



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:57 AM GMT

PDB ID : 2JBP
Title : PROTEIN KINASE MK2 IN COMPLEX WITH AN INHIBITOR (CRYSTAL FORM-2, CO-CRYSTALLIZATION)
Authors : Hillig, R.C.; Eberspaecher, U.; Monteclaro, F.; Huber, M.; Nguyen, D.; Mengel, A.; Muller-Tiemann, B.; Egner, U.
Deposited on : 2006-12-09
Resolution : 3.31 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

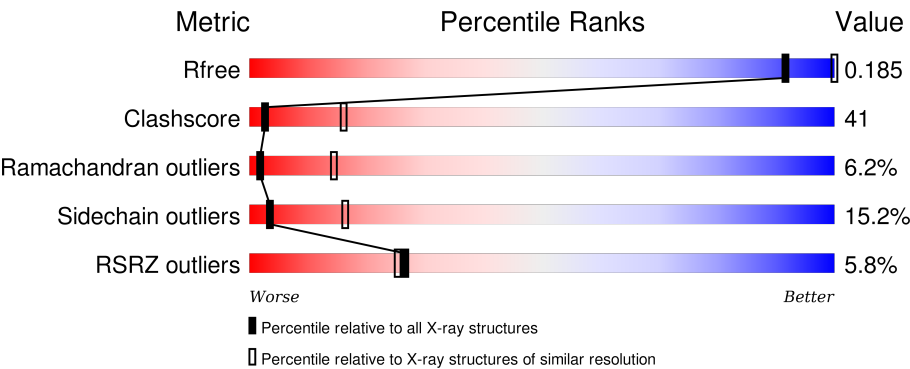
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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 $\leq 5\%$. 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	326	<div><div>45%33%8%13%</div><div></div></div>
1	B	326	<div><div>38%40%10%11%</div><div>3%</div></div>
1	C	326	<div><div>35%43%9%13%</div><div>2%</div></div>
1	D	326	<div><div>39%36%12%12%</div><div>3%</div></div>
1	E	326	<div><div>29%41%17%13%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	326	
1	G	326	
1	H	326	
1	I	326	
1	J	326	
1	K	326	
1	L	326	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P4O	B	1351	-	-	-	X
2	P4O	C	1351	-	-	-	X
2	P4O	E	1345	-	-	-	X
2	P4O	F	1350	-	-	-	X
2	P4O	H	1347	-	-	-	X
2	P4O	I	1351	-	-	-	X
2	P4O	K	1345	-	-	-	X
2	P4O	L	1345	-	-	-	X

2 Entry composition

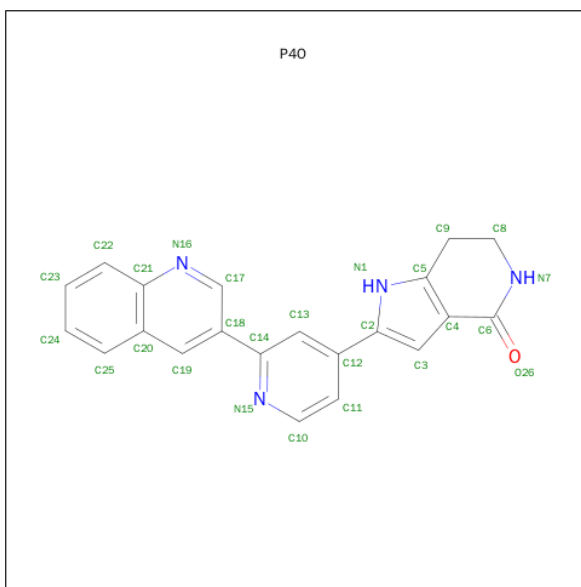
There are 3 unique types of molecules in this entry. The entry contains 27367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAP KINASE-ACTIVATED PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2298	1467	399	415	17			
1	B	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	C	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			
1	D	286	Total	C	N	O	S	0	0	0
			2325	1486	402	420	17			
1	E	283	Total	C	N	O	S	0	0	1
			2291	1467	395	412	17			
1	F	288	Total	C	N	O	S	0	0	1
			2344	1499	405	423	17			
1	G	288	Total	C	N	O	S	0	0	1
			2343	1498	405	423	17			
1	H	283	Total	C	N	O	S	0	0	1
			2289	1464	396	412	17			
1	I	289	Total	C	N	O	S	0	0	0
			2354	1503	407	427	17			
1	J	225	Total	C	N	O	S	0	0	1
			1823	1167	315	326	15			
1	K	265	Total	C	N	O	S	0	0	1
			2142	1367	374	384	17			
1	L	268	Total	C	N	O	S	0	0	1
			2177	1390	379	391	17			

- Molecule 2 is 2-(2-QUINOLIN-3-YPYRIDIN-4-YL)-1,5,6,7-TETRAHYDRO-4H-PYRROLO[3,2-C]PYRIDIN-4-ONE (three-letter code: P4O) (formula: C₂₁H₁₆N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	21	4	1		
2	B	1	Total	C	N	O	0	0
			26	21	4	1		
2	C	1	Total	C	N	O	0	0
			26	21	4	1		
2	D	1	Total	C	N	O	0	0
			26	21	4	1		
2	E	1	Total	C	N	O	0	0
			26	21	4	1		
2	F	1	Total	C	N	O	0	0
			26	21	4	1		
2	G	1	Total	C	N	O	0	0
			26	21	4	1		
2	H	1	Total	C	N	O	0	0
			26	21	4	1		
2	I	1	Total	C	N	O	0	0
			26	21	4	1		
2	K	1	Total	C	N	O	0	0
			26	21	4	1		
2	L	1	Total	C	N	O	0	0
			26	21	4	1		

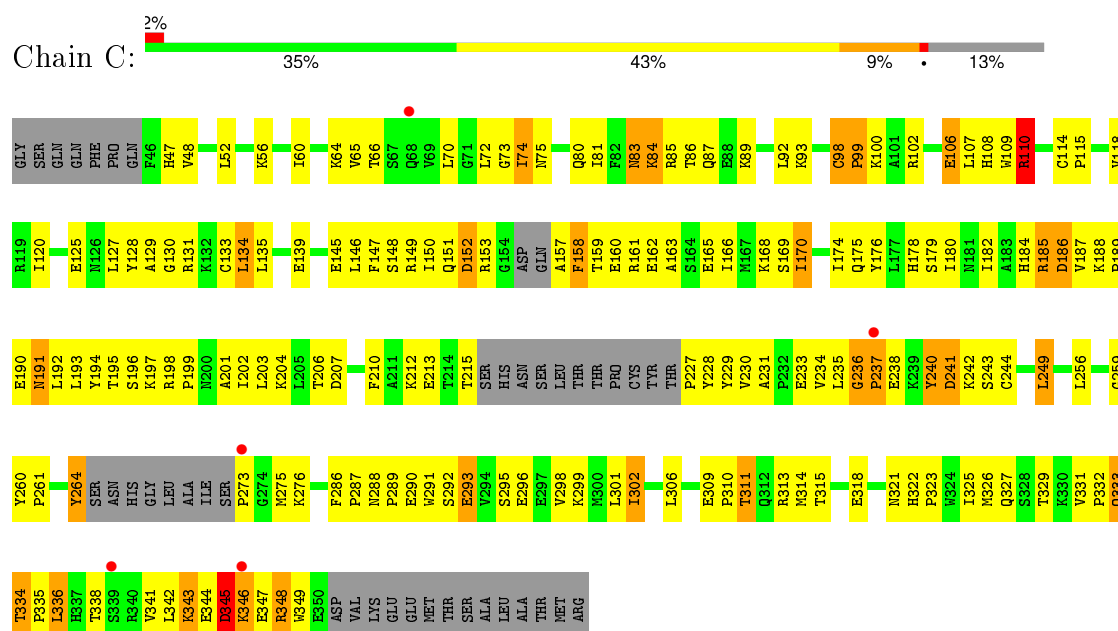
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		

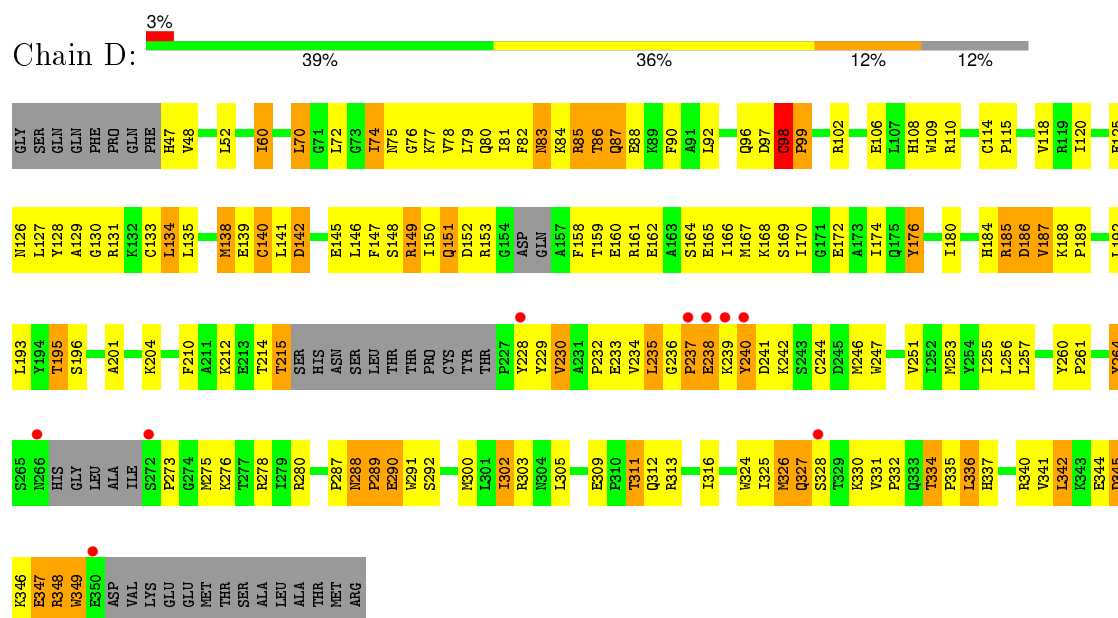
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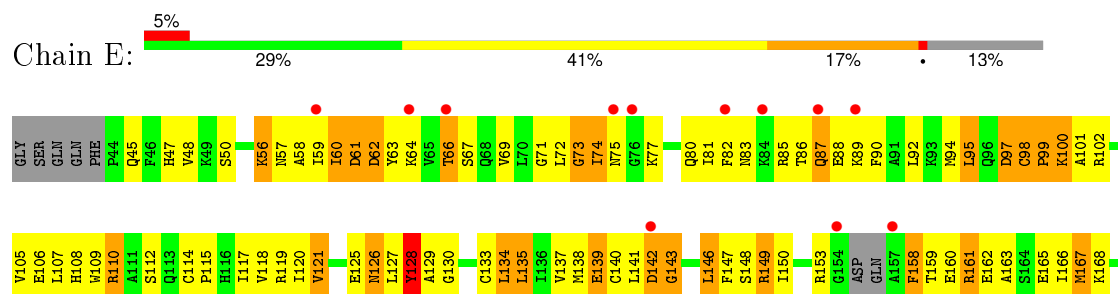
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	O 2	0	0
3	C	2	Total 2	O 2	0	0
3	D	2	Total 2	O 2	0	0
3	E	1	Total 1	O 1	0	0
3	F	2	Total 2	O 2	0	0
3	G	3	Total 3	O 3	0	0
3	I	1	Total 1	O 1	0	0
3	L	1	Total 1	O 1	0	0



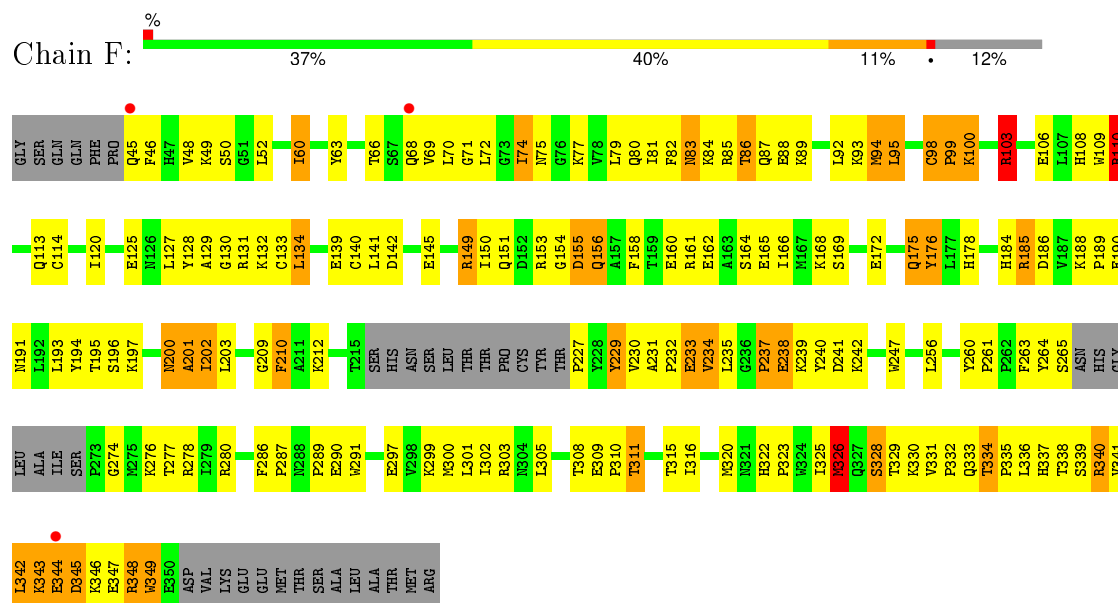
- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



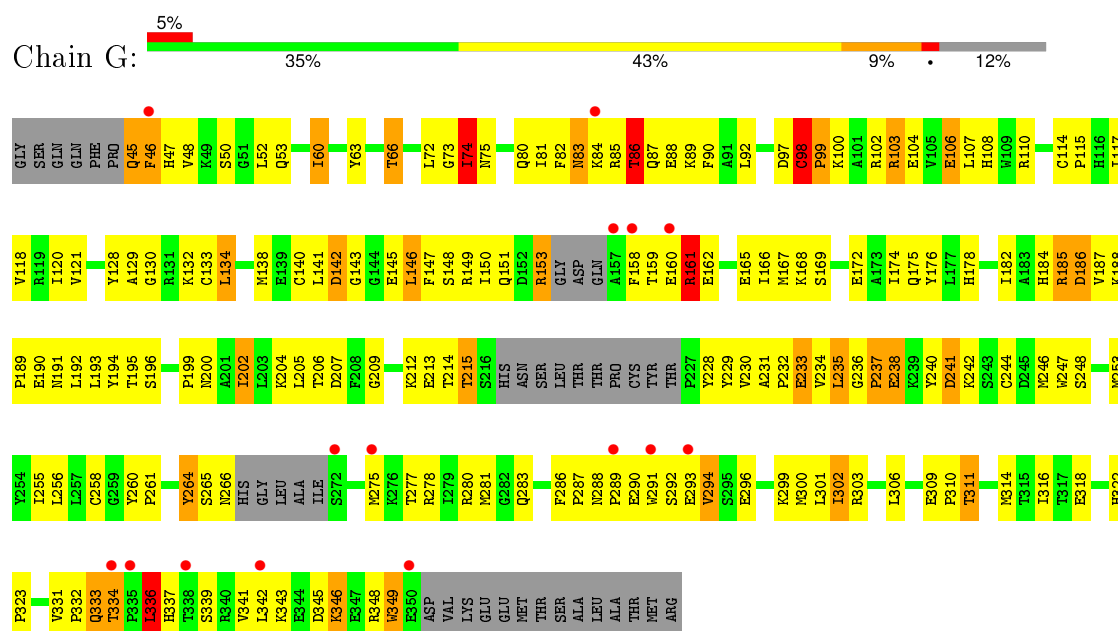
- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



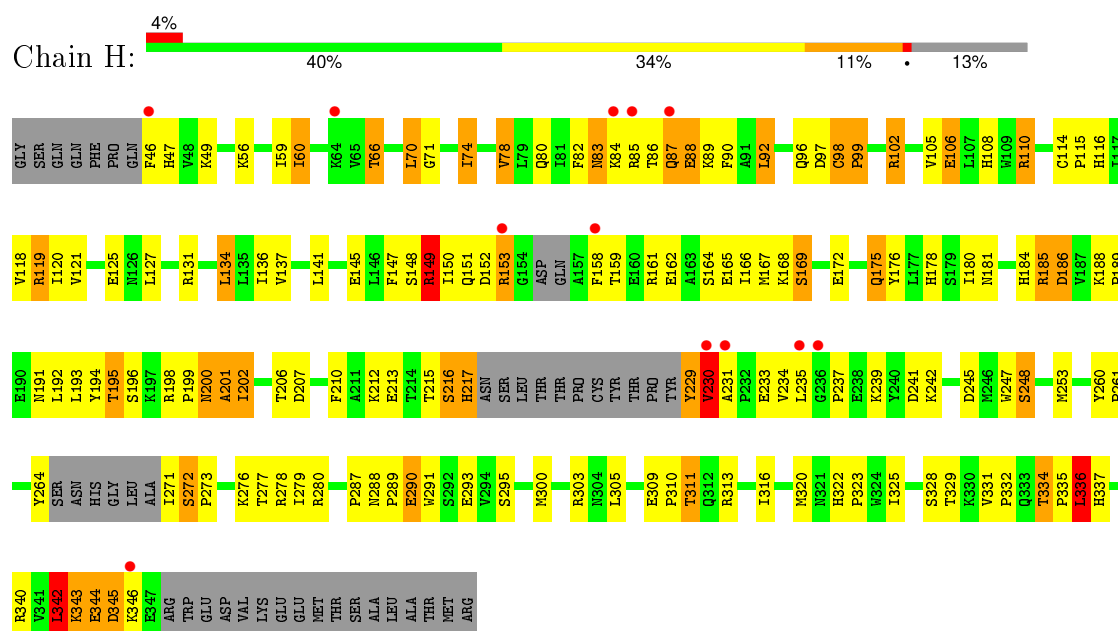
- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



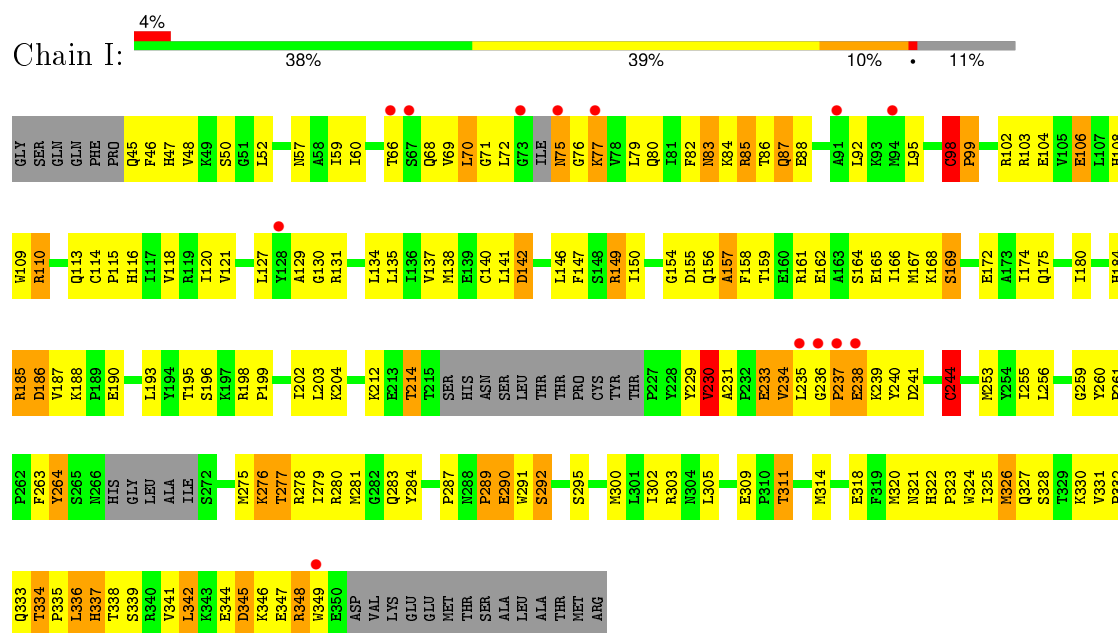
- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



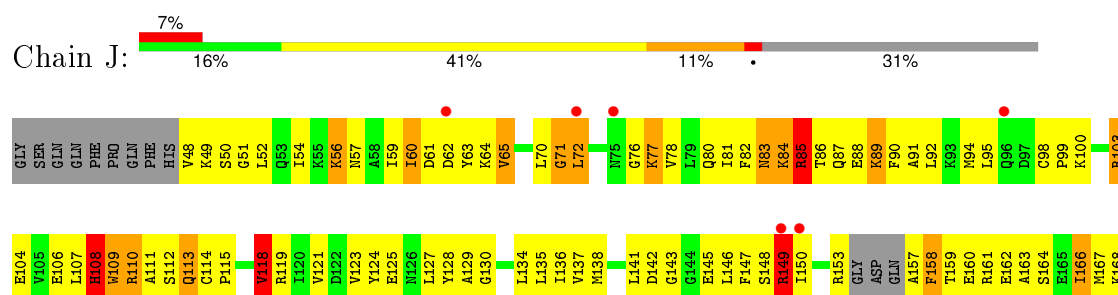
- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

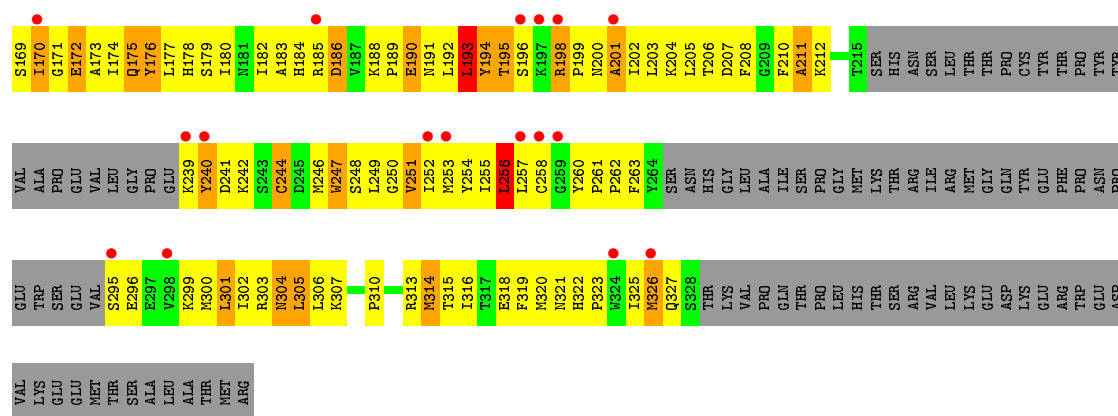


• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

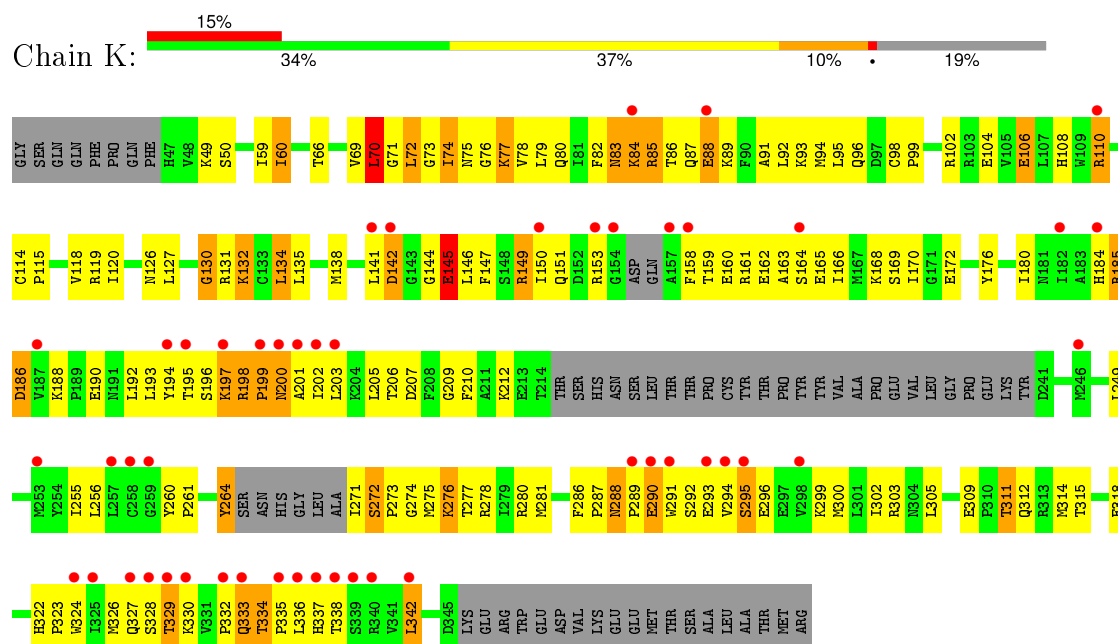


• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

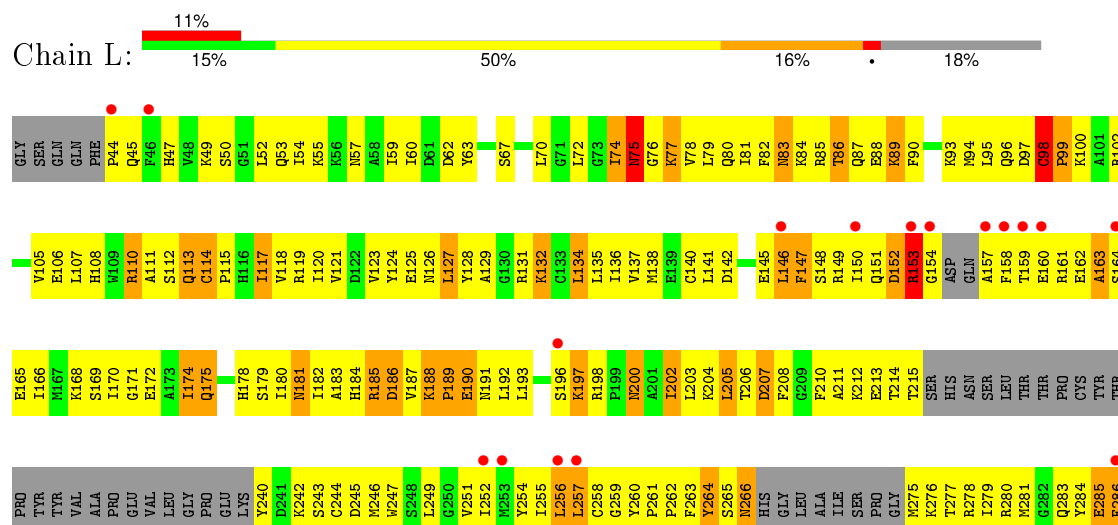


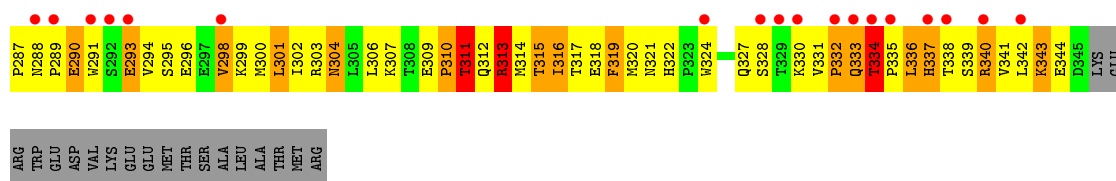


• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.98Å 215.56Å 179.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 3.31 49.08 – 3.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.08-3.31) 96.6 (49.08-3.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.33Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.215 , 0.279 0.195 , 0.185	Depositor DCC
R_{free} test set	3942 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 101.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78628 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27367	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: P4O

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	0.93	3/2346 (0.1%)	0.97	8/3160 (0.3%)
1	B	0.78	1/2413 (0.0%)	0.85	2/3254 (0.1%)
1	C	0.85	1/2367 (0.0%)	0.89	2/3189 (0.1%)
1	D	0.89	5/2375 (0.2%)	0.92	2/3201 (0.1%)
1	E	0.65	0/2341	0.83	1/3155 (0.0%)
1	F	0.94	2/2396 (0.1%)	0.97	4/3230 (0.1%)
1	G	0.77	0/2394	0.91	8/3227 (0.2%)
1	H	0.65	0/2337	0.82	6/3149 (0.2%)
1	I	0.72	1/2405 (0.0%)	0.88	3/3241 (0.1%)
1	J	0.57	0/1855	0.76	0/2493
1	K	0.55	0/2184	0.74	2/2940 (0.1%)
1	L	0.59	1/2221 (0.0%)	0.78	2/2990 (0.1%)
All	All	0.76	14/27634 (0.1%)	0.87	40/37229 (0.1%)

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	B	0	1
1	D	0	2
1	F	0	2
1	G	0	2
1	I	0	1
All	All	0	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	CYS	CB-SG	-7.21	1.70	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	320	MET	SD-CE	-7.17	1.37	1.77
1	A	98	CYS	CB-SG	-6.25	1.71	1.82
1	D	140	CYS	CB-SG	-6.21	1.71	1.82
1	I	244	CYS	CB-SG	-6.20	1.71	1.82
1	C	244	CYS	CB-SG	-5.87	1.72	1.81
1	D	133	CYS	CB-SG	-5.67	1.72	1.81
1	D	98	CYS	CB-SG	-5.66	1.72	1.81
1	D	244	CYS	CB-SG	-5.58	1.72	1.81
1	A	138	MET	SD-CE	-5.46	1.47	1.77
1	A	313	ARG	CZ-NH1	-5.30	1.26	1.33
1	D	187	VAL	CA-CB	-5.29	1.43	1.54
1	F	202	ILE	CA-CB	-5.16	1.43	1.54
1	L	98	CYS	CB-SG	-5.03	1.73	1.81

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	185	ARG	NE-CZ-NH1	-10.42	115.09	120.30
1	A	103	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	F	103	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	A	110	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	110	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	I	185	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	K	119	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	G	110	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	H	119	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	G	161	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	A	103	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	F	153	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	F	110	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	H	102	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	K	119	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	G	110	ARG	CG-CD-NE	-6.47	98.22	111.80
1	C	110	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	340	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	G	336	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	313	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	E	134	LEU	CA-CB-CG	6.20	129.57	115.30
1	B	288	ASN	C-N-CD	-5.81	107.82	120.60
1	D	76	GLY	N-CA-C	5.81	127.62	113.10
1	H	119	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	H	342	LEU	CA-CB-CG	5.72	128.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	LEU	CA-CB-CG	5.69	128.38	115.30
1	G	98	CYS	C-N-CD	5.68	140.32	128.40
1	L	127	LEU	CA-CB-CG	-5.66	102.28	115.30
1	G	133	CYS	CA-CB-SG	-5.59	103.94	114.00
1	C	110	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	G	161	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	D	288	ASN	C-N-CD	-5.51	108.48	120.60
1	A	98	CYS	C-N-CD	5.42	139.79	128.40
1	G	103	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	H	336	LEU	CA-CB-CG	5.33	127.56	115.30
1	H	102	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	103	ARG	CD-NE-CZ	5.21	130.90	123.60
1	F	340	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	L	134	LEU	CA-CB-CG	-5.12	103.52	115.30
1	I	98	CYS	C-N-CD	5.02	138.94	128.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	264	TYR	Sidechain
1	D	176	TYR	Sidechain
1	D	229	TYR	Sidechain
1	F	176	TYR	Sidechain
1	F	229	TYR	Sidechain
1	G	228	TYR	Sidechain
1	G	229	TYR	Sidechain
1	I	155	ASP	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	2298	0	2326	135	0
1	B	2361	0	2385	185	0
1	C	2316	0	2346	174	0
1	D	2325	0	2352	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2291	0	2325	238	0
1	F	2344	0	2370	172	0
1	G	2343	0	2369	186	0
1	H	2289	0	2325	157	0
1	I	2354	0	2370	176	0
1	J	1823	0	1868	267	0
1	K	2142	0	2186	156	0
1	L	2177	0	2212	321	0
2	A	26	0	16	2	0
2	B	26	0	16	1	0
2	C	26	0	16	4	0
2	D	26	0	16	5	0
2	E	26	0	16	4	0
2	F	26	0	16	5	0
2	G	26	0	16	5	0
2	H	26	0	16	4	0
2	I	26	0	16	2	0
2	K	26	0	16	3	0
2	L	26	0	16	4	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
All	All	27367	0	27610	2240	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 41.

All (2240) 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:G:45:GLN:HG3	1:G:46:PHE:H	1.03	1.17
1:L:275:MET:HA	1:L:278:ARG:NH1	1.60	1.16
1:L:275:MET:HG3	1:L:278:ARG:HH22	1.12	1.15
1:D:264:TYR:O	1:D:275:MET:HG3	1.43	1.14
1:F:151:GLN:HE22	1:F:346:LYS:HD3	1.01	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ILE:HD12	1:C:158:PHE:HE1	1.07	1.13
1:G:233:GLU:HG2	1:H:310:PRO:HG3	1.24	1.13
1:J:149:ARG:HB3	1:J:149:ARG:HH11	0.96	1.12
1:B:264:TYR:O	1:B:275:MET:HG3	1.48	1.11
1:L:300:MET:HE1	1:L:303:ARG:HH21	1.11	1.09
1:J:202:ILE:HD12	1:J:204:LYS:HE3	1.25	1.06
1:D:86:THR:HG22	1:D:88:GLU:H	1.09	1.06
1:E:343:LYS:HB2	1:E:344:GLU:OE2	1.56	1.06
1:K:86:THR:HG22	1:K:88:GLU:H	1.09	1.06
1:F:149:ARG:HG3	1:F:149:ARG:HH11	1.14	1.06
1:C:185:ARG:HH21	1:C:212:LYS:HD3	1.14	1.04
1:K:83:ASN:HD21	1:K:85:ARG:HG3	1.22	1.03
1:F:344:GLU:O	1:F:345:ASP:HB2	1.59	1.03
1:D:214:THR:O	1:D:215:THR:HG23	1.59	1.02
1:L:118:VAL:HG11	1:L:206:THR:HG22	1.40	1.02
1:G:310:PRO:HG3	1:I:233:GLU:HG2	1.39	1.02
1:F:86:THR:CG2	1:F:88:GLU:HB2	1.90	1.01
1:K:74:ILE:HG21	1:K:209:GLY:HA3	1.42	1.01
1:L:165:GLU:HG2	1:L:328:SER:HB3	1.42	1.00
1:J:83:ASN:HD21	1:J:85:ARG:HB3	1.24	1.00
1:C:150:ILE:HD12	1:C:158:PHE:CE1	1.97	1.00
1:G:74:ILE:HG21	1:G:209:GLY:HA3	1.43	1.00
1:D:230:VAL:HG11	1:D:235:LEU:HD21	1.40	1.00
1:A:149:ARG:HH11	1:A:149:ARG:HB3	1.26	1.00
1:A:149:ARG:HH11	1:A:149:ARG:CB	1.73	1.00
1:J:167:MET:HG3	1:J:253:MET:HG2	1.39	1.00
1:J:149:ARG:NH2	1:J:199:PRO:HA	1.76	0.99
1:J:195:THR:HG23	1:J:196:SER:H	1.22	0.99
1:E:246:MET:HE1	1:E:316:ILE:HD12	1.41	0.99
1:L:275:MET:CA	1:L:278:ARG:HH12	1.75	0.99
1:J:193:LEU:H	1:J:193:LEU:HD23	1.28	0.99
1:E:288:ASN:HB3	1:E:289:PRO:HA	1.44	0.98
1:J:251:VAL:HG12	1:J:252:ILE:HG13	1.41	0.98
1:E:227:PRO:HB3	1:E:229:TYR:CE2	2.00	0.97
1:J:149:ARG:HB3	1:J:149:ARG:NH1	1.79	0.97
1:E:180:ILE:HG13	1:E:182:ILE:HD12	1.47	0.97
1:L:281:MET:HB2	1:L:283:GLN:HG3	1.44	0.97
1:D:151:GLN:HE22	1:D:346:LYS:HD2	1.28	0.97
1:E:264:TYR:O	1:E:275:MET:HG3	1.64	0.96
1:J:195:THR:HG21	1:J:202:ILE:H	1.29	0.96
1:D:70:LEU:HD21	1:D:80:GLN:HB2	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:GLU:HG2	1:F:310:PRO:HG3	1.46	0.95
1:K:288:ASN:HB3	1:K:289:PRO:HA	1.49	0.95
1:K:118:VAL:HG11	1:K:206:THR:HG22	1.46	0.95
1:J:149:ARG:CB	1:J:149:ARG:HH11	1.80	0.94
1:L:263:PHE:CE2	1:L:279:ILE:HA	2.03	0.94
1:K:86:THR:HG22	1:K:88:GLU:N	1.83	0.94
1:A:310:PRO:HG3	1:C:233:GLU:CG	1.96	0.94
1:G:45:GLN:HG3	1:G:46:PHE:N	1.83	0.93
1:J:83:ASN:ND2	1:J:85:ARG:HB3	1.82	0.93
1:I:289:PRO:O	1:I:291:TRP:N	2.01	0.93
1:F:86:THR:HG21	1:F:88:GLU:HB2	1.50	0.93
1:A:310:PRO:HG3	1:C:233:GLU:HG2	1.50	0.93
1:C:348:ARG:HG2	1:C:348:ARG:HH21	1.35	0.92
1:B:227:PRO:HG2	1:B:230:VAL:HB	1.52	0.92
1:L:275:MET:HG3	1:L:278:ARG:NH2	1.84	0.91
1:B:80:GLN:NE2	1:B:89:LYS:HD2	1.83	0.91
1:L:332:PRO:HB2	1:L:334:THR:HG22	1.49	0.91
1:J:301:LEU:HD13	1:J:322:HIS:CD2	2.06	0.91
1:I:83:ASN:OD1	1:I:86:THR:HG22	1.71	0.91
1:F:151:GLN:NE2	1:F:346:LYS:HD3	1.86	0.90
1:F:149:ARG:HG3	1:F:149:ARG:NH1	1.83	0.90
1:J:107:LEU:HD22	1:J:182:ILE:CG2	2.01	0.90
1:J:198:ARG:HH11	1:J:198:ARG:HG2	1.35	0.90
1:G:143:GLY:HA3	1:G:196:SER:O	1.72	0.90
1:F:83:ASN:HD22	1:F:84:LYS:N	1.68	0.90
1:B:343:LYS:O	1:B:344:GLU:HB3	1.72	0.90
1:L:246:MET:SD	1:L:316:ILE:HB	2.12	0.90
1:F:185:ARG:HH21	1:F:212:LYS:HD3	1.37	0.89
1:H:149:ARG:HH11	1:H:149:ARG:HB3	1.36	0.89
1:L:275:MET:HA	1:L:278:ARG:HH12	0.79	0.89
1:G:74:ILE:HG23	1:G:75:ASN:H	1.35	0.89
1:C:331:VAL:HG13	1:C:332:PRO:HD2	1.54	0.89
1:E:299:LYS:O	1:E:303:ARG:HG3	1.72	0.89
1:L:181:ASN:HB3	1:L:214:THR:OG1	1.71	0.89
1:J:195:THR:HB	1:J:202:ILE:HG13	1.52	0.88
1:J:143:GLY:O	1:J:149:ARG:HD2	1.74	0.88
1:F:344:GLU:O	1:F:344:GLU:HG2	1.72	0.88
1:B:86:THR:HG23	1:B:88:GLU:HB2	1.55	0.88
1:E:235:LEU:HD13	1:F:276:LYS:HG3	1.56	0.88
1:D:238:GLU:OE1	1:D:242:LYS:HE3	1.74	0.88
1:E:66:THR:HG23	1:E:80:GLN:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:THR:O	1:L:88:GLU:N	2.08	0.87
1:L:83:ASN:C	1:L:83:ASN:HD22	1.77	0.87
1:H:74:ILE:HG21	1:H:210:PHE:CE2	2.10	0.87
1:E:227:PRO:HB3	1:E:229:TYR:CZ	2.10	0.87
1:E:73:GLY:HA3	2:E:1345:P4O:H8C2	1.57	0.87
1:K:74:ILE:CG2	1:K:209:GLY:HA3	2.05	0.86
1:K:196:SER:HB2	1:K:198:ARG:HB2	1.56	0.86
1:B:147:PHE:HD1	1:B:349:TRP:CZ2	1.93	0.86
1:L:343:LYS:H	1:L:343:LYS:HE2	1.40	0.86
1:K:83:ASN:HD21	1:K:85:ARG:CG	1.89	0.85
1:C:338:THR:O	1:C:342:LEU:HD13	1.76	0.85
1:A:233:GLU:HG2	1:B:310:PRO:HG3	1.57	0.85
1:J:114:CYS:HB2	1:J:176:TYR:CD2	2.12	0.85
1:J:110:ARG:HG2	1:J:110:ARG:HH11	1.38	0.85
1:E:60:ILE:HG12	1:E:61:ASP:H	1.40	0.85
1:B:276:LYS:O	1:B:280:ARG:HG3	1.77	0.85
1:E:60:ILE:HG12	1:E:61:ASP:N	1.92	0.85
1:H:152:ASP:O	1:H:153:ARG:HG3	1.76	0.85
1:G:185:ARG:HH21	1:G:212:LYS:HD2	1.41	0.85
1:J:114:CYS:HB2	1:J:176:TYR:HD2	1.42	0.84
1:K:160:GLU:OE1	1:K:294:VAL:HG13	1.78	0.84
1:E:121:VAL:HG23	1:E:137:VAL:O	1.77	0.84
1:E:185:ARG:CB	1:E:185:ARG:HH11	1.89	0.84
1:E:198:ARG:HH21	1:E:200:ASN:HD21	1.26	0.84
1:D:337:HIS:CD2	1:D:340:ARG:HH12	1.96	0.84
1:F:83:ASN:HD22	1:F:83:ASN:C	1.80	0.84
1:K:151:GLN:HB2	1:K:342:LEU:HD23	1.59	0.84
1:L:166:ILE:HG21	1:L:256:LEU:HD11	1.59	0.84
1:L:255:ILE:HG12	1:L:261:PRO:HA	1.59	0.83
1:E:60:ILE:O	1:E:62:ASP:N	2.11	0.83
1:E:146:LEU:HD11	1:E:166:ILE:HD13	1.59	0.83
1:E:101:ALA:O	1:E:105:VAL:HG23	1.78	0.83
1:D:86:THR:HG21	1:D:88:GLU:HB2	1.61	0.83
1:E:83:ASN:HB3	1:E:86:THR:HG22	1.59	0.83
1:C:185:ARG:NH2	1:C:212:LYS:HD3	1.93	0.83
1:I:149:ARG:HH11	1:I:149:ARG:HB3	1.43	0.83
1:I:57:ASN:HA	1:K:50:SER:OG	1.79	0.82
1:E:185:ARG:HH11	1:E:185:ARG:HB3	1.43	0.82
1:E:85:ARG:O	1:E:85:ARG:HD2	1.79	0.82
1:H:149:ARG:HH11	1:H:149:ARG:CB	1.91	0.82
1:E:195:THR:HG21	1:E:202:ILE:HG12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:275:MET:CG	1:L:278:ARG:HH22	1.92	0.82
1:H:74:ILE:HG21	1:H:210:PHE:HE2	1.44	0.82
1:D:230:VAL:CG1	1:D:235:LEU:HD21	2.09	0.82
1:D:332:PRO:HB2	1:D:334:THR:HG22	1.59	0.82
1:L:331:VAL:HG13	1:L:332:PRO:HD2	1.61	0.81
1:I:195:THR:HG23	1:I:202:ILE:O	1.80	0.81
1:F:86:THR:CG2	1:F:88:GLU:H	1.92	0.81
1:B:331:VAL:HG13	1:B:332:PRO:HD2	1.59	0.81
1:J:143:GLY:HA3	1:J:196:SER:O	1.80	0.81
1:G:151:GLN:O	1:G:343:LYS:HE2	1.81	0.81
1:B:233:GLU:HG2	1:C:310:PRO:HG3	1.61	0.81
1:J:158:PHE:HZ	1:J:163:ALA:HB2	1.46	0.81
1:J:174:ILE:HB	1:J:316:ILE:HD13	1.62	0.81
1:E:195:THR:HG23	1:E:202:ILE:O	1.81	0.80
1:G:118:VAL:HG11	1:G:206:THR:HG22	1.62	0.80
1:L:185:ARG:CB	1:L:185:ARG:HH11	1.94	0.80
1:G:233:GLU:CG	1:H:310:PRO:HG3	2.10	0.80
1:J:169:SER:C	1:J:171:GLY:H	1.85	0.80
1:J:158:PHE:CZ	1:J:163:ALA:HB2	2.17	0.79
1:A:327:GLN:HE21	1:A:330:LYS:HG3	1.47	0.79
1:L:59:ILE:HG13	1:L:124:TYR:CD1	2.16	0.79
1:G:148:SER:O	1:G:150:ILE:N	2.16	0.79
1:K:80:GLN:NE2	1:K:89:LYS:HG2	1.97	0.79
1:C:83:ASN:HD22	1:C:84:LYS:N	1.80	0.79
1:D:86:THR:O	1:D:87:GLN:HB2	1.82	0.79
1:K:271:ILE:CG2	1:K:278:ARG:HH12	1.95	0.79
1:J:304:ASN:O	1:J:307:LYS:HG2	1.83	0.79
1:K:86:THR:HG21	1:K:88:GLU:OE1	1.82	0.79
1:K:118:VAL:CG1	1:K:206:THR:HG22	2.11	0.79
1:H:331:VAL:HG13	1:H:332:PRO:HD2	1.65	0.79
1:E:260:TYR:HB2	1:E:261:PRO:HD2	1.65	0.79
1:K:83:ASN:ND2	1:K:85:ARG:HG3	1.98	0.78
1:J:107:LEU:HD22	1:J:182:ILE:HG23	1.64	0.78
1:H:260:TYR:OH	1:H:287:PRO:HG2	1.84	0.78
1:F:149:ARG:HH11	1:F:149:ARG:CG	1.95	0.78
1:H:98:CYS:HB2	1:H:99:PRO:HD3	1.64	0.78
1:E:246:MET:CE	1:E:316:ILE:HD12	2.13	0.78
1:J:149:ARG:HH21	1:J:199:PRO:HA	1.45	0.78
1:L:74:ILE:HG23	1:L:75:ASN:ND2	1.98	0.78
1:L:300:MET:CE	1:L:303:ARG:HH21	1.93	0.78
1:L:67:SER:HA	1:L:79:LEU:HD22	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:PRO:HB2	1:D:334:THR:CG2	2.12	0.78
1:G:86:THR:O	1:G:88:GLU:N	2.17	0.78
1:C:273:PRO:HB3	1:K:131:ARG:HH12	1.46	0.78
1:L:121:VAL:HB	1:L:137:VAL:HG12	1.66	0.78
1:C:227:PRO:HG2	1:C:229:TYR:CZ	2.19	0.78
1:E:198:ARG:HH21	1:E:200:ASN:ND2	1.81	0.77
1:G:192:LEU:C	1:G:193:LEU:HD23	2.04	0.77
1:E:167:MET:HG3	1:E:253:MET:HE2	1.66	0.77
1:L:74:ILE:HG23	1:L:75:ASN:H	1.49	0.77
1:H:98:CYS:HB2	1:H:99:PRO:CD	2.14	0.77
1:E:121:VAL:HG23	1:E:137:VAL:HG12	1.67	0.77
1:G:337:HIS:O	1:G:341:VAL:HG23	1.83	0.77
1:C:152:ASP:O	1:C:153:ARG:HG3	1.85	0.77
1:K:84:LYS:HD2	1:K:84:LYS:O	1.85	0.76
1:C:65:VAL:O	1:L:44:PRO:HA	1.84	0.76
1:G:99:PRO:HD2	1:G:100:LYS:H	1.50	0.76
1:C:64:LYS:HE3	1:L:44:PRO:CG	2.16	0.76
1:L:77:LYS:H	1:L:77:LYS:HD3	1.49	0.76
1:G:147:PHE:CE1	1:G:255:ILE:HG21	2.21	0.76
1:A:70:LEU:HD13	2:A:1351:P4O:C17	2.15	0.76
1:L:152:ASP:O	1:L:153:ARG:HG3	1.86	0.76
1:H:158:PHE:HD1	1:H:336:LEU:HD23	1.49	0.76
1:J:146:LEU:O	1:J:150:ILE:HG12	1.85	0.76
1:E:260:TYR:HB2	1:E:261:PRO:CD	2.15	0.76
1:D:151:GLN:NE2	1:D:346:LYS:HD2	1.99	0.76
1:J:107:LEU:HD22	1:J:182:ILE:HG21	1.68	0.76
1:K:290:GLU:OE2	1:K:337:HIS:HB2	1.86	0.76
1:E:233:GLU:CG	1:F:310:PRO:HG3	2.15	0.76
1:E:195:THR:CG2	1:E:202:ILE:HG12	2.16	0.75
1:D:96:GLN:OE1	1:D:131:ARG:HD3	1.87	0.75
1:J:189:PRO:HA	1:J:192:LEU:HD12	1.68	0.75
1:L:184:HIS:ND1	1:L:205:LEU:HD21	2.01	0.75
1:J:108:HIS:O	1:J:111:ALA:N	2.18	0.75
1:A:233:GLU:CG	1:B:310:PRO:HG3	2.17	0.75
1:I:83:ASN:CG	1:I:86:THR:HG22	2.07	0.75
1:F:276:LYS:O	1:F:280:ARG:HG3	1.87	0.75
1:E:198:ARG:NH2	1:E:200:ASN:HD21	1.84	0.75
1:E:181:ASN:HB3	1:E:214:THR:OG1	1.87	0.75
1:A:264:TYR:O	1:A:275:MET:HG3	1.85	0.75
1:D:276:LYS:O	1:D:280:ARG:HG3	1.86	0.75
1:B:83:ASN:HD22	1:B:84:LYS:N	1.82	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ILE:HD11	1:E:204:LYS:CE	2.17	0.74
1:F:239:LYS:HB2	1:F:241:ASP:OD2	1.86	0.74
1:L:82:PHE:CD1	1:L:89:LYS:HB3	2.22	0.74
1:C:260:TYR:HE1	1:C:290:GLU:HG2	1.52	0.74
1:D:70:LEU:HD12	2:D:1351:P4O:C17	2.17	0.74
1:I:332:PRO:HB2	1:I:334:THR:HG22	1.69	0.74
1:D:86:THR:HG22	1:D:88:GLU:N	1.94	0.74
1:F:86:THR:HG22	1:F:88:GLU:H	1.51	0.74
1:B:83:ASN:HD22	1:B:83:ASN:C	1.90	0.74
1:C:64:LYS:HE3	1:L:44:PRO:HG3	1.70	0.74
1:L:327:GLN:HB3	1:L:330:LYS:HB2	1.68	0.74
1:C:264:TYR:O	1:C:275:MET:HG3	1.87	0.74
1:J:189:PRO:HD2	1:J:190:GLU:OE1	1.88	0.74
1:B:300:MET:CE	1:B:303:ARG:HH21	2.00	0.74
1:J:195:THR:HG23	1:J:196:SER:N	2.01	0.73
1:J:254:TYR:HB3	1:J:262:PRO:HG3	1.70	0.73
1:L:83:ASN:HD21	1:L:85:ARG:HG3	1.53	0.73
1:I:130:GLY:HA3	1:K:180:ILE:HB	1.71	0.73
1:J:193:LEU:HD23	1:J:193:LEU:N	1.96	0.73
1:D:239:LYS:HB3	1:D:241:ASP:OD2	1.88	0.73
1:I:52:LEU:HD13	1:I:109:TRP:CE3	2.22	0.73
1:F:347:GLU:C	1:F:349:TRP:H	1.90	0.73
1:D:332:PRO:CB	1:D:334:THR:HG22	2.19	0.73
1:G:145:GLU:O	1:G:145:GLU:HG3	1.88	0.73
1:B:300:MET:HE2	1:B:303:ARG:HH21	1.52	0.73
1:F:80:GLN:NE2	1:F:89:LYS:HD3	2.03	0.73
1:C:331:VAL:CG1	1:C:332:PRO:HD2	2.18	0.73
1:E:332:PRO:HB2	1:E:334:THR:HG22	1.70	0.73
1:D:74:ILE:O	1:D:74:ILE:HD12	1.89	0.73
1:J:195:THR:CG2	1:J:202:ILE:H	2.02	0.73
1:E:141:LEU:HD13	1:E:193:LEU:HB2	1.70	0.73
1:J:118:VAL:HG12	1:J:205:LEU:O	1.89	0.73
1:L:78:VAL:HG12	1:L:79:LEU:N	2.04	0.73
1:L:82:PHE:HD1	1:L:89:LYS:HB3	1.54	0.73
1:J:175:GLN:O	1:J:177:LEU:N	2.22	0.73
1:K:332:PRO:HB2	1:K:334:THR:HG22	1.71	0.73
1:J:256:LEU:HD13	1:J:256:LEU:O	1.89	0.72
1:C:227:PRO:HB2	1:C:229:TYR:CE2	2.24	0.72
1:B:260:TYR:HB2	1:B:261:PRO:HD2	1.71	0.72
1:H:83:ASN:ND2	1:H:85:ARG:H	1.87	0.72
1:G:83:ASN:C	1:G:83:ASN:HD22	1.92	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:309:GLU:OE2	1:K:311:THR:HG23	1.89	0.72
1:A:60:ILE:HD13	1:F:48:VAL:HG23	1.72	0.72
1:K:147:PHE:CZ	1:K:255:ILE:HG21	2.24	0.72
1:L:205:LEU:HD12	1:L:206:THR:N	2.05	0.72
1:D:141:LEU:HD13	1:D:193:LEU:HB2	1.72	0.72
1:L:185:ARG:HB3	1:L:185:ARG:HH11	1.54	0.72
1:L:142:ASP:HA	2:L:1345:P4O:N16	2.04	0.72
1:L:63:TYR:CD1	1:L:81:ILE:HD12	2.25	0.72
1:J:168:LYS:O	1:J:168:LYS:HG2	1.88	0.72
1:G:45:GLN:CG	1:G:46:PHE:H	1.93	0.72
1:L:337:HIS:O	1:L:341:VAL:HG23	1.90	0.72
1:G:86:THR:CG2	1:G:86:THR:O	2.37	0.72
1:E:73:GLY:HA3	2:E:1345:P4O:C8	2.20	0.71
1:L:166:ILE:HG21	1:L:256:LEU:CD1	2.20	0.71
1:J:188:LYS:O	1:J:192:LEU:HG	1.90	0.71
1:E:60:ILE:C	1:E:62:ASP:H	1.93	0.71
1:L:98:CYS:HB2	1:L:99:PRO:CD	2.20	0.71
1:G:214:THR:O	1:G:215:THR:HB	1.90	0.71
1:I:345:ASP:O	1:I:347:GLU:N	2.23	0.71
1:D:83:ASN:HD22	1:D:83:ASN:C	1.90	0.71
1:E:233:GLU:HG2	1:F:310:PRO:CG	2.20	0.71
1:I:156:GLN:O	1:I:158:PHE:N	2.23	0.71
1:H:83:ASN:HD22	1:H:84:LYS:N	1.88	0.71
1:I:241:ASP:O	1:I:244:CYS:HB2	1.89	0.71
1:C:345:ASP:O	1:C:347:GLU:N	2.23	0.71
1:I:260:TYR:OH	1:I:287:PRO:HG2	1.90	0.71
1:L:80:GLN:NE2	1:L:89:LYS:HB2	2.05	0.71
1:F:154:GLY:O	1:F:156:GLN:OE1	2.07	0.71
1:K:83:ASN:C	1:K:83:ASN:HD22	1.93	0.71
1:B:343:LYS:O	1:B:344:GLU:CB	2.37	0.71
1:K:141:LEU:HD13	1:K:193:LEU:HB2	1.73	0.71
1:C:86:THR:O	1:C:87:GLN:HB2	1.91	0.71
1:C:322:HIS:ND1	1:C:323:PRO:HD2	2.06	0.71
1:C:83:ASN:ND2	1:C:85:ARG:H	1.89	0.71
1:J:254:TYR:CB	1:J:262:PRO:HG3	2.21	0.71
1:F:98:CYS:HB2	1:F:99:PRO:HD3	1.73	0.71
1:J:299:LYS:O	1:J:303:ARG:HG3	1.91	0.70
1:G:80:GLN:NE2	1:G:89:LYS:HG2	2.05	0.70
1:D:149:ARG:HB3	1:D:149:ARG:HH11	1.56	0.70
1:H:200:ASN:N	1:H:200:ASN:HD22	1.87	0.70
1:L:284:TYR:OH	1:L:303:ARG:HA	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:GLU:O	1:F:345:ASP:CB	2.38	0.70
1:C:309:GLU:OE2	1:C:311:THR:HG23	1.92	0.70
1:L:77:LYS:N	1:L:77:LYS:HD3	2.05	0.70
1:J:314:MET:HG3	1:J:318:GLU:OE1	1.91	0.70
1:J:195:THR:CB	1:J:202:ILE:HG13	2.20	0.70
1:L:184:HIS:CE1	1:L:205:LEU:HD11	2.26	0.70
1:L:247:TRP:HB2	1:L:313:ARG:NH1	2.06	0.70
1:H:309:GLU:OE2	1:H:311:THR:HG23	1.92	0.70
1:E:314:MET:HG3	1:E:318:GLU:HB2	1.72	0.70
1:L:255:ILE:CG1	1:L:261:PRO:HA	2.21	0.70
1:K:260:TYR:OH	1:K:287:PRO:HG2	1.90	0.70
1:J:110:ARG:NH1	1:J:110:ARG:HG2	2.03	0.70
1:E:80:GLN:HE22	1:E:89:LYS:HG2	1.56	0.70
1:G:296:GLU:OE2	1:G:303:ARG:NH2	2.24	0.70
1:C:52:LEU:HD13	1:C:109:TRP:CD2	2.27	0.70
1:L:263:PHE:HE2	1:L:279:ILE:HA	1.56	0.70
1:E:121:VAL:CG2	1:E:137:VAL:HG12	2.22	0.70
1:B:288:ASN:OD1	1:B:292:SER:HB3	1.91	0.70
1:L:77:LYS:CD	1:L:77:LYS:H	2.05	0.70
1:I:347:GLU:HG3	1:I:348:ARG:N	2.06	0.70
1:C:348:ARG:HG2	1:C:348:ARG:NH2	2.05	0.70
1:E:193:LEU:N	1:E:193:LEU:HD23	2.06	0.70
1:L:285:GLU:O	1:L:287:PRO:HD3	1.92	0.69
1:C:127:LEU:HD23	1:C:131:ARG:O	1.92	0.69
1:A:74:ILE:CG2	1:A:210:PHE:HE2	2.05	0.69
1:L:324:TRP:HE1	1:L:331:VAL:HG11	1.57	0.69
1:D:151:GLN:HE22	1:D:346:LYS:CD	2.03	0.69
1:L:78:VAL:CG1	1:L:79:LEU:N	2.54	0.69
1:D:337:HIS:O	1:D:341:VAL:HG23	1.93	0.69
1:G:141:LEU:HD13	1:G:193:LEU:HB2	1.73	0.69
1:D:313:ARG:NH1	1:F:233:GLU:OE1	2.25	0.69
1:H:276:LYS:O	1:H:280:ARG:HG3	1.92	0.69
1:E:344:GLU:H	1:E:344:GLU:CD	1.96	0.69
1:J:195:THR:HG22	1:J:202:ILE:O	1.93	0.69
1:H:74:ILE:CG2	1:H:210:PHE:HE2	2.05	0.69
1:A:74:ILE:HG21	1:A:210:PHE:CE2	2.28	0.69
1:J:166:ILE:HG21	1:J:256:LEU:HG	1.75	0.69
1:D:83:ASN:HD22	1:D:84:LYS:N	1.90	0.69
1:G:301:LEU:HD13	1:G:322:HIS:CD2	2.28	0.69
1:G:118:VAL:CG1	1:G:206:THR:HG22	2.23	0.69
1:K:185:ARG:HH11	1:K:185:ARG:HB3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:GLU:OE2	1:D:311:THR:HG23	1.93	0.68
1:E:125:GLU:C	1:E:126:ASN:HD22	1.96	0.68
1:K:276:LYS:O	1:K:280:ARG:HG3	1.92	0.68
1:E:288:ASN:CB	1:E:289:PRO:HA	2.18	0.68
1:D:234:VAL:C	1:D:236:GLY:H	1.96	0.68
1:L:70:LEU:HD22	2:L:1345:P4O:C21	2.24	0.68
1:E:278:ARG:HG3	1:E:283:GLN:HB2	1.75	0.68
1:F:337:HIS:O	1:F:339:SER:N	2.26	0.68
1:C:83:ASN:C	1:C:83:ASN:HD22	1.97	0.68
1:D:52:LEU:HD13	1:D:109:TRP:CE3	2.29	0.68
1:L:83:ASN:ND2	1:L:85:ARG:H	1.92	0.68
1:I:327:GLN:HE21	1:I:330:LYS:HD3	1.57	0.68
1:D:81:ILE:HD13	1:D:92:LEU:HB2	1.75	0.68
1:L:316:ILE:O	1:L:316:ILE:HG13	1.92	0.68
1:J:118:VAL:O	1:J:118:VAL:HG22	1.94	0.68
1:C:48:VAL:HG22	1:D:60:ILE:HD13	1.74	0.68
1:F:331:VAL:CG1	1:F:332:PRO:HD2	2.24	0.68
1:J:167:MET:SD	1:J:252:ILE:O	2.52	0.68
1:L:315:THR:OG1	1:L:317:THR:HG22	1.93	0.68
1:A:276:LYS:O	1:A:280:ARG:HG3	1.93	0.68
1:E:99:PRO:HA	1:E:102:ARG:HB2	1.76	0.67
1:E:159:THR:OG1	1:E:162:GLU:HG3	1.93	0.67
1:K:83:ASN:HD22	1:K:84:LYS:N	1.93	0.67
1:J:111:ALA:O	1:J:113:GLN:N	2.28	0.67
1:B:181:ASN:HB3	1:B:214:THR:HG22	1.76	0.67
1:F:260:TYR:HB2	1:F:261:PRO:HD2	1.76	0.67
1:H:47:HIS:HB3	1:H:49:LYS:NZ	2.09	0.67
1:A:310:PRO:HG3	1:C:233:GLU:HG3	1.75	0.67
1:C:153:ARG:NH2	1:C:157:ALA:O	2.28	0.67
1:J:86:THR:O	1:J:86:THR:HG22	1.93	0.67
1:B:260:TYR:OH	1:B:287:PRO:HG2	1.94	0.67
1:K:114:CYS:HB2	1:K:176:TYR:CD2	2.29	0.67
1:F:142:ASP:OD2	1:F:196:SER:HA	1.95	0.67
1:A:337:HIS:CD2	1:A:340:ARG:HH11	2.12	0.67
1:H:271:ILE:CD1	1:H:278:ARG:HH12	2.07	0.67
1:B:343:LYS:HG2	1:B:343:LYS:O	1.93	0.67
1:D:78:VAL:C	1:D:79:LEU:HD23	2.14	0.67
1:A:85:ARG:O	1:A:85:ARG:HG2	1.94	0.67
1:B:275:MET:HE2	1:B:279:ILE:HD12	1.77	0.67
1:E:83:ASN:CB	1:E:86:THR:HG22	2.25	0.67
1:B:233:GLU:CG	1:C:310:PRO:HG3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:291:TRP:HA	1:L:294:VAL:HG23	1.76	0.67
1:B:83:ASN:ND2	1:B:85:ARG:H	1.93	0.67
1:G:80:GLN:OE1	1:G:89:LYS:HE2	1.95	0.67
1:J:168:LYS:HB2	1:J:325:ILE:HG23	1.76	0.67
1:J:103:ARG:CB	1:J:103:ARG:HH11	2.07	0.67
1:E:148:SER:O	1:E:150:ILE:N	2.28	0.66
1:J:86:THR:CG2	1:J:88:GLU:HB2	2.26	0.66
1:L:309:GLU:OE2	1:L:310:PRO:HD2	1.96	0.66
1:C:147:PHE:CD1	1:C:189:PRO:HB3	2.30	0.66
1:I:327:GLN:HE21	1:I:330:LYS:CD	2.09	0.66
1:F:322:HIS:ND1	1:F:323:PRO:HD2	2.10	0.66
1:B:235:LEU:HD23	1:B:235:LEU:N	2.09	0.66
1:I:149:ARG:CB	1:I:149:ARG:HH11	2.08	0.66
1:I:300:MET:CE	1:I:303:ARG:HH21	2.09	0.66
1:J:167:MET:HE3	1:J:167:MET:HA	1.76	0.66
1:L:302:ILE:HG22	1:L:306:LEU:HD12	1.75	0.66
1:A:145:GLU:HA	1:A:193:LEU:CD2	2.24	0.66
1:L:184:HIS:HE1	1:L:205:LEU:HD11	1.60	0.66
1:A:310:PRO:CG	1:C:233:GLU:HG2	2.26	0.66
1:E:202:ILE:HD11	1:E:204:LYS:HE3	1.76	0.66
1:J:188:LYS:HB2	1:J:189:PRO:CD	2.25	0.66
1:J:186:ASP:OD2	1:J:188:LYS:HE3	1.96	0.66
1:K:141:LEU:CD1	1:K:193:LEU:HB2	2.25	0.66
1:L:59:ILE:HG13	1:L:124:TYR:CE1	2.30	0.66
1:E:48:VAL:HG13	1:H:60:ILE:HD13	1.77	0.66
1:E:237:PRO:O	1:E:238:GLU:HB2	1.96	0.66
1:L:118:VAL:HG11	1:L:206:THR:CG2	2.22	0.65
1:L:331:VAL:CG1	1:L:332:PRO:HD2	2.24	0.65
1:J:319:PHE:O	1:J:321:ASN:N	2.29	0.65
1:L:263:PHE:CD2	1:L:279:ILE:HG12	2.31	0.65
1:G:66:THR:HG21	1:G:82:PHE:HE2	1.60	0.65
1:L:333:GLN:O	1:L:335:PRO:HD3	1.95	0.65
1:L:192:LEU:HB3	1:L:203:LEU:HD11	1.76	0.65
1:K:288:ASN:N	1:K:288:ASN:HD22	1.92	0.65
1:F:70:LEU:HD21	1:F:80:GLN:HB2	1.76	0.65
1:A:74:ILE:HB	1:A:210:PHE:HE2	1.62	0.65
1:L:119:ARG:HB2	1:L:119:ARG:NH1	2.10	0.65
1:B:291:TRP:CE3	1:B:294:VAL:HG21	2.30	0.65
1:D:86:THR:CG2	1:D:88:GLU:H	1.96	0.65
1:D:237:PRO:O	1:D:238:GLU:HB3	1.97	0.65
1:L:247:TRP:HB2	1:L:313:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:CYS:HB2	1:D:99:PRO:HD3	1.77	0.65
1:J:185:ARG:O	1:J:186:ASP:HB2	1.96	0.65
1:A:145:GLU:HA	1:A:193:LEU:HD23	1.78	0.65
1:E:117:ILE:HD12	1:E:208:PHE:HZ	1.61	0.65
1:D:167:MET:HG3	1:D:253:MET:HG3	1.77	0.65
1:B:337:HIS:O	1:B:341:VAL:HG23	1.96	0.65
1:K:83:ASN:HB3	1:K:86:THR:HB	1.76	0.65
1:C:162:GLU:O	1:C:166:ILE:HG13	1.96	0.65
1:L:108:HIS:HD2	1:L:108:HIS:O	1.79	0.65
1:B:235:LEU:HD23	1:B:235:LEU:H	1.61	0.65
1:A:260:TYR:OH	1:A:287:PRO:HG2	1.96	0.65
1:H:328:SER:O	1:H:331:VAL:HB	1.97	0.65
1:E:202:ILE:HD11	1:E:204:LYS:HE2	1.79	0.64
1:B:260:TYR:HB2	1:B:261:PRO:CD	2.27	0.64
1:I:300:MET:HE2	1:I:303:ARG:HH21	1.63	0.64
1:H:229:TYR:O	1:H:230:VAL:HG13	1.97	0.64
1:G:238:GLU:OE1	1:G:242:LYS:HE3	1.97	0.64
1:B:185:ARG:HH11	1:B:185:ARG:HB3	1.62	0.64
1:J:148:SER:C	1:J:150:ILE:H	1.98	0.64
1:J:167:MET:HG3	1:J:253:MET:CG	2.24	0.64
1:L:83:ASN:C	1:L:83:ASN:ND2	2.50	0.64
1:L:158:PHE:CZ	1:L:163:ALA:HB2	2.33	0.64
1:K:271:ILE:HG22	1:K:278:ARG:HH12	1.60	0.64
1:L:52:LEU:HD12	1:L:53:GLN:H	1.62	0.64
1:J:310:PRO:O	1:J:313:ARG:HB3	1.97	0.64
1:C:52:LEU:HD13	1:C:109:TRP:CE3	2.33	0.64
1:F:114:CYS:HB2	1:F:176:TYR:CD2	2.32	0.64
1:L:281:MET:CB	1:L:283:GLN:HG3	2.26	0.64
1:J:296:GLU:HA	1:J:299:LYS:HD2	1.80	0.64
1:A:331:VAL:HG13	1:A:332:PRO:HD2	1.79	0.64
1:L:111:ALA:HB1	1:L:117:ILE:HD12	1.79	0.64
1:E:291:TRP:O	1:E:294:VAL:HB	1.97	0.64
1:B:114:CYS:HB2	1:B:176:TYR:CD2	2.31	0.64
1:A:309:GLU:OE2	1:A:311:THR:HG23	1.97	0.64
1:E:80:GLN:NE2	1:E:89:LYS:HG2	2.12	0.64
1:L:105:VAL:HG22	1:L:136:ILE:HD11	1.79	0.64
1:L:192:LEU:O	1:L:193:LEU:HD23	1.98	0.64
1:I:156:GLN:HB3	1:I:339:SER:HB3	1.78	0.64
1:A:237:PRO:O	1:A:238:GLU:HB3	1.98	0.64
1:L:281:MET:HG3	1:L:283:GLN:HE21	1.63	0.64
1:L:300:MET:HE1	1:L:303:ARG:NH2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:ARG:HB2	1:L:332:PRO:O	1.98	0.64
1:D:70:LEU:CD2	1:D:70:LEU:H	2.11	0.64
1:I:83:ASN:CB	1:I:86:THR:HG22	2.28	0.64
1:H:98:CYS:O	1:H:102:ARG:HG2	1.98	0.64
1:K:71:GLY:O	1:K:72:LEU:HD22	1.98	0.64
1:E:74:ILE:HG21	1:E:209:GLY:HA3	1.80	0.64
1:G:143:GLY:CA	1:G:196:SER:O	2.44	0.64
1:I:154:GLY:C	1:I:156:GLN:H	2.00	0.64
1:D:83:ASN:HD21	1:D:85:ARG:HG3	1.63	0.64
1:H:200:ASN:HD22	1:H:200:ASN:H	1.46	0.64
1:A:74:ILE:HB	1:A:210:PHE:CE2	2.33	0.64
1:J:124:TYR:HB2	1:J:135:LEU:HB2	1.80	0.64
1:I:328:SER:O	1:I:331:VAL:HB	1.98	0.63
1:H:83:ASN:C	1:H:83:ASN:HD22	2.01	0.63
1:E:291:TRP:HE3	1:E:294:VAL:HG11	1.62	0.63
1:G:291:TRP:HA	1:G:294:VAL:CG2	2.27	0.63
1:B:184:HIS:HD2	1:B:186:ASP:H	1.46	0.63
1:F:300:MET:HE2	1:F:303:ARG:HH21	1.63	0.63
1:B:201:ALA:C	1:B:202:ILE:HD13	2.18	0.63
1:B:69:VAL:HG23	1:B:77:LYS:HG3	1.80	0.63
1:L:205:LEU:HD12	1:L:206:THR:H	1.63	0.63
1:E:95:LEU:HD13	1:E:101:ALA:HB1	1.80	0.63
1:K:73:GLY:HA2	2:K:1345:P4O:H8C1	1.80	0.63
1:A:337:HIS:O	1:A:341:VAL:HG23	1.98	0.63
1:K:72:LEU:HD11	1:K:77:LYS:HE3	1.81	0.63
1:I:130:GLY:O	1:K:110:ARG:NH1	2.31	0.63
1:B:214:THR:O	1:B:214:THR:HG23	1.97	0.63
1:L:108:HIS:CD2	1:L:108:HIS:O	2.52	0.63
1:A:332:PRO:HB2	1:A:334:THR:CG2	2.28	0.63
1:B:77:LYS:HD3	1:B:77:LYS:H	1.63	0.63
1:I:142:ASP:OD2	1:I:196:SER:HA	1.99	0.63
1:A:149:ARG:NH1	1:A:149:ARG:HB3	2.07	0.63
1:D:337:HIS:CD2	1:D:340:ARG:NH1	2.65	0.63
1:B:178:HIS:CG	1:B:242:LYS:HD3	2.32	0.63
1:J:148:SER:O	1:J:150:ILE:N	2.31	0.63
1:C:153:ARG:HH21	1:C:157:ALA:C	2.02	0.63
1:I:69:VAL:C	1:I:70:LEU:HD23	2.18	0.63
1:H:344:GLU:HG2	1:H:344:GLU:O	1.99	0.63
1:G:195:THR:HG23	1:G:202:ILE:O	1.98	0.63
1:J:198:ARG:CG	1:J:198:ARG:HH11	2.10	0.63
1:L:191:ASN:O	1:L:205:LEU:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:ILE:O	1:J:252:ILE:HG22	1.97	0.63
1:L:86:THR:C	1:L:88:GLU:H	1.99	0.63
1:I:158:PHE:O	1:I:336:LEU:HD22	1.99	0.63
1:J:166:ILE:HG21	1:J:256:LEU:CG	2.29	0.63
1:A:74:ILE:HG21	1:A:210:PHE:CD2	2.33	0.63
1:L:52:LEU:HD12	1:L:53:GLN:N	2.13	0.63
1:L:301:LEU:HD13	1:L:322:HIS:CD2	2.33	0.63
1:L:49:LYS:HE3	1:L:113:GLN:OE1	1.98	0.63
1:L:168:LYS:O	1:L:172:GLU:HG3	1.98	0.63
1:C:238:GLU:OE1	1:C:242:LYS:HE3	1.99	0.63
1:G:83:ASN:ND2	1:G:85:ARG:H	1.97	0.63
1:G:260:TYR:HB2	1:G:261:PRO:HD2	1.80	0.63
1:K:96:GLN:CD	1:K:131:ARG:HH21	2.01	0.63
1:D:149:ARG:HH11	1:D:149:ARG:CB	2.12	0.63
1:I:214:THR:HB	1:I:238:GLU:HG3	1.80	0.63
1:A:128:TYR:O	1:A:129:ALA:HB3	1.99	0.63
1:B:147:PHE:HD1	1:B:349:TRP:HZ2	1.47	0.62
1:J:302:ILE:CG2	1:J:306:LEU:HD12	2.28	0.62
1:F:70:LEU:HD11	1:F:80:GLN:HA	1.80	0.62
1:G:300:MET:CE	1:G:303:ARG:HE	2.12	0.62
1:H:114:CYS:HB2	1:H:176:TYR:CD2	2.34	0.62
1:C:150:ILE:CD1	1:C:158:PHE:HE1	1.98	0.62
1:J:169:SER:C	1:J:171:GLY:N	2.52	0.62
1:L:260:TYR:HB2	1:L:261:PRO:HD2	1.80	0.62
1:G:98:CYS:HB2	1:G:99:PRO:HD3	1.82	0.62
1:L:186:ASP:OD1	1:L:188:LYS:HE3	1.98	0.62
1:A:149:ARG:HH11	1:A:149:ARG:CG	2.12	0.62
1:L:258:CYS:SG	1:L:259:GLY:N	2.73	0.62
1:J:261:PRO:HG2	1:J:263:PHE:O	1.99	0.62
1:G:86:THR:HG23	1:G:86:THR:O	2.00	0.62
1:A:83:ASN:C	1:A:83:ASN:HD22	2.00	0.62
1:A:260:TYR:HB2	1:A:261:PRO:HD2	1.81	0.62
1:G:264:TYR:O	1:G:275:MET:HG3	1.99	0.62
1:J:103:ARG:HB2	1:J:103:ARG:HH11	1.62	0.62
1:E:69:VAL:HG12	1:E:71:GLY:H	1.64	0.62
1:F:86:THR:CG2	1:F:88:GLU:CB	2.73	0.62
1:D:165:GLU:HG2	1:D:328:SER:OG	1.98	0.62
1:J:255:ILE:HD11	1:J:261:PRO:HA	1.81	0.62
1:B:338:THR:O	1:B:342:LEU:HB2	1.99	0.62
1:L:260:TYR:OH	1:L:287:PRO:HG2	1.99	0.62
1:J:149:ARG:HH22	1:J:199:PRO:HA	1.59	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:PRO:HB2	1:B:334:THR:CG2	2.29	0.62
1:L:312:GLN:O	1:L:313:ARG:O	2.18	0.62
1:D:195:THR:HG22	1:D:196:SER:N	2.14	0.62
1:L:154:GLY:HA3	1:L:157:ALA:HB2	1.82	0.62
1:G:74:ILE:HG23	1:G:75:ASN:N	2.12	0.62
1:L:83:ASN:HD22	1:L:85:ARG:H	1.46	0.62
1:L:344:GLU:CD	1:L:344:GLU:N	2.53	0.62
1:K:158:PHE:HD2	1:K:159:THR:N	1.97	0.62
1:L:80:GLN:HE21	1:L:89:LYS:HB2	1.64	0.62
1:G:193:LEU:HD23	1:G:193:LEU:N	2.14	0.62
1:K:332:PRO:HB2	1:K:334:THR:CG2	2.29	0.62
1:G:214:THR:O	1:G:215:THR:CB	2.48	0.62
1:L:108:HIS:CD2	1:L:120:ILE:HD11	2.35	0.62
1:L:174:ILE:HD11	1:L:187:VAL:HG21	1.81	0.62
1:J:121:VAL:HB	1:J:137:VAL:HG12	1.81	0.62
1:E:99:PRO:O	1:E:102:ARG:N	2.33	0.62
1:L:44:PRO:O	1:L:45:GLN:HG2	1.99	0.62
1:B:237:PRO:O	1:B:238:GLU:HB3	1.98	0.62
1:L:94:MET:C	1:L:95:LEU:HD23	2.20	0.62
1:D:86:THR:CG2	1:D:88:GLU:HB2	2.30	0.61
1:J:255:ILE:HG12	1:J:260:TYR:O	1.99	0.61
1:I:332:PRO:HB2	1:I:334:THR:CG2	2.30	0.61
1:K:83:ASN:ND2	1:K:85:ARG:CG	2.58	0.61
1:I:83:ASN:HB3	1:I:86:THR:HG22	1.80	0.61
1:J:108:HIS:HA	1:J:208:PHE:CD2	2.34	0.61
1:A:74:ILE:CG2	1:A:210:PHE:CE2	2.83	0.61
1:D:246:MET:HE1	1:D:316:ILE:HA	1.82	0.61
1:L:184:HIS:O	1:L:184:HIS:CD2	2.53	0.61
1:C:160:GLU:O	1:C:163:ALA:HB3	2.00	0.61
1:E:300:MET:HA	1:E:300:MET:HE2	1.81	0.61
1:F:330:LYS:O	1:F:332:PRO:HD3	2.01	0.61
1:C:260:TYR:CE1	1:C:290:GLU:HG2	2.34	0.61
1:B:238:GLU:OE1	1:B:242:LYS:HE3	1.99	0.61
1:A:99:PRO:HD2	1:A:100:LYS:H	1.64	0.61
1:G:74:ILE:HD13	1:G:75:ASN:HB2	1.82	0.61
1:D:108:HIS:CG	1:D:120:ILE:HD11	2.35	0.61
1:D:185:ARG:HH11	1:D:185:ARG:CB	2.13	0.61
1:A:86:THR:HG22	1:A:88:GLU:H	1.65	0.61
1:E:337:HIS:O	1:E:341:VAL:HG23	2.00	0.61
1:G:145:GLU:O	1:G:147:PHE:N	2.34	0.61
1:E:130:GLY:HA3	1:J:180:ILE:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ILE:HG13	1:D:75:ASN:N	2.16	0.61
1:K:69:VAL:HG12	1:K:69:VAL:O	1.98	0.61
1:E:278:ARG:CG	1:E:283:GLN:HB2	2.30	0.61
1:J:260:TYR:HB2	1:J:261:PRO:HD2	1.81	0.61
1:D:115:PRO:O	1:D:204:LYS:HE2	2.01	0.61
1:I:180:ILE:O	1:I:180:ILE:HG13	1.99	0.61
1:F:347:GLU:O	1:F:349:TRP:N	2.33	0.61
1:J:108:HIS:HA	1:J:208:PHE:CE2	2.36	0.61
1:B:344:GLU:O	1:B:344:GLU:HG2	2.00	0.61
1:C:259:GLY:HA2	1:C:342:LEU:HD11	1.82	0.61
1:K:158:PHE:HD2	1:K:159:THR:H	1.49	0.61
1:H:102:ARG:HD2	1:H:134:LEU:HD21	1.82	0.61
1:E:58:ALA:N	1:J:50:SER:HB3	2.16	0.61
1:G:332:PRO:HB2	1:G:334:THR:HG22	1.82	0.61
1:J:255:ILE:CG1	1:J:261:PRO:HA	2.31	0.60
1:D:289:PRO:O	1:D:291:TRP:N	2.34	0.60
1:L:146:LEU:O	1:L:148:SER:N	2.33	0.60
1:D:251:VAL:O	1:D:255:ILE:HG13	2.00	0.60
1:C:333:GLN:HE21	1:C:333:GLN:HA	1.66	0.60
1:L:151:GLN:HG3	1:L:151:GLN:O	2.01	0.60
1:E:82:PHE:HA	1:E:88:GLU:O	2.01	0.60
1:H:288:ASN:HB3	1:H:289:PRO:HA	1.83	0.60
1:F:129:ALA:O	1:F:131:ARG:N	2.34	0.60
1:H:234:VAL:CG1	1:H:234:VAL:O	2.49	0.60
1:K:288:ASN:HB3	1:K:289:PRO:CA	2.28	0.60
1:E:133:CYS:HB3	1:E:135:LEU:HD21	1.83	0.60
1:G:291:TRP:HA	1:G:294:VAL:HG21	1.84	0.60
1:B:309:GLU:OE2	1:B:311:THR:HG23	2.01	0.60
1:C:118:VAL:HG11	1:C:206:THR:HG22	1.83	0.60
1:I:86:THR:C	1:I:88:GLU:H	2.04	0.60
1:E:60:ILE:C	1:E:62:ASP:N	2.50	0.60
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.66	0.60
1:A:74:ILE:CB	1:A:210:PHE:HE2	2.15	0.60
1:H:47:HIS:HB3	1:H:49:LYS:HZ3	1.66	0.60
1:G:128:TYR:O	1:G:129:ALA:HB3	2.01	0.60
1:G:292:SER:HB2	1:G:293:GLU:OE2	2.02	0.60
1:E:343:LYS:HD3	1:E:343:LYS:N	2.16	0.60
1:L:332:PRO:CB	1:L:334:THR:HG22	2.27	0.60
1:L:171:GLY:O	1:L:175:GLN:HB3	2.02	0.60
1:C:322:HIS:CE1	1:C:323:PRO:HD2	2.37	0.60
1:I:147:PHE:HE1	1:I:256:LEU:HD23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:196:SER:CB	1:K:198:ARG:HB2	2.30	0.60
1:A:233:GLU:OE1	1:B:313:ARG:NH2	2.35	0.60
1:L:337:HIS:N	1:L:337:HIS:ND1	2.50	0.60
1:A:237:PRO:O	1:A:238:GLU:CB	2.49	0.60
1:D:186:ASP:OD2	1:D:188:LYS:NZ	2.34	0.60
1:F:86:THR:HG23	1:F:88:GLU:H	1.67	0.60
1:D:341:VAL:O	1:D:345:ASP:HB2	2.01	0.60
1:L:112:SER:OG	1:L:119:ARG:HA	2.01	0.60
1:I:263:PHE:CZ	1:I:284:TYR:HD1	2.19	0.60
1:D:86:THR:O	1:D:87:GLN:CB	2.49	0.60
1:I:82:PHE:HA	1:I:88:GLU:O	2.02	0.60
1:I:198:ARG:HB3	1:I:199:PRO:HD2	1.83	0.60
1:L:314:MET:SD	1:L:319:PHE:HB2	2.42	0.59
1:F:155:ASP:O	1:F:156:GLN:HB2	2.01	0.59
1:F:260:TYR:OH	1:F:287:PRO:HG2	2.02	0.59
1:A:185:ARG:HH21	1:A:212:LYS:CD	2.15	0.59
1:A:52:LEU:HD13	1:A:109:TRP:CE3	2.37	0.59
1:H:116:HIS:CE1	1:H:169:SER:HB3	2.37	0.59
1:F:86:THR:HG22	1:F:88:GLU:N	2.17	0.59
1:B:233:GLU:OE1	1:C:313:ARG:NH1	2.34	0.59
1:L:119:ARG:CB	1:L:119:ARG:HH11	2.15	0.59
1:D:278:ARG:HH11	1:D:278:ARG:HG3	1.67	0.59
1:K:82:PHE:HD1	1:K:88:GLU:O	1.85	0.59
1:E:246:MET:HE2	1:E:316:ILE:HA	1.85	0.59
1:E:64:LYS:N	1:E:82:PHE:O	2.31	0.59
1:C:70:LEU:HD22	2:C:1351:P4O:N16	2.17	0.59
1:I:185:ARG:HH21	1:I:212:LYS:HD3	1.67	0.59
1:L:127:LEU:HD23	1:L:132:LYS:HA	1.84	0.59
1:F:82:PHE:CE1	1:F:89:LYS:HG2	2.37	0.59
1:D:289:PRO:HG2	1:D:290:GLU:H	1.68	0.59
1:C:93:LYS:HE3	2:C:1351:P4O:O26	2.03	0.59
1:D:47:HIS:ND1	1:D:47:HIS:O	2.35	0.59
1:L:180:ILE:O	1:L:182:ILE:HG13	2.03	0.59
1:J:70:LEU:HD23	1:J:70:LEU:O	2.02	0.59
1:J:158:PHE:HA	1:J:162:GLU:OE2	2.03	0.59
1:F:300:MET:CE	1:F:303:ARG:HH21	2.14	0.59
1:H:168:LYS:O	1:H:172:GLU:HG3	2.03	0.59
1:F:69:VAL:HG12	1:F:71:GLY:H	1.68	0.59
1:L:184:HIS:CD2	1:L:184:HIS:C	2.75	0.59
1:K:260:TYR:HB2	1:K:261:PRO:HD2	1.84	0.59
1:E:60:ILE:CG1	1:E:61:ASP:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:75:ASN:ND2	1:L:75:ASN:H	2.00	0.59
1:L:99:PRO:HD2	1:L:100:LYS:H	1.67	0.59
1:J:128:TYR:O	1:J:129:ALA:HB3	2.02	0.59
1:H:191:ASN:ND2	2:H:1347:P4O:H8C2	2.17	0.59
1:E:190:GLU:N	1:E:190:GLU:OE1	2.31	0.59
1:L:324:TRP:NE1	1:L:331:VAL:HG11	2.17	0.59
1:B:83:ASN:ND2	1:B:83:ASN:C	2.55	0.59
1:H:344:GLU:O	1:H:344:GLU:CG	2.51	0.59
1:H:162:GLU:O	1:H:166:ILE:HG13	2.02	0.59
1:K:314:MET:HG3	1:K:318:GLU:HB2	1.85	0.59
1:C:146:LEU:HD12	1:C:146:LEU:O	2.02	0.59
1:J:246:MET:HA	1:J:246:MET:HE3	1.83	0.59
1:I:345:ASP:O	1:I:348:ARG:N	2.35	0.59
1:D:79:LEU:N	1:D:79:LEU:HD23	2.15	0.59
1:B:321:ASN:O	1:B:326:MET:HG3	2.03	0.59
1:I:264:TYR:O	1:I:275:MET:HG3	2.03	0.59
1:J:64:LYS:HB2	1:J:84:LYS:HG3	1.85	0.59
1:E:143:GLY:CA	1:E:196:SER:O	2.51	0.59
1:G:88:GLU:CG	1:G:89:LYS:H	2.16	0.59
1:F:301:LEU:HD13	1:F:322:HIS:CD2	2.38	0.59
1:E:237:PRO:O	1:E:238:GLU:CB	2.50	0.59
1:J:319:PHE:C	1:J:321:ASN:H	2.05	0.59
1:F:227:PRO:HB3	1:F:229:TYR:CZ	2.38	0.59
1:J:86:THR:O	1:J:86:THR:CG2	2.50	0.58
1:J:86:THR:HG22	1:J:88:GLU:HB2	1.85	0.58
1:A:235:LEU:HB2	1:B:280:ARG:NH1	2.18	0.58
1:G:147:PHE:HD1	1:G:349:TRP:CZ2	2.20	0.58
1:L:94:MET:HE3	1:L:135:LEU:HD21	1.85	0.58
1:I:276:LYS:O	1:I:280:ARG:HG3	2.02	0.58
1:I:322:HIS:ND1	1:I:323:PRO:HD2	2.18	0.58
1:J:248:SER:O	1:J:250:GLY:N	2.36	0.58
1:D:239:LYS:HG3	1:D:240:TYR:H	1.68	0.58
1:G:288:ASN:HB3	1:G:289:PRO:HA	1.85	0.58
1:H:159:THR:OG1	1:H:162:GLU:HG3	2.03	0.58
1:I:275:MET:O	1:I:279:ILE:HG13	2.03	0.58
1:A:114:CYS:HB2	1:A:176:TYR:CD2	2.38	0.58
1:H:88:GLU:HG2	1:H:90:PHE:CE1	2.38	0.58
1:F:168:LYS:O	1:F:172:GLU:HG3	2.03	0.58
1:D:214:THR:O	1:D:215:THR:CG2	2.43	0.58
1:D:150:ILE:CD1	1:D:158:PHE:HE2	2.16	0.58
1:C:150:ILE:HG23	1:C:158:PHE:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:160:GLU:O	1:J:162:GLU:N	2.37	0.58
1:I:260:TYR:HB2	1:I:261:PRO:HD2	1.85	0.58
1:A:98:CYS:HB2	1:A:99:PRO:HD3	1.85	0.58
1:I:278:ARG:HB3	1:I:283:GLN:HB2	1.85	0.58
1:F:110:ARG:HG2	1:F:110:ARG:HH11	1.68	0.58
1:G:310:PRO:HG3	1:I:233:GLU:CG	2.26	0.58
1:E:274:GLY:O	1:E:278:ARG:HB2	2.03	0.58
1:E:235:LEU:HD13	1:F:276:LYS:CG	2.32	0.58
1:H:233:GLU:HG2	1:H:233:GLU:O	2.02	0.58
1:I:86:THR:O	1:I:88:GLU:N	2.35	0.58
1:J:158:PHE:HZ	1:J:163:ALA:CB	2.17	0.58
1:C:83:ASN:C	1:C:83:ASN:ND2	2.55	0.58
1:G:80:GLN:CD	1:G:89:LYS:HE2	2.23	0.58
1:L:310:PRO:N	1:L:313:ARG:HH21	2.01	0.58
1:A:141:LEU:HD13	1:A:193:LEU:HB2	1.86	0.58
1:K:108:HIS:CG	1:K:120:ILE:HD11	2.39	0.58
1:L:188:LYS:HB3	1:L:189:PRO:CD	2.34	0.58
1:F:83:ASN:ND2	1:F:83:ASN:C	2.51	0.58
1:K:192:LEU:C	1:K:193:LEU:HD23	2.24	0.58
1:L:178:HIS:CE1	1:L:242:LYS:HB3	2.39	0.58
1:I:195:THR:CG2	1:I:202:ILE:HB	2.33	0.58
1:H:97:ASP:OD1	1:H:102:ARG:NH2	2.26	0.58
1:I:327:GLN:NE2	1:I:330:LYS:HD3	2.19	0.58
1:E:287:PRO:O	1:E:291:TRP:HD1	1.87	0.58
1:I:72:LEU:HG	1:I:77:LYS:HB3	1.85	0.58
1:H:110:ARG:HH11	1:H:110:ARG:HG2	1.69	0.58
1:I:82:PHE:HB3	1:I:87:GLN:O	2.03	0.57
1:J:175:GLN:C	1:J:177:LEU:H	2.06	0.57
1:L:119:ARG:HB2	1:L:119:ARG:HH11	1.68	0.57
1:F:74:ILE:O	1:F:74:ILE:HD12	2.04	0.57
1:J:63:TYR:HE1	1:J:90:PHE:CD1	2.22	0.57
1:J:205:LEU:HD12	1:J:206:THR:H	1.69	0.57
1:L:146:LEU:C	1:L:148:SER:H	2.07	0.57
1:I:234:VAL:HG12	1:I:235:LEU:HD23	1.86	0.57
1:G:159:THR:OG1	1:G:162:GLU:HG3	2.05	0.57
1:J:56:LYS:HZ1	1:J:125:GLU:CD	2.07	0.57
1:J:65:VAL:HA	1:J:81:ILE:HG22	1.87	0.57
1:E:63:TYR:CB	1:E:81:ILE:HD12	2.35	0.57
1:E:185:ARG:HH11	1:E:185:ARG:CG	2.14	0.57
1:J:316:ILE:O	1:J:316:ILE:HG13	2.02	0.57
1:H:271:ILE:HD11	1:H:278:ARG:HH12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:VAL:O	1:C:236:GLY:N	2.34	0.57
1:A:178:HIS:CG	1:A:242:LYS:HD3	2.38	0.57
1:L:174:ILE:O	1:L:178:HIS:HD2	1.88	0.57
1:F:349:TRP:HA	1:F:349:TRP:CE3	2.39	0.57
1:J:149:ARG:NH2	1:J:199:PRO:CA	2.60	0.57
1:D:313:ARG:NH2	1:F:233:GLU:OE1	2.36	0.57
1:D:147:PHE:HE2	1:D:256:LEU:HD23	1.69	0.57
1:L:285:GLU:C	1:L:287:PRO:HD3	2.25	0.57
1:L:332:PRO:HB2	1:L:334:THR:CG2	2.29	0.57
1:G:74:ILE:CG2	1:G:209:GLY:HA3	2.27	0.57
1:E:57:ASN:ND2	1:E:58:ALA:O	2.38	0.57
1:H:141:LEU:CD1	1:H:193:LEU:HB2	2.35	0.57
1:H:260:TYR:HB2	1:H:261:PRO:HD2	1.86	0.57
1:J:254:TYR:CD1	1:J:262:PRO:HD3	2.40	0.57
1:D:278:ARG:HG3	1:D:278:ARG:NH1	2.18	0.57
1:K:197:LYS:CE	1:K:197:LYS:H	2.17	0.57
1:D:164:SER:HA	1:D:324:TRP:CH2	2.39	0.57
1:B:126:ASN:HB3	1:I:48:VAL:CG2	2.34	0.57
1:J:195:THR:HG21	1:J:202:ILE:N	2.09	0.57
1:A:332:PRO:CB	1:A:334:THR:HG22	2.35	0.57
1:L:189:PRO:HD2	1:L:190:GLU:OE1	2.05	0.57
1:L:83:ASN:O	1:L:85:ARG:N	2.38	0.57
1:L:291:TRP:HA	1:L:294:VAL:CG2	2.34	0.57
1:I:149:ARG:O	1:I:150:ILE:C	2.43	0.57
1:F:128:TYR:O	1:F:129:ALA:HB3	2.05	0.57
1:J:183:ALA:O	1:J:211:ALA:HA	2.04	0.57
1:E:246:MET:CE	1:E:316:ILE:HA	2.35	0.56
1:C:227:PRO:HG2	1:C:229:TYR:CE1	2.40	0.56
1:C:322:HIS:ND1	1:C:323:PRO:CD	2.68	0.56
1:I:168:LYS:O	1:I:172:GLU:HG3	2.05	0.56
1:I:289:PRO:C	1:I:291:TRP:H	2.03	0.56
1:B:69:VAL:CG2	1:B:77:LYS:HG3	2.34	0.56
1:G:231:ALA:O	1:G:234:VAL:HB	2.05	0.56
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.86	0.56
1:L:212:LYS:HG2	1:L:213:GLU:O	2.04	0.56
1:E:168:LYS:HD2	1:E:325:ILE:O	2.05	0.56
1:J:178:HIS:HD2	1:J:182:ILE:O	1.88	0.56
1:L:86:THR:O	1:L:86:THR:CG2	2.53	0.56
1:G:212:LYS:HG2	1:G:213:GLU:O	2.05	0.56
1:D:280:ARG:HG2	1:F:235:LEU:HD12	1.87	0.56
1:F:200:ASN:HD22	1:F:201:ALA:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLU:OE1	1:A:242:LYS:HE3	2.04	0.56
1:D:185:ARG:HH11	1:D:185:ARG:HB3	1.70	0.56
1:C:118:VAL:CG1	1:C:206:THR:HG22	2.35	0.56
1:C:108:HIS:CG	1:C:120:ILE:HD11	2.40	0.56
1:H:184:HIS:HD2	1:H:186:ASP:H	1.52	0.56
1:L:304:ASN:HD22	1:L:307:LYS:HE2	1.70	0.56
1:J:296:GLU:CD	1:J:296:GLU:H	2.09	0.56
1:H:195:THR:HG22	1:H:201:ALA:HB1	1.86	0.56
1:L:95:LEU:HD23	1:L:95:LEU:N	2.21	0.56
1:D:146:LEU:HD11	1:D:166:ILE:HD13	1.87	0.56
1:A:162:GLU:O	1:A:166:ILE:HG13	2.06	0.56
1:J:255:ILE:HG12	1:J:260:TYR:C	2.25	0.56
1:H:234:VAL:HG12	1:H:234:VAL:O	2.05	0.56
1:I:141:LEU:HD21	1:I:204:LYS:HD2	1.88	0.56
1:F:52:LEU:HD13	1:F:109:TRP:CD2	2.40	0.56
1:C:107:LEU:HD22	1:C:182:ILE:HD13	1.87	0.56
1:G:45:GLN:O	1:G:46:PHE:HB2	2.05	0.56
1:J:252:ILE:O	1:J:252:ILE:CG2	2.54	0.56
1:I:314:MET:HG3	1:I:318:GLU:HB2	1.88	0.56
1:I:337:HIS:O	1:I:341:VAL:HG23	2.05	0.56
1:L:128:TYR:O	1:L:129:ALA:HB3	2.03	0.56
1:J:195:THR:CG2	1:J:196:SER:H	2.05	0.56
1:J:251:VAL:HG12	1:J:252:ILE:N	2.21	0.56
1:C:345:ASP:C	1:C:347:GLU:H	2.08	0.56
1:F:274:GLY:O	1:F:278:ARG:HG3	2.06	0.56
1:H:147:PHE:CD1	1:H:189:PRO:HB3	2.41	0.56
1:F:158:PHE:CZ	1:F:256:LEU:HD22	2.41	0.56
1:L:189:PRO:HA	1:L:192:LEU:HD12	1.88	0.56
1:E:291:TRP:CE3	1:E:294:VAL:HG11	2.41	0.56
1:I:70:LEU:HD13	2:I:1351:P4O:C17	2.36	0.56
1:E:174:ILE:HG21	1:E:316:ILE:HD13	1.87	0.56
1:G:83:ASN:HD22	1:G:84:LYS:N	2.04	0.56
1:E:125:GLU:O	1:E:126:ASN:ND2	2.26	0.56
1:H:141:LEU:HD13	1:H:193:LEU:HB2	1.87	0.56
1:K:197:LYS:H	1:K:197:LYS:HE2	1.70	0.56
1:C:195:THR:OG1	1:C:201:ALA:HB1	2.06	0.56
1:G:107:LEU:HD22	1:G:182:ILE:HD13	1.87	0.56
1:E:110:ARG:HG2	1:E:110:ARG:HH11	1.70	0.56
1:H:198:ARG:HB3	1:H:199:PRO:HD2	1.87	0.56
1:F:184:HIS:O	1:F:185:ARG:HB2	2.06	0.55
1:I:68:GLN:HG2	1:I:70:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:ILE:HD11	1:G:187:VAL:HG21	1.87	0.55
1:J:198:ARG:HD3	1:J:201:ALA:HB2	1.87	0.55
1:E:143:GLY:HA3	1:E:196:SER:O	2.06	0.55
1:K:72:LEU:HD13	1:K:77:LYS:HA	1.88	0.55
1:I:77:LYS:HD2	1:I:79:LEU:HD21	1.87	0.55
1:I:230:VAL:HG21	1:I:235:LEU:HD21	1.87	0.55
1:L:254:TYR:CD1	1:L:262:PRO:HD3	2.42	0.55
1:G:310:PRO:CG	1:I:233:GLU:HG2	2.24	0.55
1:G:184:HIS:HD2	1:G:186:ASP:H	1.54	0.55
1:E:273:PRO:HB3	1:L:131:ARG:NH2	2.21	0.55
1:J:143:GLY:HA3	1:J:196:SER:C	2.26	0.55
1:E:264:TYR:O	1:E:275:MET:CG	2.49	0.55
1:H:74:ILE:HG21	1:H:210:PHE:CD2	2.41	0.55
1:L:344:GLU:CD	1:L:344:GLU:H	2.10	0.55
1:J:166:ILE:HG21	1:J:256:LEU:HD11	1.88	0.55
1:B:178:HIS:CD2	1:B:242:LYS:HD3	2.41	0.55
1:I:259:GLY:HA2	1:I:342:LEU:HD13	1.89	0.55
1:L:275:MET:O	1:L:279:ILE:HG13	2.06	0.55
1:J:166:ILE:HG21	1:J:256:LEU:CD1	2.36	0.55
1:F:239:LYS:N	1:F:239:LYS:HE2	2.22	0.55
1:D:83:ASN:ND2	1:D:83:ASN:C	2.60	0.55
1:G:300:MET:HE2	1:G:303:ARG:HH21	1.72	0.55
1:I:121:VAL:HB	1:I:137:VAL:HG12	1.88	0.55
1:L:162:GLU:C	1:L:164:SER:H	2.10	0.55
1:J:171:GLY:C	1:J:173:ALA:H	2.07	0.55
1:C:227:PRO:CG	1:C:229:TYR:CZ	2.90	0.55
1:I:344:GLU:O	1:I:345:ASP:OD1	2.25	0.55
1:L:174:ILE:HG22	1:L:178:HIS:CD2	2.41	0.55
1:G:280:ARG:HH12	1:I:236:GLY:HA3	1.70	0.55
1:J:88:GLU:HG3	1:J:89:LYS:N	2.21	0.55
1:E:73:GLY:CA	2:E:1345:P4O:H8C2	2.34	0.55
1:E:119:ARG:HG2	1:E:120:ILE:N	2.22	0.55
1:J:148:SER:C	1:J:150:ILE:N	2.60	0.55
1:D:260:TYR:OH	1:D:287:PRO:HG2	2.06	0.55
1:E:210:PHE:CD2	1:E:210:PHE:N	2.75	0.55
1:L:343:LYS:HE2	1:L:343:LYS:N	2.15	0.55
1:L:53:GLN:HA	1:L:53:GLN:NE2	2.22	0.55
1:D:184:HIS:CD2	1:D:184:HIS:O	2.60	0.55
1:H:235:LEU:HD12	1:I:280:ARG:HG2	1.88	0.55
1:F:140:CYS:SG	2:F:1350:P4O:H17	2.47	0.55
1:F:60:ILE:HD13	1:G:48:VAL:CG1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:HG2	1:C:310:PRO:CG	2.36	0.55
1:J:188:LYS:HB2	1:J:189:PRO:HD2	1.87	0.55
1:G:247:TRP:O	1:G:248:SER:C	2.45	0.55
1:G:161:ARG:O	1:G:165:GLU:HG3	2.07	0.55
1:B:348:ARG:O	1:B:350:GLU:N	2.31	0.55
1:A:295:SER:OG	1:A:297:GLU:HB3	2.06	0.55
1:E:344:GLU:N	1:E:344:GLU:CD	2.61	0.54
1:D:141:LEU:CD1	1:D:193:LEU:HB2	2.36	0.54
1:A:233:GLU:HG2	1:B:310:PRO:CG	2.34	0.54
1:G:151:GLN:HB2	1:G:342:LEU:HB3	1.88	0.54
1:G:148:SER:C	1:G:150:ILE:H	2.10	0.54
1:G:147:PHE:HE1	1:G:255:ILE:HG21	1.69	0.54
1:B:265:SER:O	1:B:271:ILE:O	2.24	0.54
1:L:278:ARG:O	1:L:283:GLN:HB2	2.06	0.54
1:L:160:GLU:O	1:L:160:GLU:HG2	2.08	0.54
1:K:300:MET:HE2	1:K:303:ARG:HH21	1.71	0.54
1:E:121:VAL:HG23	1:E:137:VAL:C	2.27	0.54
1:I:83:ASN:HD22	1:I:84:LYS:N	2.05	0.54
1:L:258:CYS:HB3	1:L:291:TRP:CZ2	2.43	0.54
1:H:71:GLY:O	1:H:78:VAL:HG23	2.07	0.54
1:G:74:ILE:HG21	1:G:209:GLY:CA	2.28	0.54
1:E:229:TYR:N	1:E:229:TYR:CD2	2.71	0.54
1:F:200:ASN:O	1:F:201:ALA:O	2.25	0.54
1:H:145:GLU:O	1:H:148:SER:HB2	2.07	0.54
1:B:278:ARG:HB3	1:B:283:GLN:HB2	1.88	0.54
1:L:277:THR:O	1:L:280:ARG:N	2.41	0.54
1:J:149:ARG:C	1:J:150:ILE:HD13	2.28	0.54
1:D:83:ASN:ND2	1:D:85:ARG:H	2.06	0.54
1:E:255:ILE:O	1:E:257:LEU:N	2.41	0.54
1:G:289:PRO:HD2	1:G:290:GLU:OE2	2.07	0.54
1:B:326:MET:HA	1:B:326:MET:HE3	1.90	0.54
1:F:74:ILE:HG21	1:F:209:GLY:HA3	1.87	0.54
1:B:141:LEU:HD13	1:B:193:LEU:HB2	1.89	0.54
1:I:321:ASN:HA	1:I:326:MET:HG3	1.90	0.54
1:C:145:GLU:HA	1:C:193:LEU:HD23	1.88	0.54
1:J:170:ILE:O	1:J:170:ILE:HG22	2.07	0.54
1:E:265:SER:O	1:E:266:ASN:HB2	2.08	0.54
1:D:142:ASP:HA	2:D:1351:P4O:N16	2.23	0.54
1:B:227:PRO:HG2	1:B:230:VAL:CB	2.34	0.54
1:I:159:THR:C	1:I:336:LEU:HD21	2.27	0.54
1:E:159:THR:HB	1:E:333:GLN:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:VAL:HG13	1:G:332:PRO:HD2	1.88	0.54
1:H:151:GLN:O	1:H:343:LYS:HE3	2.07	0.54
1:F:210:PHE:CD2	1:F:210:PHE:N	2.76	0.54
1:E:159:THR:HG23	1:E:162:GLU:OE2	2.08	0.54
1:A:168:LYS:O	1:A:172:GLU:HG3	2.08	0.54
1:C:315:THR:OG1	1:C:318:GLU:HG3	2.08	0.54
1:G:281:MET:HB2	1:G:283:GLN:HG3	1.88	0.54
1:L:277:THR:HG22	1:L:280:ARG:HD3	1.90	0.54
1:L:246:MET:HG3	1:L:314:MET:O	2.08	0.54
1:G:185:ARG:NH2	1:G:212:LYS:HD2	2.18	0.54
1:E:83:ASN:OD1	1:E:86:THR:N	2.41	0.54
1:I:154:GLY:C	1:I:156:GLN:N	2.60	0.54
1:B:69:VAL:HG13	1:B:69:VAL:O	2.08	0.54
1:B:74:ILE:HG13	1:B:75:ASN:CG	2.28	0.54
1:D:327:GLN:HG3	1:D:330:LYS:HG2	1.89	0.54
1:D:70:LEU:CD2	1:D:80:GLN:HB2	2.31	0.54
1:D:337:HIS:HD2	1:D:340:ARG:NH1	2.05	0.54
1:E:98:CYS:HB2	1:E:99:PRO:CD	2.38	0.54
1:C:301:LEU:HD13	1:C:322:HIS:CD2	2.43	0.54
1:K:296:GLU:OE2	1:K:299:LYS:HD2	2.07	0.54
1:B:168:LYS:O	1:B:172:GLU:HG3	2.08	0.54
1:B:86:THR:C	1:B:88:GLU:H	2.11	0.54
1:E:300:MET:HA	1:E:300:MET:CE	2.36	0.54
1:E:300:MET:HE2	1:E:303:ARG:HE	1.72	0.54
1:L:85:ARG:HD2	1:L:85:ARG:O	2.08	0.54
1:F:99:PRO:HD2	1:F:100:LYS:H	1.73	0.54
1:F:323:PRO:HA	1:F:326:MET:HB2	1.90	0.54
1:E:74:ILE:HD12	1:E:74:ILE:O	2.07	0.54
1:G:309:GLU:OE2	1:G:310:PRO:HD2	2.08	0.53
1:F:86:THR:O	1:F:87:GLN:CB	2.56	0.53
1:E:146:LEU:HD13	1:E:203:LEU:HD22	1.89	0.53
1:J:160:GLU:C	1:J:162:GLU:H	2.11	0.53
1:G:300:MET:HE2	1:G:303:ARG:HE	1.73	0.53
1:A:48:VAL:HG13	1:G:60:ILE:HD13	1.90	0.53
1:L:255:ILE:HG12	1:L:261:PRO:CA	2.36	0.53
1:J:83:ASN:HD22	1:J:83:ASN:C	2.10	0.53
1:G:99:PRO:CD	1:G:100:LYS:H	2.21	0.53
1:B:185:ARG:HH11	1:B:185:ARG:CB	2.20	0.53
1:G:86:THR:C	1:G:88:GLU:H	2.12	0.53
1:K:332:PRO:CB	1:K:334:THR:HG22	2.37	0.53
1:F:237:PRO:O	1:F:238:GLU:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:HIS:CG	1:F:120:ILE:HD11	2.43	0.53
1:H:87:GLN:HA	1:H:87:GLN:NE2	2.24	0.53
1:E:341:VAL:O	1:E:344:GLU:OE1	2.26	0.53
1:B:147:PHE:CD1	1:B:349:TRP:CZ2	2.86	0.53
1:K:141:LEU:H	2:K:1345:P4O:C10	2.21	0.53
1:F:322:HIS:ND1	1:F:323:PRO:CD	2.72	0.53
1:D:150:ILE:O	1:D:152:ASP:N	2.41	0.53
1:B:272:SER:H	1:B:273:PRO:CD	2.21	0.53
1:I:309:GLU:OE2	1:I:311:THR:HG23	2.08	0.53
1:F:289:PRO:HD2	1:F:290:GLU:OE2	2.08	0.53
1:L:277:THR:C	1:L:279:ILE:N	2.62	0.53
1:I:83:ASN:C	1:I:83:ASN:HD22	2.10	0.53
1:L:86:THR:HG22	1:L:88:GLU:HB2	1.89	0.53
1:E:134:LEU:C	1:E:135:LEU:HD23	2.29	0.53
1:D:239:LYS:C	1:D:241:ASP:H	2.10	0.53
1:J:59:ILE:C	1:J:61:ASP:H	2.12	0.53
1:I:69:VAL:HG11	1:I:72:LEU:HD11	1.89	0.53
1:H:147:PHE:HB3	1:H:342:LEU:HD11	1.89	0.53
1:F:195:THR:HG23	1:F:202:ILE:O	2.09	0.53
1:J:195:THR:HG21	1:J:201:ALA:HB3	1.91	0.53
1:H:200:ASN:O	1:H:201:ALA:O	2.26	0.53
1:F:260:TYR:HB2	1:F:261:PRO:CD	2.39	0.53
1:L:150:ILE:HG23	1:L:151:GLN:N	2.22	0.53
1:F:110:ARG:HG2	1:F:110:ARG:NH1	2.24	0.53
1:K:195:THR:HG22	1:K:202:ILE:H	1.74	0.53
1:B:129:ALA:O	1:B:131:ARG:N	2.41	0.53
1:F:86:THR:HG21	1:F:88:GLU:CB	2.29	0.53
1:J:108:HIS:O	1:J:110:ARG:N	2.41	0.53
1:H:200:ASN:C	1:H:201:ALA:O	2.46	0.53
1:K:84:LYS:C	1:K:85:ARG:HG2	2.29	0.53
1:J:189:PRO:C	1:J:191:ASN:H	2.12	0.53
1:A:74:ILE:CB	1:A:210:PHE:CE2	2.92	0.53
1:E:59:ILE:N	1:E:126:ASN:OD1	2.42	0.53
1:J:103:ARG:HA	1:J:106:GLU:HB2	1.89	0.53
1:I:300:MET:CE	1:I:303:ARG:HE	2.21	0.53
1:C:114:CYS:HB2	1:C:176:TYR:CD2	2.44	0.53
1:I:174:ILE:HD11	1:I:187:VAL:HG21	1.91	0.53
1:J:119:ARG:CZ	1:J:119:ARG:HB2	2.39	0.53
1:J:62:ASP:O	1:J:84:LYS:N	2.42	0.53
1:F:98:CYS:HB2	1:F:99:PRO:CD	2.38	0.53
1:G:264:TYR:C	1:G:278:ARG:HH21	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:LYS:HB2	1:I:325:ILE:HG23	1.89	0.53
1:B:59:ILE:HG13	1:B:124:TYR:CE1	2.44	0.53
1:C:302:ILE:HG22	1:C:306:LEU:HD12	1.91	0.53
1:B:86:THR:CG2	1:B:88:GLU:HB2	2.35	0.53
1:H:289:PRO:O	1:H:290:GLU:C	2.48	0.53
1:F:191:ASN:ND2	2:F:1350:P4O:H8C2	2.24	0.53
1:B:164:SER:HA	1:B:324:TRP:CH2	2.44	0.53
1:L:78:VAL:CG1	1:L:79:LEU:H	2.21	0.52
1:I:337:HIS:ND1	1:I:337:HIS:N	2.56	0.52
1:G:114:CYS:HB2	1:G:176:TYR:CD2	2.43	0.52
1:C:158:PHE:O	1:C:336:LEU:HD22	2.09	0.52
1:A:148:SER:O	1:A:149:ARG:C	2.45	0.52
1:L:90:PHE:HA	1:L:140:CYS:HB2	1.91	0.52
1:L:340:ARG:H	1:L:340:ARG:HD3	1.74	0.52
1:K:118:VAL:HG12	1:K:205:LEU:O	2.09	0.52
1:E:97:ASP:HB2	1:E:134:LEU:HD22	1.92	0.52
1:C:147:PHE:HD1	1:C:189:PRO:HB3	1.74	0.52
1:L:108:HIS:CG	1:L:120:ILE:HD11	2.45	0.52
1:I:164:SER:HA	1:I:324:TRP:CH2	2.44	0.52
1:J:239:LYS:O	1:J:241:ASP:N	2.43	0.52
1:F:239:LYS:HE2	1:F:239:LYS:CA	2.39	0.52
1:I:237:PRO:O	1:I:238:GLU:HB3	2.10	0.52
1:A:195:THR:HG23	1:A:202:ILE:O	2.09	0.52
1:I:98:CYS:HB2	1:I:99:PRO:CD	2.39	0.52
1:C:150:ILE:HG23	1:C:158:PHE:HD1	1.73	0.52
1:E:185:ARG:NH1	1:E:185:ARG:CG	2.72	0.52
1:K:158:PHE:CD2	1:K:159:THR:N	2.77	0.52
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.92	0.52
1:G:240:TYR:O	1:G:241:ASP:C	2.47	0.52
1:F:346:LYS:HZ2	1:F:349:TRP:HD1	1.58	0.52
1:K:86:THR:O	1:K:87:GLN:HB2	2.09	0.52
1:I:83:ASN:ND2	1:I:83:ASN:C	2.62	0.52
1:L:310:PRO:HA	1:L:313:ARG:NH2	2.25	0.52
1:C:333:GLN:CA	1:C:333:GLN:HE21	2.22	0.52
1:L:145:GLU:O	1:L:147:PHE:N	2.42	0.52
1:L:255:ILE:HA	1:L:260:TYR:O	2.09	0.52
1:G:309:GLU:OE2	1:G:311:THR:HG23	2.09	0.52
1:D:239:LYS:HG3	1:D:240:TYR:N	2.25	0.52
1:L:310:PRO:CA	1:L:313:ARG:HH21	2.22	0.52
1:E:110:ARG:HG2	1:E:110:ARG:NH1	2.24	0.52
1:B:272:SER:N	1:B:273:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:HIS:CG	1:C:47:HIS:O	2.62	0.52
1:F:345:ASP:OD1	1:F:348:ARG:HB2	2.08	0.52
1:C:147:PHE:CE1	1:C:189:PRO:HB3	2.44	0.52
1:J:48:VAL:O	1:J:48:VAL:HG13	2.09	0.52
1:H:185:ARG:HH21	1:H:212:LYS:CD	2.23	0.52
1:I:338:THR:HG22	1:I:342:LEU:HD22	1.91	0.52
1:B:129:ALA:C	1:B:131:ARG:H	2.13	0.52
1:I:75:ASN:HD22	1:I:75:ASN:N	2.07	0.52
1:J:149:ARG:O	1:J:150:ILE:HD13	2.10	0.52
1:B:275:MET:HE2	1:B:279:ILE:CD1	2.40	0.52
1:J:83:ASN:HD21	1:J:85:ARG:HE	1.58	0.52
1:E:198:ARG:O	1:E:201:ALA:N	2.43	0.52
1:I:202:ILE:HG22	1:I:203:LEU:N	2.25	0.52
1:B:341:VAL:O	1:B:345:ASP:HB2	2.10	0.52
1:A:185:ARG:HH21	1:A:212:LYS:HD3	1.74	0.52
1:E:210:PHE:HD2	1:E:210:PHE:N	2.07	0.52
1:A:151:GLN:O	1:A:343:LYS:HE3	2.10	0.52
1:L:208:PHE:O	1:L:210:PHE:N	2.43	0.52
1:K:164:SER:HA	1:K:324:TRP:CH2	2.45	0.52
1:F:151:GLN:HG3	1:F:342:LEU:HB3	1.90	0.52
1:B:147:PHE:HD1	1:B:349:TRP:CH2	2.27	0.52
1:K:49:LYS:HD2	1:K:50:SER:H	1.74	0.52
1:J:321:ASN:HA	1:J:326:MET:HG2	1.92	0.52
1:G:168:LYS:O	1:G:172:GLU:HG3	2.10	0.52
1:B:159:THR:OG1	1:B:162:GLU:HG3	2.09	0.52
1:A:277:THR:HG21	1:C:179:SER:O	2.10	0.52
1:E:338:THR:O	1:E:342:LEU:HB2	2.10	0.52
1:D:192:LEU:C	1:D:193:LEU:HD23	2.31	0.51
1:I:156:GLN:HB3	1:I:339:SER:CB	2.41	0.51
1:B:332:PRO:CB	1:B:334:THR:HG22	2.39	0.51
1:J:255:ILE:CD1	1:J:261:PRO:HA	2.41	0.51
1:A:83:ASN:HD22	1:A:84:LYS:N	2.07	0.51
1:E:127:LEU:O	1:E:128:TYR:HB2	2.10	0.51
1:B:110:ARG:NH1	1:B:110:ARG:HG2	2.26	0.51
1:A:151:GLN:O	1:A:151:GLN:HG2	2.09	0.51
1:C:74:ILE:HG13	1:C:75:ASN:ND2	2.25	0.51
1:J:78:VAL:HG11	1:J:91:ALA:HB1	1.92	0.51
1:K:83:ASN:CB	1:K:86:THR:HB	2.40	0.51
1:L:188:LYS:O	1:L:192:LEU:HD12	2.09	0.51
1:E:230:VAL:HG22	1:E:231:ALA:N	2.25	0.51
1:I:83:ASN:OD1	1:I:86:THR:CG2	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:TYR:O	1:D:129:ALA:HB3	2.10	0.51
1:D:114:CYS:HB2	1:D:176:TYR:CD2	2.45	0.51
1:D:150:ILE:C	1:D:152:ASP:H	2.14	0.51
1:D:159:THR:O	1:D:160:GLU:C	2.47	0.51
1:H:151:GLN:HG3	1:H:342:LEU:HB3	1.91	0.51
1:F:162:GLU:O	1:F:166:ILE:HG13	2.11	0.51
1:F:309:GLU:OE2	1:F:311:THR:HG23	2.10	0.51
1:I:83:ASN:HB3	1:I:86:THR:CG2	2.40	0.51
1:E:302:ILE:O	1:E:302:ILE:HG22	2.09	0.51
1:C:260:TYR:OH	1:C:287:PRO:HG2	2.11	0.51
1:D:52:LEU:HD13	1:D:109:TRP:CD2	2.46	0.51
1:K:69:VAL:O	1:K:71:GLY:N	2.44	0.51
1:H:70:LEU:HD22	1:H:80:GLN:HB2	1.92	0.51
1:B:150:ILE:C	1:B:152:ASP:H	2.12	0.51
1:F:349:TRP:HA	1:F:349:TRP:HE3	1.73	0.51
1:J:195:THR:HG21	1:J:201:ALA:CB	2.40	0.51
1:L:180:ILE:O	1:L:180:ILE:HG13	2.11	0.51
1:K:146:LEU:HD13	1:K:203:LEU:HD11	1.93	0.51
1:B:74:ILE:O	1:B:74:ILE:HD12	2.10	0.51
1:L:184:HIS:O	1:L:184:HIS:HD2	1.94	0.51
1:F:86:THR:HG23	1:F:88:GLU:HB2	1.86	0.51
1:D:98:CYS:HB2	1:D:99:PRO:CD	2.39	0.51
1:H:105:VAL:HG22	1:H:136:ILE:HD11	1.92	0.51
1:I:195:THR:CG2	1:I:202:ILE:H	2.23	0.51
1:C:227:PRO:CG	1:C:229:TYR:OH	2.58	0.51
1:G:97:ASP:O	1:G:98:CYS:HB3	2.10	0.51
1:G:147:PHE:CE1	1:G:255:ILE:CG2	2.93	0.51
1:L:153:ARG:CZ	1:L:153:ARG:CB	2.88	0.51
1:D:92:LEU:HD11	1:D:135:LEU:HB3	1.92	0.51
1:G:247:TRP:NE1	1:I:230:VAL:O	2.44	0.51
1:C:145:GLU:HA	1:C:193:LEU:CD2	2.40	0.51
1:E:240:TYR:O	1:E:241:ASP:C	2.48	0.51
1:E:158:PHE:HE1	1:E:256:LEU:HD22	1.75	0.51
1:D:70:LEU:N	1:D:70:LEU:HD22	2.26	0.51
1:K:288:ASN:N	1:K:288:ASN:ND2	2.57	0.51
1:J:158:PHE:HA	1:J:162:GLU:CD	2.30	0.51
1:C:168:LYS:HB2	1:C:325:ILE:HG23	1.93	0.51
1:J:176:TYR:CD2	1:J:176:TYR:O	2.64	0.51
1:J:179:SER:HA	1:L:281:MET:SD	2.51	0.51
1:F:86:THR:O	1:F:87:GLN:HB2	2.10	0.51
1:K:74:ILE:HG22	1:K:207:ASP:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:300:MET:O	1:J:302:ILE:N	2.44	0.51
1:C:152:ASP:N	1:C:152:ASP:OD1	2.44	0.51
1:E:160:GLU:O	1:E:163:ALA:N	2.44	0.51
1:G:83:ASN:ND2	1:G:83:ASN:C	2.63	0.51
1:I:347:GLU:HG3	1:I:348:ARG:H	1.74	0.51
1:I:345:ASP:HB3	1:I:348:ARG:HG3	1.92	0.51
1:J:103:ARG:HG3	1:J:104:GLU:N	2.24	0.51
1:E:127:LEU:HB2	1:J:49:LYS:HB2	1.91	0.51
1:A:146:LEU:HD11	1:A:166:ILE:HD13	1.93	0.51
1:G:241:ASP:O	1:G:244:CYS:HB3	2.11	0.51
1:B:48:VAL:HG13	1:K:60:ILE:HD13	1.92	0.51
1:I:290:GLU:CD	1:I:290:GLU:H	2.14	0.51
1:L:160:GLU:HB3	1:L:334:THR:HG23	1.93	0.51
1:J:302:ILE:HG22	1:J:306:LEU:HD12	1.91	0.51
1:D:158:PHE:O	1:D:336:LEU:HD22	2.10	0.51
1:E:118:VAL:CG1	1:E:206:THR:HG22	2.41	0.51
1:C:170:ILE:CD1	1:C:192:LEU:HD13	2.41	0.51
1:J:167:MET:CE	1:J:167:MET:HA	2.41	0.51
1:G:185:ARG:HH11	1:G:185:ARG:HB3	1.74	0.51
1:E:115:PRO:O	1:E:204:LYS:HE2	2.10	0.51
1:C:237:PRO:O	1:C:238:GLU:HB3	2.11	0.51
1:B:314:MET:HG3	1:B:318:GLU:HB2	1.93	0.51
1:C:341:VAL:O	1:C:341:VAL:HG12	2.10	0.51
1:J:193:LEU:CD2	1:J:193:LEU:N	2.68	0.50
1:H:83:ASN:C	1:H:83:ASN:ND2	2.64	0.50
1:D:234:VAL:C	1:D:236:GLY:N	2.63	0.50
1:A:87:GLN:HA	1:A:87:GLN:NE2	2.26	0.50
1:H:184:HIS:HD2	1:H:186:ASP:N	2.09	0.50
1:K:102:ARG:O	1:K:106:GLU:HB2	2.11	0.50
1:K:93:LYS:NZ	1:K:104:GLU:OE1	2.36	0.50
1:K:168:LYS:O	1:K:172:GLU:HG3	2.12	0.50
1:E:89:LYS:O	1:E:90:PHE:CD2	2.64	0.50
1:K:196:SER:CB	1:K:198:ARG:HD3	2.41	0.50
1:G:88:GLU:HG3	1:G:89:LYS:H	1.77	0.50
1:G:147:PHE:CZ	1:G:255:ILE:CG2	2.95	0.50
1:H:110:ARG:NH1	1:H:110:ARG:HG2	2.26	0.50
1:J:56:LYS:NZ	1:J:125:GLU:CD	2.65	0.50
1:C:202:ILE:N	1:C:202:ILE:HD13	2.25	0.50
1:J:71:GLY:O	1:J:72:LEU:C	2.49	0.50
1:A:149:ARG:CG	1:A:149:ARG:NH1	2.72	0.50
1:D:96:GLN:CD	1:D:131:ARG:HD3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:THR:CG2	1:G:202:ILE:HB	2.41	0.50
1:L:255:ILE:HG12	1:L:260:TYR:O	2.12	0.50
1:J:301:LEU:HD22	1:J:322:HIS:CE1	2.47	0.50
1:E:99:PRO:O	1:E:101:ALA:N	2.44	0.50
1:C:129:ALA:O	1:C:131:ARG:HG3	2.12	0.50
1:F:331:VAL:HG13	1:F:332:PRO:HD2	1.91	0.50
1:C:196:SER:OG	1:C:201:ALA:HB2	2.11	0.50
1:G:166:ILE:HG21	1:G:256:LEU:HD11	1.94	0.50
1:H:272:SER:H	1:H:273:PRO:CD	2.25	0.50
1:K:329:THR:CG2	1:K:330:LYS:HE2	2.41	0.50
1:A:118:VAL:O	1:A:118:VAL:HG13	2.12	0.50
1:C:158:PHE:HD2	1:C:158:PHE:C	2.15	0.50
1:L:118:VAL:HG13	1:L:118:VAL:O	2.11	0.50
1:L:189:PRO:O	1:L:191:ASN:N	2.45	0.50
1:E:180:ILE:CG1	1:E:182:ILE:HD12	2.31	0.50
1:K:110:ARG:HH11	1:K:110:ARG:HG2	1.76	0.50
1:F:80:GLN:HE22	1:F:89:LYS:HD3	1.73	0.50
1:D:74:ILE:C	1:D:74:ILE:HD12	2.32	0.50
1:F:290:GLU:N	1:F:290:GLU:OE2	2.41	0.50
1:J:62:ASP:HB2	1:J:63:TYR:CD2	2.47	0.50
1:H:149:ARG:HH11	1:H:149:ARG:CG	2.25	0.50
1:L:158:PHE:CE1	1:L:163:ALA:HB2	2.47	0.50
1:L:90:PHE:CD2	1:L:121:VAL:HG21	2.47	0.50
1:G:63:TYR:C	1:G:84:LYS:HG3	2.31	0.50
1:C:288:ASN:OD1	1:C:288:ASN:N	2.45	0.50
1:A:56:LYS:O	1:F:50:SER:HB2	2.11	0.50
1:L:251:VAL:HG13	1:L:262:PRO:HD2	1.94	0.50
1:L:175:GLN:O	1:L:175:GLN:HG3	2.09	0.50
1:L:153:ARG:NH1	1:L:153:ARG:HB3	2.26	0.50
1:H:200:ASN:N	1:H:200:ASN:ND2	2.57	0.50
1:E:48:VAL:O	1:E:48:VAL:HG13	2.11	0.50
1:G:286:PHE:O	1:G:291:TRP:HB2	2.11	0.50
1:I:71:GLY:O	1:I:72:LEU:HD12	2.12	0.50
1:I:338:THR:O	1:I:342:LEU:HB2	2.11	0.50
1:L:202:ILE:HG22	1:L:204:LYS:HG3	1.94	0.50
1:B:190:GLU:CD	1:B:190:GLU:H	2.16	0.50
1:C:151:GLN:HE22	1:C:346:LYS:HG3	1.76	0.50
1:K:338:THR:O	1:K:342:LEU:HB2	2.12	0.50
1:L:335:PRO:C	1:L:336:LEU:HD13	2.32	0.50
1:G:48:VAL:O	1:G:48:VAL:HG13	2.12	0.50
1:C:198:ARG:HB3	1:C:199:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:240:TYR:CD2	1:J:240:TYR:N	2.79	0.50
1:B:323:PRO:HA	1:B:326:MET:HB2	1.93	0.49
1:D:159:THR:C	1:D:336:LEU:HD21	2.32	0.49
1:C:74:ILE:HD12	1:C:74:ILE:O	2.12	0.49
1:D:192:LEU:O	1:D:193:LEU:HD23	2.12	0.49
1:D:340:ARG:O	1:D:344:GLU:HB2	2.12	0.49
1:I:195:THR:HG21	1:I:202:ILE:HB	1.94	0.49
1:B:233:GLU:OE1	1:C:313:ARG:NH2	2.45	0.49
1:J:303:ARG:O	1:J:306:LEU:O	2.30	0.49
1:F:227:PRO:HB2	1:F:230:VAL:HB	1.94	0.49
1:K:146:LEU:HD12	1:K:194:TYR:CE2	2.46	0.49
1:C:343:LYS:C	1:C:345:ASP:H	2.15	0.49
1:A:83:ASN:C	1:A:83:ASN:ND2	2.65	0.49
1:F:139:GLU:O	2:F:1350:P4O:H10	2.12	0.49
1:A:165:GLU:HG2	1:A:328:SER:HB3	1.93	0.49
1:D:300:MET:HE2	1:D:303:ARG:HH21	1.77	0.49
1:C:174:ILE:HD11	1:C:187:VAL:HG21	1.94	0.49
1:L:192:LEU:C	1:L:193:LEU:HD23	2.32	0.49
1:J:248:SER:C	1:J:250:GLY:N	2.66	0.49
1:G:88:GLU:CG	1:G:89:LYS:N	2.75	0.49
1:C:333:GLN:NE2	1:C:333:GLN:HA	2.27	0.49
1:E:239:LYS:HE3	1:E:240:TYR:HE1	1.77	0.49
1:E:118:VAL:HA	1:E:139:GLU:OE1	2.12	0.49
1:H:161:ARG:O	1:H:164:SER:HB3	2.10	0.49
1:F:277:THR:HA	1:F:280:ARG:HG3	1.94	0.49
1:K:80:GLN:NE2	1:K:89:LYS:CG	2.71	0.49
1:L:98:CYS:O	1:L:102:ARG:HG2	2.13	0.49
1:F:332:PRO:HB2	1:F:334:THR:CG2	2.43	0.49
1:B:74:ILE:CG2	1:B:210:PHE:HE2	2.25	0.49
1:H:105:VAL:CG2	1:H:136:ILE:HD11	2.43	0.49
1:D:168:LYS:O	1:D:172:GLU:HG3	2.13	0.49
1:J:251:VAL:CG1	1:J:252:ILE:HG13	2.29	0.49
1:I:83:ASN:O	1:I:87:GLN:N	2.45	0.49
1:B:147:PHE:CD1	1:B:349:TRP:CH2	3.01	0.49
1:L:158:PHE:HE1	1:L:256:LEU:O	1.96	0.49
1:L:258:CYS:O	1:L:338:THR:HA	2.12	0.49
1:K:70:LEU:HG	2:K:1345:P4O:C17	2.43	0.49
1:F:286:PHE:CE1	1:F:299:LYS:HB3	2.48	0.49
1:L:208:PHE:C	1:L:210:PHE:H	2.15	0.49
1:C:80:GLN:NE2	1:C:89:LYS:HB2	2.28	0.49
1:L:125:GLU:O	1:L:126:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:TRP:CZ2	1:F:263:PHE:HE1	2.31	0.49
1:D:237:PRO:O	1:D:238:GLU:CB	2.60	0.49
1:J:302:ILE:HG23	1:J:306:LEU:HD12	1.94	0.49
1:J:254:TYR:HD1	1:J:262:PRO:HD3	1.75	0.49
1:A:83:ASN:ND2	1:A:85:ARG:H	2.11	0.49
1:A:52:LEU:HD13	1:A:109:TRP:CD2	2.47	0.49
1:G:166:ILE:CG2	1:G:256:LEU:HD11	2.43	0.49
1:B:151:GLN:HG3	1:B:151:GLN:O	2.13	0.49
1:F:331:VAL:HG12	1:F:332:PRO:HD2	1.95	0.49
1:E:148:SER:C	1:E:150:ILE:H	2.16	0.49
1:H:207:ASP:HB2	2:H:1347:P4O:N7	2.28	0.49
1:F:60:ILE:HD13	1:G:48:VAL:HG12	1.95	0.49
1:B:74:ILE:HB	1:B:210:PHE:HE2	1.77	0.49
1:J:119:ARG:NH1	1:J:119:ARG:HB2	2.28	0.49
1:K:329:THR:HG23	1:K:330:LYS:HE2	1.93	0.49
1:G:246:MET:HE1	1:G:316:ILE:HA	1.94	0.49
1:I:156:GLN:O	1:I:157:ALA:C	2.51	0.49
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.93	0.49
1:C:227:PRO:HG2	1:C:229:TYR:OH	2.12	0.49
1:B:198:ARG:O	1:B:201:ALA:HB2	2.13	0.49
1:H:172:GLU:HG2	1:H:320:MET:CE	2.43	0.49
1:D:150:ILE:C	1:D:152:ASP:N	2.66	0.49
1:J:72:LEU:HD23	1:J:72:LEU:C	2.33	0.49
1:G:199:PRO:HD2	1:G:200:ASN:OD1	2.12	0.49
1:L:277:THR:HA	1:L:280:ARG:CD	2.42	0.48
1:L:319:PHE:O	1:L:319:PHE:CG	2.66	0.48
1:E:80:GLN:HE21	1:E:81:ILE:N	2.10	0.48
1:L:291:TRP:CE3	1:L:294:VAL:HG21	2.48	0.48
1:E:133:CYS:HB3	1:E:135:LEU:CD2	2.43	0.48
1:J:261:PRO:HB2	1:J:263:PHE:O	2.12	0.48
1:G:66:THR:HG21	1:G:82:PHE:CE2	2.45	0.48
1:K:314:MET:CG	1:K:318:GLU:HB2	2.43	0.48
1:F:191:ASN:HD21	2:F:1350:P4O:H8C2	1.78	0.48
1:B:59:ILE:HG13	1:B:124:TYR:CD1	2.47	0.48
1:D:118:VAL:HG13	1:D:118:VAL:O	2.13	0.48
1:C:158:PHE:CD2	1:C:158:PHE:C	2.85	0.48
1:L:161:ARG:O	1:L:165:GLU:HG3	2.12	0.48
1:J:81:ILE:HG13	1:J:90:PHE:O	2.12	0.48
1:L:316:ILE:CG1	1:L:316:ILE:O	2.59	0.48
1:L:180:ILE:O	1:L:181:ASN:C	2.51	0.48
1:F:196:SER:OG	1:F:201:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:ARG:NH2	1:K:197:LYS:O	2.46	0.48
1:K:194:TYR:HB3	1:K:201:ALA:HB1	1.96	0.48
1:J:76:GLY:O	1:J:77:LYS:HB2	2.13	0.48
1:A:58:ALA:H	1:F:50:SER:HB3	1.77	0.48
1:I:108:HIS:CG	1:I:120:ILE:HD11	2.48	0.48
1:A:147:PHE:HE2	1:A:256:LEU:HD23	1.78	0.48
1:L:277:THR:C	1:L:279:ILE:H	2.16	0.48
1:J:60:ILE:HG22	1:J:65:VAL:HG21	1.96	0.48
1:K:287:PRO:C	1:K:288:ASN:HD22	2.16	0.48
1:F:184:HIS:HD2	1:F:186:ASP:H	1.60	0.48
1:E:142:ASP:HA	2:E:1345:P4O:N16	2.27	0.48
1:C:345:ASP:C	1:C:347:GLU:N	2.64	0.48
1:C:309:GLU:OE2	1:C:311:THR:CG2	2.59	0.48
1:B:271:ILE:CG1	1:B:273:PRO:HD2	2.43	0.48
1:D:330:LYS:N	1:D:330:LYS:HD3	2.27	0.48
1:G:191:ASN:ND2	2:G:1350:P4O:H8C2	2.29	0.48
1:C:240:TYR:O	1:C:243:SER:N	2.46	0.48
1:A:108:HIS:CG	1:A:120:ILE:HD11	2.48	0.48
1:B:340:ARG:O	1:B:343:LYS:O	2.31	0.48
1:E:83:ASN:OD1	1:E:85:ARG:HB3	2.13	0.48
1:G:148:SER:C	1:G:150:ILE:N	2.65	0.48
1:K:274:GLY:O	1:K:278:ARG:HG3	2.12	0.48
1:E:253:MET:HB2	1:E:253:MET:HE2	1.65	0.48
1:E:147:PHE:CE1	1:E:255:ILE:HG21	2.47	0.48
1:A:185:ARG:HH21	1:A:212:LYS:HD2	1.78	0.48
1:D:159:THR:OG1	1:D:162:GLU:HG3	2.14	0.48
1:G:115:PRO:O	1:G:204:LYS:HE2	2.14	0.48
1:F:178:HIS:CG	1:F:242:LYS:HD3	2.48	0.48
1:H:178:HIS:CG	1:H:242:LYS:HD3	2.48	0.48
1:I:150:ILE:CD1	1:I:158:PHE:CE2	2.97	0.48
1:F:155:ASP:O	1:F:156:GLN:O	2.32	0.48
1:B:188:LYS:HB2	1:B:189:PRO:CD	2.42	0.48
1:C:228:TYR:C	1:C:228:TYR:CD1	2.86	0.48
1:L:47:HIS:O	1:L:47:HIS:CG	2.66	0.48
1:L:86:THR:O	1:L:86:THR:HG22	2.13	0.48
1:K:196:SER:HB3	1:K:198:ARG:HD3	1.96	0.48
1:E:193:LEU:O	1:E:203:LEU:HD12	2.14	0.48
1:L:185:ARG:CG	1:L:185:ARG:HH11	2.25	0.48
1:G:291:TRP:CE3	1:G:294:VAL:HG21	2.49	0.48
1:F:289:PRO:O	1:F:290:GLU:C	2.52	0.48
1:H:121:VAL:HB	1:H:137:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:LEU:HD23	1:F:79:LEU:N	2.28	0.48
1:C:190:GLU:CD	1:C:190:GLU:H	2.17	0.48
1:G:141:LEU:CD1	1:G:193:LEU:HB2	2.41	0.48
1:F:230:VAL:HG13	1:F:230:VAL:O	2.14	0.48
1:F:52:LEU:HD13	1:F:109:TRP:CE3	2.49	0.48
1:I:45:GLN:O	1:I:46:PHE:CD2	2.67	0.48
1:L:278:ARG:HB2	1:L:278:ARG:CZ	2.40	0.48
1:D:70:LEU:CD2	1:D:70:LEU:N	2.75	0.48
1:G:192:LEU:O	1:G:193:LEU:HD23	2.13	0.48
1:G:289:PRO:O	1:G:292:SER:OG	2.30	0.48
1:H:78:VAL:HA	1:H:92:LEU:O	2.14	0.48
1:F:202:ILE:HG22	1:F:203:LEU:N	2.28	0.48
1:J:123:VAL:HG22	1:J:136:ILE:HA	1.94	0.48
1:L:183:ALA:O	1:L:211:ALA:HA	2.13	0.48
1:L:188:LYS:O	1:L:192:LEU:CD1	2.61	0.48
1:D:145:GLU:HA	1:D:193:LEU:CD2	2.44	0.48
1:C:332:PRO:HB2	1:C:334:THR:CG2	2.44	0.48
1:E:66:THR:OG1	1:E:67:SER:N	2.44	0.48
1:J:255:ILE:C	1:J:257:LEU:H	2.17	0.48
1:L:309:GLU:HG3	1:L:311:THR:HG23	1.96	0.48
1:B:74:ILE:HG21	1:B:210:PHE:CE2	2.49	0.48
1:I:98:CYS:HB2	1:I:99:PRO:HD3	1.96	0.48
1:G:146:LEU:HA	1:G:194:TYR:HE2	1.79	0.48
1:F:68:GLN:O	1:F:79:LEU:HA	2.14	0.48
1:I:146:LEU:HD11	1:I:166:ILE:HD13	1.95	0.48
1:E:304:ASN:HA	1:E:307:LYS:HE2	1.94	0.48
1:C:161:ARG:O	1:C:165:GLU:HG3	2.13	0.48
1:F:151:GLN:O	1:F:151:GLN:HG2	2.14	0.48
1:J:250:GLY:O	1:J:251:VAL:C	2.52	0.48
1:K:300:MET:CE	1:K:303:ARG:HE	2.27	0.48
1:C:130:GLY:HA3	1:L:180:ILE:CG2	2.44	0.48
1:L:86:THR:HG22	1:L:88:GLU:CB	2.44	0.48
1:J:174:ILE:HB	1:J:316:ILE:CD1	2.39	0.48
1:J:304:ASN:O	1:J:307:LYS:N	2.47	0.48
1:D:129:ALA:O	1:D:131:ARG:N	2.47	0.48
1:F:239:LYS:C	1:F:241:ASP:H	2.16	0.48
1:B:300:MET:HE2	1:B:303:ARG:NH2	2.25	0.48
1:E:117:ILE:HD12	1:E:208:PHE:CZ	2.47	0.48
1:E:252:ILE:O	1:E:256:LEU:HB2	2.14	0.48
1:E:138:MET:O	1:E:139:GLU:O	2.32	0.48
1:F:190:GLU:H	1:F:190:GLU:CD	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ILE:CG2	1:E:316:ILE:HD13	2.43	0.47
1:E:233:GLU:CD	1:F:310:PRO:HG3	2.33	0.47
1:L:159:THR:C	1:L:336:LEU:CD2	2.83	0.47
1:F:256:LEU:HD23	1:F:256:LEU:HA	1.66	0.47
1:A:58:ALA:N	1:F:50:SER:HB3	2.29	0.47
1:F:175:GLN:HA	1:F:316:ILE:HG12	1.96	0.47
1:K:199:PRO:HG2	1:K:200:ASN:H	1.79	0.47
1:I:277:THR:O	1:I:281:MET:HG2	2.14	0.47
1:E:341:VAL:O	1:E:341:VAL:HG12	2.14	0.47
1:F:276:LYS:O	1:F:280:ARG:CG	2.61	0.47
1:L:158:PHE:CE2	1:L:162:GLU:HB2	2.49	0.47
1:L:169:SER:C	1:L:171:GLY:N	2.67	0.47
1:J:171:GLY:C	1:J:173:ALA:N	2.67	0.47
1:J:254:TYR:HB3	1:J:262:PRO:CG	2.42	0.47
1:A:212:LYS:HG2	1:A:213:GLU:O	2.14	0.47
1:B:150:ILE:O	1:B:152:ASP:N	2.39	0.47
1:J:72:LEU:HG	1:J:77:LYS:HG2	1.94	0.47
1:D:125:GLU:C	1:D:126:ASN:HD22	2.17	0.47
1:L:284:TYR:OH	1:L:303:ARG:HG3	2.14	0.47
1:K:86:THR:O	1:K:87:GLN:CB	2.61	0.47
1:L:343:LYS:HB2	1:L:344:GLU:OE2	2.13	0.47
1:J:304:ASN:C	1:J:306:LEU:N	2.63	0.47
1:H:212:LYS:HG2	1:H:213:GLU:O	2.14	0.47
1:F:93:LYS:HE3	2:F:1350:P4O:O26	2.13	0.47
1:I:59:ILE:HG21	1:I:135:LEU:CD1	2.44	0.47
1:D:233:GLU:CB	1:E:310:PRO:HG3	2.44	0.47
1:B:82:PHE:CD1	1:B:89:LYS:HG2	2.48	0.47
1:L:249:LEU:HD21	1:L:319:PHE:CE2	2.49	0.47
1:E:253:MET:HG2	1:E:302:ILE:HD11	1.96	0.47
1:L:317:THR:O	1:L:321:ASN:ND2	2.47	0.47
1:L:333:GLN:O	1:L:335:PRO:CD	2.61	0.47
1:B:125:GLU:C	1:B:126:ASN:HD22	2.17	0.47
1:A:265:SER:O	1:A:266:ASN:HB2	2.15	0.47
1:D:70:LEU:HD12	2:D:1351:P4O:N16	2.29	0.47
1:L:180:ILE:O	1:L:182:ILE:N	2.48	0.47
1:L:86:THR:CG2	1:L:88:GLU:HB2	2.44	0.47
1:J:255:ILE:HD11	1:J:261:PRO:CA	2.44	0.47
1:C:128:TYR:O	1:C:129:ALA:HB3	2.14	0.47
1:J:100:LYS:O	1:J:103:ARG:HG2	2.14	0.47
1:A:129:ALA:C	1:A:131:ARG:H	2.17	0.47
1:B:271:ILE:HG12	1:B:273:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:CD1	1:C:75:ASN:ND2	2.77	0.47
1:E:309:GLU:HG3	1:E:311:THR:HG23	1.96	0.47
1:B:106:GLU:OE2	1:K:132:LYS:NZ	2.47	0.47
1:I:190:GLU:OE1	1:I:190:GLU:N	2.43	0.47
1:C:56:LYS:O	1:L:50:SER:HB2	2.15	0.47
1:H:300:MET:CE	1:H:303:ARG:HE	2.28	0.47
1:C:185:ARG:HB3	1:C:185:ARG:HH11	1.79	0.47
1:J:261:PRO:CG	1:J:263:PHE:O	2.60	0.47
1:G:118:VAL:HG12	1:G:205:LEU:O	2.15	0.47
1:I:255:ILE:HG12	1:I:261:PRO:HA	1.96	0.47
1:B:202:ILE:CG2	1:B:203:LEU:N	2.77	0.47
1:I:185:ARG:HB3	1:I:185:ARG:HE	1.57	0.47
1:H:172:GLU:HG2	1:H:320:MET:HE1	1.96	0.47
1:B:145:GLU:HA	1:B:193:LEU:CD2	2.45	0.47
1:G:90:PHE:CE2	1:G:121:VAL:HG21	2.49	0.47
1:E:340:ARG:HA	1:E:343:LYS:HE2	1.96	0.47
1:K:83:ASN:CG	1:K:86:THR:HB	2.35	0.47
1:I:83:ASN:ND2	1:I:85:ARG:H	2.13	0.47
1:H:149:ARG:HG3	1:H:194:TYR:CD2	2.50	0.47
1:G:345:ASP:O	1:G:346:LYS:C	2.52	0.47
1:C:230:VAL:HG22	1:C:231:ALA:H	1.79	0.47
1:G:63:TYR:CB	1:G:81:ILE:HD12	2.45	0.47
1:I:141:LEU:CD1	1:I:193:LEU:HB2	2.45	0.47
1:E:108:HIS:O	1:E:109:TRP:C	2.52	0.47
1:B:74:ILE:CB	1:B:210:PHE:HE2	2.27	0.47
1:F:202:ILE:CG2	1:F:203:LEU:N	2.78	0.47
1:G:146:LEU:HA	1:G:194:TYR:CE2	2.50	0.47
1:G:140:CYS:SG	2:G:1350:P4O:H17	2.55	0.47
1:G:52:LEU:HD12	1:G:53:GLN:N	2.29	0.47
1:E:230:VAL:O	1:F:247:TRP:NE1	2.48	0.47
1:B:83:ASN:OD1	1:B:86:THR:HG22	2.14	0.47
1:F:83:ASN:ND2	1:F:85:ARG:H	2.13	0.47
1:G:178:HIS:CG	1:G:242:LYS:HD3	2.49	0.47
1:A:96:GLN:OE1	1:A:131:ARG:HD2	2.13	0.47
1:I:147:PHE:HD2	1:I:349:TRP:HZ2	1.61	0.47
1:H:191:ASN:HD21	2:H:1347:P4O:H8C2	1.79	0.47
1:D:233:GLU:HB3	1:E:310:PRO:HG3	1.97	0.47
1:A:300:MET:HE2	1:A:303:ARG:HH21	1.79	0.47
1:L:288:ASN:HB3	1:L:289:PRO:HA	1.97	0.47
1:K:127:LEU:HA	1:K:127:LEU:HD23	1.60	0.47
1:L:189:PRO:C	1:L:191:ASN:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:LEU:HB3	2:L:1345:P4O:C19	2.45	0.47
1:K:162:GLU:O	1:K:166:ILE:HG13	2.15	0.47
1:B:77:LYS:HE3	1:B:79:LEU:HD21	1.96	0.47
1:L:150:ILE:CG2	1:L:151:GLN:N	2.78	0.47
1:B:127:LEU:HD13	1:I:113:GLN:HE21	1.79	0.47
1:E:210:PHE:O	1:E:211:ALA:C	2.52	0.47
1:I:75:ASN:HD22	1:I:76:GLY:N	2.13	0.47
1:G:316:ILE:O	1:G:316:ILE:HG13	2.15	0.47
1:H:167:MET:HG3	1:H:253:MET:HG3	1.97	0.47
1:G:108:HIS:CG	1:G:120:ILE:HD11	2.50	0.47
1:H:289:PRO:CD	1:H:290:GLU:H	2.27	0.47
1:H:96:GLN:NE2	1:H:131:ARG:HH21	2.13	0.47
1:B:118:VAL:O	1:B:118:VAL:HG13	2.13	0.47
1:H:185:ARG:HH11	1:H:185:ARG:HB3	1.79	0.46
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.49	0.46
1:E:191:ASN:ND2	1:E:207:ASP:HB2	2.30	0.46
1:L:107:LEU:HD23	1:L:110:ARG:HH21	1.80	0.46
1:E:72:LEU:HD13	1:E:77:LYS:HG2	1.98	0.46
1:F:149:ARG:O	1:F:150:ILE:C	2.52	0.46
1:E:230:VAL:CG2	1:E:231:ALA:N	2.78	0.46
1:B:80:GLN:CD	1:B:89:LYS:HD2	2.34	0.46
1:E:98:CYS:HB2	1:E:99:PRO:HD3	1.96	0.46
1:J:256:LEU:CD1	1:J:256:LEU:O	2.61	0.46
1:L:55:LYS:HD2	1:L:124:TYR:CE2	2.50	0.46
1:H:97:ASP:OD1	1:H:102:ARG:HD3	2.16	0.46
1:K:78:VAL:C	1:K:79:LEU:HD23	2.36	0.46
1:D:196:SER:O	1:D:201:ALA:HB2	2.15	0.46
1:G:331:VAL:CG1	1:G:332:PRO:HD2	2.45	0.46
1:E:309:GLU:OE2	1:E:310:PRO:HD2	2.15	0.46
1:H:293:GLU:OE2	1:H:293:GLU:HA	2.15	0.46
1:G:343:LYS:O	1:G:346:LYS:HB2	2.15	0.46
1:J:258:CYS:SG	1:J:260:TYR:CE1	3.09	0.46
1:H:196:SER:H	1:H:201:ALA:HB1	1.80	0.46
1:D:147:PHE:HE2	1:D:256:LEU:CD2	2.28	0.46
1:A:159:THR:OG1	1:A:162:GLU:HG3	2.15	0.46
1:G:241:ASP:O	1:G:244:CYS:CB	2.63	0.46
1:D:82:PHE:HD1	1:D:87:GLN:O	1.98	0.46
1:J:82:PHE:HA	1:J:88:GLU:O	2.15	0.46
1:D:70:LEU:HD22	1:D:70:LEU:H	1.77	0.46
1:H:102:ARG:O	1:H:106:GLU:HB2	2.16	0.46
1:I:331:VAL:HA	1:I:332:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:VAL:HA	1:E:332:PRO:HD3	1.67	0.46
1:K:72:LEU:CD1	1:K:77:LYS:HA	2.45	0.46
1:D:289:PRO:CG	1:D:290:GLU:H	2.28	0.46
1:G:188:LYS:HB2	1:G:189:PRO:CD	2.45	0.46
1:G:189:PRO:HD2	1:G:190:GLU:OE1	2.15	0.46
1:B:60:ILE:O	1:B:61:ASP:C	2.53	0.46
1:E:234:VAL:O	1:E:234:VAL:HG12	2.15	0.46
1:J:295:SER:O	1:J:299:LYS:HE3	2.14	0.46
1:A:74:ILE:HG12	1:A:209:GLY:HA3	1.96	0.46
1:A:332:PRO:HB3	1:A:334:THR:HG22	1.97	0.46
1:G:265:SER:O	1:G:266:ASN:HB2	2.15	0.46
1:H:70:LEU:HG	2:H:1347:P4O:C17	2.46	0.46
1:K:330:LYS:N	1:K:330:LYS:HD3	2.31	0.46
1:I:188:LYS:HD2	1:I:190:GLU:OE2	2.16	0.46
1:K:188:LYS:HD2	1:K:190:GLU:OE2	2.15	0.46
1:L:184:HIS:CE1	1:L:205:LEU:HD21	2.50	0.46
1:D:70:LEU:HD21	1:D:80:GLN:CB	2.33	0.46
1:K:300:MET:CE	1:K:303:ARG:HH21	2.29	0.46
1:B:151:GLN:HE21	1:B:343:LYS:HB3	1.80	0.46
1:E:286:PHE:CD1	1:E:299:LYS:HD3	2.51	0.46
1:J:153:ARG:NH2	1:J:162:GLU:OE1	2.49	0.46
1:J:190:GLU:O	1:J:191:ASN:ND2	2.49	0.46
1:I:345:ASP:C	1:I:347:GLU:N	2.69	0.46
1:C:321:ASN:O	1:C:326:MET:HG3	2.16	0.46
1:F:200:ASN:H	1:F:200:ASN:HD22	1.63	0.46
1:B:237:PRO:O	1:B:238:GLU:CB	2.64	0.46
1:B:145:GLU:HA	1:B:193:LEU:HD23	1.96	0.46
1:L:47:HIS:ND1	1:L:47:HIS:O	2.47	0.46
1:A:326:MET:HE3	1:A:326:MET:HB3	1.87	0.46
1:C:72:LEU:HD12	1:C:73:GLY:H	1.80	0.46
1:G:232:PRO:HB3	1:H:279:ILE:HG22	1.97	0.46
1:H:59:ILE:HG12	1:H:59:ILE:O	2.15	0.46
1:K:287:PRO:O	1:K:291:TRP:HD1	1.97	0.46
1:J:301:LEU:HD22	1:J:322:HIS:CG	2.51	0.46
1:K:294:VAL:O	1:K:295:SER:C	2.54	0.46
1:J:296:GLU:O	1:J:300:MET:N	2.39	0.46
1:E:257:LEU:HD13	1:E:291:TRP:HZ3	1.81	0.46
1:G:278:ARG:HG3	1:G:278:ARG:HH11	1.81	0.46
1:H:148:SER:O	1:H:150:ILE:N	2.49	0.46
1:B:188:LYS:HD2	1:B:190:GLU:OE2	2.16	0.46
1:E:191:ASN:ND2	1:E:207:ASP:CB	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LYS:HG2	1:E:213:GLU:O	2.16	0.46
1:K:256:LEU:HA	1:K:256:LEU:HD23	1.79	0.46
1:L:240:TYR:C	1:L:240:TYR:CD1	2.89	0.46
1:I:127:LEU:HA	1:I:127:LEU:HD23	1.68	0.46
1:H:119:ARG:HG2	1:H:120:ILE:N	2.30	0.46
1:L:324:TRP:CD1	1:L:331:VAL:HG21	2.50	0.46
1:B:233:GLU:HG2	1:C:310:PRO:HD3	1.98	0.46
1:G:300:MET:CE	1:G:303:ARG:HH21	2.28	0.46
1:L:178:HIS:ND1	1:L:242:LYS:CD	2.79	0.46
1:H:186:ASP:OD1	1:H:188:LYS:HE3	2.15	0.46
1:G:207:ASP:HB2	2:G:1350:P4O:N7	2.31	0.46
1:B:167:MET:HG3	1:B:253:MET:HG3	1.97	0.46
1:D:90:PHE:HA	1:D:140:CYS:HB2	1.96	0.46
1:G:302:ILE:HG22	1:G:306:LEU:HD12	1.98	0.46
1:E:264:TYR:CB	1:E:278:ARG:HH22	2.28	0.46
1:K:286:PHE:HE1	1:K:303:ARG:NH1	2.13	0.46
1:D:340:ARG:HG2	1:D:344:GLU:OE1	2.16	0.46
1:I:162:GLU:O	1:I:166:ILE:HG13	2.16	0.46
1:F:145:GLU:HA	1:F:193:LEU:HD23	1.98	0.46
1:K:49:LYS:CD	1:K:50:SER:H	2.28	0.46
1:I:195:THR:HG23	1:I:202:ILE:N	2.31	0.46
1:H:331:VAL:HG13	1:H:332:PRO:CD	2.41	0.46
1:L:149:ARG:O	1:L:153:ARG:HD3	2.16	0.46
1:I:140:CYS:SG	2:I:1351:P4O:H17	2.56	0.46
1:E:130:GLY:HA3	1:J:180:ILE:CG2	2.45	0.46
1:H:108:HIS:CG	1:H:120:ILE:HD11	2.51	0.46
1:B:161:ARG:O	1:B:165:GLU:HG3	2.15	0.46
1:C:256:LEU:HA	1:C:256:LEU:HD23	1.66	0.46
1:F:134:LEU:HA	1:F:134:LEU:HD12	1.60	0.46
1:L:189:PRO:C	1:L:191:ASN:N	2.69	0.45
1:E:300:MET:HE2	1:E:300:MET:CA	2.45	0.45
1:B:349:TRP:O	1:B:349:TRP:CG	2.69	0.45
1:J:300:MET:C	1:J:302:ILE:N	2.70	0.45
1:G:147:PHE:CZ	1:G:255:ILE:HG22	2.51	0.45
1:L:315:THR:HG1	1:L:317:THR:HG22	1.81	0.45
1:B:181:ASN:CB	1:B:214:THR:HG22	2.45	0.45
1:C:139:GLU:O	2:C:1351:P4O:H10	2.15	0.45
1:D:150:ILE:CD1	1:D:158:PHE:CE2	2.98	0.45
1:L:304:ASN:HD22	1:L:307:LYS:CE	2.29	0.45
1:A:94:MET:SD	1:F:46:PHE:HZ	2.40	0.45
1:G:134:LEU:HA	1:G:134:LEU:HD12	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:252:ILE:CG2	1:L:252:ILE:O	2.64	0.45
1:L:63:TYR:CG	1:L:81:ILE:HD12	2.51	0.45
1:L:120:ILE:HD13	1:L:138:MET:CE	2.47	0.45
1:L:53:GLN:HA	1:L:53:GLN:HE21	1.80	0.45
1:B:202:ILE:N	1:B:202:ILE:HD13	2.27	0.45
1:I:70:LEU:HD21	1:I:80:GLN:HB2	1.98	0.45
1:A:131:ARG:HH11	1:D:273:PRO:HB3	1.81	0.45
1:A:185:ARG:HB3	1:A:185:ARG:HH11	1.80	0.45
1:G:159:THR:O	1:G:160:GLU:C	2.54	0.45
1:K:194:TYR:HA	1:K:202:ILE:O	2.17	0.45
1:I:141:LEU:HD13	1:I:193:LEU:HB2	1.98	0.45
1:A:343:LYS:C	1:A:345:ASP:H	2.20	0.45
1:L:170:ILE:HG22	1:L:170:ILE:O	2.16	0.45
1:L:141:LEU:HB2	1:L:193:LEU:HD12	1.98	0.45
1:K:159:THR:OG1	1:K:162:GLU:HG3	2.16	0.45
1:H:332:PRO:CB	1:H:334:THR:HG22	2.45	0.45
1:J:189:PRO:O	1:J:191:ASN:N	2.47	0.45
1:B:286:PHE:HE1	1:B:303:ARG:NH1	2.13	0.45
1:E:48:VAL:CG1	1:H:60:ILE:HD13	2.43	0.45
1:D:264:TYR:HE2	1:D:348:ARG:HH12	1.63	0.45
1:K:271:ILE:HG12	1:K:274:GLY:H	1.82	0.45
1:H:331:VAL:HA	1:H:332:PRO:HD3	1.72	0.45
1:G:86:THR:HG22	1:G:88:GLU:HB2	1.99	0.45
1:C:287:PRO:O	1:C:291:TRP:HD1	1.99	0.45
1:E:210:PHE:O	1:E:211:ALA:O	2.34	0.45
1:B:174:ILE:HD11	1:B:187:VAL:HG21	1.97	0.45
1:E:171:GLY:O	1:E:175:GLN:HB3	2.16	0.45
1:L:255:ILE:CD1	1:L:261:PRO:HA	2.46	0.45
1:I:150:ILE:HD12	1:I:158:PHE:CE2	2.52	0.45
1:J:166:ILE:CG2	1:J:256:LEU:HD11	2.46	0.45
1:K:311:THR:HG21	1:L:311:THR:OG1	2.17	0.45
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.79	0.45
1:B:181:ASN:HD22	1:B:214:THR:CG2	2.29	0.45
1:H:247:TRP:O	1:H:248:SER:C	2.55	0.45
1:B:158:PHE:HE1	1:B:256:LEU:HD22	1.82	0.45
1:I:167:MET:HG3	1:I:253:MET:HE2	1.99	0.45
1:B:229:TYR:N	1:B:229:TYR:CD2	2.82	0.45
1:J:60:ILE:CG1	1:J:60:ILE:O	2.62	0.45
1:G:184:HIS:HD2	1:G:186:ASP:N	2.14	0.45
1:C:227:PRO:HD2	1:C:230:VAL:HB	1.98	0.45
1:F:100:LYS:O	1:F:103:ARG:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:TYR:HD1	1:E:129:ALA:N	2.14	0.45
1:A:134:LEU:HA	1:A:134:LEU:HD12	1.72	0.45
1:J:107:LEU:O	1:J:108:HIS:C	2.55	0.45
1:C:334:THR:HA	1:C:335:PRO:HD3	1.67	0.45
1:D:161:ARG:O	1:D:165:GLU:HG3	2.16	0.45
1:C:260:TYR:HB2	1:C:261:PRO:HD2	1.99	0.45
1:H:271:ILE:CD1	1:H:278:ARG:NH1	2.79	0.45
1:L:94:MET:O	1:L:95:LEU:HD23	2.16	0.45
1:H:88:GLU:HG3	1:H:89:LYS:N	2.32	0.45
1:G:161:ARG:NH1	1:G:333:GLN:OE1	2.50	0.45
1:H:87:GLN:CA	1:H:87:GLN:NE2	2.78	0.45
1:I:164:SER:HA	1:I:324:TRP:CZ3	2.51	0.45
1:G:142:ASP:HA	2:G:1350:P4O:N16	2.32	0.45
1:B:158:PHE:CE1	1:B:256:LEU:HD22	2.52	0.45
1:B:98:CYS:HB2	1:B:99:PRO:CD	2.46	0.45
1:I:116:HIS:CE1	1:I:169:SER:HB3	2.52	0.45
1:F:125:GLU:HA	1:F:133:CYS:O	2.17	0.45
1:G:314:MET:CG	1:G:318:GLU:HB2	2.47	0.45
1:J:301:LEU:HD22	1:J:322:HIS:ND1	2.32	0.45
1:J:302:ILE:O	1:J:306:LEU:HB2	2.17	0.45
1:K:110:ARG:NH1	1:K:110:ARG:HG2	2.31	0.45
1:E:160:GLU:HB2	1:E:334:THR:HG23	1.97	0.45
1:C:343:LYS:O	1:C:345:ASP:N	2.46	0.45
1:K:72:LEU:HD13	1:K:72:LEU:HA	1.52	0.45
1:A:128:TYR:O	1:A:129:ALA:CB	2.65	0.45
1:I:278:ARG:HA	1:I:283:GLN:HG3	1.99	0.45
1:G:158:PHE:O	1:G:336:LEU:HD22	2.17	0.45
1:A:110:ARG:NH1	1:G:130:GLY:O	2.47	0.45
1:F:343:LYS:O	1:F:346:LYS:HB2	2.17	0.45
1:F:70:LEU:HD11	1:F:80:GLN:CA	2.44	0.45
1:F:334:THR:HA	1:F:335:PRO:HD3	1.75	0.45
1:G:286:PHE:CE1	1:G:299:LYS:HB3	2.51	0.45
1:H:151:GLN:NE2	1:H:346:LYS:HD2	2.32	0.45
1:C:74:ILE:HD11	1:C:75:ASN:HD21	1.82	0.45
1:J:71:GLY:O	1:J:72:LEU:O	2.34	0.45
1:L:202:ILE:CD1	1:L:202:ILE:N	2.80	0.45
1:L:251:VAL:O	1:L:255:ILE:HG13	2.16	0.45
1:L:169:SER:C	1:L:171:GLY:H	2.19	0.45
1:B:56:LYS:NZ	1:I:52:LEU:O	2.50	0.45
1:D:278:ARG:HH11	1:D:278:ARG:CG	2.30	0.45
1:F:74:ILE:CG2	1:F:209:GLY:HA3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ASN:ND2	1:I:75:ASN:N	2.64	0.45
1:F:49:LYS:HG3	1:F:113:GLN:CD	2.37	0.45
1:D:247:TRP:CE2	1:F:231:ALA:HA	2.52	0.45
1:D:86:THR:HG21	1:D:88:GLU:CB	2.39	0.44
1:B:86:THR:O	1:B:88:GLU:N	2.50	0.44
1:L:338:THR:O	1:L:339:SER:C	2.56	0.44
1:J:157:ALA:O	1:J:158:PHE:HB3	2.17	0.44
1:J:304:ASN:OD1	1:J:304:ASN:N	2.49	0.44
1:A:74:ILE:O	1:A:74:ILE:HD12	2.17	0.44
1:H:344:GLU:O	1:H:345:ASP:HB2	2.17	0.44
1:E:158:PHE:O	1:E:335:PRO:HA	2.16	0.44
1:D:174:ILE:HD11	1:D:187:VAL:HG21	1.99	0.44
1:F:160:GLU:HA	1:F:336:LEU:HD11	1.99	0.44
1:L:266:ASN:HA	1:L:266:ASN:HD22	1.53	0.44
1:B:247:TRP:O	1:B:248:SER:C	2.55	0.44
1:A:333:GLN:HE21	1:A:333:GLN:HB3	1.43	0.44
1:J:198:ARG:CG	1:J:198:ARG:NH1	2.74	0.44
1:B:86:THR:HG23	1:B:88:GLU:CB	2.36	0.44
1:I:86:THR:HG23	1:I:88:GLU:H	1.82	0.44
1:B:147:PHE:CE1	1:B:255:ILE:HG21	2.52	0.44
1:E:60:ILE:O	1:E:61:ASP:C	2.56	0.44
1:E:108:HIS:CD2	1:E:120:ILE:HD11	2.53	0.44
1:A:239:LYS:C	1:A:241:ASP:H	2.21	0.44
1:K:170:ILE:HG22	1:K:249:LEU:HD11	1.99	0.44
1:I:110:ARG:HG2	1:I:110:ARG:HH11	1.82	0.44
1:L:277:THR:O	1:L:279:ILE:N	2.50	0.44
1:J:194:TYR:O	1:J:195:THR:C	2.55	0.44
1:F:86:THR:CG2	1:F:88:GLU:N	2.71	0.44
1:B:331:VAL:HA	1:B:332:PRO:HD3	1.81	0.44
1:L:74:ILE:HG13	1:L:75:ASN:N	2.31	0.44
1:B:296:GLU:O	1:B:300:MET:HB2	2.17	0.44
1:C:343:LYS:HG2	1:C:343:LYS:H	1.63	0.44
1:D:313:ARG:CZ	1:F:233:GLU:OE1	2.65	0.44
1:L:111:ALA:O	1:L:113:GLN:N	2.50	0.44
1:B:201:ALA:O	1:B:202:ILE:HD13	2.18	0.44
1:D:246:MET:CE	1:D:316:ILE:HA	2.46	0.44
1:B:118:VAL:HG11	1:B:206:THR:HG22	2.00	0.44
1:G:230:VAL:HG21	1:G:235:LEU:HD23	1.97	0.44
1:K:75:ASN:CB	1:K:95:LEU:HD22	2.47	0.44
1:D:232:PRO:HD3	1:E:247:TRP:CZ2	2.52	0.44
1:H:309:GLU:OE2	1:H:310:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:244:CYS:O	1:J:247:TRP:HB3	2.17	0.44
1:J:113:GLN:HG2	1:J:113:GLN:H	1.58	0.44
1:E:83:ASN:O	1:E:87:GLN:N	2.51	0.44
1:L:74:ILE:O	1:L:75:ASN:O	2.34	0.44
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.80	0.44
1:G:84:LYS:HE2	1:G:84:LYS:HB3	1.55	0.44
1:G:63:TYR:CA	1:G:84:LYS:HG3	2.48	0.44
1:A:74:ILE:C	1:A:74:ILE:HD12	2.38	0.44
1:H:114:CYS:HA	1:H:115:PRO:HD3	1.75	0.44
1:C:159:THR:O	1:C:160:GLU:C	2.56	0.44
1:G:332:PRO:HB2	1:G:334:THR:CG2	2.45	0.44
1:E:108:HIS:CG	1:E:120:ILE:HD11	2.52	0.44
1:E:336:LEU:HA	1:E:336:LEU:HD13	1.56	0.44
1:L:115:PRO:O	1:L:204:LYS:HG2	2.17	0.44
1:F:231:ALA:HB1	1:F:232:PRO:HD2	2.00	0.44
1:K:272:SER:H	1:K:273:PRO:CD	2.30	0.44
1:H:66:THR:HG21	1:H:82:PHE:HE2	1.81	0.44
1:D:97:ASP:OD1	1:D:102:ARG:NH2	2.45	0.44
1:E:178:HIS:CG	1:E:242:LYS:HD3	2.53	0.44
1:H:217:HIS:CD2	1:H:217:HIS:N	2.85	0.44
1:J:247:TRP:O	1:J:248:SER:C	2.56	0.44
1:E:227:PRO:HB2	1:E:230:VAL:HB	1.98	0.44
1:I:86:THR:HG23	1:I:88:GLU:CB	2.47	0.44
1:J:178:HIS:CD2	1:J:182:ILE:O	2.69	0.44
1:L:166:ILE:O	1:L:169:SER:HB2	2.18	0.44
1:G:80:GLN:NE2	1:G:89:LYS:HE2	2.33	0.44
1:A:70:LEU:HD13	2:A:1351:P4O:C18	2.46	0.44
1:H:85:ARG:HG2	1:H:85:ARG:O	2.18	0.44
1:K:309:GLU:HB3	1:K:312:GLN:HB2	1.99	0.44
1:G:237:PRO:O	1:G:238:GLU:CB	2.66	0.44
1:B:212:LYS:HG2	1:B:213:GLU:O	2.17	0.44
1:I:69:VAL:HG11	1:I:72:LEU:CD1	2.48	0.44
1:H:184:HIS:HE1	1:H:206:THR:O	2.00	0.44
1:B:158:PHE:HZ	1:B:166:ILE:HD12	1.82	0.44
1:A:190:GLU:H	1:A:190:GLU:CD	2.21	0.44
1:J:195:THR:CG2	1:J:201:ALA:HB3	2.47	0.44
1:F:86:THR:HG22	1:F:87:GLN:N	2.32	0.44
1:E:180:ILE:HG13	1:E:180:ILE:O	2.16	0.44
1:K:158:PHE:HE2	1:K:163:ALA:N	2.16	0.44
1:I:195:THR:HG21	1:I:202:ILE:CB	2.47	0.44
1:L:89:LYS:O	1:L:140:CYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:PRO:O	1:L:45:GLN:CG	2.65	0.44
1:J:313:ARG:O	1:J:314:MET:O	2.35	0.44
1:J:72:LEU:HA	1:J:77:LYS:HA	1.99	0.44
1:E:234:VAL:O	1:E:234:VAL:CG1	2.65	0.44
1:A:174:ILE:HD11	1:A:187:VAL:HG21	1.99	0.44
1:E:107:LEU:HA	1:E:107:LEU:HD23	1.52	0.44
1:L:165:GLU:HG2	1:L:328:SER:CB	2.31	0.44
1:A:233:GLU:OE1	1:B:313:ARG:NH1	2.47	0.44
1:A:233:GLU:CD	1:B:313:ARG:HH22	2.21	0.44
1:L:72:LEU:HD12	1:L:77:LYS:HB3	1.99	0.44
1:L:99:PRO:HA	1:L:102:ARG:HB2	2.00	0.44
1:E:148:SER:C	1:E:150:ILE:N	2.70	0.44
1:H:110:ARG:NH1	1:J:130:GLY:O	2.51	0.44
1:B:81:ILE:HD13	1:B:92:LEU:HB2	1.99	0.44
1:H:175:GLN:HA	1:H:316:ILE:HG12	2.00	0.44
1:D:230:VAL:HG11	1:D:235:LEU:CD2	2.30	0.44
1:E:264:TYR:HB3	1:E:278:ARG:HH22	1.82	0.44
1:I:86:THR:C	1:I:88:GLU:N	2.71	0.44
1:C:331:VAL:HA	1:C:332:PRO:HD3	1.61	0.44
1:J:147:PHE:CZ	1:J:255:ILE:HG21	2.53	0.44
1:E:302:ILE:O	1:E:302:ILE:CG2	2.65	0.44
1:J:315:THR:OG1	1:J:318:GLU:HG3	2.17	0.44
1:C:178:HIS:CE1	1:C:242:LYS:HB3	2.53	0.44
1:H:147:PHE:O	1:H:151:GLN:HB2	2.17	0.44
1:H:87:GLN:CA	1:H:87:GLN:HE21	2.30	0.44
1:C:74:ILE:CG2	1:C:207:ASP:OD2	2.66	0.44
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.76	0.44
1:E:175:GLN:O	1:E:175:GLN:HG3	2.18	0.44
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.35	0.44
1:H:56:LYS:HD3	1:H:125:GLU:HB3	1.98	0.44
1:L:145:GLU:O	1:L:145:GLU:HG3	2.17	0.44
1:K:86:THR:HG21	1:K:88:GLU:HB2	2.00	0.44
1:L:290:GLU:HA	1:L:337:HIS:CE1	2.53	0.44
1:I:156:GLN:HE21	1:I:156:GLN:HB2	1.55	0.44
1:D:334:THR:HA	1:D:335:PRO:HD3	1.74	0.44
1:J:300:MET:C	1:J:302:ILE:H	2.21	0.44
1:G:322:HIS:ND1	1:G:323:PRO:HD2	2.32	0.44
1:I:79:LEU:HD23	1:I:79:LEU:N	2.33	0.44
1:I:322:HIS:CE1	1:I:323:PRO:HD2	2.52	0.44
1:I:190:GLU:CD	1:I:190:GLU:H	2.19	0.44
1:C:134:LEU:C	1:C:135:LEU:HD23	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:ARG:O	1:G:104:GLU:C	2.55	0.44
1:C:191:ASN:HA	1:C:191:ASN:HD22	1.50	0.44
1:C:293:GLU:OE2	1:C:293:GLU:N	2.47	0.44
1:H:46:PHE:HE2	1:J:65:VAL:HG11	1.83	0.43
1:E:179:SER:OG	1:E:180:ILE:HG23	2.18	0.43
1:I:85:ARG:HG3	1:I:85:ARG:O	2.17	0.43
1:A:233:GLU:CD	1:B:310:PRO:HG3	2.39	0.43
1:L:337:HIS:O	1:L:338:THR:C	2.56	0.43
1:I:154:GLY:O	1:I:156:GLN:N	2.50	0.43
1:B:233:GLU:HG3	1:B:233:GLU:H	1.08	0.43
1:K:271:ILE:CG2	1:K:278:ARG:NH1	2.74	0.43
1:D:309:GLU:HB3	1:D:312:GLN:HB2	2.00	0.43
1:D:114:CYS:SG	1:D:115:PRO:HD2	2.58	0.43
1:L:96:GLN:HG2	1:L:97:ASP:N	2.33	0.43
1:C:240:TYR:O	1:C:241:ASP:C	2.56	0.43
1:L:298:VAL:HG12	1:L:298:VAL:O	2.18	0.43
1:K:134:LEU:HD12	1:K:134:LEU:HA	1.59	0.43
1:A:325:ILE:HD12	1:A:325:ILE:HG23	1.74	0.43
1:J:176:TYR:HA	1:J:179:SER:OG	2.18	0.43
1:J:163:ALA:CB	1:J:257:LEU:HG	2.48	0.43
1:D:129:ALA:C	1:D:131:ARG:H	2.22	0.43
1:D:134:LEU:HA	1:D:134:LEU:HD12	1.84	0.43
1:H:47:HIS:HB3	1:H:49:LYS:HZ1	1.82	0.43
1:B:202:ILE:HG22	1:B:203:LEU:N	2.32	0.43
1:F:210:PHE:N	1:F:210:PHE:HD2	2.15	0.43
1:A:161:ARG:O	1:A:165:GLU:HG3	2.18	0.43
1:C:110:ARG:HG2	1:C:110:ARG:HH11	1.84	0.43
1:I:184:HIS:HD2	1:I:186:ASP:H	1.65	0.43
1:D:180:ILE:HG13	1:D:180:ILE:O	2.18	0.43
1:F:127:LEU:HA	1:F:127:LEU:HD23	1.82	0.43
1:E:66:THR:HG21	1:E:82:PHE:HE2	1.83	0.43
1:L:257:LEU:HD23	1:L:336:LEU:HG	1.98	0.43
1:H:88:GLU:HG2	1:H:90:PHE:CZ	2.52	0.43
1:E:110:ARG:HD3	1:H:127:LEU:HD21	1.99	0.43
1:A:184:HIS:HD2	1:A:186:ASP:H	1.66	0.43
1:H:305:LEU:O	1:H:313:ARG:HD3	2.18	0.43
1:L:262:PRO:C	1:L:263:PHE:CD1	2.92	0.43
1:L:170:ILE:CD1	1:L:192:LEU:HD22	2.48	0.43
1:L:214:THR:O	1:L:215:THR:HG23	2.18	0.43
1:L:341:VAL:O	1:L:341:VAL:HG12	2.17	0.43
1:E:202:ILE:HG13	1:E:203:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:THR:CG2	1:G:88:GLU:HB2	2.47	0.43
1:L:152:ASP:C	1:L:153:ARG:HG3	2.39	0.43
1:D:280:ARG:HG2	1:F:235:LEU:CD1	2.47	0.43
1:I:130:GLY:CA	1:K:180:ILE:HB	2.46	0.43
1:D:52:LEU:HA	1:D:52:LEU:HD12	1.65	0.43
1:E:287:PRO:O	1:E:291:TRP:CD1	2.70	0.43
1:E:257:LEU:HD13	1:E:291:TRP:CZ3	2.54	0.43
1:K:77:LYS:HE2	1:K:77:LYS:HB3	1.37	0.43
1:B:57:ASN:O	1:B:58:ALA:C	2.57	0.43
1:A:164:SER:HA	1:A:324:TRP:CH2	2.54	0.43
1:J:143:GLY:CA	1:J:196:SER:O	2.59	0.43
1:H:46:PHE:CE2	1:J:65:VAL:HG11	2.54	0.43
1:E:230:VAL:CG2	1:E:231:ALA:H	2.31	0.43
1:L:249:LEU:HD21	1:L:319:PHE:CZ	2.54	0.43
1:H:332:PRO:HB2	1:H:334:THR:HG22	1.99	0.43
1:J:254:TYR:CD1	1:J:262:PRO:CD	3.02	0.43
1:G:63:TYR:CG	1:G:81:ILE:HD12	2.54	0.43
1:K:281:MET:HE2	1:L:179:SER:HB3	2.00	0.43
1:I:98:CYS:CB	1:I:99:PRO:CD	2.95	0.43
1:C:148:SER:O	1:C:149:ARG:C	2.54	0.43
1:L:243:SER:C	1:L:245:ASP:H	2.21	0.43
1:K:83:ASN:ND2	1:K:85:ARG:HG2	2.33	0.43
1:D:346:LYS:O	1:D:347:GLU:O	2.37	0.43
1:D:70:LEU:HD12	2:D:1351:P4O:C18	2.48	0.43
1:L:291:TRP:O	1:L:299:LYS:NZ	2.49	0.43
1:E:134:LEU:O	1:E:135:LEU:HD23	2.18	0.43
1:L:304:ASN:HA	1:L:304:ASN:HD22	1.66	0.43
1:H:127:LEU:HA	1:H:127:LEU:HD23	1.75	0.43
1:H:242:LYS:O	1:H:245:ASP:N	2.52	0.43
1:K:161:ARG:O	1:K:165:GLU:HG3	2.17	0.43
1:L:170:ILE:HG12	1:L:192:LEU:CD2	2.49	0.43
1:L:314:MET:HG3	1:L:318:GLU:HB2	2.00	0.43
1:G:83:ASN:HD22	1:G:85:ARG:H	1.65	0.43
1:K:70:LEU:HD22	1:K:79:LEU:C	2.39	0.43
1:C:323:PRO:HA	1:C:326:MET:HB2	2.01	0.43
1:A:74:ILE:HG13	1:A:75:ASN:N	2.33	0.43
1:H:271:ILE:HD11	1:H:278:ARG:NH1	2.33	0.43
1:A:129:ALA:O	1:A:131:ARG:N	2.52	0.43
1:A:86:THR:O	1:A:87:GLN:HB2	2.18	0.43
1:B:127:LEU:O	1:I:48:VAL:HG23	2.19	0.43
1:G:146:LEU:HD11	1:G:166:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:HIS:HA	1:H:323:PRO:HD3	1.80	0.43
1:E:56:LYS:O	1:J:51:GLY:N	2.50	0.43
1:I:161:ARG:O	1:I:165:GLU:HG3	2.18	0.43
1:J:127:LEU:HA	1:J:127:LEU:HD23	1.68	0.43
1:K:150:ILE:O	1:K:150:ILE:HG12	2.19	0.43
1:I:103:ARG:O	1:I:104:GLU:C	2.55	0.43
1:G:45:GLN:CG	1:G:46:PHE:N	2.63	0.43
1:J:89:LYS:O	1:J:90:PHE:CD2	2.71	0.43
1:J:247:TRP:CE3	1:J:247:TRP:HA	2.54	0.43
1:E:301:LEU:CD1	1:E:314:MET:HE1	2.48	0.43
1:I:195:THR:HG21	1:I:202:ILE:CG1	2.49	0.43
1:L:75:ASN:HB2	1:L:76:GLY:H	1.69	0.43
1:K:70:LEU:HD23	1:K:91:ALA:CB	2.49	0.43
1:E:58:ALA:HA	1:E:126:ASN:OD1	2.19	0.43
1:F:322:HIS:CE1	1:F:323:PRO:HD2	2.54	0.43
1:J:59:ILE:O	1:J:61:ASP:N	2.43	0.43
1:F:129:ALA:C	1:F:131:ARG:H	2.21	0.43
1:G:290:GLU:H	1:G:290:GLU:CD	2.22	0.43
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.54	0.43
1:H:337:HIS:CD2	1:H:340:ARG:NH1	2.86	0.43
1:G:102:ARG:O	1:G:106:GLU:HB2	2.19	0.43
1:E:305:LEU:HD23	1:E:305:LEU:HA	1.82	0.43
1:G:73:GLY:O	1:G:74:ILE:C	2.57	0.43
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.79	0.43
1:J:157:ALA:O	1:J:158:PHE:CB	2.66	0.43
1:J:160:GLU:C	1:J:162:GLU:N	2.72	0.43
1:H:134:LEU:HD12	1:H:134:LEU:HA	1.62	0.43
1:D:74:ILE:HB	1:D:210:PHE:CE2	2.54	0.43
1:B:114:CYS:HA	1:B:115:PRO:HD3	1.91	0.43
1:E:168:LYS:O	1:E:172:GLU:HG3	2.19	0.43
1:C:134:LEU:HA	1:C:134:LEU:HD12	1.85	0.43
1:I:114:CYS:HA	1:I:115:PRO:HD3	1.87	0.43
1:K:142:ASP:C	1:K:144:GLY:H	2.22	0.43
1:C:99:PRO:HD2	1:C:100:LYS:H	1.83	0.43
1:J:247:TRP:HE3	1:J:247:TRP:HA	1.84	0.43
1:J:166:ILE:HD13	1:J:203:LEU:HD21	2.01	0.43
1:F:287:PRO:O	1:F:291:TRP:HB2	2.19	0.43
1:K:114:CYS:HA	1:K:115:PRO:HD3	1.84	0.43
1:H:289:PRO:O	1:H:291:TRP:N	2.51	0.43
1:L:97:ASP:HB2	1:L:132:LYS:O	2.19	0.43
1:H:185:ARG:HH21	1:H:212:LYS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:CB	1:C:210:PHE:HE2	2.32	0.43
1:C:98:CYS:HB2	1:C:99:PRO:HD3	2.00	0.43
1:H:118:VAL:O	1:H:118:VAL:HG13	2.18	0.43
1:J:83:ASN:HB3	1:J:88:GLU:H	1.84	0.42
1:E:180:ILE:HG13	1:E:182:ILE:CD1	2.32	0.42
1:D:145:GLU:O	1:D:148:SER:HB2	2.19	0.42
1:B:82:PHE:HA	1:B:88:GLU:O	2.19	0.42
1:J:108:HIS:CA	1:J:208:PHE:CD2	3.02	0.42
1:I:150:ILE:HA	1:I:150:ILE:HD13	1.85	0.42
1:L:55:LYS:HB2	1:L:124:TYR:CD2	2.54	0.42
1:D:74:ILE:HG21	1:D:210:PHE:CE2	2.55	0.42
1:A:60:ILE:HD13	1:F:48:VAL:CG2	2.47	0.42
1:E:153:ARG:NH2	1:E:162:GLU:OE1	2.50	0.42
1:C:74:ILE:HG22	1:C:207:ASP:OD2	2.19	0.42
1:L:265:SER:OG	1:L:266:ASN:N	2.50	0.42
1:B:121:VAL:HB	1:B:137:VAL:HG12	2.00	0.42
1:L:200:ASN:OD1	1:L:200:ASN:N	2.46	0.42
1:F:305:LEU:HA	1:F:305:LEU:HD23	1.74	0.42
1:J:176:TYR:CG	1:J:176:TYR:O	2.72	0.42
1:L:285:GLU:O	1:L:287:PRO:CD	2.63	0.42
1:J:146:LEU:C	1:J:148:SER:H	2.23	0.42
1:L:78:VAL:HG13	1:L:79:LEU:H	1.83	0.42
1:J:108:HIS:O	1:J:109:TRP:C	2.58	0.42
1:H:332:PRO:HB2	1:H:334:THR:CG2	2.48	0.42
1:G:99:PRO:CD	1:G:100:LYS:N	2.82	0.42
1:I:147:PHE:HE1	1:I:256:LEU:CD2	2.31	0.42
1:I:147:PHE:CE1	1:I:256:LEU:HD23	2.51	0.42
1:C:195:THR:HG23	1:C:202:ILE:O	2.19	0.42
1:B:192:LEU:O	1:B:193:LEU:HD23	2.19	0.42
1:J:78:VAL:CG1	1:J:91:ALA:HB1	2.48	0.42
1:C:150:ILE:CG2	1:C:158:PHE:CD1	3.02	0.42
1:J:198:ARG:NH1	1:J:198:ARG:HG2	2.15	0.42
1:J:198:ARG:HH22	1:J:200:ASN:HD22	1.67	0.42
1:J:83:ASN:O	1:J:85:ARG:N	2.49	0.42
1:J:107:LEU:CD2	1:J:182:ILE:HG23	2.42	0.42
1:E:300:MET:O	1:E:303:ARG:HB2	2.19	0.42
1:J:184:HIS:O	1:J:185:ARG:HB2	2.19	0.42
1:I:331:VAL:HG13	1:I:332:PRO:HD2	2.00	0.42
1:L:310:PRO:HA	1:L:313:ARG:HH21	1.80	0.42
1:I:241:ASP:O	1:I:244:CYS:CB	2.65	0.42
1:I:69:VAL:O	1:I:70:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:HIS:CG	1:C:242:LYS:HD3	2.54	0.42
1:A:98:CYS:HB2	1:A:99:PRO:CD	2.50	0.42
1:C:197:LYS:C	1:C:198:ARG:O	2.56	0.42
1:I:184:HIS:HD2	1:I:186:ASP:N	2.17	0.42
1:D:288:ASN:OD1	1:D:292:SER:HB3	2.19	0.42
1:B:289:PRO:HG2	1:B:290:GLU:N	2.35	0.42
1:F:94:MET:HE3	1:F:94:MET:HB3	1.85	0.42
1:A:79:LEU:N	1:A:79:LEU:HD23	2.34	0.42
1:F:234:VAL:O	1:F:234:VAL:CG1	2.67	0.42
1:L:331:VAL:O	1:L:332:PRO:O	2.37	0.42
1:E:300:MET:CA	1:E:300:MET:CE	2.97	0.42
1:C:259:GLY:HA2	1:C:342:LEU:CD1	2.48	0.42
1:K:293:GLU:HG3	1:K:294:VAL:HG23	2.01	0.42
1:H:331:VAL:CG1	1:H:332:PRO:N	2.82	0.42
1:H:195:THR:HB	1:H:202:ILE:H	1.84	0.42
1:B:337:HIS:N	1:B:337:HIS:ND1	2.66	0.42
1:G:195:THR:HG21	1:G:202:ILE:HB	2.01	0.42
1:C:286:PHE:CE1	1:C:299:LYS:HB3	2.55	0.42
1:L:191:ASN:HD22	1:L:191:ASN:N	2.17	0.42
1:J:178:HIS:HB3	1:J:242:LYS:HD3	2.01	0.42
1:F:184:HIS:HD2	1:F:186:ASP:N	2.17	0.42
1:L:180:ILE:O	1:L:180:ILE:CG1	2.67	0.42
1:J:314:MET:HG2	1:J:315:THR:N	2.34	0.42
1:L:54:ILE:CG2	1:L:125:GLU:HB2	2.49	0.42
1:A:150:ILE:CD1	1:A:158:PHE:CE2	3.03	0.42
1:A:184:HIS:HD2	1:A:186:ASP:N	2.18	0.42
1:C:296:GLU:HA	1:C:296:GLU:OE1	2.20	0.42
1:K:59:ILE:O	1:K:59:ILE:HG12	2.19	0.42
1:L:57:ASN:N	1:L:57:ASN:OD1	2.50	0.42
1:F:72:LEU:HD12	1:F:72:LEU:HA	1.60	0.42
1:J:80:GLN:O	1:J:81:ILE:HG23	2.19	0.42
1:F:308:THR:O	1:F:310:PRO:HD3	2.20	0.42
1:L:59:ILE:CG2	1:L:60:ILE:N	2.79	0.42
1:A:145:GLU:HA	1:A:193:LEU:HD22	2.02	0.42
1:J:59:ILE:HG21	1:J:135:LEU:CD1	2.50	0.42
1:B:184:HIS:HD2	1:B:186:ASP:N	2.15	0.42
1:I:180:ILE:O	1:I:180:ILE:CG1	2.67	0.42
1:G:331:VAL:HA	1:G:332:PRO:HD3	1.78	0.42
1:D:184:HIS:C	1:D:184:HIS:CD2	2.92	0.42
1:C:74:ILE:HD11	1:C:75:ASN:ND2	2.35	0.42
1:B:48:VAL:CG1	1:K:60:ILE:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:HG13	1:C:249:LEU:HD13	2.01	0.42
1:B:98:CYS:CB	1:B:99:PRO:CD	2.98	0.42
1:F:161:ARG:O	1:F:165:GLU:HG3	2.20	0.42
1:H:325:ILE:HD12	1:H:325:ILE:HG23	1.76	0.42
1:J:89:LYS:HA	1:J:89:LYS:HD3	1.73	0.42
1:E:88:GLU:HG2	1:E:89:LYS:N	2.35	0.42
1:G:184:HIS:O	1:G:185:ARG:HB2	2.19	0.42
1:D:326:MET:O	1:D:328:SER:N	2.44	0.42
1:J:166:ILE:CG2	1:J:256:LEU:HG	2.46	0.42
1:H:329:THR:C	1:H:331:VAL:H	2.22	0.42
1:L:197:LYS:O	1:L:198:ARG:C	2.58	0.42
1:J:185:ARG:HE	1:J:212:LYS:HB2	1.83	0.42
1:L:313:ARG:HB2	1:L:313:ARG:HE	1.75	0.42
1:D:134:LEU:C	1:D:135:LEU:HD23	2.40	0.42
1:H:114:CYS:SG	1:H:115:PRO:HD2	2.60	0.42
1:D:184:HIS:HD2	1:D:186:ASP:N	2.17	0.42
1:D:188:LYS:HB2	1:D:189:PRO:CD	2.49	0.42
1:H:192:LEU:C	1:H:193:LEU:HD23	2.40	0.42
1:L:304:ASN:HA	1:L:307:LYS:HE2	2.02	0.42
1:G:190:GLU:H	1:G:190:GLU:CD	2.21	0.42
1:A:338:THR:O	1:A:342:LEU:HB2	2.19	0.42
1:J:98:CYS:O	1:J:99:PRO:C	2.57	0.42
1:F:63:TYR:HB3	1:F:81:ILE:HD12	2.01	0.42
1:C:102:ARG:O	1:C:106:GLU:HB2	2.19	0.42
1:D:347:GLU:O	1:D:349:TRP:N	2.52	0.42
1:K:286:PHE:O	1:K:291:TRP:HB2	2.20	0.42
1:H:185:ARG:HH21	1:H:212:LYS:HD3	1.83	0.42
1:B:159:THR:O	1:B:160:GLU:C	2.57	0.42
1:A:300:MET:CE	1:A:303:ARG:HH21	2.33	0.42
1:E:247:TRP:O	1:E:248:SER:C	2.56	0.42
1:F:75:ASN:HB2	1:F:95:LEU:HD22	2.01	0.42
1:K:49:LYS:CG	1:K:50:SER:N	2.82	0.42
1:C:83:ASN:ND2	1:C:84:LYS:N	2.59	0.42
1:J:296:GLU:O	1:J:299:LYS:N	2.45	0.42
1:G:215:THR:CG2	1:G:215:THR:O	2.67	0.42
1:K:281:MET:O	1:L:317:THR:HG21	2.19	0.42
1:B:185:ARG:HH21	1:B:212:LYS:HD2	1.85	0.42
1:I:276:LYS:O	1:I:279:ILE:HB	2.19	0.42
1:G:114:CYS:HA	1:G:115:PRO:HD3	1.85	0.42
1:B:48:VAL:HG23	1:K:126:ASN:HB3	2.02	0.42
1:B:315:THR:OG1	1:B:318:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:CG1	1:B:206:THR:HG22	2.50	0.42
1:C:295:SER:OG	1:C:298:VAL:HG23	2.20	0.42
1:J:200:ASN:O	1:J:200:ASN:OD1	2.38	0.42
1:J:158:PHE:HZ	1:J:163:ALA:CA	2.33	0.42
1:H:260:TYR:HB2	1:H:261:PRO:CD	2.50	0.42
1:K:145:GLU:HA	1:K:193:LEU:HD22	2.02	0.42
1:G:238:GLU:CD	1:G:242:LYS:HE3	2.40	0.42
1:I:320:MET:O	1:I:326:MET:HG2	2.20	0.42
1:C:74:ILE:HB	1:C:210:PHE:HE2	1.85	0.42
1:C:288:ASN:HB3	1:C:289:PRO:HA	2.02	0.42
1:L:114:CYS:HA	1:L:115:PRO:HD3	1.69	0.42
1:H:216:SER:HB2	1:H:217:HIS:HD2	1.84	0.42
1:H:337:HIS:CD2	1:H:340:ARG:HH12	2.38	0.42
1:E:165:GLU:HG3	1:E:328:SER:HB3	2.00	0.42
1:L:293:GLU:HA	1:L:293:GLU:OE2	2.18	0.42
1:E:341:VAL:C	1:E:343:LYS:H	2.22	0.41
1:I:289:PRO:O	1:I:292:SER:N	2.45	0.41
1:L:314:MET:SD	1:L:319:PHE:CA	3.08	0.41
1:E:80:GLN:NE2	1:E:89:LYS:CG	2.83	0.41
1:E:99:PRO:O	1:E:100:LYS:C	2.58	0.41
1:I:203:LEU:HA	1:I:203:LEU:HD12	1.82	0.41
1:B:331:VAL:CG1	1:B:332:PRO:HD2	2.40	0.41
1:I:334:THR:HA	1:I:335:PRO:HD3	1.73	0.41
1:B:69:VAL:CG1	1:B:69:VAL:O	2.68	0.41
1:A:86:THR:CG2	1:A:88:GLU:HB3	2.50	0.41
1:D:162:GLU:O	1:D:166:ILE:HG13	2.20	0.41
1:B:150:ILE:HD13	1:B:150:ILE:HG23	1.71	0.41
1:L:107:LEU:HD23	1:L:110:ARG:NH2	2.35	0.41
1:B:229:TYR:CZ	1:C:188:LYS:HD3	2.55	0.41
1:D:138:MET:C	1:D:139:GLU:O	2.58	0.41
1:G:74:ILE:HG12	1:G:75:ASN:N	2.33	0.41
1:J:301:LEU:CD1	1:J:322:HIS:CD2	2.93	0.41
1:C:227:PRO:HB2	1:C:229:TYR:CZ	2.53	0.41
1:D:305:LEU:O	1:D:313:ARG:HD3	2.19	0.41
1:F:194:TYR:CZ	1:F:203:LEU:HD13	2.55	0.41
1:K:184:HIS:HD2	1:K:186:ASP:H	1.66	0.41
1:I:129:ALA:C	1:I:131:ARG:H	2.23	0.41
1:K:322:HIS:HA	1:K:323:PRO:HD3	1.94	0.41
1:F:325:ILE:HD13	1:F:325:ILE:HA	1.80	0.41
1:C:203:LEU:HD12	1:C:203:LEU:HA	1.76	0.41
1:K:264:TYR:O	1:K:275:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:207:ASP:HB2	2:L:1345:P4O:N7	2.34	0.41
1:B:86:THR:HG23	1:B:88:GLU:H	1.85	0.41
1:B:343:LYS:CG	1:B:343:LYS:O	2.67	0.41
1:E:64:LYS:HD3	1:E:64:LYS:C	2.40	0.41
1:E:95:LEU:HD12	1:E:134:LEU:HB2	2.01	0.41
1:H:102:ARG:HD2	1:H:134:LEU:CD2	2.48	0.41
1:K:311:THR:CG2	1:L:311:THR:OG1	2.69	0.41
1:L:333:GLN:HE21	1:L:333:GLN:HB3	1.56	0.41
1:D:98:CYS:CB	1:D:99:PRO:CD	2.98	0.41
1:I:68:GLN:HG2	1:I:70:LEU:HD21	2.01	0.41
1:A:86:THR:HG22	1:A:88:GLU:HB3	2.02	0.41
1:E:127:LEU:O	1:J:48:VAL:HA	2.20	0.41
1:F:74:ILE:C	1:F:74:ILE:HD12	2.41	0.41
1:A:158:PHE:CZ	1:A:256:LEU:HD22	2.56	0.41
1:G:232:PRO:HD3	1:H:247:TRP:CZ2	2.55	0.41
1:K:75:ASN:HB2	1:K:95:LEU:HD22	2.02	0.41
1:C:184:HIS:HD2	1:C:186:ASP:N	2.18	0.41
1:H:309:GLU:CD	1:H:310:PRO:HD2	2.40	0.41
1:B:89:LYS:O	1:B:90:PHE:CD1	2.73	0.41
1:G:151:GLN:HB2	1:G:342:LEU:HD23	2.02	0.41
1:K:147:PHE:HZ	1:K:255:ILE:HG21	1.79	0.41
1:L:62:ASP:O	1:L:63:TYR:CD2	2.73	0.41
1:L:98:CYS:CB	1:L:99:PRO:CD	2.92	0.41
1:H:161:ARG:O	1:H:165:GLU:HG3	2.19	0.41
1:I:305:LEU:HA	1:I:305:LEU:HD23	1.79	0.41
1:A:149:ARG:HG3	1:A:194:TYR:CD2	2.56	0.41
1:C:331:VAL:CG1	1:C:332:PRO:CD	2.93	0.41
1:L:158:PHE:HD1	1:L:338:THR:CB	2.33	0.41
1:K:141:LEU:HD12	1:K:193:LEU:HB2	2.02	0.41
1:L:257:LEU:O	1:L:336:LEU:HG	2.19	0.41
1:G:265:SER:HA	1:G:275:MET:HB2	2.01	0.41
1:C:115:PRO:O	1:C:204:LYS:HE2	2.21	0.41
1:I:98:CYS:O	1:I:102:ARG:HG2	2.21	0.41
1:B:58:ALA:HB3	1:B:61:ASP:OD2	2.20	0.41
1:A:93:LYS:HD3	1:A:95:LEU:HD21	2.01	0.41
1:B:70:LEU:HD22	2:B:1351:P4O:C17	2.51	0.41
1:J:172:GLU:H	1:J:172:GLU:HG3	1.58	0.41
1:J:254:TYR:HB3	1:J:262:PRO:HD3	2.02	0.41
1:K:334:THR:HA	1:K:335:PRO:HD3	1.82	0.41
1:B:71:GLY:O	1:B:77:LYS:HB2	2.20	0.41
1:L:146:LEU:C	1:L:148:SER:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ARG:NH2	1:D:162:GLU:OE1	2.54	0.41
1:K:149:ARG:HG3	1:K:194:TYR:CD2	2.56	0.41
1:E:158:PHE:O	1:E:336:LEU:N	2.52	0.41
1:E:118:VAL:HG11	1:E:206:THR:HG22	2.00	0.41
1:C:135:LEU:N	1:C:135:LEU:HD23	2.36	0.41
1:J:248:SER:C	1:J:250:GLY:H	2.24	0.41
1:B:83:ASN:CG	1:B:86:THR:HG22	2.41	0.41
1:D:161:ARG:HA	1:D:331:VAL:CG1	2.51	0.41
1:I:195:THR:CG2	1:I:202:ILE:CB	2.98	0.41
1:B:260:TYR:CB	1:B:261:PRO:CD	2.93	0.41
1:F:155:ASP:O	1:F:156:GLN:CB	2.64	0.41
1:E:237:PRO:HB2	1:E:238:GLU:H	1.68	0.41
1:A:86:THR:CG2	1:A:88:GLU:CB	2.98	0.41
1:H:184:HIS:O	1:H:185:ARG:HB2	2.20	0.41
1:I:102:ARG:O	1:I:106:GLU:HB2	2.20	0.41
1:E:342:LEU:HD12	1:E:342:LEU:HA	1.92	0.41
1:H:180:ILE:O	1:H:181:ASN:HB2	2.19	0.41
1:L:206:THR:HB	1:L:207:ASP:H	1.54	0.41
1:L:334:THR:OG1	1:L:334:THR:O	2.33	0.41
1:B:89:LYS:C	1:B:90:PHE:CD1	2.94	0.41
1:L:318:GLU:O	1:L:320:MET:N	2.53	0.41
1:E:286:PHE:CE1	1:E:299:LYS:HB3	2.55	0.41
1:E:64:LYS:HB3	1:E:82:PHE:HB2	2.03	0.41
1:J:255:ILE:HG22	1:J:256:LEU:N	2.36	0.41
1:J:304:ASN:O	1:J:305:LEU:C	2.58	0.41
1:C:322:HIS:ND1	1:C:323:PRO:N	2.69	0.41
1:F:286:PHE:HA	1:F:287:PRO:HD2	1.82	0.41
1:A:331:VAL:CG1	1:A:332:PRO:HD2	2.49	0.41
1:C:70:LEU:HD22	2:C:1351:P4O:C21	2.51	0.41
1:F:191:ASN:HA	1:F:191:ASN:HD22	1.67	0.41
1:G:158:PHE:HE1	1:G:256:LEU:O	2.04	0.41
1:J:52:LEU:HG	1:J:54:ILE:CD1	2.51	0.41
1:D:257:LEU:HA	1:D:257:LEU:HD23	1.90	0.41
1:K:86:THR:HG22	1:K:87:GLN:N	2.36	0.41
1:L:162:GLU:C	1:L:164:SER:N	2.75	0.41
1:L:286:PHE:HD2	1:L:291:TRP:CE3	2.38	0.41
1:J:147:PHE:CZ	1:J:255:ILE:CG2	3.04	0.41
1:J:255:ILE:HG13	1:J:261:PRO:HA	2.03	0.41
1:B:300:MET:CE	1:B:303:ARG:HE	2.34	0.41
1:E:160:GLU:HB3	1:E:331:VAL:CG1	2.51	0.41
1:L:63:TYR:CD1	1:L:81:ILE:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:HIS:C	1:F:341:VAL:HG23	2.41	0.41
1:L:127:LEU:CD2	1:L:132:LYS:HA	2.48	0.41
1:D:256:LEU:HA	1:D:256:LEU:HD23	1.77	0.41
1:J:210:PHE:O	1:J:211:ALA:C	2.59	0.41
1:E:168:LYS:HB2	1:E:325:ILE:HG23	2.01	0.41
1:I:338:THR:CG2	1:I:342:LEU:HD22	2.51	0.41
1:B:128:TYR:O	1:B:129:ALA:HB3	2.21	0.41
1:C:110:ARG:NH2	1:C:213:GLU:OE1	2.53	0.41
1:C:149:ARG:HD3	1:C:194:TYR:CD2	2.55	0.41
1:K:184:HIS:HD2	1:K:186:ASP:N	2.19	0.41
1:F:164:SER:OG	1:F:328:SER:HB2	2.20	0.41
1:B:149:ARG:NH1	1:B:149:ARG:HG3	2.36	0.41
1:J:95:LEU:HA	1:J:95:LEU:HD23	1.82	0.41
1:L:244:CYS:O	1:L:244:CYS:SG	2.79	0.41
1:D:302:ILE:HG22	1:D:302:ILE:O	2.21	0.41
1:J:141:LEU:HD22	1:J:195:THR:HA	2.03	0.41
1:K:158:PHE:CD1	1:K:338:THR:HB	2.56	0.41
1:H:158:PHE:O	1:H:335:PRO:HA	2.20	0.41
1:A:337:HIS:CD2	1:A:340:ARG:NH1	2.84	0.41
1:L:138:MET:HE3	1:L:138:MET:HB3	1.72	0.41
1:G:128:TYR:O	1:G:129:ALA:CB	2.67	0.41
1:D:150:ILE:HG12	1:D:158:PHE:CE2	2.56	0.41
1:G:247:TRP:CD1	1:I:231:ALA:HB2	2.55	0.41
1:L:295:SER:HB2	1:L:298:VAL:HG23	2.01	0.41
1:K:161:ARG:NH1	1:K:333:GLN:OE1	2.54	0.41
1:G:167:MET:HG3	1:G:253:MET:HE2	2.03	0.41
1:C:180:ILE:O	1:C:180:ILE:HG13	2.21	0.41
1:L:264:TYR:O	1:L:278:ARG:NH2	2.54	0.40
1:L:275:MET:O	1:L:277:THR:N	2.54	0.40
1:L:70:LEU:HB2	1:L:78:VAL:CG1	2.51	0.40
1:L:256:LEU:CD2	1:L:256:LEU:O	2.70	0.40
1:E:195:THR:OG1	1:E:196:SER:N	2.54	0.40
1:G:278:ARG:HG3	1:G:278:ARG:NH1	2.35	0.40
1:E:128:TYR:C	1:E:130:GLY:N	2.74	0.40
1:G:332:PRO:CB	1:G:334:THR:HG22	2.51	0.40
1:J:56:LYS:HG3	1:J:56:LYS:HZ3	1.56	0.40
1:C:114:CYS:HA	1:C:115:PRO:HD3	1.88	0.40
1:C:80:GLN:HG3	1:C:81:ILE:N	2.34	0.40
1:F:234:VAL:O	1:F:234:VAL:HG13	2.21	0.40
1:J:52:LEU:HG	1:J:54:ILE:HD13	2.03	0.40
1:J:142:ASP:OD2	1:J:196:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:ILE:CG1	1:G:75:ASN:N	2.80	0.40
1:J:322:HIS:HA	1:J:323:PRO:HD3	1.90	0.40
1:H:149:ARG:NH1	1:H:149:ARG:CG	2.81	0.40
1:A:232:PRO:HB3	1:B:280:ARG:HA	2.03	0.40
1:J:159:THR:N	1:J:162:GLU:HG3	2.36	0.40
1:G:260:TYR:OH	1:G:287:PRO:HG2	2.20	0.40
1:G:191:ASN:HD21	2:G:1350:P4O:H8C2	1.86	0.40
1:C:286:PHE:CD1	1:C:299:LYS:HD3	2.56	0.40
1:F:325:ILE:HD12	1:F:325:ILE:HG23	1.69	0.40
1:F:188:LYS:HB2	1:F:189:PRO:HD2	2.02	0.40
1:C:125:GLU:HA	1:C:133:CYS:O	2.21	0.40
1:I:118:VAL:HG13	1:I:118:VAL:O	2.20	0.40
1:L:147:PHE:CZ	1:L:255:ILE:CG2	3.04	0.40
1:E:343:LYS:O	1:E:344:GLU:C	2.60	0.40
1:E:246:MET:HG3	1:E:314:MET:O	2.21	0.40
1:C:130:GLY:HA3	1:L:180:ILE:HG22	2.03	0.40
1:E:63:TYR:HB3	1:E:81:ILE:HD12	2.03	0.40
1:C:151:GLN:HG2	1:C:342:LEU:HB3	2.03	0.40
1:J:153:ARG:HD2	1:J:157:ALA:HB3	2.02	0.40
1:J:158:PHE:CZ	1:J:163:ALA:N	2.90	0.40
1:L:149:ARG:HH11	1:L:197:LYS:HA	1.86	0.40
1:B:235:LEU:CD2	1:B:235:LEU:H	2.28	0.40
1:B:110:ARG:CG	1:K:130:GLY:O	2.69	0.40
1:D:159:THR:C	1:D:336:LEU:CD2	2.90	0.40
1:C:314:MET:HG3	1:C:318:GLU:HB2	2.03	0.40
1:G:114:CYS:SG	1:G:117:ILE:HG13	2.61	0.40
1:I:45:GLN:O	1:I:45:GLN:HG2	2.20	0.40
1:K:134:LEU:C	1:K:135:LEU:HD23	2.41	0.40
1:G:153:ARG:HH11	1:G:153:ARG:CG	2.35	0.40
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.74	0.40
1:A:59:ILE:HG12	1:A:59:ILE:O	2.21	0.40
1:E:192:LEU:C	1:E:193:LEU:HD23	2.42	0.40
1:J:153:ARG:HH22	1:J:158:PHE:HD2	1.70	0.40
1:H:85:ARG:O	1:H:86:THR:HG23	2.21	0.40
1:L:247:TRP:CZ3	1:L:306:LEU:HA	2.57	0.40
1:D:185:ARG:HH21	1:D:212:LYS:HD3	1.86	0.40
1:K:305:LEU:HD23	1:K:314:MET:HB3	2.04	0.40
1:B:321:ASN:HA	1:B:326:MET:HG2	2.02	0.40
1:I:342:LEU:HA	1:I:342:LEU:HD12	1.71	0.40
1:A:151:GLN:O	1:A:151:GLN:CG	2.69	0.40
1:A:320:MET:O	1:A:326:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ARG:HB2	1:G:339:SER:OG	2.21	0.40
1:D:325:ILE:HG23	1:D:325:ILE:HD12	1.73	0.40
1:L:147:PHE:CZ	1:L:255:ILE:HG21	2.56	0.40
1:K:74:ILE:HG12	1:K:210:PHE:CE2	2.56	0.40
1:D:141:LEU:O	2:D:1351:P4O:C17	2.69	0.40
1:E:198:ARG:O	1:E:199:PRO:C	2.59	0.40
1:E:195:THR:HG23	1:E:202:ILE:HG12	2.01	0.40
1:J:258:CYS:HB2	1:J:260:TYR:CE1	2.57	0.40
1:K:145:GLU:OE1	1:K:147:PHE:HB2	2.22	0.40
1:D:83:ASN:ND2	1:D:85:ARG:HG3	2.34	0.40
1:E:333:GLN:HB3	1:E:333:GLN:HE21	1.62	0.40
1:H:230:VAL:HB	1:H:231:ALA:H	1.59	0.40
1:A:99:PRO:CD	1:A:100:LYS:H	2.32	0.40
1:H:290:GLU:H	1:H:290:GLU:HG2	1.73	0.40
1:J:128:TYR:O	1:J:129:ALA:CB	2.68	0.40
1:G:234:VAL:C	1:G:236:GLY:N	2.75	0.40
1:E:239:LYS:HG3	1:E:240:TYR:CD1	2.57	0.40
1:A:147:PHE:CD1	1:A:189:PRO:HB3	2.57	0.40
1:I:277:THR:O	1:I:281:MET:HB2	2.22	0.40
1:A:191:ASN:HA	1:A:191:ASN:HD22	1.62	0.40
1:D:342:LEU:HA	1:D:342:LEU:HD12	1.96	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	275/326 (84%)	244 (89%)	23 (8%)	8 (3%)	6	34
1	B	284/326 (87%)	238 (84%)	32 (11%)	14 (5%)	3	20
1	C	276/326 (85%)	245 (89%)	19 (7%)	12 (4%)	3	24
1	D	278/326 (85%)	236 (85%)	26 (9%)	16 (6%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	275/326 (84%)	210 (76%)	47 (17%)	18 (6%)	1	13
1	F	282/326 (86%)	248 (88%)	21 (7%)	13 (5%)	3	22
1	G	280/326 (86%)	238 (85%)	26 (9%)	16 (6%)	2	16
1	H	275/326 (84%)	239 (87%)	23 (8%)	13 (5%)	3	21
1	I	281/326 (86%)	245 (87%)	22 (8%)	14 (5%)	3	20
1	J	217/326 (67%)	142 (65%)	40 (18%)	35 (16%)	0	1
1	K	257/326 (79%)	221 (86%)	22 (9%)	14 (5%)	2	18
1	L	260/326 (80%)	187 (72%)	44 (17%)	29 (11%)	0	3
All	All	3240/3912 (83%)	2693 (83%)	345 (11%)	202 (6%)	2	14

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	237	PRO
1	B	98	CYS
1	B	156	GLN
1	B	235	LEU
1	B	349	TRP
1	C	235	LEU
1	C	237	PRO
1	C	241	ASP
1	D	98	CYS
1	D	237	PRO
1	D	290	GLU
1	D	327	GLN
1	D	347	GLU
1	E	61	ASP
1	E	98	CYS
1	E	139	GLU
1	E	149	ARG
1	E	211	ALA
1	E	237	PRO
1	E	238	GLU
1	E	241	ASP
1	E	256	LEU
1	F	98	CYS
1	F	99	PRO
1	F	201	ALA

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Mol	Chain	Res	Type
1	F	338	THR
1	F	345	ASP
1	F	348	ARG
1	G	46	PHE
1	G	74	ILE
1	G	87	GLN
1	G	98	CYS
1	G	146	LEU
1	G	149	ARG
1	G	215	THR
1	G	238	GLU
1	G	241	ASP
1	G	349	TRP
1	H	98	CYS
1	H	99	PRO
1	H	149	ARG
1	H	201	ALA
1	H	230	VAL
1	I	87	GLN
1	I	98	CYS
1	I	157	ALA
1	I	229	TYR
1	J	60	ILE
1	J	72	LEU
1	J	85	ARG
1	J	112	SER
1	J	145	GLU
1	J	175	GLN
1	J	176	TYR
1	J	186	ASP
1	J	190	GLU
1	J	193	LEU
1	J	195	THR
1	J	201	ALA
1	J	211	ALA
1	J	240	TYR
1	J	314	MET
1	J	320	MET
1	K	70	LEU
1	K	85	ARG
1	K	88	GLU
1	K	98	CYS

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Mol	Chain	Res	Type
1	K	145	GLU
1	K	295	SER
1	L	75	ASN
1	L	86	THR
1	L	87	GLN
1	L	146	LEU
1	L	147	PHE
1	L	181	ASN
1	L	207	ASP
1	L	313	ARG
1	L	332	PRO
1	A	99	PRO
1	A	238	GLU
1	A	346	LYS
1	B	236	GLY
1	B	344	GLU
1	C	152	ASP
1	C	345	ASP
1	C	346	LYS
1	D	86	THR
1	D	130	GLY
1	D	186	ASP
1	D	238	GLU
1	E	99	PRO
1	E	344	GLU
1	F	130	GLY
1	F	240	TYR
1	G	99	PRO
1	G	235	LEU
1	G	237	PRO
1	H	345	ASP
1	I	290	GLU
1	I	346	LYS
1	J	109	TRP
1	J	149	ARG
1	J	161	ARG
1	J	170	ILE
1	J	207	ASP
1	J	251	VAL
1	J	256	LEU
1	J	301	LEU
1	K	130	GLY

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Mol	Chain	Res	Type
1	L	84	LYS
1	L	113	GLN
1	L	152	ASP
1	L	311	THR
1	L	319	PHE
1	A	186	ASP
1	B	151	GLN
1	C	186	ASP
1	C	344	GLU
1	D	87	GLN
1	D	99	PRO
1	D	151	GLN
1	D	326	MET
1	D	349	TRP
1	E	73	GLY
1	E	128	TYR
1	E	143	GLY
1	E	186	ASP
1	F	156	GLN
1	G	186	ASP
1	H	290	GLU
1	I	99	PRO
1	I	237	PRO
1	I	239	LYS
1	J	71	GLY
1	J	108	HIS
1	J	158	PHE
1	J	164	SER
1	K	99	PRO
1	K	186	ASP
1	L	98	CYS
1	L	190	GLU
1	L	316	ILE
1	A	347	GLU
1	B	87	GLN
1	B	233	GLU
1	D	235	LEU
1	D	289	PRO
1	F	238	GLU
1	F	326	MET
1	G	86	THR
1	H	216	SER

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Mol	Chain	Res	Type
1	H	237	PRO
1	H	272	SER
1	I	186	ASP
1	J	77	LYS
1	J	84	LYS
1	J	247	TRP
1	L	153	ARG
1	L	163	ALA
1	L	186	ASP
1	L	189	PRO
1	A	61	ASP
1	B	238	GLU
1	B	326	MET
1	C	98	CYS
1	C	236	GLY
1	C	349	TRP
1	E	87	GLN
1	E	97	ASP
1	E	161	ARG
1	F	237	PRO
1	G	346	LYS
1	H	186	ASP
1	H	215	THR
1	I	238	GLU
1	I	345	ASP
1	J	87	GLN
1	K	292	SER
1	L	99	PRO
1	L	188	LYS
1	L	286	PHE
1	L	301	LEU
1	L	334	THR
1	B	99	PRO
1	F	343	LYS
1	H	153	ARG
1	J	172	GLU
1	K	76	GLY
1	K	199	PRO
1	L	276	LYS
1	L	298	VAL
1	C	99	PRO
1	K	198	ARG

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Mol	Chain	Res	Type
1	K	272	SER
1	L	310	PRO
1	J	118	VAL
1	B	237	PRO
1	B	272	SER
1	I	230	VAL
1	J	115	PRO
1	I	289	PRO

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	255/294 (87%)	218 (86%)	37 (14%)	4	18
1	B	262/294 (89%)	218 (83%)	44 (17%)	2	12
1	C	256/294 (87%)	224 (88%)	32 (12%)	6	24
1	D	258/294 (88%)	228 (88%)	30 (12%)	7	28
1	E	255/294 (87%)	198 (78%)	57 (22%)	1	4
1	F	260/294 (88%)	218 (84%)	42 (16%)	3	14
1	G	261/294 (89%)	229 (88%)	32 (12%)	6	25
1	H	255/294 (87%)	221 (87%)	34 (13%)	5	21
1	I	261/294 (89%)	222 (85%)	39 (15%)	4	17
1	J	202/294 (69%)	175 (87%)	27 (13%)	5	21
1	K	239/294 (81%)	199 (83%)	40 (17%)	3	13
1	L	243/294 (83%)	201 (83%)	42 (17%)	2	11
All	All	3007/3528 (85%)	2551 (85%)	456 (15%)	3	16

All (456) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	48	VAL

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Mol	Chain	Res	Type
1	A	50	SER
1	A	60	ILE
1	A	66	THR
1	A	72	LEU
1	A	74	ILE
1	A	75	ASN
1	A	77	LYS
1	A	83	ASN
1	A	86	THR
1	A	92	LEU
1	A	106	GLU
1	A	110	ARG
1	A	134	LEU
1	A	138	MET
1	A	142	ASP
1	A	145	GLU
1	A	149	ARG
1	A	152	ASP
1	A	169	SER
1	A	175	GLN
1	A	185	ARG
1	A	233	GLU
1	A	264	TYR
1	A	277	THR
1	A	292	SER
1	A	293	GLU
1	A	295	SER
1	A	302	ILE
1	A	311	THR
1	A	326	MET
1	A	333	GLN
1	A	334	THR
1	A	336	LEU
1	A	342	LEU
1	A	348	ARG
1	B	46	PHE
1	B	60	ILE
1	B	66	THR
1	B	70	LEU
1	B	74	ILE
1	B	75	ASN
1	B	77	LYS

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Mol	Chain	Res	Type
1	B	83	ASN
1	B	92	LEU
1	B	106	GLU
1	B	110	ARG
1	B	134	LEU
1	B	142	ASP
1	B	146	LEU
1	B	148	SER
1	B	149	ARG
1	B	150	ILE
1	B	152	ASP
1	B	155	ASP
1	B	169	SER
1	B	185	ARG
1	B	197	LYS
1	B	200	ASN
1	B	233	GLU
1	B	235	LEU
1	B	240	TYR
1	B	256	LEU
1	B	264	TYR
1	B	266	ASN
1	B	296	GLU
1	B	302	ILE
1	B	311	THR
1	B	326	MET
1	B	329	THR
1	B	333	GLN
1	B	334	THR
1	B	336	LEU
1	B	337	HIS
1	B	339	SER
1	B	342	LEU
1	B	343	LYS
1	B	344	GLU
1	B	345	ASP
1	B	348	ARG
1	C	60	ILE
1	C	66	THR
1	C	74	ILE
1	C	83	ASN
1	C	84	LYS

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Mol	Chain	Res	Type
1	C	92	LEU
1	C	106	GLU
1	C	110	ARG
1	C	134	LEU
1	C	158	PHE
1	C	169	SER
1	C	170	ILE
1	C	175	GLN
1	C	185	ARG
1	C	191	ASN
1	C	215	THR
1	C	240	TYR
1	C	249	LEU
1	C	264	TYR
1	C	276	LYS
1	C	292	SER
1	C	293	GLU
1	C	302	ILE
1	C	311	THR
1	C	327	GLN
1	C	329	THR
1	C	333	GLN
1	C	334	THR
1	C	336	LEU
1	C	343	LYS
1	C	345	ASP
1	C	348	ARG
1	D	48	VAL
1	D	60	ILE
1	D	70	LEU
1	D	72	LEU
1	D	74	ILE
1	D	77	LYS
1	D	83	ASN
1	D	85	ARG
1	D	106	GLU
1	D	110	ARG
1	D	134	LEU
1	D	138	MET
1	D	142	ASP
1	D	149	ARG
1	D	169	SER

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Mol	Chain	Res	Type
1	D	170	ILE
1	D	185	ARG
1	D	195	THR
1	D	215	THR
1	D	228	TYR
1	D	230	VAL
1	D	240	TYR
1	D	264	TYR
1	D	302	ILE
1	D	311	THR
1	D	334	THR
1	D	336	LEU
1	D	342	LEU
1	D	345	ASP
1	D	348	ARG
1	E	45	GLN
1	E	47	HIS
1	E	50	SER
1	E	56	LYS
1	E	60	ILE
1	E	62	ASP
1	E	66	THR
1	E	74	ILE
1	E	75	ASN
1	E	92	LEU
1	E	94	MET
1	E	95	LEU
1	E	100	LYS
1	E	106	GLU
1	E	110	ARG
1	E	112	SER
1	E	114	CYS
1	E	121	VAL
1	E	126	ASN
1	E	128	TYR
1	E	135	LEU
1	E	140	CYS
1	E	142	ASP
1	E	146	LEU
1	E	149	ARG
1	E	158	PHE
1	E	161	ARG

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Mol	Chain	Res	Type
1	E	167	MET
1	E	175	GLN
1	E	179	SER
1	E	181	ASN
1	E	185	ARG
1	E	187	VAL
1	E	198	ARG
1	E	202	ILE
1	E	210	PHE
1	E	228	TYR
1	E	233	GLU
1	E	240	TYR
1	E	246	MET
1	E	252	ILE
1	E	256	LEU
1	E	261	PRO
1	E	264	TYR
1	E	275	MET
1	E	278	ARG
1	E	288	ASN
1	E	292	SER
1	E	297	GLU
1	E	311	THR
1	E	314	MET
1	E	333	GLN
1	E	334	THR
1	E	336	LEU
1	E	337	HIS
1	E	340	ARG
1	E	343	LYS
1	F	45	GLN
1	F	60	ILE
1	F	66	THR
1	F	74	ILE
1	F	77	LYS
1	F	83	ASN
1	F	86	THR
1	F	92	LEU
1	F	94	MET
1	F	95	LEU
1	F	100	LYS
1	F	103	ARG

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Mol	Chain	Res	Type
1	F	106	GLU
1	F	110	ARG
1	F	132	LYS
1	F	134	LEU
1	F	141	LEU
1	F	149	ARG
1	F	155	ASP
1	F	169	SER
1	F	175	GLN
1	F	185	ARG
1	F	197	LYS
1	F	200	ASN
1	F	210	PHE
1	F	233	GLU
1	F	234	VAL
1	F	264	TYR
1	F	265	SER
1	F	297	GLU
1	F	302	ILE
1	F	311	THR
1	F	315	THR
1	F	326	MET
1	F	328	SER
1	F	329	THR
1	F	333	GLN
1	F	334	THR
1	F	340	ARG
1	F	342	LEU
1	F	344	GLU
1	F	349	TRP
1	G	45	GLN
1	G	47	HIS
1	G	50	SER
1	G	60	ILE
1	G	66	THR
1	G	72	LEU
1	G	74	ILE
1	G	83	ASN
1	G	86	THR
1	G	92	LEU
1	G	106	GLU
1	G	132	LYS

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Mol	Chain	Res	Type
1	G	134	LEU
1	G	138	MET
1	G	142	ASP
1	G	153	ARG
1	G	161	ARG
1	G	169	SER
1	G	175	GLN
1	G	185	ARG
1	G	202	ILE
1	G	233	GLU
1	G	258	CYS
1	G	264	TYR
1	G	277	THR
1	G	294	VAL
1	G	302	ILE
1	G	311	THR
1	G	333	GLN
1	G	334	THR
1	G	336	LEU
1	G	348	ARG
1	H	60	ILE
1	H	66	THR
1	H	70	LEU
1	H	74	ILE
1	H	78	VAL
1	H	83	ASN
1	H	87	GLN
1	H	88	GLU
1	H	92	LEU
1	H	106	GLU
1	H	110	ARG
1	H	134	LEU
1	H	149	ARG
1	H	169	SER
1	H	175	GLN
1	H	185	ARG
1	H	195	THR
1	H	200	ASN
1	H	202	ILE
1	H	217	HIS
1	H	229	TYR
1	H	230	VAL

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Mol	Chain	Res	Type
1	H	239	LYS
1	H	241	ASP
1	H	248	SER
1	H	264	TYR
1	H	277	THR
1	H	295	SER
1	H	311	THR
1	H	334	THR
1	H	336	LEU
1	H	342	LEU
1	H	343	LYS
1	H	344	GLU
1	I	47	HIS
1	I	50	SER
1	I	60	ILE
1	I	66	THR
1	I	70	LEU
1	I	75	ASN
1	I	77	LYS
1	I	83	ASN
1	I	85	ARG
1	I	92	LEU
1	I	95	LEU
1	I	106	GLU
1	I	110	ARG
1	I	134	LEU
1	I	138	MET
1	I	142	ASP
1	I	149	ARG
1	I	169	SER
1	I	175	GLN
1	I	214	THR
1	I	230	VAL
1	I	233	GLU
1	I	234	VAL
1	I	240	TYR
1	I	244	CYS
1	I	264	TYR
1	I	276	LYS
1	I	277	THR
1	I	292	SER
1	I	295	SER

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Mol	Chain	Res	Type
1	I	302	ILE
1	I	311	THR
1	I	326	MET
1	I	333	GLN
1	I	334	THR
1	I	336	LEU
1	I	337	HIS
1	I	342	LEU
1	I	348	ARG
1	J	56	LYS
1	J	57	ASN
1	J	65	VAL
1	J	83	ASN
1	J	85	ARG
1	J	89	LYS
1	J	92	LEU
1	J	94	MET
1	J	103	ARG
1	J	108	HIS
1	J	110	ARG
1	J	113	GLN
1	J	118	VAL
1	J	134	LEU
1	J	138	MET
1	J	149	ARG
1	J	166	ILE
1	J	193	LEU
1	J	194	TYR
1	J	198	ARG
1	J	244	CYS
1	J	249	LEU
1	J	256	LEU
1	J	304	ASN
1	J	305	LEU
1	J	326	MET
1	J	327	GLN
1	K	60	ILE
1	K	66	THR
1	K	70	LEU
1	K	72	LEU
1	K	74	ILE
1	K	77	LYS

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Mol	Chain	Res	Type
1	K	83	ASN
1	K	84	LYS
1	K	92	LEU
1	K	94	MET
1	K	106	GLU
1	K	110	ARG
1	K	132	LYS
1	K	134	LEU
1	K	138	MET
1	K	142	ASP
1	K	145	GLU
1	K	149	ARG
1	K	153	ARG
1	K	169	SER
1	K	185	ARG
1	K	197	LYS
1	K	200	ASN
1	K	212	LYS
1	K	264	TYR
1	K	276	LYS
1	K	277	THR
1	K	288	ASN
1	K	290	GLU
1	K	302	ILE
1	K	311	THR
1	K	315	THR
1	K	326	MET
1	K	327	GLN
1	K	328	SER
1	K	329	THR
1	K	333	GLN
1	K	334	THR
1	K	336	LEU
1	K	342	LEU
1	L	74	ILE
1	L	75	ASN
1	L	77	LYS
1	L	83	ASN
1	L	89	LYS
1	L	93	LYS
1	L	98	CYS
1	L	106	GLU

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Mol	Chain	Res	Type
1	L	110	ARG
1	L	114	CYS
1	L	117	ILE
1	L	123	VAL
1	L	132	LYS
1	L	134	LEU
1	L	153	ARG
1	L	174	ILE
1	L	175	GLN
1	L	185	ARG
1	L	196	SER
1	L	197	LYS
1	L	200	ASN
1	L	202	ILE
1	L	205	LEU
1	L	256	LEU
1	L	257	LEU
1	L	264	TYR
1	L	266	ASN
1	L	285	GLU
1	L	290	GLU
1	L	293	GLU
1	L	296	GLU
1	L	304	ASN
1	L	311	THR
1	L	313	ARG
1	L	315	THR
1	L	333	GLN
1	L	334	THR
1	L	336	LEU
1	L	337	HIS
1	L	340	ARG
1	L	342	LEU
1	L	343	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	83	ASN
1	A	87	GLN
1	A	184	HIS

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Mol	Chain	Res	Type
1	A	191	ASN
1	A	327	GLN
1	A	333	GLN
1	A	337	HIS
1	B	80	GLN
1	B	83	ASN
1	B	96	GLN
1	B	151	GLN
1	B	181	ASN
1	B	184	HIS
1	B	191	ASN
1	B	266	ASN
1	B	333	GLN
1	C	53	GLN
1	C	75	ASN
1	C	80	GLN
1	C	83	ASN
1	C	96	GLN
1	C	151	GLN
1	C	184	HIS
1	C	191	ASN
1	C	327	GLN
1	C	333	GLN
1	D	68	GLN
1	D	83	ASN
1	D	96	GLN
1	D	126	ASN
1	D	151	GLN
1	D	184	HIS
1	D	191	ASN
1	D	200	ASN
1	D	337	HIS
1	E	45	GLN
1	E	96	GLN
1	E	184	HIS
1	E	191	ASN
1	E	200	ASN
1	E	266	ASN
1	E	283	GLN
1	E	288	ASN
1	E	333	GLN
1	F	80	GLN

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Mol	Chain	Res	Type
1	F	83	ASN
1	F	151	GLN
1	F	184	HIS
1	F	191	ASN
1	F	200	ASN
1	F	333	GLN
1	G	45	GLN
1	G	47	HIS
1	G	83	ASN
1	G	96	GLN
1	G	184	HIS
1	G	191	ASN
1	G	288	ASN
1	H	80	GLN
1	H	83	ASN
1	H	87	GLN
1	H	96	GLN
1	H	184	HIS
1	H	200	ASN
1	H	217	HIS
1	H	337	HIS
1	I	45	GLN
1	I	75	ASN
1	I	80	GLN
1	I	83	ASN
1	I	96	GLN
1	I	113	GLN
1	I	151	GLN
1	I	156	GLN
1	I	184	HIS
1	I	191	ASN
1	I	327	GLN
1	J	75	ASN
1	J	83	ASN
1	J	96	GLN
1	J	178	HIS
1	J	200	ASN
1	K	68	GLN
1	K	80	GLN
1	K	83	ASN
1	K	96	GLN
1	K	181	ASN

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Mol	Chain	Res	Type
1	K	184	HIS
1	K	288	ASN
1	K	337	HIS
1	L	53	GLN
1	L	75	ASN
1	L	83	ASN
1	L	108	HIS
1	L	181	ASN
1	L	184	HIS
1	L	191	ASN
1	L	266	ASN
1	L	283	GLN
1	L	304	ASN
1	L	321	ASN
1	L	333	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P4O	A	1351	-	28,30,30	2.46	6 (21%)	35,43,43	2.29	11 (31%)
2	P4O	B	1351	-	28,30,30	2.52	6 (21%)	35,43,43	2.15	12 (34%)
2	P4O	C	1351	-	28,30,30	2.49	6 (21%)	35,43,43	2.06	10 (28%)
2	P4O	D	1351	-	28,30,30	2.52	6 (21%)	35,43,43	2.19	9 (25%)
2	P4O	E	1345	-	28,30,30	2.50	6 (21%)	35,43,43	2.26	11 (31%)
2	P4O	F	1350	-	28,30,30	2.52	6 (21%)	35,43,43	2.22	9 (25%)
2	P4O	G	1350	-	28,30,30	2.51	6 (21%)	35,43,43	2.19	9 (25%)
2	P4O	H	1347	-	28,30,30	2.51	6 (21%)	35,43,43	2.11	8 (22%)
2	P4O	I	1351	-	28,30,30	2.50	6 (21%)	35,43,43	2.15	10 (28%)
2	P4O	K	1345	-	28,30,30	2.51	6 (21%)	35,43,43	2.23	10 (28%)
2	P4O	L	1345	-	28,30,30	2.52	6 (21%)	35,43,43	2.21	9 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P4O	A	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	B	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	C	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	D	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	E	1345	-	-	0/8/18/18	0/5/5/5
2	P4O	F	1350	-	-	0/8/18/18	0/5/5/5
2	P4O	G	1350	-	-	0/8/18/18	0/5/5/5
2	P4O	H	1347	-	-	0/8/18/18	0/5/5/5
2	P4O	I	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	K	1345	-	-	0/8/18/18	0/5/5/5
2	P4O	L	1345	-	-	0/8/18/18	0/5/5/5

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1350	P4O	C12-C2	-6.24	1.39	1.48
2	B	1351	P4O	C12-C2	-6.13	1.39	1.48
2	D	1351	P4O	C12-C2	-6.12	1.39	1.48
2	F	1350	P4O	C18-C14	-6.11	1.39	1.48
2	K	1345	P4O	C12-C2	-6.08	1.39	1.48
2	C	1351	P4O	C12-C2	-6.08	1.39	1.48
2	E	1345	P4O	C12-C2	-6.06	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1351	P4O	C18-C14	-6.06	1.39	1.48
2	K	1345	P4O	C18-C14	-6.05	1.39	1.48
2	H	1347	P4O	C12-C2	-6.05	1.39	1.48
2	D	1351	P4O	C18-C14	-6.05	1.39	1.48
2	I	1351	P4O	C18-C14	-6.05	1.39	1.48
2	H	1347	P4O	C18-C14	-6.04	1.39	1.48
2	I	1351	P4O	C12-C2	-6.04	1.39	1.48
2	L	1345	P4O	C18-C14	-6.04	1.39	1.48
2	B	1351	P4O	C18-C14	-6.02	1.39	1.48
2	G	1350	P4O	C18-C14	-6.00	1.39	1.48
2	A	1351	P4O	C12-C2	-5.99	1.39	1.48
2	L	1345	P4O	C12-C2	-5.97	1.39	1.48
2	G	1350	P4O	C12-C2	-5.97	1.39	1.48
2	E	1345	P4O	C18-C14	-5.93	1.39	1.48
2	A	1351	P4O	C18-C14	-5.85	1.40	1.48
2	A	1351	P4O	C4-C6	-4.76	1.39	1.47
2	L	1345	P4O	C4-C6	-4.75	1.39	1.47
2	B	1351	P4O	C4-C6	-4.75	1.39	1.47
2	K	1345	P4O	C4-C6	-4.73	1.39	1.47
2	D	1351	P4O	C4-C6	-4.72	1.39	1.47
2	I	1351	P4O	C4-C6	-4.72	1.39	1.47
2	E	1345	P4O	C4-C6	-4.71	1.39	1.47
2	F	1350	P4O	C4-C6	-4.69	1.39	1.47
2	C	1351	P4O	C4-C6	-4.69	1.39	1.47
2	H	1347	P4O	C4-C6	-4.65	1.39	1.47
2	G	1350	P4O	C4-C6	-4.65	1.39	1.47
2	F	1350	P4O	C3-C2	-3.70	1.33	1.40
2	I	1351	P4O	C3-C2	-3.63	1.33	1.40
2	L	1345	P4O	C3-C2	-3.63	1.33	1.40
2	D	1351	P4O	C3-C2	-3.61	1.33	1.40
2	G	1350	P4O	C3-C2	-3.61	1.33	1.40
2	B	1351	P4O	C3-C2	-3.61	1.33	1.40
2	C	1351	P4O	C3-C2	-3.60	1.33	1.40
2	A	1351	P4O	C3-C2	-3.60	1.33	1.40
2	H	1347	P4O	C3-C2	-3.59	1.33	1.40
2	E	1345	P4O	C3-C2	-3.58	1.33	1.40
2	K	1345	P4O	C3-C2	-3.56	1.33	1.40
2	L	1345	P4O	C3-C4	-3.30	1.33	1.40
2	F	1350	P4O	C3-C4	-3.29	1.33	1.40
2	B	1351	P4O	C3-C4	-3.29	1.33	1.40
2	K	1345	P4O	C3-C4	-3.28	1.33	1.40
2	E	1345	P4O	C3-C4	-3.26	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1351	P4O	C3-C4	-3.26	1.33	1.40
2	H	1347	P4O	C3-C4	-3.22	1.33	1.40
2	I	1351	P4O	C3-C4	-3.22	1.33	1.40
2	G	1350	P4O	C3-C4	-3.21	1.33	1.40
2	C	1351	P4O	C3-C4	-3.20	1.33	1.40
2	A	1351	P4O	C3-C4	-3.18	1.33	1.40
2	A	1351	P4O	C6-N7	5.66	1.40	1.34
2	F	1350	P4O	C6-N7	5.82	1.40	1.34
2	C	1351	P4O	C6-N7	5.86	1.40	1.34
2	I	1351	P4O	C6-N7	5.90	1.40	1.34
2	K	1345	P4O	C6-N7	5.94	1.40	1.34
2	H	1347	P4O	C6-N7	6.04	1.40	1.34
2	B	1351	P4O	C6-N7	6.05	1.40	1.34
2	E	1345	P4O	C6-N7	6.07	1.40	1.34
2	D	1351	P4O	C6-N7	6.07	1.40	1.34
2	L	1345	P4O	C6-N7	6.19	1.41	1.34
2	G	1350	P4O	C6-N7	6.21	1.41	1.34

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1345	P4O	C18-C17-N16	-3.71	120.77	125.46
2	D	1351	P4O	C18-C17-N16	-3.61	120.89	125.46
2	B	1351	P4O	C18-C17-N16	-3.54	120.98	125.46
2	F	1350	P4O	C18-C17-N16	-3.52	121.01	125.46
2	I	1351	P4O	C18-C17-N16	-3.44	121.12	125.46
2	G	1350	P4O	C18-C17-N16	-3.43	121.12	125.46
2	E	1345	P4O	C11-C10-N15	-3.42	120.00	123.90
2	H	1347	P4O	C18-C17-N16	-3.39	121.17	125.46
2	C	1351	P4O	C18-C17-N16	-3.39	121.17	125.46
2	L	1345	P4O	C18-C17-N16	-3.34	121.24	125.46
2	L	1345	P4O	C11-C10-N15	-3.33	120.10	123.90
2	E	1345	P4O	C18-C17-N16	-3.30	121.28	125.46
2	G	1350	P4O	C11-C10-N15	-3.28	120.15	123.90
2	K	1345	P4O	C11-C10-N15	-3.20	120.25	123.90
2	F	1350	P4O	C3-C2-C12	-3.18	124.98	129.40
2	A	1351	P4O	C18-C17-N16	-3.09	121.56	125.46
2	I	1351	P4O	C11-C10-N15	-3.02	120.45	123.90
2	A	1351	P4O	C11-C10-N15	-3.01	120.47	123.90
2	D	1351	P4O	C3-C2-C12	-2.95	125.29	129.40
2	H	1347	P4O	C11-C10-N15	-2.89	120.60	123.90
2	D	1351	P4O	C11-C10-N15	-2.85	120.64	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1350	P4O	C11-C10-N15	-2.78	120.72	123.90
2	L	1345	P4O	C3-C2-C12	-2.76	125.56	129.40
2	B	1351	P4O	C11-C10-N15	-2.68	120.85	123.90
2	C	1351	P4O	C11-C10-N15	-2.56	120.97	123.90
2	C	1351	P4O	C8-C9-C5	-2.56	108.72	113.15
2	E	1345	P4O	C3-C2-C12	-2.53	125.88	129.40
2	K	1345	P4O	C3-C2-C12	-2.52	125.89	129.40
2	D	1351	P4O	C8-C9-C5	-2.51	108.82	113.15
2	B	1351	P4O	C3-C2-C12	-2.50	125.92	129.40
2	B	1351	P4O	C8-C9-C5	-2.43	108.95	113.15
2	H	1347	P4O	C3-C2-C12	-2.41	126.05	129.40
2	A	1351	P4O	C13-C14-N15	-2.25	119.05	122.02
2	A	1351	P4O	O26-C6-N7	-2.24	118.53	122.78
2	I	1351	P4O	C3-C2-C12	-2.21	126.32	129.40
2	C	1351	P4O	C13-C14-N15	-2.21	119.11	122.02
2	E	1345	P4O	C13-C14-N15	-2.18	119.15	122.02
2	E	1345	P4O	C8-C9-C5	-2.17	109.40	113.15
2	I	1351	P4O	C8-C9-C5	-2.15	109.43	113.15
2	A	1351	P4O	C3-C2-C12	-2.12	126.45	129.40
2	B	1351	P4O	C13-C14-N15	-2.09	119.27	122.02
2	L	1345	P4O	C8-C9-C5	-2.05	109.61	113.15
2	G	1350	P4O	C3-C2-C12	-2.02	126.58	129.40
2	K	1345	P4O	C8-C9-C5	-2.01	109.68	113.15
2	C	1351	P4O	C3-C4-C5	2.00	106.75	104.10
2	B	1351	P4O	C9-C8-N7	2.03	112.10	109.69
2	K	1345	P4O	C3-C4-C5	2.07	106.85	104.10
2	E	1345	P4O	C9-C8-N7	2.09	112.16	109.69
2	I	1351	P4O	C3-C4-C5	2.09	106.88	104.10
2	B	1351	P4O	C3-C4-C5	2.12	106.92	104.10
2	F	1350	P4O	C9-C8-N7	2.46	112.60	109.69
2	G	1350	P4O	C9-C8-N7	2.54	112.70	109.69
2	C	1351	P4O	C12-C2-N1	2.60	124.17	120.62
2	A	1351	P4O	C9-C8-N7	2.62	112.80	109.69
2	I	1351	P4O	C12-C2-N1	3.04	124.78	120.62
2	B	1351	P4O	C12-C2-N1	3.09	124.85	120.62
2	G	1350	P4O	C12-C2-N1	3.15	124.93	120.62
2	H	1347	P4O	C12-C2-N1	3.26	125.07	120.62
2	K	1345	P4O	C12-C2-N1	3.49	125.39	120.62
2	B	1351	P4O	C4-C3-C2	3.50	108.36	105.98
2	E	1345	P4O	C12-C2-N1	3.57	125.50	120.62
2	A	1351	P4O	C12-C2-N1	3.62	125.56	120.62
2	D	1351	P4O	C12-C2-N1	3.73	125.72	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1351	P4O	C4-C3-C2	3.73	108.52	105.98
2	F	1350	P4O	C12-C2-N1	3.75	125.75	120.62
2	D	1351	P4O	C10-N15-C14	3.82	122.46	117.20
2	L	1345	P4O	C12-C2-N1	3.82	125.85	120.62
2	C	1351	P4O	C10-N15-C14	3.83	122.48	117.20
2	A	1351	P4O	C10-N15-C14	3.83	122.48	117.20
2	K	1345	P4O	C10-N15-C14	3.84	122.49	117.20
2	I	1351	P4O	C4-C3-C2	3.85	108.59	105.98
2	I	1351	P4O	C10-N15-C14	3.85	122.50	117.20
2	H	1347	P4O	C10-N15-C14	3.85	122.51	117.20
2	F	1350	P4O	C10-N15-C14	3.87	122.53	117.20
2	G	1350	P4O	C10-N15-C14	3.91	122.59	117.20
2	B	1351	P4O	C10-N15-C14	3.92	122.60	117.20
2	F	1350	P4O	C4-C3-C2	3.98	108.69	105.98
2	L	1345	P4O	C10-N15-C14	4.00	122.72	117.20
2	K	1345	P4O	C4-C3-C2	4.02	108.71	105.98
2	D	1351	P4O	C4-C3-C2	4.10	108.77	105.98
2	H	1347	P4O	C4-C3-C2	4.30	108.90	105.98
2	E	1345	P4O	C4-C3-C2	4.30	108.90	105.98
2	E	1345	P4O	C10-N15-C14	4.31	123.13	117.20
2	L	1345	P4O	C4-C3-C2	4.35	108.94	105.98
2	G	1350	P4O	C4-C3-C2	4.36	108.94	105.98
2	C	1351	P4O	C17-N16-C21	4.36	121.92	116.95
2	L	1345	P4O	C17-N16-C21	4.38	121.94	116.95
2	G	1350	P4O	C17-N16-C21	4.39	121.95	116.95
2	F	1350	P4O	C17-N16-C21	4.46	122.03	116.95
2	I	1351	P4O	C17-N16-C21	4.46	122.03	116.95
2	A	1351	P4O	C17-N16-C21	4.47	122.04	116.95
2	H	1347	P4O	C17-N16-C21	4.53	122.11	116.95
2	E	1345	P4O	C17-N16-C21	4.54	122.12	116.95
2	D	1351	P4O	C17-N16-C21	4.65	122.24	116.95
2	K	1345	P4O	C17-N16-C21	4.65	122.25	116.95
2	B	1351	P4O	C17-N16-C21	4.66	122.26	116.95
2	A	1351	P4O	C4-C3-C2	5.09	109.44	105.98
2	H	1347	P4O	C4-C6-N7	5.93	119.39	115.81
2	D	1351	P4O	C4-C6-N7	6.11	119.50	115.81
2	C	1351	P4O	C4-C6-N7	6.22	119.57	115.81
2	L	1345	P4O	C4-C6-N7	6.23	119.58	115.81
2	B	1351	P4O	C4-C6-N7	6.24	119.58	115.81
2	F	1350	P4O	C4-C6-N7	6.40	119.68	115.81
2	I	1351	P4O	C4-C6-N7	6.55	119.77	115.81
2	G	1350	P4O	C4-C6-N7	6.58	119.78	115.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1345	P4O	C4-C6-N7	6.75	119.89	115.81
2	K	1345	P4O	C4-C6-N7	6.82	119.93	115.81
2	A	1351	P4O	C4-C6-N7	7.37	120.26	115.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1351	P4O	2	0
2	B	1351	P4O	1	0
2	C	1351	P4O	4	0
2	D	1351	P4O	5	0
2	E	1345	P4O	4	0
2	F	1350	P4O	5	0
2	G	1350	P4O	5	0
2	H	1347	P4O	4	0
2	I	1351	P4O	2	0
2	K	1345	P4O	3	0
2	L	1345	P4O	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	283/326 (86%)	-0.15	4 (1%) 78 78	13, 40, 110, 170	0
1	B	290/326 (88%)	0.06	10 (3%) 49 48	20, 63, 141, 173	0
1	C	284/326 (87%)	0.07	5 (1%) 71 70	19, 54, 127, 169	0
1	D	286/326 (87%)	0.06	9 (3%) 52 52	16, 51, 125, 171	0
1	E	283/326 (86%)	0.20	16 (5%) 27 26	33, 81, 140, 174	0
1	F	288/326 (88%)	-0.02	3 (1%) 84 84	13, 47, 116, 156	0
1	G	288/326 (88%)	0.24	15 (5%) 31 29	19, 74, 150, 194	0
1	H	283/326 (86%)	0.23	12 (4%) 40 37	36, 76, 137, 186	0
1	I	289/326 (88%)	0.20	13 (4%) 37 35	31, 72, 152, 180	0
1	J	225/326 (69%)	0.53	23 (10%) 9 9	51, 120, 170, 198	0
1	K	265/326 (81%)	0.85	49 (18%) 2 2	50, 127, 177, 198	0
1	L	268/326 (82%)	0.54	35 (13%) 5 4	35, 113, 174, 188	0
All	All	3332/3912 (85%)	0.22	194 (5%) 26 25	13, 73, 157, 198	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	201	ALA	5.8
1	G	338	THR	5.5
1	K	289	PRO	5.0
1	H	235	LEU	4.8
1	H	231	ALA	4.8
1	A	266	ASN	4.8
1	G	350	GLU	4.6
1	J	298	VAL	4.6
1	E	157	ALA	4.5
1	K	329	THR	4.5
1	K	338	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	272	SER	4.4
1	D	266	ASN	4.4
1	H	230	VAL	4.3
1	H	236	GLY	4.3
1	L	257	LEU	4.2
1	K	337	HIS	4.2
1	L	328	SER	4.1
1	K	340	ARG	4.1
1	K	202	ILE	4.0
1	L	164	SER	4.0
1	J	201	ALA	3.9
1	J	72	LEU	3.9
1	L	158	PHE	3.9
1	L	340	ARG	3.8
1	K	199	PRO	3.8
1	L	154	GLY	3.8
1	H	64	LYS	3.8
1	K	257	LEU	3.8
1	K	294	VAL	3.7
1	I	128	TYR	3.7
1	K	158	PHE	3.7
1	K	150	ILE	3.7
1	L	44	PRO	3.6
1	K	327	GLN	3.6
1	K	328	SER	3.6
1	L	342	LEU	3.6
1	K	197	LYS	3.6
1	K	324	TRP	3.6
1	L	150	ILE	3.5
1	G	158	PHE	3.5
1	L	46	PHE	3.4
1	I	94	MET	3.4
1	G	46	PHE	3.4
1	J	253	MET	3.3
1	B	85	ARG	3.3
1	K	333	GLN	3.3
1	I	91	ALA	3.3
1	K	142	ASP	3.2
1	I	66	THR	3.2
1	L	160	GLU	3.2
1	E	154	GLY	3.2
1	I	75	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	87	GLN	3.2
1	J	197	LYS	3.2
1	K	335	PRO	3.2
1	K	336	LEU	3.2
1	K	293	GLU	3.2
1	L	332	PRO	3.2
1	L	146	LEU	3.2
1	E	75	ASN	3.1
1	B	237	PRO	3.1
1	F	68	GLN	3.1
1	K	330	LYS	3.1
1	L	291	TRP	3.1
1	E	89	LYS	3.1
1	E	76	GLY	3.1
1	K	153	ARG	3.1
1	K	342	LEU	3.1
1	L	289	PRO	3.1
1	K	141	LEU	3.0
1	L	338	THR	3.0
1	H	85	ARG	3.0
1	J	326	MET	3.0
1	L	333	GLN	2.9
1	L	293	GLU	2.9
1	K	290	GLU	2.9
1	K	295	SER	2.9
1	J	258	CYS	2.9
1	K	325	ILE	2.9
1	E	197	LYS	2.9
1	I	237	PRO	2.8
1	B	87	GLN	2.8
1	C	346	LYS	2.8
1	L	159	THR	2.8
1	L	256	LEU	2.8
1	K	187	VAL	2.8
1	K	291	TRP	2.8
1	K	154	GLY	2.8
1	K	332	PRO	2.8
1	E	66	THR	2.8
1	H	158	PHE	2.7
1	I	349	TRP	2.7
1	J	196	SER	2.7
1	J	324	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	238	GLU	2.7
1	G	342	LEU	2.7
1	I	73	GLY	2.7
1	D	237	PRO	2.7
1	C	339	SER	2.7
1	E	64	LYS	2.7
1	B	86	THR	2.7
1	K	194	TYR	2.6
1	G	157	ALA	2.6
1	L	337	HIS	2.6
1	B	64	LYS	2.6
1	G	160	GLU	2.6
1	J	240	TYR	2.6
1	I	67	SER	2.6
1	E	342	LEU	2.6
1	L	153	ARG	2.6
1	G	293	GLU	2.5
1	K	258	CYS	2.5
1	K	200	ASN	2.5
1	J	257	LEU	2.5
1	A	237	PRO	2.5
1	L	196	SER	2.5
1	E	199	PRO	2.5
1	I	236	GLY	2.5
1	L	288	ASN	2.5
1	D	239	LYS	2.5
1	D	350	GLU	2.5
1	E	82	PHE	2.5
1	G	289	PRO	2.5
1	H	84	LYS	2.5
1	H	153	ARG	2.4
1	I	77	LYS	2.4
1	G	291	TRP	2.4
1	J	96	GLN	2.4
1	L	324	TRP	2.4
1	J	150	ILE	2.4
1	C	237	PRO	2.4
1	K	298	VAL	2.4
1	G	334	THR	2.4
1	J	295	SER	2.4
1	L	292	SER	2.3
1	C	273	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	259	GLY	2.3
1	L	157	ALA	2.3
1	K	184	HIS	2.3
1	I	238	GLU	2.3
1	J	239	LYS	2.3
1	J	259	GLY	2.3
1	J	62	ASP	2.3
1	G	84	LYS	2.3
1	H	46	PHE	2.3
1	I	235	LEU	2.3
1	K	203	LEU	2.3
1	K	88	GLU	2.3
1	D	272	SER	2.3
1	L	252	ILE	2.3
1	K	195	THR	2.2
1	L	329	THR	2.2
1	A	272	SER	2.2
1	E	84	LYS	2.2
1	D	240	TYR	2.2
1	L	253	MET	2.2
1	J	252	ILE	2.2
1	B	83	ASN	2.2
1	J	198	ARG	2.2
1	E	59	ILE	2.2
1	K	110	ARG	2.2
1	J	75	ASN	2.2
1	B	240	TYR	2.1
1	K	84	LYS	2.1
1	D	328	SER	2.1
1	E	87	GLN	2.1
1	F	45	GLN	2.1
1	L	286	PHE	2.1
1	K	164	SER	2.1
1	D	228	TYR	2.1
1	K	339	SER	2.1
1	A	235	LEU	2.1
1	G	275	MET	2.1
1	K	157	ALA	2.1
1	L	335	PRO	2.1
1	J	149	ARG	2.1
1	G	335	PRO	2.1
1	B	155	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	298	VAL	2.1
1	C	68	GLN	2.1
1	K	182	ILE	2.1
1	L	334	THR	2.1
1	F	344	GLU	2.1
1	B	66	THR	2.0
1	J	185	ARG	2.0
1	J	170	ILE	2.0
1	K	246	MET	2.0
1	E	142	ASP	2.0
1	H	346	LYS	2.0
1	K	253	MET	2.0
1	B	70	LEU	2.0
1	E	196	SER	2.0
1	L	330	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	P4O	H	1347	26/26	0.90	0.50	3.71	37,88,111,116	0
2	P4O	C	1351	26/26	0.92	0.53	3.59	55,84,118,136	0
2	P4O	B	1351	26/26	0.85	0.55	3.01	54,105,135,142	0
2	P4O	F	1350	26/26	0.93	0.44	2.54	28,79,116,121	0
2	P4O	L	1345	26/26	0.80	0.41	2.06	125,139,158,161	0
2	P4O	D	1351	26/26	0.92	0.35	2.00	42,78,99,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	P4O	E	1345	26/26	0.83	0.42	1.85	79,115,138,145	0
2	P4O	I	1351	26/26	0.78	0.51	1.83	117,137,150,162	0
2	P4O	K	1345	26/26	0.73	0.51	1.51	133,152,162,171	0
2	P4O	G	1350	26/26	0.91	0.28	1.07	39,98,121,130	0
2	P4O	A	1351	26/26	0.96	0.22	0.69	25,57,77,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.