ASP:HB3	1:C:233:PRO:HD3	2.00	0.42
2:K:330:GLU:HA	2:K:386:TRP:HB3	2.01	0.42
2:L:361:THR:OG1	2:L:363:ASP:OD1	2.21	0.42
2:O:348:SER:HB3	2:O:362:LYS:HA	2.00	0.42
2:J:194:TYR:HE1	2:J:228:CYS:HB2	1.84	0.42
1:A:116:LEU:CD2	1:A:142:ILE:HD13	2.47	0.42
1:E:221:THR:HG22	1:E:250:LEU:HD13	2.02	0.42
2:I:208:PRO:HB3	2:I:282:ILE:HD11	2.01	0.42
2:O:303:GLN:HG3	2:O:304:HIS:ND1	2.35	0.42
2:P:36:LEU:O	2:P:414:LEU:HD12	2.20	0.42
2:J:395:GLN:OE1	2:J:399:ARG:NH1	2.52	0.42
1:D:229:ARG:NH1	1:D:268:TYR:OH	2.53	0.42
1:D:348:TRP:O	1:D:351:SER:OG	2.25	0.42
1:F:195:VAL:HG12	1:F:200:VAL:HG11	2.00	0.42
2:K:119:GLU:HG3	2:K:141:PHE:CE2	2.54	0.42
2:P:117:LEU:HD11	2:P:141:PHE:CE2	2.55	0.42
1:E:289:LEU:HD12	1:E:292:LEU:HD12	2.00	0.42
1:F:461:LYS:O	1:F:465:LEU:HG	2.19	0.42
1:G:463:GLU:O	1:G:466:GLN:HG2	2.18	0.42
1:H:308:VAL:HG12	1:H:349:PHE:HE1	1.84	0.42
1:A:390:TRP:CE3	2:K:9:ARG:HD2	2.55	0.42
1:E:348:TRP:O	1:E:351:SER:OG	2.26	0.42
1:G:310:ASN:O	1:G:313:THR:OG1	2.27	0.42
1:G:449:ILE:HA	1:G:452:LEU:HD12	2.02	0.42
2:O:330:GLU:HA	2:O:386:TRP:HB3	2.01	0.42
1:G:462:ILE:HG22	1:G:481:ILE:HD11	2.02	0.42
1:H:137:TRP:HE1	2:O:26:SER:HB2	1.85	0.42
2:L:174:VAL:HA	2:L:188:THR:HA	2.01	0.42
2:L:330:GLU:HA	2:L:386:TRP:HB3	2.01	0.42
2:M:117:LEU:HD11	2:M:141:PHE:CE2	2.55	0.42
2:P:10:ARG:HG2	2:P:11:SER:N	2.34	0.42
2:P:348:SER:HB3	2:P:362:LYS:HA	2.01	0.42
1:A:104:ASN:OD1	2:K:257:HIS:CD2	2.72	0.42
1:A:289:LEU:HD12	1:A:292:LEU:HD12	2.01	0.42
1:C:390:TRP:CE3	2:J:9:ARG:HD2	2.54	0.42
1:F:105:PRO:N	1:F:106:PRO:CD	2.83	0.42
1:F:231:LYS:HD3	1:F:271:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:206:ARG:HB3	2:I:229:VAL:HG22	2.02	0.42
2:K:152:VAL:HG12	2:K:154:GLY:H	1.85	0.42
2:M:302:GLY:HA3	2:M:305:HIS:CE1	2.54	0.42
2:K:207:VAL:HB	2:K:211:PHE:CE1	2.54	0.41
2:M:3:PRO:HB2	2:M:4:LYS:H	1.65	0.41
2:M:208:PRO:HB3	2:M:282:ILE:HD11	2.01	0.41
2:P:402:LEU:HD11	2:P:416:LYS:HB2	2.01	0.41
1:A:256:VAL:O	1:A:260:VAL:HG23	2.20	0.41
1:A:308:VAL:HA	1:A:311:ILE:HD12	2.02	0.41
1:B:208:ILE:HD11	1:B:224:MET:HE1	2.02	0.41
1:G:407:LEU:HG	1:G:412:VAL:HG11	2.02	0.41
2:L:201:GLN:HB3	2:L:266:LEU:HB2	2.01	0.41
2:L:402:LEU:HD11	2:L:416:LYS:HB2	2.01	0.41
2:N:302:GLY:HA3	2:N:305:HIS:CE1	2.55	0.41
2:O:248:GLY:HA3	2:O:251:PHE:CE2	2.55	0.41
2:O:324:GLY:HA2	2:O:386:TRP:CE3	2.54	0.41
1:C:76:ILE:HG21	1:C:95:ALA:HB2	2.01	0.41
1:D:96:ARG:HG2	1:D:137:TRP:CG	2.55	0.41
1:D:125:ARG:O	1:D:132:GLN:NE2	2.48	0.41
1:F:352:ASN:O	2:M:8:LYS:HE3	2.19	0.41
1:G:328:LEU:HA	1:G:331:PHE:CD2	2.56	0.41
2:I:348:SER:HB3	2:I:362:LYS:HA	2.01	0.41
2:K:132:ALA:HB2	2:K:142:LEU:HD13	2.02	0.41
2:L:152:VAL:HG12	2:L:154:GLY:H	1.86	0.41
2:L:358:TYR:OH	2:L:376:GLN:O	2.29	0.41
2:M:10:ARG:HG3	2:M:11:SER:H	1.85	0.41
2:M:248:GLY:HA3	2:M:251:PHE:CE2	2.55	0.41
2:M:371:MET:HG2	2:M:373:THR:H	1.85	0.41
2:O:174:VAL:HA	2:O:188:THR:HA	2.01	0.41
1:A:420:LEU:HB3	1:A:465:LEU:HD11	2.02	0.41
1:B:120:VAL:O	1:B:123:LEU:HB3	2.20	0.41
1:B:232:ASP:HB3	1:B:233:PRO:CD	2.50	0.41
1:D:95:ALA:O	1:D:97:LYS:N	2.53	0.41
1:E:229:ARG:NH2	2:L:20:SER:HB3	2.36	0.41
2:L:244:ASP:OD1	2:L:245:ALA:N	2.49	0.41
2:M:330:GLU:HA	2:M:386:TRP:HB3	2.02	0.41
2:N:174:VAL:HA	2:N:188:THR:HA	2.01	0.41
2:O:67:GLU:OE1	2:O:85:SER:OG	2.36	0.41
2:J:324:GLY:HA2	2:J:386:TRP:CE3	2.55	0.41
2:J:347:VAL:HA	2:J:361:THR:HA	2.02	0.41
1:C:466:GLN:OE1	2:O:58:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:ILE:HD11	1:H:224:MET:HE1	2.02	0.41
2:K:19:LYS:O	2:K:20:SER:HB3	2.20	0.41
2:K:47:GLN:HG3	2:K:410:HIS:ND1	2.36	0.41
2:K:202:GLY:HA3	2:K:281:PHE:CD1	2.56	0.41
2:K:376:GLN:NE2	2:K:408:GLY:O	2.53	0.41
2:L:47:GLN:HG3	2:L:410:HIS:ND1	2.35	0.41
2:L:371:MET:HG2	2:L:373:THR:H	1.86	0.41
2:N:47:GLN:HG3	2:N:410:HIS:ND1	2.36	0.41
2:P:38:LEU:HB2	2:P:413:LEU:HB2	2.03	0.41
2:J:36:LEU:O	2:J:414:LEU:HD12	2.21	0.41
1:B:194:TYR:O	1:B:197:SER:OG	2.28	0.41
1:F:115:ILE:HA	1:F:118:ILE:HG12	2.02	0.41
2:I:347:VAL:HA	2:I:361:THR:HA	2.02	0.41
2:K:348:SER:HB3	2:K:362:LYS:HA	2.02	0.41
2:L:38:LEU:HB2	2:L:413:LEU:HB2	2.02	0.41
2:M:310:ASP:OD1	2:M:314:LYS:N	2.54	0.41
2:O:119:GLU:HG3	2:O:141:PHE:CE2	2.55	0.41
1:B:416:PHE:CZ	1:B:431:VAL:HA	2.55	0.41
1:D:99:LEU:HD12	2:P:25:VAL:HA	2.02	0.41
1:E:328:LEU:HA	1:E:331:PHE:CD2	2.55	0.41
1:H:115:ILE:HG22	1:H:119:LEU:HD23	2.03	0.41
1:H:144:SER:HB2	2:O:23:VAL:HG22	2.03	0.41
2:K:378:GLY:HA3	2:K:391:MET:HE3	2.03	0.41
2:L:6:ILE:HG22	2:L:7:ALA:H	1.86	0.41
2:M:127:GLY:HA3	2:M:130:HIS:NE2	2.35	0.41
2:N:119:GLU:HG3	2:N:141:PHE:CE2	2.56	0.41
2:N:282:ILE:O	2:N:284:GLN:N	2.54	0.41
2:O:119:GLU:HG3	2:O:141:PHE:HE2	1.85	0.41
2:J:14:ALA:HB3	2:J:17:ILE:HG13	2.03	0.41
1:A:137:TRP:CH2	2:K:24:LYS:HE3	2.56	0.41
1:B:126:ASP:OD2	1:B:164:ARG:NH2	2.53	0.41
1:B:461:LYS:O	1:B:465:LEU:HG	2.21	0.41
1:D:115:ILE:HA	1:D:118:ILE:HD12	2.03	0.41
1:F:92:VAL:HG11	1:F:131:LEU:HD12	2.02	0.41
1:F:96:ARG:HD2	1:F:137:TRP:CG	2.56	0.41
1:F:310:ASN:O	1:F:313:THR:OG1	2.28	0.41
2:I:45:VAL:HG21	2:I:93:CYS:HB2	2.03	0.41
2:L:135:THR:OG1	2:L:137:ASP:OD1	2.34	0.41
2:M:174:VAL:HA	2:M:188:THR:HA	2.03	0.41
2:N:201:GLN:HB3	2:N:266:LEU:HB2	2.02	0.41
2:P:303:GLN:HG3	2:P:304:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:6:ILE:HG22	2:J:7:ALA:N	2.36	0.41
2:J:45:VAL:HG21	2:J:93:CYS:HB2	2.03	0.41
1:C:420:LEU:HB3	1:C:465:LEU:HD11	2.02	0.41
1:D:229:ARG:HG2	1:D:230:HIS:N	2.36	0.41
2:I:201:GLN:HB3	2:I:266:LEU:HB2	2.03	0.41
2:I:243:GLN:HE21	2:I:257:HIS:HA	1.86	0.41
2:N:152:VAL:HG12	2:N:154:GLY:H	1.84	0.41
2:O:91:PHE:HB3	2:O:112:PRO:HA	2.02	0.41
2:O:282:ILE:O	2:O:284:GLN:N	2.54	0.41
2:P:201:GLN:HB3	2:P:266:LEU:HB2	2.02	0.41
1:C:176:GLN:HE22	2:J:24:LYS:HD3	1.86	0.40
1:C:390:TRP:HZ2	1:C:426:GLN:HE21	1.67	0.40
1:D:328:LEU:HA	1:D:331:PHE:CD2	2.55	0.40
1:F:229:ARG:HG2	1:F:230:HIS:N	2.36	0.40
2:O:402:LEU:HD11	2:O:416:LYS:HB2	2.03	0.40
1:B:241:GLN:NE2	1:B:279:MET:SD	2.93	0.40
1:D:96:ARG:HB2	1:D:134:GLU:OE1	2.21	0.40
2:I:206:ARG:NH2	2:I:225:VAL:O	2.54	0.40
2:K:402:LEU:HD11	2:K:416:LYS:HB2	2.03	0.40
2:L:91:PHE:HB3	2:L:112:PRO:HA	2.03	0.40
2:M:282:ILE:O	2:M:284:GLN:N	2.53	0.40
2:M:303:GLN:HG3	2:M:304:HIS:ND1	2.36	0.40
2:N:38:LEU:HB2	2:N:413:LEU:HB2	2.02	0.40
2:J:202:GLY:HA3	2:J:281:PHE:CD1	2.56	0.40
1:B:144:SER:CB	2:I:23:VAL:HG22	2.52	0.40
1:D:221:THR:HG21	1:D:258:ILE:HG23	2.03	0.40
1:G:115:ILE:CG2	1:G:119:LEU:CD1	2.99	0.40
1:H:100:SER:OG	2:O:26:SER:HB3	2.22	0.40
2:K:146:PHE:CE2	2:K:155:LEU:HD12	2.56	0.40
2:L:194:TYR:CE1	2:L:228:CYS:HB2	2.56	0.40
2:L:233:SER:N	2:L:236:SER:OG	2.28	0.40
2:M:201:GLN:HB3	2:M:266:LEU:HB2	2.02	0.40
1:B:115:ILE:O	1:B:119:LEU:HG	2.22	0.40
1:C:208:ILE:HD11	1:C:224:MET:HE1	2.03	0.40
1:C:241:GLN:HA	1:C:241:GLN:OE1	2.22	0.40
1:F:100:SER:HB2	1:F:141:ASN:HD22	1.86	0.40
1:G:416:PHE:CZ	1:G:431:VAL:HA	2.56	0.40
2:I:308:CYS:SG	2:I:316:TYR:HB2	2.62	0.40
2:K:282:ILE:O	2:K:284:GLN:N	2.55	0.40
2:L:67:GLU:OE1	2:L:85:SER:OG	2.38	0.40
2:L:303:GLN:HG3	2:L:304:HIS:ND1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:308:CYS:SG	2:O:316:TYR:HB2	2.62	0.40
2:J:348:SER:HB3	2:J:362:LYS:HA	2.03	0.40
1:B:395:LEU:HD22	1:B:407:LEU:HD22	2.03	0.40
1:C:125:ARG:O	1:C:132:GLN:NE2	2.53	0.40
1:E:202:LYS:HB3	1:E:203:PRO:HD3	2.04	0.40
1:F:413:ILE:HB	1:F:414:PRO:HD3	2.03	0.40
2:I:117:LEU:HD11	2:I:141:PHE:CE2	2.56	0.40
2:I:282:ILE:O	2:I:284:GLN:N	2.54	0.40
2:L:282:ILE:O	2:L:284:GLN:N	2.54	0.40
2:M:206:ARG:NH2	2:M:225:VAL:O	2.54	0.40
2:N:148:ASP:C	2:N:150:ASN:H	2.30	0.40
2:P:152:VAL:HG12	2:P:154:GLY:H	1.87	0.40
2:P:206:ARG:NH2	2:P:225:VAL:O	2.54	0.40
2:P:378:GLY:HA3	2:P:391:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/521 (80%)	404 (97%)	11 (3%)	0	100	100
1	B	413/521 (79%)	400 (97%)	13 (3%)	0	100	100
1	C	415/521 (80%)	402 (97%)	13 (3%)	0	100	100
1	D	413/521 (79%)	406 (98%)	7 (2%)	0	100	100
1	E	414/521 (80%)	401 (97%)	13 (3%)	0	100	100
1	F	414/521 (80%)	400 (97%)	14 (3%)	0	100	100
1	G	415/521 (80%)	404 (97%)	11 (3%)	0	100	100
1	H	415/521 (80%)	403 (97%)	12 (3%)	0	100	100
2	I	417/421 (99%)	396 (95%)	21 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	416/421 (99%)	394 (95%)	22 (5%)	0	100	100
2	K	416/421 (99%)	395 (95%)	21 (5%)	0	100	100
2	L	416/421 (99%)	395 (95%)	21 (5%)	0	100	100
2	M	417/421 (99%)	396 (95%)	21 (5%)	0	100	100
2	N	416/421 (99%)	396 (95%)	20 (5%)	0	100	100
2	O	416/421 (99%)	394 (95%)	22 (5%)	0	100	100
2	P	417/421 (99%)	394 (94%)	23 (6%)	0	100	100
All	All	6645/7536 (88%)	6380 (96%)	265 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/460 (79%)	365 (100%)	0	100	100
1	B	357/460 (78%)	357 (100%)	0	100	100
1	C	359/460 (78%)	359 (100%)	0	100	100
1	D	363/460 (79%)	363 (100%)	0	100	100
1	E	358/460 (78%)	358 (100%)	0	100	100
1	F	358/460 (78%)	358 (100%)	0	100	100
1	G	359/460 (78%)	359 (100%)	0	100	100
1	H	359/460 (78%)	359 (100%)	0	100	100
2	I	339/341 (99%)	339 (100%)	0	100	100
2	J	338/341 (99%)	338 (100%)	0	100	100
2	K	338/341 (99%)	338 (100%)	0	100	100
2	L	338/341 (99%)	338 (100%)	0	100	100
2	M	339/341 (99%)	339 (100%)	0	100	100
2	N	338/341 (99%)	338 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	338/341 (99%)	338 (100%)	0	100	100
2	P	339/341 (99%)	339 (100%)	0	100	100
All	All	5585/6408 (87%)	5585 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	170	HIS
1	A	257	ASN
1	A	426	GLN
1	B	151	GLN
1	B	170	HIS
1	C	151	GLN
1	C	170	HIS
1	C	257	ASN
1	C	320	GLN
1	C	426	GLN
1	D	121	HIS
1	D	151	GLN
1	D	170	HIS
1	D	257	ASN
1	D	362	GLN
1	D	403	GLN
1	D	470	ASN
1	E	151	GLN
1	E	170	HIS
1	E	257	ASN
1	E	324	ASN
1	E	426	GLN
1	F	151	GLN
1	F	170	HIS
1	F	426	GLN
1	G	151	GLN
1	G	170	HIS
1	G	324	ASN
1	H	151	GLN
1	H	170	HIS
1	H	257	ASN
1	H	320	GLN

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Mol	Chain	Res	Type
1	H	426	GLN
2	I	30	HIS
2	I	243	GLN
2	I	409	GLN
2	K	71	GLN
2	K	257	HIS
2	K	376	GLN
2	K	409	GLN
2	L	71	GLN
2	L	409	GLN
2	M	71	GLN
2	M	257	HIS
2	M	376	GLN
2	N	71	GLN
2	N	409	GLN
2	O	149	ASN
2	O	409	GLN
2	P	71	GLN
2	P	409	GLN
2	J	71	GLN
2	J	118	GLN
2	J	123	GLN
2	J	257	HIS
2	J	409	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	417/521 (80%)	0.11	15 (3%)	46	27	23, 67, 143, 273	0
1	B	415/521 (79%)	0.27	19 (4%)	37	21	38, 103, 178, 245	0
1	C	417/521 (80%)	0.12	12 (2%)	53	32	30, 76, 142, 224	0
1	D	415/521 (79%)	0.35	26 (6%)	26	17	52, 105, 196, 263	0
1	E	416/521 (79%)	0.23	20 (4%)	35	21	54, 108, 196, 292	0
1	F	416/521 (79%)	0.15	15 (3%)	46	27	57, 92, 162, 213	0
1	G	417/521 (80%)	0.24	13 (3%)	51	31	64, 103, 170, 241	0
1	H	417/521 (80%)	0.19	5 (1%)	76	53	58, 106, 211, 289	0
2	I	419/421 (99%)	0.63	34 (8%)	18	13	88, 157, 289, 394	0
2	J	418/421 (99%)	0.10	6 (1%)	73	49	61, 102, 169, 241	0
2	K	418/421 (99%)	0.15	11 (2%)	57	34	60, 108, 170, 220	0
2	L	418/421 (99%)	0.51	28 (6%)	24	16	89, 175, 288, 361	0
2	M	419/421 (99%)	0.37	20 (4%)	35	21	63, 129, 277, 346	0
2	N	418/421 (99%)	0.38	20 (4%)	35	21	85, 155, 274, 342	0
2	O	418/421 (99%)	0.38	17 (4%)	41	24	54, 154, 279, 341	0
2	P	419/421 (99%)	0.75	51 (12%)	8	7	90, 169, 296, 368	0
All	All	6677/7536 (88%)	0.31	312 (4%)	36	21	23, 116, 246, 394	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	223	LEU	7.1
1	D	105	PRO	7.0
2	N	155	LEU	6.2
1	F	394	ASN	6.0
2	L	155	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
2	O	223	LEU	5.6
2	P	223	LEU	5.6
2	P	25	VAL	5.3
2	I	272	LEU	5.2
1	A	72	SER	5.0
2	O	155	LEU	4.9
2	N	272	LEU	4.9
2	P	155	LEU	4.9
1	B	303	ALA	4.7
1	H	290	VAL	4.7
2	I	155	LEU	4.7
1	E	261	ASP	4.4
2	O	272	LEU	4.3
2	L	401	VAL	4.2
1	F	269	LEU	4.2
1	F	311	ILE	4.1
2	I	220	LEU	4.1
2	P	154	GLY	4.0
2	M	197	GLY	3.9
2	P	120	LYS	3.8
2	K	351	ALA	3.8
1	C	78	GLN	3.7
1	D	230	HIS	3.7
2	L	21	LYS	3.7
1	G	109	ASP	3.6
2	L	223	LEU	3.6
2	P	242	PHE	3.6
1	B	299	LYS	3.6
1	A	110	LEU	3.5
1	D	345	GLU	3.5
1	F	109	ASP	3.5
2	P	213	ASN	3.4
2	I	327	GLY	3.4
1	D	417	CYS	3.4
2	N	250	TYR	3.4
2	O	250	TYR	3.4
2	M	155	LEU	3.4
1	F	486	SER	3.4
2	L	299	PHE	3.4
1	G	476	LEU	3.4
2	L	133	ALA	3.4
2	P	212	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	I	203	GLN	3.4
2	P	173	PRO	3.3
2	K	325	ARG	3.3
1	C	72	SER	3.3
2	I	242	PHE	3.3
2	P	207	VAL	3.3
2	P	126	ALA	3.3
2	L	220	LEU	3.2
1	A	91	ALA	3.2
2	P	355	SER	3.2
1	D	279	MET	3.2
1	D	267	SER	3.2
1	F	111	ILE	3.2
1	E	455	GLU	3.2
2	I	213	ASN	3.2
1	D	100	SER	3.2
2	P	24	LYS	3.1
2	P	272	LEU	3.1
2	I	245	ALA	3.1
1	C	111	ILE	3.1
2	P	77	MET	3.1
2	K	50	LEU	3.1
2	L	23	VAL	3.1
2	O	220	LEU	3.1
2	I	404	VAL	3.1
1	D	261	ASP	3.1
1	A	105	PRO	3.1
2	P	250	TYR	3.1
2	K	272	LEU	3.0
1	F	318	GLN	3.0
2	L	159	MET	3.0
2	P	81	CYS	3.0
2	M	263	GLY	3.0
1	E	111	ILE	3.0
1	B	105	PRO	3.0
2	P	48	LEU	3.0
2	P	299	PHE	3.0
1	A	242	GLU	3.0
2	I	173	PRO	3.0
2	L	262	TYR	3.0
1	F	433	ASP	3.0
2	N	223	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	199	GLY	2.9
1	A	401	LYS	2.9
2	I	20	SER	2.9
2	M	81	CYS	2.9
2	I	297	VAL	2.9
2	N	78	HIS	2.9
1	E	419	LEU	2.9
2	K	118	GLN	2.9
2	L	156	LEU	2.9
2	P	211	PHE	2.9
1	F	73	LEU	2.9
2	I	212	ALA	2.9
2	O	81	CYS	2.9
2	K	205	GLY	2.9
2	P	380	GLY	2.9
1	B	462	ILE	2.9
2	P	266	LEU	2.9
2	P	3	PRO	2.8
2	I	25	VAL	2.8
1	C	401	LYS	2.8
1	F	273	GLY	2.8
2	M	204	LEU	2.8
2	P	220	LEU	2.8
2	P	215	GLY	2.8
1	D	303	ALA	2.8
2	P	217	ARG	2.8
1	E	235	PRO	2.8
1	D	376	LEU	2.8
1	A	73	LEU	2.7
2	N	328	LEU	2.7
1	F	390	TRP	2.7
1	D	122	CYS	2.7
2	I	270	HIS	2.7
2	J	118	GLN	2.7
1	G	471	GLU	2.7
1	D	72	SER	2.7
2	L	20	SER	2.7
1	A	95	ALA	2.7
2	L	78	HIS	2.7
2	M	6	ILE	2.7
2	N	77	MET	2.7
1	E	259	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	108	ASP	2.7
2	P	18	PRO	2.6
2	I	216	GLY	2.6
2	L	154	GLY	2.6
1	D	228	CYS	2.6
2	P	210	LEU	2.6
2	L	58	LYS	2.6
2	O	78	HIS	2.6
1	A	466	GLN	2.6
2	L	153	ILE	2.6
1	B	230	HIS	2.6
1	E	486	SER	2.6
1	B	381	ASP	2.6
1	B	80	ALA	2.6
1	G	474	TYR	2.6
2	P	358	TYR	2.6
2	O	327	GLY	2.6
2	L	174	VAL	2.6
1	C	262	THR	2.6
1	B	465	LEU	2.5
2	L	272	LEU	2.5
1	D	94	ALA	2.5
1	D	384	THR	2.5
2	L	296	TRP	2.5
2	M	296	TRP	2.5
1	D	248	CYS	2.5
2	N	184	LEU	2.5
1	E	79	ASN	2.5
2	O	266	LEU	2.5
2	P	385	ALA	2.5
2	N	266	LEU	2.5
2	P	216	GLY	2.5
1	D	92	VAL	2.5
2	M	303	GLN	2.5
2	L	132	ALA	2.5
1	C	242	GLU	2.5
1	G	187	ASP	2.5
1	E	465	LEU	2.5
1	F	244	LEU	2.5
2	I	389	VAL	2.5
1	B	417	CYS	2.4
1	E	463	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	275	GLU	2.4
2	I	77	MET	2.4
1	D	420	LEU	2.4
2	I	215	GLY	2.4
2	O	199	GLY	2.4
1	C	228	CYS	2.4
2	I	125	SER	2.4
1	F	476	LEU	2.4
2	M	326	LEU	2.4
1	C	109	ASP	2.4
2	L	408	GLY	2.4
1	D	73	LEU	2.4
2	P	150	ASN	2.4
2	N	152	VAL	2.4
2	P	261	VAL	2.4
2	P	197	GLY	2.4
1	H	80	ALA	2.4
2	P	110	MET	2.4
2	I	299	PHE	2.4
2	M	266	LEU	2.4
1	E	425	ALA	2.4
1	D	299	LYS	2.4
2	M	223	LEU	2.4
2	P	152	VAL	2.4
2	I	198	CYS	2.4
2	O	273	GLY	2.3
1	C	403	GLN	2.3
1	F	471	GLU	2.3
2	P	39	THR	2.3
2	M	134	LEU	2.3
2	N	156	LEU	2.3
1	B	463	GLU	2.3
1	C	474	TYR	2.3
1	E	89	LEU	2.3
2	I	217	ARG	2.3
2	N	217	ARG	2.3
1	G	123	LEU	2.3
1	G	269	LEU	2.3
2	M	78	HIS	2.3
1	H	122	CYS	2.3
2	P	19	LYS	2.3
2	O	154	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	51	GLY	2.3
2	O	296	TRP	2.3
2	I	224	LEU	2.3
2	N	220	LEU	2.3
2	I	355	SER	2.3
1	B	474	TYR	2.3
2	P	389	VAL	2.3
2	L	17	ILE	2.2
2	M	153	ILE	2.2
2	M	14	ALA	2.2
1	D	99	LEU	2.2
1	G	354	THR	2.2
1	E	478	TYR	2.2
1	A	248	CYS	2.2
2	L	207	VAL	2.2
2	N	197	GLY	2.2
1	B	416	PHE	2.2
1	C	487	SER	2.2
2	P	405	SER	2.2
1	H	111	ILE	2.2
2	I	17	ILE	2.2
2	K	81	CYS	2.2
1	F	420	LEU	2.2
2	L	24	LYS	2.2
2	P	270	HIS	2.2
1	A	478	TYR	2.2
2	O	262	TYR	2.2
2	K	23	VAL	2.2
2	I	266	LEU	2.2
2	K	266	LEU	2.2
2	O	326	LEU	2.2
2	P	99	LEU	2.2
1	B	307	ALA	2.2
2	N	332	ALA	2.2
2	P	198	CYS	2.2
2	P	199	GLY	2.2
2	P	205	GLY	2.2
2	J	351	ALA	2.2
2	M	177	VAL	2.2
1	D	465	LEU	2.2
1	E	452	LEU	2.2
1	H	387	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	391	MET	2.2
1	G	235	PRO	2.2
2	N	388	PRO	2.2
2	P	151	GLY	2.2
2	P	253	PHE	2.2
1	E	290	VAL	2.1
2	I	175	VAL	2.1
2	L	261	VAL	2.1
1	E	247	LEU	2.1
2	P	328	LEU	2.1
2	M	403	SER	2.1
1	B	384	THR	2.1
1	B	305	LEU	2.1
2	I	218	GLN	2.1
2	N	199	GLY	2.1
1	E	153	VAL	2.1
2	J	25	VAL	2.1
1	D	377	LEU	2.1
2	J	326	LEU	2.1
1	C	391	ALA	2.1
1	D	466	GLN	2.1
1	B	380	GLY	2.1
2	M	92	GLY	2.1
2	N	18	PRO	2.1
2	P	356	VAL	2.1
2	N	17	ILE	2.1
2	I	221	GLU	2.1
1	B	100	SER	2.1
2	L	25	VAL	2.1
2	M	37	VAL	2.1
1	D	461	LYS	2.1
1	A	98	LEU	2.1
2	K	326	LEU	2.1
1	G	230	HIS	2.1
2	L	14	ALA	2.1
1	G	431	VAL	2.0
2	L	297	VAL	2.0
2	J	317	SER	2.0
1	D	305	LEU	2.0
1	G	384	THR	2.0
2	K	182	ASP	2.0
1	E	331	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	211	PHE	2.0
2	O	401	VAL	2.0
1	A	353	ILE	2.0
1	E	135	ALA	2.0
2	I	14	ALA	2.0
2	M	262	TYR	2.0
1	B	228	CYS	2.0
2	N	211	PHE	2.0
2	J	327	GLY	2.0
1	A	403	GLN	2.0
1	A	275	GLU	2.0
2	I	200	GLU	2.0
1	B	435	LEU	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 oligosaccharides 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.