



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 09:00 AM EDT

PDB ID : 4YG2
Title : X-ray crystal structur of Escherichia coli RNA polymerase sigma70 holoenzyme
Authors : Murakami, K.S.
Deposited on : unknown
Resolution : 3.70 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

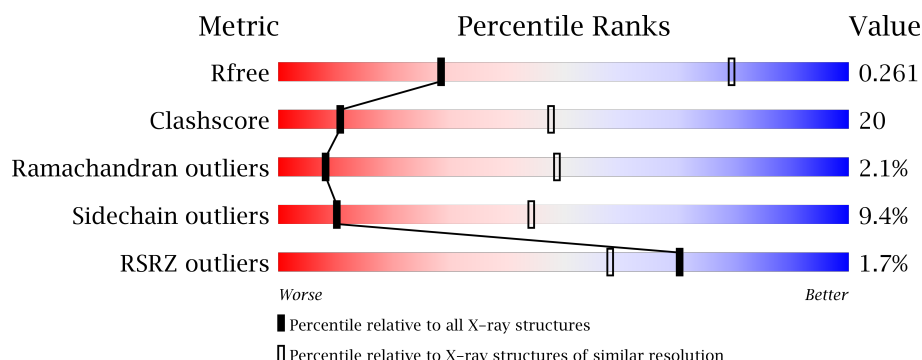
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.





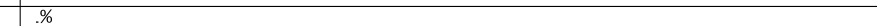
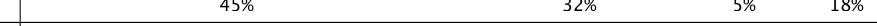


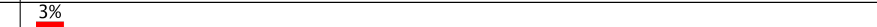
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	 <div>3% 59% 37% .</div>
3	D	1407	 <div>44% 33% 5% 17%</div>
3	J	1407	 <div>1% 45% 32% 5% 18%</div>
4	E	91	 <div>62% 27% 9% .</div>
4	K	91	 <div>1% 47% 33% 7% 13%</div>
5	F	613	 <div>3% 41% 33% . 24%</div>
5	L	613	 <div>2% 40% 33% . 23%</div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55741 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9060	5697	1621	1696	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

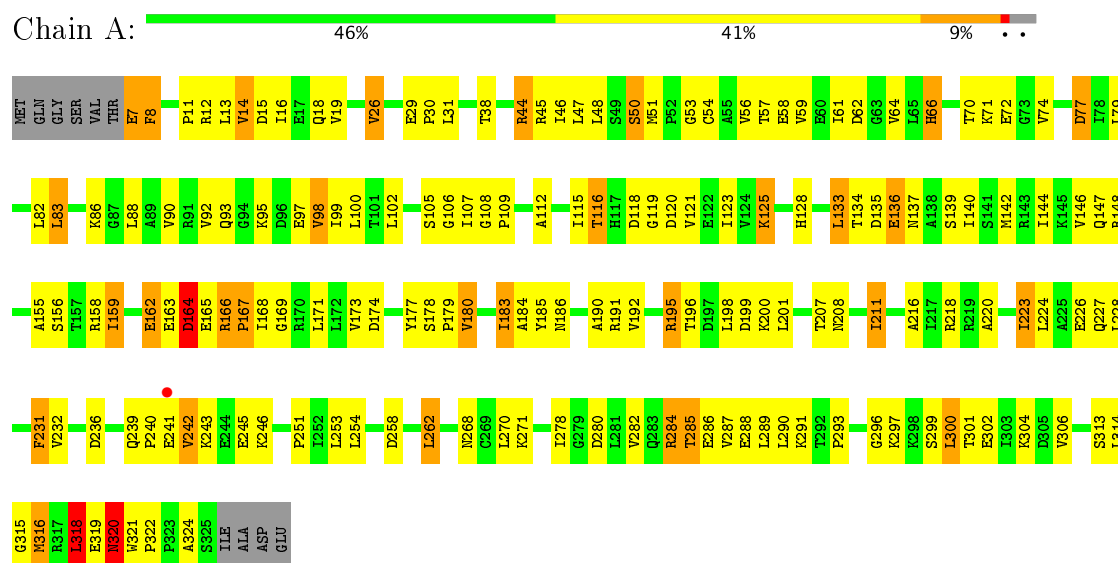
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

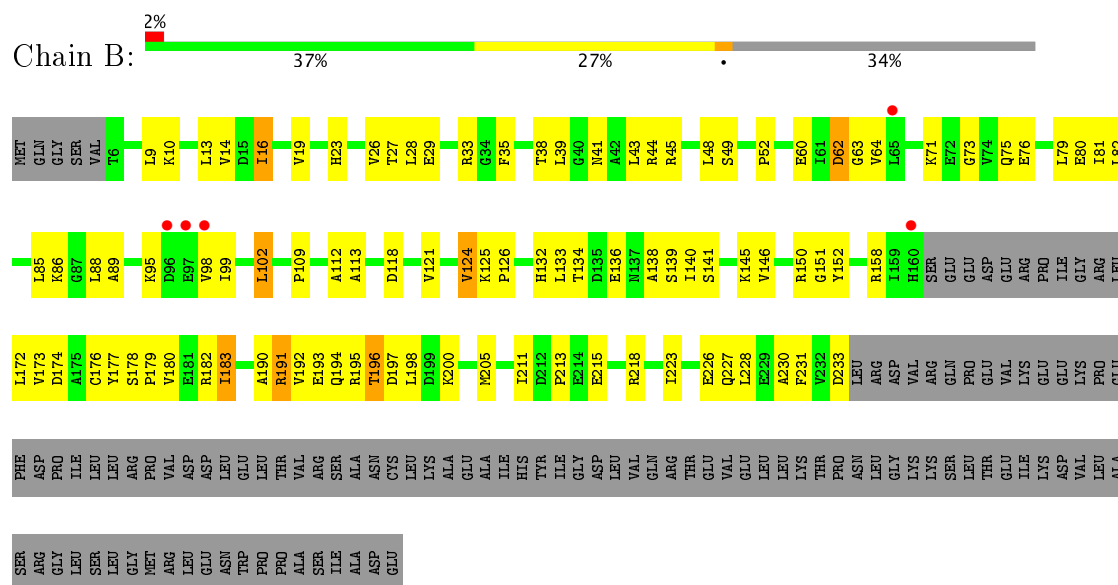
3 Residue-property plots

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

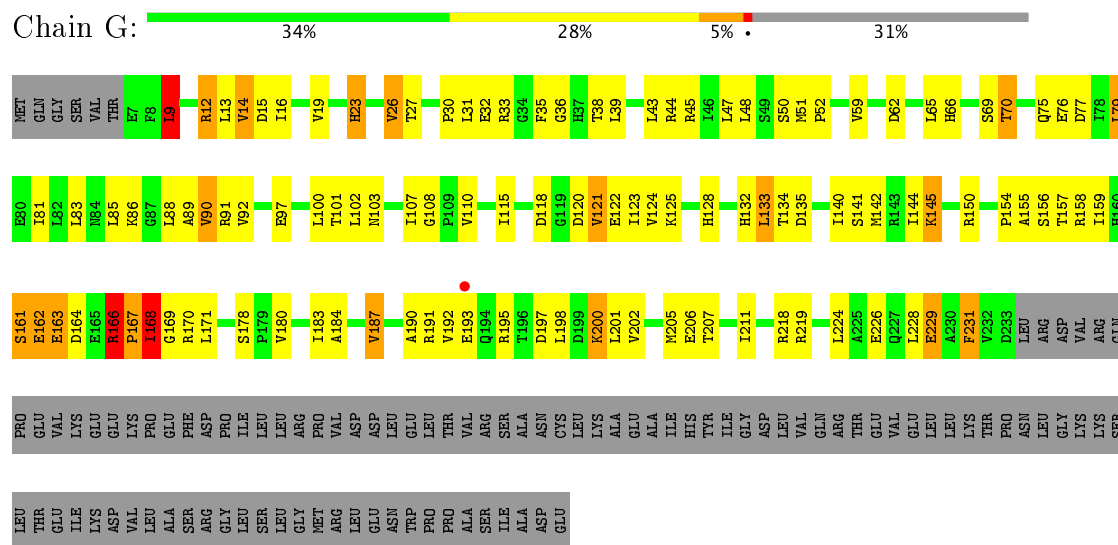
- Molecule 1: DNA-directed RNA polymerase subunit alpha

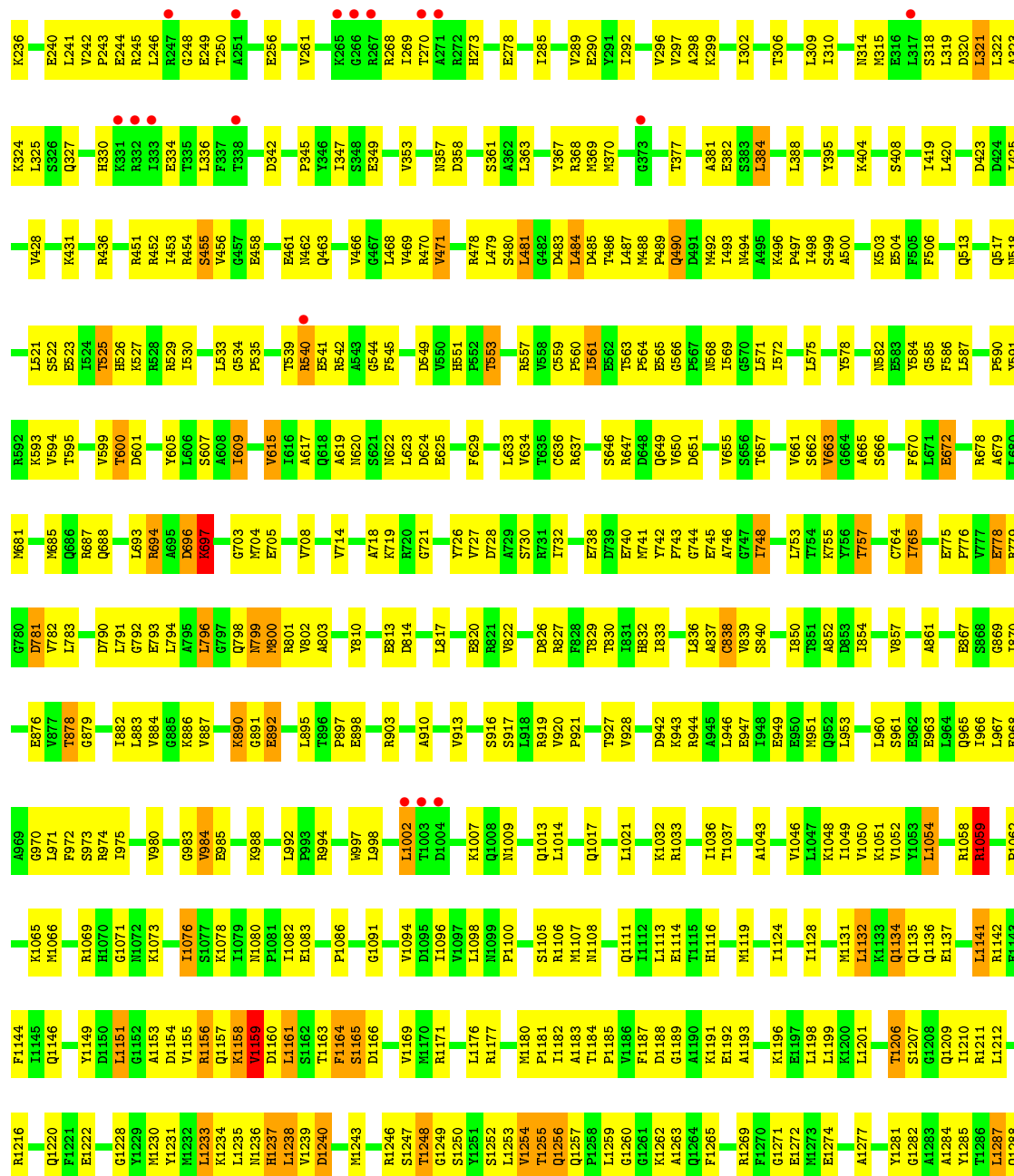


- Molecule 1: DNA-directed RNA polymerase subunit alpha



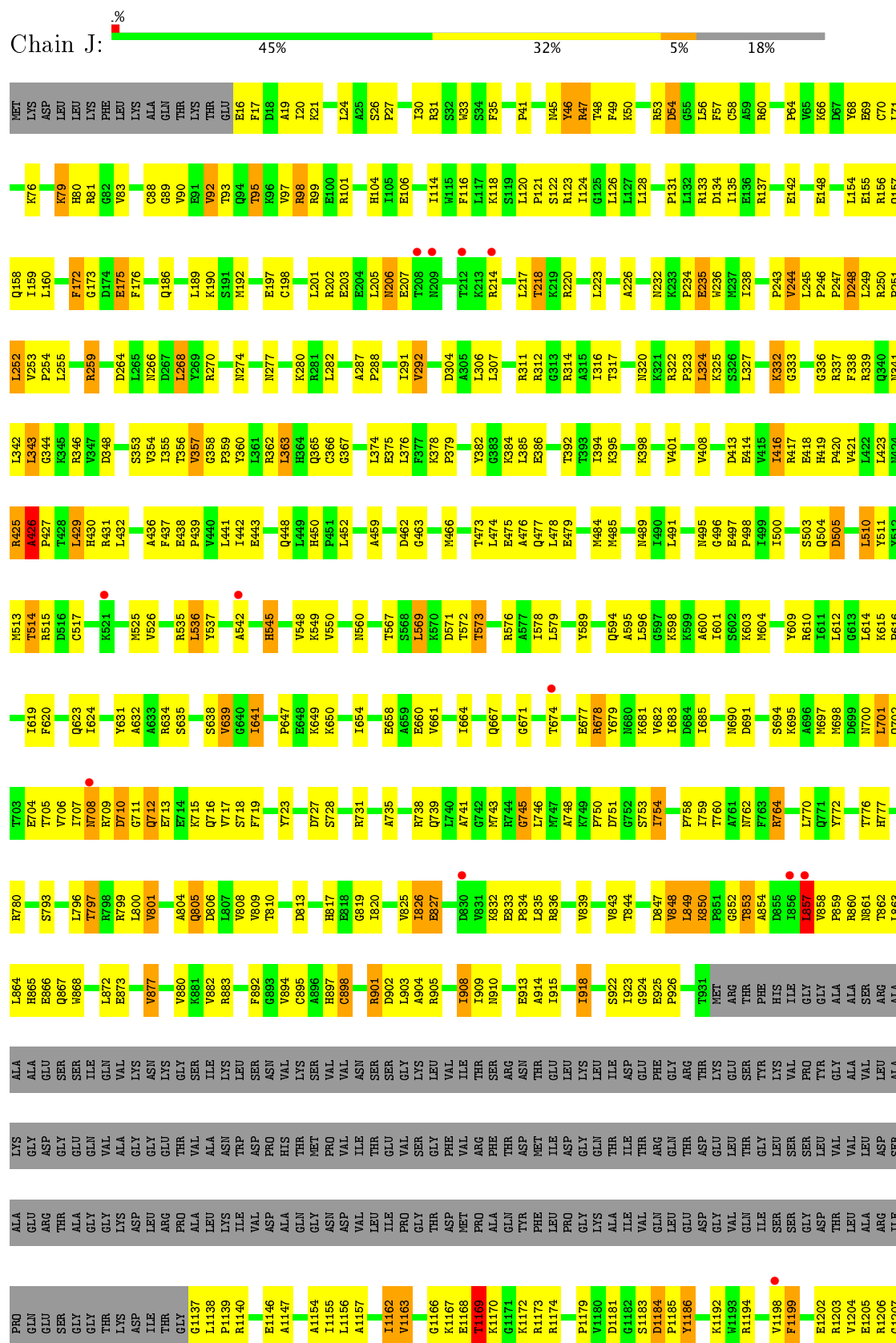
- Molecule 1: DNA-directed RNA polymerase subunit alpha



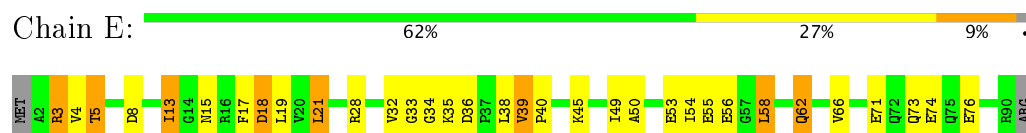




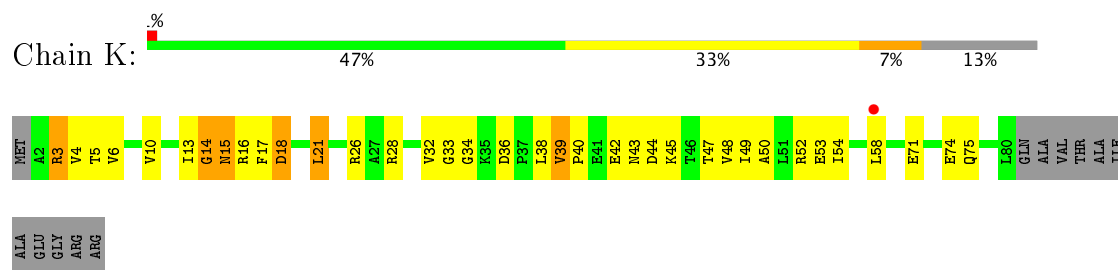
● Molecule 3: DNA-directed RNA polymerase subunit beta'



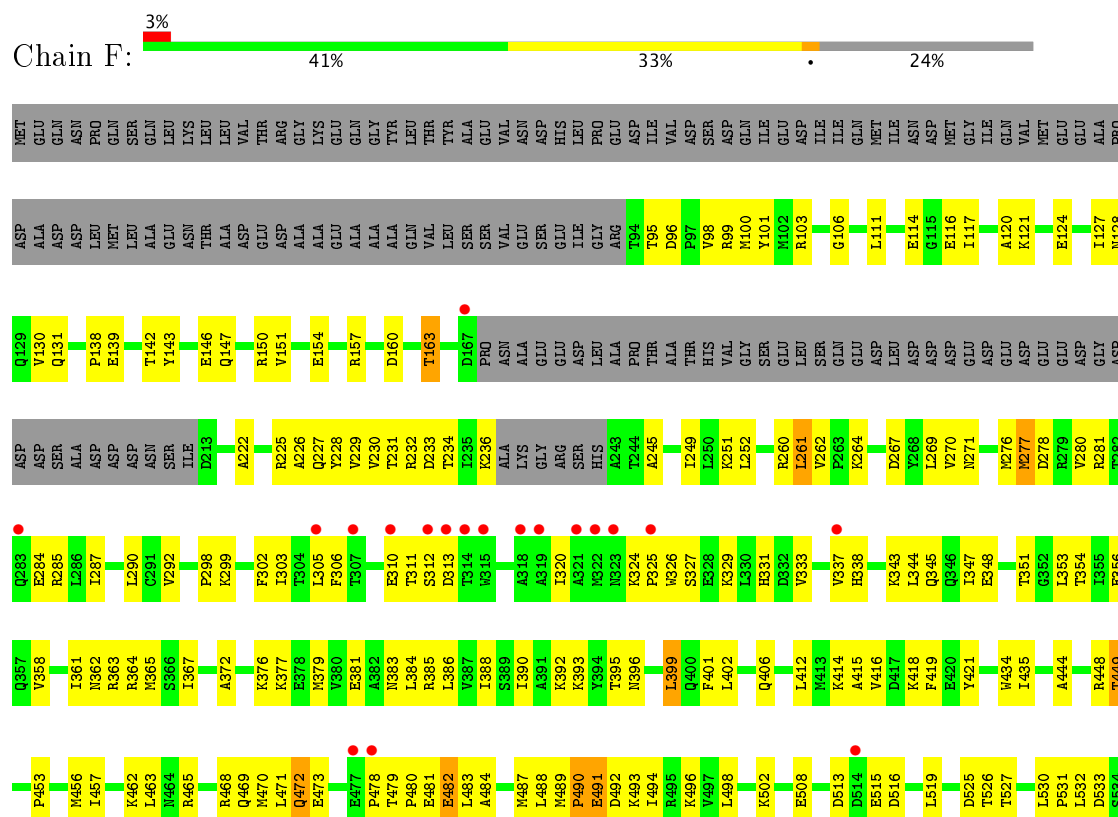
- Molecule 4: DNA-directed RNA polymerase subunit omega

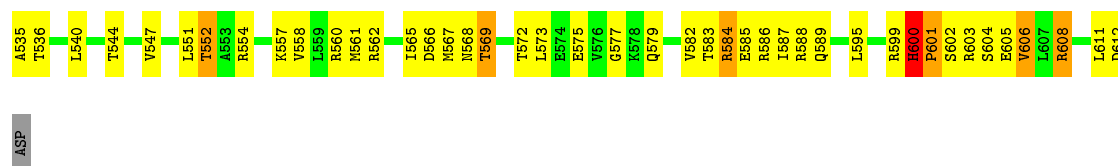


- Molecule 4: DNA-directed RNA polymerase subunit omega

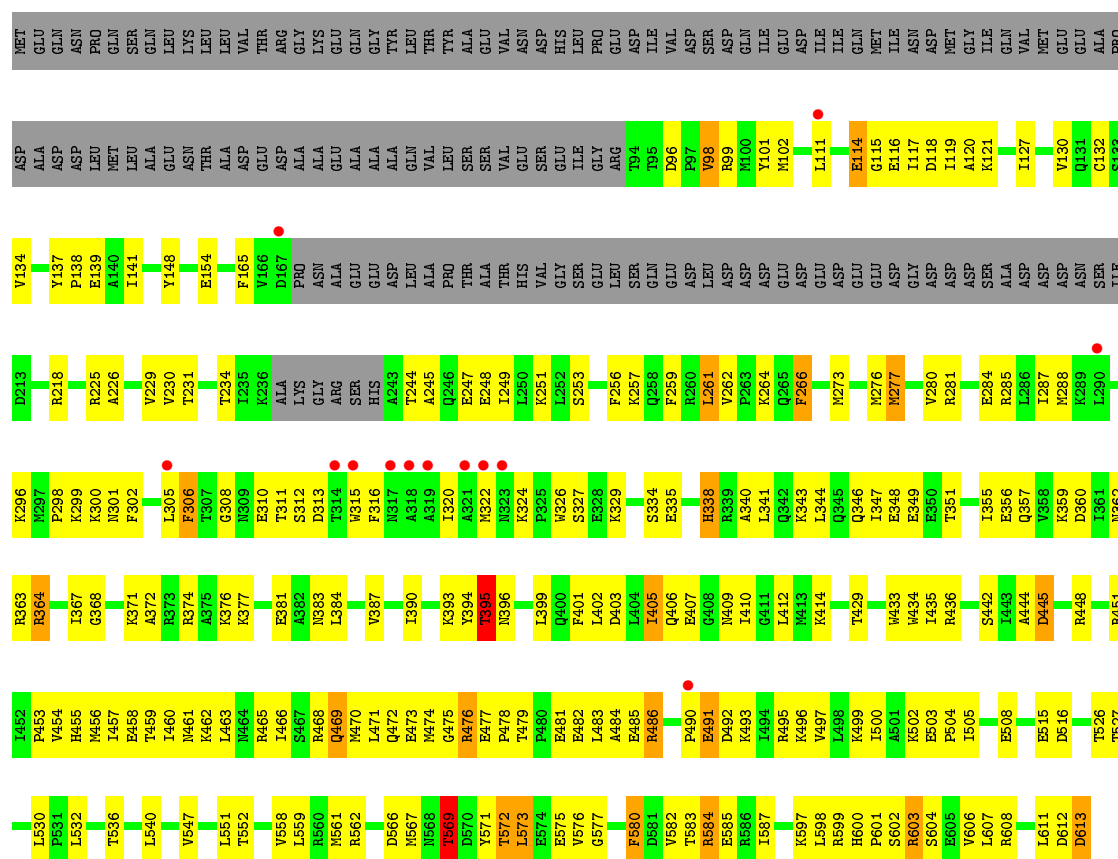


- Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.31Å 205.90Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.70 29.98 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.98-3.70) 92.5 (29.98-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.260 0.194 , 0.261	Depositor DCC
R_{free} test set	5897 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	114.6	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55741	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, MG

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	0.62	0/2524	0.81	2/3421 (0.1%)
1	B	0.58	0/1697	0.84	0/2300
1	G	0.57	0/1777	0.78	0/2408
1	H	0.51	0/1681	0.83	3/2278 (0.1%)
2	C	0.69	2/10739 (0.0%)	0.86	7/14489 (0.0%)
2	I	0.57	0/10735	0.77	3/14484 (0.0%)
3	D	0.70	0/9200	0.90	12/12423 (0.1%)
3	J	0.64	0/9140	0.83	5/12341 (0.0%)
4	E	0.66	0/693	0.82	0/935
4	K	0.61	0/629	0.77	0/847
5	F	0.56	0/3864	0.81	3/5194 (0.1%)
5	L	0.52	0/3872	0.71	1/5205 (0.0%)
All	All	0.63	2/56551 (0.0%)	0.82	36/76325 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	3
5	F	0	2
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	949	GLU	CB-CG	6.52	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	838	CYS	CB-SG	-6.02	1.72	1.82

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	484	LEU	CA-CB-CG	9.03	136.06	115.30
2	C	796	LEU	CB-CG-CD2	-8.02	97.36	111.00
2	C	1161	LEU	CA-CB-CG	-7.43	98.22	115.30
3	D	268	LEU	CA-CB-CG	-7.05	99.09	115.30
2	C	544	GLY	N-CA-C	-6.83	96.01	113.10
2	C	1326	LEU	CB-CG-CD2	-6.73	99.55	111.00
2	C	145	ILE	CG1-CB-CG2	-6.52	97.05	111.40
5	F	608	ARG	NE-CZ-NH1	6.52	123.56	120.30
3	J	1221	LEU	CA-CB-CG	6.48	130.20	115.30
3	D	426	ALA	C-N-CD	6.45	141.95	128.40
1	H	65	LEU	CA-CB-CG	6.32	129.82	115.30
5	F	600	HIS	C-N-CD	6.26	141.54	128.40
3	J	217	LEU	CA-CB-CG	6.16	129.46	115.30
1	H	29	GLU	C-N-CD	-6.11	107.17	120.60
3	D	344	GLY	N-CA-C	-6.04	98.01	113.10
2	I	817	LEU	CA-CB-CG	5.95	128.99	115.30
1	H	13	LEU	CA-CB-CG	5.90	128.86	115.30
3	D	376	LEU	CA-CB-CG	-5.87	101.81	115.30
3	D	1243	LEU	CA-CB-CG	-5.81	101.94	115.30
3	D	217	LEU	CA-CB-CG	5.73	128.48	115.30
3	J	426	ALA	C-N-CD	5.65	140.27	128.40
1	A	318	LEU	CA-CB-CG	5.64	128.28	115.30
2	C	1151	LEU	CA-CB-CG	-5.63	102.34	115.30
2	C	1132	LEU	CA-CB-CG	5.54	128.03	115.30
3	D	1344	LEU	CA-CB-CG	-5.42	102.84	115.30
3	D	120	LEU	CA-CB-CG	5.38	127.67	115.30
3	D	123	ARG	CG-CD-NE	-5.23	100.83	111.80
2	I	1327	LEU	CA-CB-CG	-5.19	103.35	115.30
5	F	519	LEU	CB-CG-CD1	-5.18	102.20	111.00
3	J	857	LEU	CA-CB-CG	5.18	127.21	115.30
3	D	701	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	177	TYR	CA-CB-CG	5.09	123.08	113.40
3	D	239	LEU	CA-CB-CG	-5.09	103.59	115.30
3	J	268	LEU	CB-CG-CD2	-5.05	102.42	111.00
5	L	530	LEU	CA-CB-CG	5.04	126.89	115.30
3	D	515	ARG	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	600	HIS	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	853	THR	Peptide
3	J	901	ARG	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	2490	0	2542	129	0
1	B	1677	0	1703	75	0
1	G	1755	0	1773	96	0
1	H	1662	0	1687	79	0
2	C	10570	0	10582	460	0
2	I	10566	0	10576	403	1
3	D	9060	0	9209	451	1
3	J	9001	0	9168	412	0
4	E	691	0	695	24	0
4	K	627	0	634	27	0
5	F	3813	0	3880	150	0
5	L	3821	0	3884	163	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	55741	0	56333	2271	1

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 20.

All (2271) 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:190:ALA:HB2	1:G:200:LYS:HB2	1.42	1.01
1:A:296:GLY:H	1:A:299:SER:HB2	1.26	1.00
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.41	0.99
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.47	0.97
3:D:1183:SER:HA	3:J:206:ASN:HD21	1.29	0.96
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.32	0.95
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.29	0.94
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.31	0.94
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.49	0.94
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.33	0.93
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.50	0.92
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.52	0.92
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.50	0.92
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.36	0.90
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.55	0.89
1:G:12:ARG:H	1:G:30:PRO:HD2	1.38	0.88
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.55	0.87
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.56	0.87
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.10	0.87
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.56	0.87
2:I:148:GLN:NE2	2:I:535:PRO:O	2.08	0.87
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.54	0.86
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.23	0.86
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.09	0.86
1:A:45:ARG:HG2	1:B:38:THR:HB	1.55	0.85
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.57	0.85
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.58	0.85
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.56	0.85
2:C:1161:LEU:HD21	2:C:1165:SER:HB3	1.59	0.84
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.59	0.84
2:I:151:ARG:HH22	2:I:175:ARG:HD2	1.43	0.84
2:C:324:LYS:O	2:C:327:GLN:NE2	2.11	0.83
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.59	0.83
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.14	0.83
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.44	0.82
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.10	0.82
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.43	0.82
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.60	0.82
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.60	0.81
1:B:35:PHE:HA	1:B:38:THR:HG22	1.59	0.81
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.61	0.81
1:G:45:ARG:HG2	1:H:38:THR:HB	1.63	0.81
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.61	0.81
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.62	0.80
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.29	0.80
3:J:48:THR:O	3:J:50:LYS:N	2.13	0.80
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.17	0.79
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.79
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.17	0.79
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.65	0.79
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.65	0.79
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.17	0.78
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.66	0.78
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.65	0.78
3:D:48:THR:O	3:D:50:LYS:N	2.16	0.78
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.65	0.78
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.66	0.78
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.64	0.78
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.49	0.78
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.19	0.77
3:D:156:ARG:NH2	3:D:191:SER:OG	2.16	0.77
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.46	0.77
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.66	0.77
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.16	0.77
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.66	0.77
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.18	0.77
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.66	0.77
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.66	0.77
4:K:32:VAL:O	4:K:34:GLY:N	2.17	0.77
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.67	0.77
2:I:5:TYR:HD1	2:I:8:LYS:HD3	1.51	0.76
3:D:490:ILE:HD13	3:D:490:ILE:H	1.50	0.76
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.65	0.76
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.66	0.76
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.67	0.76
1:H:35:PHE:HA	1:H:38:THR:HG22	1.66	0.76
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.67	0.76
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.50	0.76
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.51	0.75
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.66	0.75
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.19	0.75
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.51	0.75
1:H:134:THR:HG23	1:H:135:ASP:H	1.50	0.75
3:D:418:GLU:HG3	4:E:45:LYS:H	1.52	0.75
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.69	0.75
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.68	0.75
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.67	0.75
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.50	0.74
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.70	0.74
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.21	0.74
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.70	0.74
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.87	0.74
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.68	0.74
2:I:170:VAL:HG21	2:I:172:TYR:CZ	2.23	0.74
2:I:30:ILE:HD12	2:I:30:ILE:H	1.52	0.74
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.15	0.74
3:D:252:LEU:HD23	3:D:262:THR:HB	1.70	0.74
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.69	0.74
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.69	0.73
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.70	0.73
2:C:890:LYS:NZ	2:C:891:GLY:O	2.17	0.73
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.69	0.73
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.69	0.73
2:I:560:PRO:O	3:J:780:ARG:NH2	2.21	0.73
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.70	0.73
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.70	0.73
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.68	0.73
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.70	0.73
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.52	0.73
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.88	0.73
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	1.70	0.73
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.68	0.73
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.71	0.73
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.02	0.73
4:E:32:VAL:O	4:E:34:GLY:N	2.22	0.73
3:J:700:ASN:O	3:J:704:GLU:HB2	1.88	0.72
3:J:797:THR:O	3:J:801:VAL:HG12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:NH1	1:A:198:LEU:O	2.22	0.72
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.71	0.72
3:D:495:ASN:O	3:D:497:GLU:N	2.21	0.72
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.71	0.72
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.22	0.72
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.71	0.72
5:L:244:THR:O	5:L:247:GLU:HG2	1.89	0.72
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.18	0.72
2:I:4:SER:OG	2:I:5:TYR:N	2.20	0.72
3:J:1290:ARG:HD2	3:J:1295:ASN:HD22	1.53	0.72
1:B:63:GLY:HA3	1:B:71:LYS:HE3	1.69	0.72
2:C:703:GLY:N	2:C:705:GLU:OE2	2.17	0.72
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.69	0.72
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.71	0.72
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.22	0.72
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.72	0.72
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.72	0.72
1:A:14:VAL:HG22	1:A:15:ASP:H	1.55	0.72
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.55	0.72
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.21	0.71
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.04	0.71
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.72	0.71
1:B:52:PRO:HG3	1:B:150:ARG:HG2	1.71	0.71
2:C:582:ASN:HB3	2:C:586:PHE:H	1.56	0.71
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.71	0.71
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.70	0.71
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.23	0.71
3:D:849:LEU:H	3:D:849:LEU:HD22	1.56	0.71
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.54	0.71
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.73	0.71
1:A:77:ASP:N	1:A:77:ASP:OD1	2.23	0.71
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.72	0.71
3:J:47:ARG:HH12	5:L:500:ILE:HD11	1.56	0.71
2:C:1131:MET:HE1	2:C:1141:LEU:HD12	1.73	0.71
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.25	0.71
2:I:324:LYS:O	2:I:327:GLN:NE2	2.24	0.71
3:D:317:THR:HG22	3:D:322:ARG:O	1.91	0.70
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.73	0.70
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.71	0.70
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.06	0.70
3:D:694:SER:OG	3:D:738:ARG:NE	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1013:GLN:O	2:I:1017:GLN:HG2	1.91	0.70
5:L:561:MET:HA	5:L:567:MET:HE1	1.73	0.70
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.72	0.70
3:D:1280:VAL:HG21	3:D:1304:ARG:NH2	2.05	0.70
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.74	0.70
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.74	0.70
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.74	0.69
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.23	0.69
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.75	0.69
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.74	0.69
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.73	0.69
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.22	0.69
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.74	0.69
2:C:566:GLY:O	2:C:569:ILE:HG13	1.92	0.69
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.74	0.69
3:D:1183:SER:HA	3:J:206:ASN:ND2	2.06	0.69
2:I:1124:ILE:O	2:I:1128:ILE:HG13	1.92	0.69
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.75	0.69
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.75	0.69
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.73	0.69
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.74	0.69
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.74	0.69
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.75	0.68
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.75	0.68
1:G:167:PRO:O	1:G:169:GLY:N	2.25	0.68
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.28	0.68
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.73	0.68
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.09	0.68
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.75	0.68
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.28	0.68
2:I:620:ASN:ND2	2:I:620:ASN:O	2.27	0.68
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.75	0.68
3:J:495:ASN:O	3:J:497:GLU:N	2.25	0.68
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.75	0.68
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.75	0.68
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.75	0.68
2:I:892:GLU:OE1	3:J:66:LYS:NZ	2.27	0.68
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.23	0.68
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.57	0.68
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.28	0.68
3:D:425:ARG:HG2	3:D:426:ALA:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.74	0.68
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.76	0.68
3:D:325:LYS:HE2	3:D:330:MET:HG3	1.74	0.68
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.56	0.68
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.73	0.68
2:I:138:ILE:O	2:I:139:ASN:ND2	2.27	0.68
2:I:347:ILE:HD11	2:I:433:ILE:HD11	1.74	0.68
1:B:191:ARG:NH2	3:D:410:ASP:OD2	2.25	0.67
3:J:709:ARG:O	3:J:711:GLY:N	2.26	0.67
1:B:102:LEU:O	1:B:141:SER:HA	1.93	0.67
2:C:201:ARG:NH2	2:C:370:MET:O	2.27	0.67
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	1.74	0.67
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.28	0.67
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.27	0.67
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.60	0.67
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.58	0.67
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.74	0.67
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.75	0.67
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.28	0.67
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.77	0.67
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.09	0.67
2:C:705:GLU:HB2	2:C:794:LEU:H	1.59	0.67
3:D:797:THR:O	3:D:801:VAL:HG12	1.95	0.67
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.67
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.59	0.67
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.77	0.67
2:I:963:GLU:O	2:I:967:LEU:HB2	1.95	0.66
3:D:708:ASN:N	3:D:708:ASN:OD1	2.23	0.66
5:F:532:LEU:O	5:F:536:THR:HG23	1.96	0.66
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.27	0.66
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.60	0.66
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.76	0.66
1:G:166:ARG:HH11	1:G:168:ILE:HG12	1.61	0.66
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.61	0.66
3:D:638:SER:OG	3:D:639:VAL:N	2.28	0.66
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.76	0.66
3:D:259:ARG:HG3	5:F:502:LYS:HD2	1.78	0.66
3:D:425:ARG:HG2	3:D:426:ALA:N	2.10	0.66
5:F:281:ARG:O	5:F:285:ARG:HG3	1.95	0.66
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.60	0.66
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.60	0.66
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.30	0.66
3:D:647:PRO:HD3	3:D:697:MET:HB3	1.78	0.66
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.77	0.66
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.29	0.66
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.77	0.66
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.77	0.66
3:J:1137:GLY:O	3:J:1140:ARG:HB3	1.96	0.65
5:L:573:LEU:H	5:L:573:LEU:HD23	1.59	0.65
2:C:1289:GLU:OE1	2:C:1294:LYS:HE2	1.95	0.65
3:D:1282:TYR:HD2	3:D:1286:LYS:HZ1	1.43	0.65
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.78	0.65
4:K:14:GLY:O	4:K:16:ARG:N	2.29	0.65
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.29	0.65
2:C:624:ASP:OD1	2:C:625:GLU:N	2.27	0.65
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.77	0.65
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.78	0.65
3:D:363:LEU:HG	3:D:363:LEU:O	1.96	0.65
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.32	0.65
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.20	0.65
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.79	0.65
3:D:515:ARG:O	3:D:545:HIS:HB3	1.97	0.65
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.17	0.65
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.78	0.65
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.31	0.65
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.29	0.65
3:D:56:LEU:HD12	3:D:56:LEU:H	1.60	0.65
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.65
1:A:227:GLN:HG3	1:B:39:LEU:HD11	1.79	0.65
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.61	0.65
2:C:617:ALA:HA	2:C:636:CYS:SG	2.37	0.65
2:I:705:GLU:HB2	2:I:794:LEU:H	1.62	0.65
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.76	0.65
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.28	0.65
3:D:504:GLN:HG3	3:D:505:ASP:H	1.61	0.65
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.78	0.65
1:G:9:LEU:O	1:H:227:GLN:NE2	2.30	0.65
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.77	0.65
3:J:632:ALA:O	3:J:635:SER:OG	2.15	0.64
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.79	0.64
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.78	0.64
1:A:92:VAL:O	1:A:148:ARG:NH1	2.22	0.64
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.79	0.64
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.79	0.64
4:K:40:PRO:O	4:K:52:ARG:NH2	2.30	0.64
3:D:88:CYS:O	3:D:90:VAL:N	2.30	0.64
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.80	0.64
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.79	0.64
2:C:726:TYR:HE2	2:C:728:ASP:HB2	1.63	0.64
3:D:1183:SER:CA	3:J:206:ASN:HD21	2.07	0.64
2:I:1247:SER:HB3	3:J:375:GLU:O	1.98	0.64
3:J:600:ALA:O	3:J:603:LYS:HG2	1.98	0.64
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.62	0.64
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.26	0.64
2:C:1243:MET:HA	3:D:353:SER:HB3	1.80	0.64
3:D:262:THR:OG1	3:D:263:SER:N	2.30	0.64
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.80	0.64
5:L:316:PHE:HZ	5:L:334:SER:HA	1.63	0.64
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.62	0.63
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.16	0.63
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.80	0.63
2:I:201:ARG:NH2	2:I:370:MET:O	2.30	0.63
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.63	0.63
1:G:97:GLU:OE2	1:G:145:LYS:HE2	1.99	0.63
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.63
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.79	0.63
1:B:35:PHE:HA	1:B:38:THR:CG2	2.28	0.63
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.81	0.63
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	1.80	0.63
2:I:655:VAL:N	2:I:659:GLN:OE1	2.32	0.63
2:C:197:ARG:NH1	2:C:201:ARG:O	2.32	0.63
2:C:250:THR:HA	2:C:268:ARG:HA	1.80	0.63
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.81	0.63
1:H:79:LEU:HA	1:H:82:LEU:HD12	1.80	0.63
1:A:51:MET:HE2	1:A:220:ALA:HB2	1.80	0.63
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.62	0.63
2:C:168:GLY:O	2:C:170:VAL:N	2.26	0.63
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.80	0.63
1:G:27:THR:HG23	1:G:202:VAL:HG22	1.81	0.63
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.80	0.63
2:I:250:THR:HA	2:I:268:ARG:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:392:THR:HG21	5:F:606:VAL:HA	1.81	0.63
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.81	0.63
1:A:12:ARG:H	1:A:30:PRO:HD2	1.64	0.62
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.80	0.62
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.27	0.62
2:C:744:GLY:C	2:C:746:ALA:H	2.02	0.62
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.34	0.62
1:A:241:GLU:HG3	1:A:242:VAL:H	1.65	0.62
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.80	0.62
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.13	0.62
1:G:229:GLU:HA	1:G:231:PHE:CZ	2.34	0.62
3:D:1281:GLU:O	3:D:1285:VAL:HG13	1.99	0.62
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.82	0.62
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.81	0.62
1:H:49:SER:O	1:H:151:GLY:HA2	1.99	0.62
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.33	0.62
2:I:169:LYS:O	2:I:170:VAL:HG22	2.00	0.62
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.81	0.62
5:F:354:THR:O	5:F:358:VAL:HG23	1.99	0.62
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.80	0.62
2:C:1032:LYS:O	2:C:1036:ILE:HG13	1.99	0.62
2:C:1149:TYR:CB	2:C:1159:VAL:HG21	2.30	0.62
3:J:848:VAL:HG21	3:J:880:VAL:HG22	1.82	0.62
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.81	0.62
3:D:598:LYS:O	3:D:601:ILE:HG22	1.99	0.62
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	1.81	0.62
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.81	0.61
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.30	0.61
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.15	0.61
2:C:886:LYS:H	2:C:917:SER:HB3	1.65	0.61
3:D:48:THR:C	3:D:50:LYS:H	2.03	0.61
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.82	0.61
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.65	0.61
4:E:62:GLN:O	4:E:66:VAL:HG23	2.00	0.61
2:I:975:ILE:O	2:I:979:LEU:HB2	2.01	0.61
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.81	0.61
2:C:521:LEU:O	2:C:525:THR:HB	2.01	0.61
3:D:395:LYS:HG2	5:F:536:THR:HG21	1.83	0.61
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.82	0.61
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.36	0.61
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.36	0.61
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.36	0.61
2:C:147:SER:OG	2:C:455:SER:HB3	2.01	0.61
3:D:697:MET:SD	3:D:741:ALA:HB3	2.40	0.61
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.83	0.61
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.82	0.61
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.35	0.61
1:A:59:VAL:HG22	1:A:144:ILE:HA	1.83	0.61
1:A:95:LYS:O	1:A:148:ARG:NH2	2.34	0.61
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.81	0.61
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.34	0.61
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.82	0.61
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.35	0.61
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.82	0.61
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.82	0.61
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.16	0.61
3:J:661:VAL:HG12	3:J:685:ILE:HD11	1.83	0.61
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.81	0.61
1:A:166:ARG:O	1:A:168:ILE:N	2.34	0.60
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.82	0.60
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.83	0.60
3:J:425:ARG:HG2	3:J:426:ALA:H	1.65	0.60
2:C:1164:PHE:O	2:C:1166:ASP:N	2.33	0.60
3:D:709:ARG:O	3:D:711:GLY:N	2.34	0.60
3:D:848:VAL:HG13	3:D:857:LEU:HB2	1.81	0.60
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.83	0.60
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.66	0.60
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	1.83	0.60
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.34	0.60
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.81	0.60
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.66	0.60
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.35	0.60
3:D:825:VAL:HG13	3:D:833:GLU:HB3	1.83	0.60
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.84	0.60
2:I:998:LEU:HD12	2:I:998:LEU:H	1.67	0.60
5:L:463:LEU:HA	5:L:466:ILE:HD12	1.83	0.60
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.64	0.60
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.36	0.60
5:F:348:GLU:HG2	5:F:354:THR:HA	1.84	0.60
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.84	0.60
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.83	0.60
5:L:469:GLN:O	5:L:473:GLU:HB2	2.02	0.60
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.32	0.60
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.82	0.60
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.84	0.60
3:D:43:THR:OG1	5:F:449:THR:O	2.12	0.60
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.01	0.60
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.84	0.60
2:I:582:ASN:HB3	2:I:586:PHE:H	1.66	0.60
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.82	0.60
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.66	0.60
1:A:135:ASP:O	1:A:137:ASN:N	2.35	0.60
1:B:48:LEU:HA	1:B:180:VAL:HG21	1.84	0.60
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.17	0.60
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.35	0.60
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.84	0.60
1:H:62:ASP:OD1	1:H:62:ASP:N	2.27	0.60
2:I:168:GLY:O	2:I:170:VAL:N	2.34	0.60
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.84	0.59
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.83	0.59
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.84	0.59
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.66	0.59
3:J:114:ILE:HD11	3:J:311:ARG:HB2	1.82	0.59
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.35	0.59
1:B:99:ILE:HD12	1:B:145:LYS:HB2	1.85	0.59
2:C:685:MET:HE1	2:C:1071:GLY:HA2	1.83	0.59
2:C:41:GLN:NE2	2:C:73:TYR:O	2.35	0.59
3:D:27:PRO:O	3:D:31:ARG:HG3	2.01	0.59
5:F:600:HIS:CG	5:F:601:PRO:HD3	2.37	0.59
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.12	0.59
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.84	0.59
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.17	0.59
1:A:61:ILE:HB	1:A:64:VAL:HG21	1.84	0.59
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.17	0.59
3:D:203:GLU:O	3:D:207:GLU:HG2	2.01	0.59
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.83	0.59
3:J:598:LYS:O	3:J:601:ILE:HG22	2.03	0.59
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.84	0.59
1:A:224:LEU:HD23	1:B:228:LEU:HD11	1.84	0.59
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.37	0.59
3:J:418:GLU:HG3	4:K:45:LYS:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.84	0.59
1:A:54:CYS:HA	1:A:148:ARG:HA	1.84	0.59
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.18	0.59
3:J:801:VAL:O	3:J:805:GLN:HB2	2.02	0.59
1:A:290:LEU:HB3	1:A:291:LYS:HE2	1.85	0.59
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.02	0.59
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.37	0.59
3:D:491:LEU:HD22	3:D:496:GLY:O	2.02	0.59
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.37	0.59
3:J:1290:ARG:HD2	3:J:1295:ASN:ND2	2.17	0.59
3:J:362:ARG:H	3:J:365:GLN:HE21	1.51	0.59
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.84	0.59
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.16	0.59
3:D:355:ILE:HG12	3:D:464:ASP:O	2.03	0.59
2:I:596:ASP:CG	2:I:597:GLY:H	2.06	0.59
5:L:281:ARG:O	5:L:285:ARG:HG3	2.02	0.59
5:L:312:SER:OG	5:L:313:ASP:N	2.34	0.59
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.84	0.58
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.84	0.58
1:A:169:GLY:O	1:A:171:LEU:HD22	2.03	0.58
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.85	0.58
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.03	0.58
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.85	0.58
5:F:462:LYS:HD2	5:F:487:MET:SD	2.43	0.58
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.37	0.58
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.30	0.58
3:D:709:ARG:HD2	3:D:710:ASP:H	1.68	0.58
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.84	0.58
1:G:161:SER:O	1:G:163:GLU:N	2.36	0.58
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.85	0.58
1:H:60:GLU:OE2	1:H:143:ARG:HB2	2.03	0.58
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.03	0.58
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.85	0.58
3:J:683:ILE:HD11	3:J:754:ILE:HD13	1.84	0.58
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.03	0.58
1:G:102:LEU:HD11	1:G:110:VAL:HG11	1.83	0.58
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.85	0.58
2:C:746:ALA:CB	2:C:974:ARG:HE	2.16	0.58
3:D:647:PRO:HG3	3:D:697:MET:CA	2.34	0.58
2:I:206:ALA:O	2:I:209:ILE:HG22	2.04	0.58
2:I:524:ILE:HD12	2:I:712:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:OD1	1:B:62:ASP:N	2.34	0.58
3:D:836:ARG:HD2	3:D:873:GLU:OE1	2.04	0.58
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.84	0.58
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.04	0.58
2:I:494:ASN:HB3	2:I:497:PRO:HG2	1.85	0.58
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	1.86	0.58
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.36	0.58
1:A:218:ARG:HG3	1:B:231:PHE:O	2.04	0.58
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.38	0.58
3:D:1282:TYR:O	3:D:1285:VAL:HG22	2.04	0.58
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.24	0.58
1:H:35:PHE:HA	1:H:38:THR:CG2	2.33	0.58
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.85	0.58
2:C:1211:ARG:HE	2:C:1220:GLN:NE2	2.01	0.58
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.87	0.58
2:C:796:LEU:H	2:C:796:LEU:HD12	1.67	0.58
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.86	0.58
3:D:510:LEU:O	3:D:514:THR:HG22	2.04	0.58
5:F:311:THR:HB	5:F:345:GLN:HG2	1.85	0.58
5:F:584:ARG:O	5:F:588:ARG:HG3	2.04	0.58
3:D:1264:ALA:O	3:D:1277:GLY:HA2	2.04	0.58
3:D:473:THR:HG23	3:D:476:ALA:H	1.69	0.58
3:D:1227:HIS:HB2	3:J:1293:GLU:OE1	2.03	0.58
5:L:296:LYS:HB2	5:L:329:LYS:HD3	1.86	0.58
1:A:7:GLU:HB3	1:B:150:ARG:HH12	1.69	0.57
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.86	0.57
3:D:854:ALA:HB1	3:J:1372:ARG:CZ	2.34	0.57
4:E:49:ILE:O	4:E:53:GLU:HG3	2.04	0.57
5:F:222:ALA:O	5:F:226:ALA:N	2.35	0.57
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.86	0.57
3:J:1168:GLU:OE2	3:J:1169:THR:OG1	2.21	0.57
3:J:1206:ARG:NH2	3:J:1223:LEU:O	2.37	0.57
1:G:92:VAL:HA	1:G:120:ASP:O	2.03	0.57
1:H:101:THR:H	1:H:116:THR:HG22	1.69	0.57
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.38	0.57
5:F:267:ASP:O	5:F:271:ASN:N	2.32	0.57
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.86	0.57
3:J:197:GLU:O	3:J:201:LEU:HG	2.05	0.57
3:J:473:THR:HG23	3:J:476:ALA:H	1.70	0.57
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.86	0.57
2:I:490:GLN:HG3	5:L:472:GLN:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.85	0.57
2:I:1063:GLY:O	3:J:354:VAL:HG11	2.03	0.57
3:J:809:VAL:HA	3:J:894:VAL:O	2.04	0.57
1:A:118:ASP:H	1:A:121:VAL:HB	1.68	0.57
2:I:1106:ARG:O	2:I:1108:ASN:N	2.36	0.57
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.05	0.57
1:A:318:LEU:O	1:A:320:ASN:N	2.34	0.57
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.25	0.57
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.21	0.57
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.19	0.57
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.39	0.57
3:J:69:GLU:HG3	3:J:76:LYS:HG2	1.85	0.57
3:J:902:ASP:OD1	3:J:903:LEU:N	2.38	0.57
3:D:227:PHE:O	3:D:230:SER:HB3	2.03	0.57
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.86	0.57
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.04	0.57
2:I:170:VAL:HG21	2:I:172:TYR:OH	2.04	0.57
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.86	0.57
2:C:953:LEU:HD13	2:C:1036:ILE:HD12	1.87	0.57
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.40	0.57
5:F:612:ASP:OD1	5:F:612:ASP:N	2.36	0.57
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.86	0.57
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.40	0.57
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.39	0.57
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.86	0.57
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.04	0.57
2:C:748:ILE:HD11	2:C:966:ILE:HG22	1.85	0.57
5:F:343:LYS:H	5:F:343:LYS:HD2	1.70	0.57
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.86	0.57
2:I:1075:VAL:HG21	3:J:463:GLY:HA2	1.87	0.57
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.85	0.57
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.05	0.57
2:C:615:VAL:HG13	2:C:651:ASP:H	1.70	0.57
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.87	0.57
3:D:678:ARG:O	3:D:682:VAL:HG23	2.04	0.57
5:F:261:LEU:H	5:F:261:LEU:HD12	1.70	0.57
2:I:1263:ALA:O	2:I:1265:PHE:HD1	1.88	0.57
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.86	0.57
3:J:1203:ARG:NH2	3:J:1205:GLU:HG2	2.19	0.57
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.87	0.57
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:908:ILE:HG12	3:J:909:ILE:N	2.20	0.57
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.87	0.56
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.87	0.56
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.05	0.56
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.70	0.56
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.86	0.56
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.87	0.56
3:D:11:GLN:HG2	3:D:15:GLU:CG	2.35	0.56
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.35	0.56
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.24	0.56
1:G:75:GLN:HA	2:I:729:ALA:N	2.19	0.56
2:I:1116:HIS:HE1	3:J:641:ILE:N	1.96	0.56
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.37	0.56
3:J:16:GLU:HG3	3:J:17:PHE:H	1.69	0.56
5:L:465:ARG:HB3	5:L:468:ARG:HH12	1.70	0.56
2:C:246:LEU:HB2	2:C:269:ILE:HG21	1.86	0.56
3:D:1285:VAL:HG23	3:D:1286:LYS:HG3	1.85	0.56
1:G:13:LEU:H	1:G:13:LEU:HD23	1.69	0.56
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.87	0.56
5:L:612:ASP:OD1	5:L:612:ASP:N	2.33	0.56
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.20	0.56
2:C:1274:GLU:O	2:C:1277:ALA:HB3	2.06	0.56
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.88	0.56
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.41	0.56
3:D:549:LYS:HD3	3:D:569:LEU:HD23	1.87	0.56
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.88	0.56
5:F:226:ALA:O	5:F:229:VAL:HG22	2.06	0.56
1:G:76:GLU:OE1	1:G:132:HIS:N	2.32	0.56
2:I:1131:MET:HB3	2:I:1141:LEU:HD11	1.88	0.56
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.88	0.56
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.05	0.56
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.86	0.56
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.40	0.56
5:L:470:MET:O	5:L:478:PRO:HD3	2.05	0.56
2:C:1160:ASP:HB2	2:C:1161:LEU:HD12	1.87	0.56
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.40	0.56
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.88	0.56
2:I:601:ASP:OD1	2:I:601:ASP:N	2.37	0.56
3:J:70:CYS:SG	3:J:90:VAL:HB	2.46	0.56
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.20	0.56
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.39	0.56
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.88	0.56
5:L:245:ALA:O	5:L:249:ILE:HG13	2.05	0.56
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.88	0.56
2:C:325:LEU:O	2:C:330:HIS:HB2	2.05	0.56
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.86	0.56
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.88	0.56
2:I:1017:GLN:O	2:I:1021:LEU:HG	2.05	0.56
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.06	0.56
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.36	0.56
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.87	0.56
5:F:127:ILE:O	5:F:130:VAL:HG22	2.05	0.56
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.87	0.56
2:I:672:GLU:HB3	2:I:1187:PHE:HD2	1.70	0.56
2:I:499:SER:O	2:I:503:LYS:HB2	2.06	0.56
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.88	0.56
3:J:277:ASN:HA	3:J:280:LYS:HG3	1.88	0.56
5:L:455:HIS:O	5:L:459:THR:OG1	2.16	0.56
1:A:137:ASN:OD1	1:A:137:ASN:N	2.39	0.56
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.71	0.56
2:C:499:SER:O	2:C:503:LYS:HB2	2.06	0.56
3:D:770:LEU:H	3:D:770:LEU:HD22	1.70	0.56
3:D:825:VAL:HG22	3:D:833:GLU:H	1.71	0.56
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.87	0.56
2:I:1253:LEU:HD11	3:J:253:VAL:HG11	1.87	0.56
3:J:1168:GLU:OE1	3:J:1173:ARG:HG3	2.06	0.56
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.20	0.56
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.38	0.56
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.87	0.56
3:J:903:LEU:HD21	3:J:913:GLU:OE1	2.06	0.56
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.87	0.56
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.86	0.56
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.88	0.56
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.88	0.56
5:L:515:GLU:HG2	5:L:516:ASP:N	2.21	0.56
1:A:300:LEU:HD13	1:A:304:LYS:HE2	1.87	0.56
2:C:138:ILE:O	2:C:139:ASN:ND2	2.39	0.56
3:D:103:GLY:C	3:D:244:VAL:HG22	2.27	0.56
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.71	0.56
3:D:709:ARG:HD2	3:D:710:ASP:N	2.21	0.56
1:A:268:ASN:O	1:A:271:LYS:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.21	0.55
3:D:81:ARG:C	3:D:83:VAL:H	2.09	0.55
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.88	0.55
2:I:941:LYS:HD3	2:I:949:GLU:OE1	2.06	0.55
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.87	0.55
3:D:322:ARG:HB2	3:D:322:ARG:NH1	2.21	0.55
3:J:770:LEU:HD22	3:J:770:LEU:H	1.71	0.55
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.22	0.55
5:F:147:GLN:O	5:F:151:VAL:HG23	2.07	0.55
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.88	0.55
2:I:499:SER:HA	2:I:502:VAL:HG12	1.88	0.55
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.41	0.55
1:A:159:ILE:HG13	1:A:162:GLU:HG3	1.88	0.55
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.41	0.55
2:C:778:GLU:O	2:C:781:ASP:HB2	2.06	0.55
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.71	0.55
3:J:245:LEU:O	3:J:250:ARG:NE	2.37	0.55
3:J:836:ARG:HD2	3:J:873:GLU:OE1	2.07	0.55
1:A:115:ILE:HG22	1:A:116:THR:H	1.70	0.55
2:C:61:SER:O	2:C:63:SER:N	2.38	0.55
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.88	0.55
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.42	0.55
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.22	0.55
5:L:476:ARG:HH11	5:L:476:ARG:HB3	1.71	0.55
1:A:226:GLU:HB3	1:B:10:LYS:HE2	1.89	0.55
2:C:149:LEU:HD12	2:C:452:ARG:O	2.07	0.55
2:C:452:ARG:HH12	2:C:585:GLY:HA3	1.71	0.55
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.37	0.55
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.88	0.55
5:F:575:GLU:O	5:F:579:GLN:HG2	2.07	0.55
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.88	0.55
2:C:541:GLU:OE1	2:C:541:GLU:N	2.39	0.55
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.87	0.55
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.07	0.55
2:I:1072:ASN:N	2:I:1072:ASN:OD1	2.40	0.55
2:I:168:GLY:C	2:I:170:VAL:H	2.10	0.55
1:A:14:VAL:HG22	1:A:15:ASP:N	2.23	0.55
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.87	0.55
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.88	0.55
1:G:159:ILE:HG13	1:G:162:GLU:HG3	1.89	0.55
3:J:251:PRO:HB2	3:J:253:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:56:LEU:H	3:J:56:LEU:HD12	1.71	0.55
3:J:515:ARG:NH2	3:J:718:SER:O	2.27	0.55
3:J:793:SER:O	3:J:797:THR:HG23	2.07	0.55
5:L:474:MET:C	5:L:476:ARG:H	2.11	0.55
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.89	0.54
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.88	0.54
2:C:228:VAL:HG22	2:C:245:ARG:HE	1.72	0.54
4:E:58:LEU:H	4:E:58:LEU:HD12	1.71	0.54
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.12	0.54
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.88	0.54
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.88	0.54
5:L:347:ILE:HB	5:L:355:ILE:HD11	1.88	0.54
2:C:1255:THR:O	2:C:1257:GLN:N	2.40	0.54
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.88	0.54
5:F:245:ALA:O	5:F:249:ILE:HG13	2.07	0.54
1:H:101:THR:H	1:H:116:THR:CG2	2.21	0.54
1:H:27:THR:HB	1:H:202:VAL:HG22	1.87	0.54
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.89	0.54
1:A:112:ALA:O	1:A:115:ILE:HG13	2.07	0.54
1:B:192:VAL:O	1:B:194:GLN:N	2.41	0.54
2:C:1066:MET:HG2	2:C:1234:LYS:HA	1.90	0.54
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.72	0.54
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.42	0.54
3:J:436:ALA:HB3	3:J:485:MET:HA	1.89	0.54
5:L:601:PRO:HA	5:L:604:SER:HB3	1.88	0.54
1:A:297:LYS:O	1:A:301:THR:OG1	2.14	0.54
3:D:1344:LEU:O	3:D:1346:GLY:N	2.36	0.54
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.73	0.54
2:I:637:ARG:HA	2:I:642:SER:HA	1.88	0.54
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.89	0.54
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.07	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.71	0.54
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.37	0.54
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.07	0.54
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.73	0.54
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.07	0.54
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.90	0.54
2:C:607:SER:OG	2:C:609:ILE:HG13	2.06	0.54
5:F:392:LYS:O	5:F:395:THR:HG23	2.06	0.54
2:C:211:ARG:NH1	2:C:357:ASN:O	2.41	0.54
2:C:980:VAL:O	2:C:984:VAL:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1361:THR:HG22	4:E:21:LEU:HD22	1.90	0.54
3:J:128:LEU:HA	3:J:192:MET:HE1	1.88	0.54
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.90	0.54
2:C:1207:SER:HB2	2:C:1209:GLN:H	1.72	0.54
2:C:730:SER:O	2:C:753:LEU:HB2	2.08	0.54
3:D:1372:ARG:O	3:D:1375:ALA:HB3	2.08	0.54
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.89	0.54
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.73	0.54
1:H:59:VAL:HG23	1:H:173:VAL:HG21	1.89	0.54
2:I:149:LEU:HD12	2:I:452:ARG:O	2.08	0.54
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.90	0.54
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.23	0.54
3:J:514:THR:O	3:J:514:THR:OG1	2.17	0.54
3:D:1376:GLY:O	3:J:852:GLY:HA2	2.08	0.54
2:C:466:VAL:O	2:C:470:ARG:HG2	2.06	0.54
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.89	0.54
1:G:107:ILE:HG12	1:G:135:ASP:O	2.08	0.54
2:C:367:TYR:HA	2:C:384:LEU:HD22	1.90	0.54
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.89	0.54
2:C:998:LEU:HD12	2:C:998:LEU:H	1.73	0.54
3:D:197:GLU:O	3:D:201:LEU:HG	2.07	0.54
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.88	0.54
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.90	0.54
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.90	0.54
2:C:297:VAL:HG12	2:C:315:MET:O	2.09	0.53
3:J:478:LEU:HG	4:K:47:THR:HG23	1.89	0.53
5:L:476:ARG:HD2	5:L:477:GLU:HG2	1.89	0.53
1:A:115:ILE:HG22	1:A:116:THR:N	2.23	0.53
2:C:242:VAL:HG12	2:C:244:GLU:H	1.74	0.53
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.43	0.53
5:F:377:LYS:O	5:F:381:GLU:HG3	2.08	0.53
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.73	0.53
2:I:577:VAL:HG23	2:I:661:VAL:O	2.08	0.53
5:L:127:ILE:O	5:L:130:VAL:HG22	2.08	0.53
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	1.91	0.53
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.39	0.53
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.53
2:C:738:GLU:HA	2:C:741:MET:HE2	1.90	0.53
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.90	0.53
3:D:336:GLY:HA3	3:D:1324:SER:O	2.08	0.53
4:E:15:ASN:HB3	4:E:18:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:882:ILE:H	2:C:882:ILE:HD12	1.73	0.53
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.89	0.53
3:D:1280:VAL:CG2	3:D:1304:ARG:HH21	2.11	0.53
5:F:469:GLN:O	5:F:473:GLU:HB2	2.08	0.53
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.91	0.53
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.43	0.53
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.43	0.53
1:A:7:GLU:HB3	1:B:150:ARG:NH1	2.22	0.53
1:A:92:VAL:HG11	1:A:98:VAL:HG11	1.91	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.73	0.53
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.73	0.53
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.74	0.53
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.89	0.53
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.44	0.53
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.74	0.53
3:D:1266:ILE:HD11	3:D:1276:GLU:HB3	1.91	0.53
3:D:128:LEU:HA	3:D:192:MET:HE1	1.90	0.53
1:H:102:LEU:O	1:H:141:SER:HA	2.09	0.53
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.90	0.53
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.09	0.53
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.74	0.53
1:B:81:ILE:O	1:B:85:LEU:HG	2.09	0.53
2:C:1107:MET:HG2	3:D:740:LEU:HD11	1.90	0.53
2:C:198:ILE:O	2:C:201:ARG:HB2	2.09	0.53
1:A:134:THR:HG21	2:C:727:VAL:O	2.09	0.53
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.89	0.53
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.74	0.53
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.72	0.53
5:F:225:ARG:O	5:F:229:VAL:HG13	2.09	0.53
5:F:228:TYR:CE2	5:F:232:ARG:HD3	2.44	0.53
3:J:358:GLY:N	3:J:359:PRO:HD3	2.24	0.53
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.90	0.53
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.90	0.53
2:C:202:ARG:HH12	2:C:368:ARG:HH22	1.56	0.53
3:D:266:ASN:O	3:D:270:ARG:HB2	2.09	0.53
3:D:647:PRO:CG	3:D:697:MET:HB3	2.38	0.53
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.74	0.53
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.91	0.53
2:I:724:VAL:HG23	2:I:775:GLU:H	1.74	0.53
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.39	0.53
1:A:296:GLY:N	1:A:299:SER:HB2	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1270:GLY:HA3	3:D:1297:LYS:O	2.09	0.53
5:F:312:SER:OG	5:F:313:ASP:N	2.42	0.53
1:A:251:PRO:HD2	5:F:605:GLU:HG3	1.91	0.53
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.89	0.53
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.74	0.53
2:I:310:ILE:HD13	2:I:325:LEU:HB3	1.91	0.53
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.74	0.53
3:J:425:ARG:HG2	3:J:426:ALA:N	2.24	0.53
3:J:697:MET:SD	3:J:741:ALA:HB3	2.49	0.53
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.28	0.53
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.91	0.52
3:D:398:LYS:HE2	5:F:532:LEU:CD2	2.39	0.52
3:D:787:ALA:O	3:D:790:THR:HB	2.09	0.52
1:G:12:ARG:H	1:G:30:PRO:CD	2.14	0.52
1:G:14:VAL:HG13	1:G:15:ASP:H	1.74	0.52
4:K:50:ALA:O	4:K:54:ILE:HG12	2.09	0.52
1:B:76:GLU:OE2	1:B:132:HIS:N	2.40	0.52
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.73	0.52
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.91	0.52
2:I:37:LYS:HD2	2:I:46:GLN:HE21	1.74	0.52
3:J:525:MET:O	3:J:548:VAL:HG13	2.09	0.52
3:J:825:VAL:C	3:J:826:ILE:HG13	2.28	0.52
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.73	0.52
2:C:746:ALA:HB2	2:C:974:ARG:HE	1.72	0.52
3:D:885:VAL:HG12	3:D:894:VAL:CG1	2.40	0.52
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.90	0.52
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.16	0.52
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.40	0.52
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.41	0.52
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.42	0.52
3:D:79:LYS:HB2	5:F:568:ASN:OD1	2.09	0.52
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.44	0.52
3:J:697:MET:HG3	3:J:698:MET:N	2.24	0.52
5:L:395:THR:OG1	5:L:396:ASN:N	2.42	0.52
1:A:47:LEU:O	1:A:180:VAL:HG21	2.10	0.52
1:A:190:ALA:H	1:A:199:ASP:HA	1.74	0.52
2:C:169:LYS:O	2:C:170:VAL:HG22	2.09	0.52
2:C:620:ASN:O	2:C:620:ASN:ND2	2.43	0.52
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.92	0.52
3:D:81:ARG:HG3	3:D:82:GLY:H	1.74	0.52
1:H:65:LEU:HD13	1:H:171:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.91	0.52
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.09	0.52
2:C:928:VAL:HG22	2:C:1054:LEU:HD11	1.91	0.52
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.45	0.52
2:I:607:SER:N	2:I:610:GLU:HB2	2.25	0.52
2:I:617:ALA:HA	2:I:636:CYS:SG	2.50	0.52
2:I:726:TYR:CE2	2:I:728:ASP:HB2	2.45	0.52
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.10	0.52
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.24	0.52
3:D:356:THR:OG1	3:D:357:VAL:N	2.43	0.52
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.45	0.52
2:I:384:LEU:O	2:I:388:LEU:HG	2.10	0.52
2:I:96:LEU:HD23	2:I:124:MET:HG3	1.92	0.52
3:J:366:CYS:HB3	3:J:437:PHE:CD1	2.44	0.52
5:L:343:LYS:O	5:L:347:ILE:HG13	2.10	0.52
2:C:453:ILE:HD12	2:C:587:LEU:HG	1.92	0.52
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.92	0.52
5:F:267:ASP:HA	5:F:270:VAL:HB	1.92	0.52
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.90	0.52
5:F:117:ILE:HA	5:F:120:ALA:HB3	1.92	0.52
5:F:299:LYS:O	5:F:303:ILE:HG12	2.10	0.52
5:F:311:THR:HG21	5:F:348:GLU:CD	2.30	0.52
3:J:220:ARG:O	3:J:223:LEU:HB3	2.10	0.52
3:J:517:CYS:HB3	3:J:719:PHE:CE2	2.45	0.52
1:A:31:LEU:HB2	1:A:199:ASP:O	2.10	0.51
2:C:345:PRO:O	2:C:349:GLU:HG2	2.10	0.51
3:D:707:ILE:H	3:D:707:ILE:HD12	1.75	0.51
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.92	0.51
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.10	0.51
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.38	0.51
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.46	0.51
2:I:896:THR:HB	2:I:897:PRO:HD2	1.92	0.51
2:C:1106:ARG:HD2	2:C:1106:ARG:H	1.75	0.51
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.93	0.51
2:C:903:ARG:HE	2:C:910:ALA:HB2	1.75	0.51
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.92	0.51
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.75	0.51
3:J:311:ARG:O	3:J:312:ARG:HD3	2.09	0.51
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.46	0.51
3:J:432:LEU:HD21	3:J:489:ASN:HB3	1.92	0.51
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.40	0.51
2:C:122:VAL:HG11	2:C:493:ILE:HG21	1.93	0.51
2:C:198:ILE:HD13	2:C:388:LEU:HD13	1.91	0.51
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.40	0.51
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.92	0.51
3:D:825:VAL:C	3:D:826:ILE:HG13	2.30	0.51
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.91	0.51
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.75	0.51
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.75	0.51
3:J:549:LYS:HD3	3:J:569:LEU:HD23	1.91	0.51
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.93	0.51
5:L:226:ALA:O	5:L:229:VAL:HG22	2.10	0.51
2:C:105:TYR:HD1	2:C:112:GLY:H	1.58	0.51
2:C:1211:ARG:HE	2:C:1220:GLN:HE21	1.59	0.51
5:F:453:PRO:O	5:F:456:MET:HB2	2.10	0.51
2:I:151:ARG:NH2	2:I:177:ILE:HD11	2.26	0.51
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.10	0.51
4:K:3:ARG:HA	4:K:3:ARG:NE	2.25	0.51
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.92	0.51
3:D:1177:ILE:HG13	3:D:1186:TYR:HB3	1.93	0.51
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.92	0.51
5:F:585:GLU:HA	5:F:588:ARG:HD3	1.92	0.51
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.93	0.51
3:J:363:LEU:HG	3:J:363:LEU:O	2.11	0.51
3:J:594:GLN:HG3	3:J:596:LEU:HD22	1.92	0.51
3:J:903:LEU:HB3	3:J:905:ARG:H	1.74	0.51
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.40	0.51
3:D:252:LEU:CD2	3:D:262:THR:HB	2.38	0.51
2:I:1131:MET:HB3	2:I:1141:LEU:CD1	2.40	0.51
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.73	0.51
2:I:739:ASP:N	2:I:739:ASP:OD1	2.40	0.51
1:G:77:ASP:OD2	2:I:755:LYS:NZ	2.44	0.51
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.76	0.51
3:J:850:LYS:HB2	3:J:852:GLY:O	2.11	0.51
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.91	0.51
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.26	0.51
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.93	0.51
3:D:80:HIS:CB	3:D:83:VAL:HG11	2.38	0.51
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.93	0.51
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.41	0.51
2:I:810:TYR:HE2	3:J:359:PRO:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.51	0.51
1:A:285:THR:OG1	1:A:287:VAL:HG23	2.10	0.51
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.92	0.51
3:D:500:ILE:O	3:D:500:ILE:HG22	2.11	0.51
3:D:54:ASP:N	3:D:54:ASP:OD1	2.43	0.51
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.51
5:F:561:MET:HA	5:F:567:MET:HE1	1.93	0.51
2:I:5:TYR:O	2:I:8:LYS:HG2	2.10	0.51
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.93	0.51
2:C:13:LYS:HD3	2:C:1149:TYR:HA	1.93	0.51
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.92	0.51
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.93	0.51
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.92	0.51
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.93	0.51
3:J:1167:LYS:CE	3:J:1174:ARG:HD2	2.39	0.51
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.76	0.51
1:A:285:THR:OG1	1:A:286:GLU:N	2.44	0.50
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.46	0.50
2:C:169:LYS:HE2	2:C:190:PRO:O	2.11	0.50
2:C:961:SER:O	2:C:965:GLN:HG3	2.10	0.50
3:D:647:PRO:CD	3:D:697:MET:HB3	2.40	0.50
3:D:72:CYS:SG	3:D:73:GLY:N	2.84	0.50
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.92	0.50
2:I:125:GLY:CA	2:I:499:SER:HB2	2.38	0.50
2:C:1124:ILE:HG21	2:C:1180:MET:CE	2.41	0.50
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.93	0.50
3:D:226:ALA:O	3:D:230:SER:N	2.42	0.50
2:I:1210:ILE:HD11	2:I:1227:VAL:HG21	1.91	0.50
4:K:15:ASN:C	4:K:17:PHE:H	2.15	0.50
1:A:156:SER:HB3	2:C:1059:ARG:NH2	2.26	0.50
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.25	0.50
3:D:69:GLU:HG3	3:D:76:LYS:HG2	1.93	0.50
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.93	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.93	0.50
1:G:91:ARG:HB3	1:G:122:GLU:HB3	1.93	0.50
1:H:64:VAL:HG12	1:H:66:HIS:H	1.77	0.50
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.92	0.50
3:J:223:LEU:O	3:J:226:ALA:HB3	2.11	0.50
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.26	0.50
5:F:487:MET:HA	5:F:487:MET:CE	2.41	0.50
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:15:ASN:HB3	4:K:18:ASP:H	1.76	0.50
5:L:141:ILE:HD13	5:L:256:PHE:CD1	2.46	0.50
1:A:228:LEU:HD21	1:B:43:LEU:HD11	1.94	0.50
2:C:1106:ARG:O	2:C:1108:ASN:N	2.42	0.50
2:C:719:LYS:O	2:C:779:ARG:HG3	2.12	0.50
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.77	0.50
5:F:147:GLN:HE22	5:F:150:ARG:HH11	1.58	0.50
5:F:354:THR:OG1	5:F:356:GLU:HB3	2.11	0.50
1:G:125:LYS:HG3	1:G:128:HIS:HB2	1.94	0.50
2:C:1282:GLY:O	2:C:1284:ALA:N	2.44	0.50
3:D:75:TYR:HB3	3:D:80:HIS:HD2	1.76	0.50
2:I:1286:THR:O	2:I:1290:MET:HB2	2.11	0.50
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.77	0.50
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.93	0.50
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.10	0.50
3:J:515:ARG:O	3:J:545:HIS:HB3	2.12	0.50
5:L:483:LEU:H	5:L:483:LEU:HD12	1.76	0.50
1:B:76:GLU:HB3	1:B:80:GLU:HG2	1.93	0.50
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.41	0.50
1:G:103:ASN:OD1	1:G:141:SER:HB2	2.12	0.50
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.94	0.50
3:J:647:PRO:HG3	3:J:697:MET:CA	2.42	0.50
5:L:414:LYS:HD3	5:L:434:TRP:HZ3	1.76	0.50
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.93	0.50
2:C:408:SER:O	2:C:431:LYS:NZ	2.45	0.50
2:C:494:ASN:O	2:C:498:ILE:HD13	2.12	0.50
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.29	0.50
5:F:320:ILE:HG23	5:F:327:SER:O	2.11	0.50
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.92	0.50
2:I:757:THR:O	2:I:765:ILE:HG23	2.12	0.50
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.94	0.50
3:J:844:THR:OG1	3:J:860:ARG:O	2.21	0.50
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.94	0.50
2:C:1269:ARG:HD3	3:D:343:LEU:HD23	1.94	0.50
2:C:92:TYR:CD2	2:C:129:LEU:HB2	2.47	0.50
2:C:796:LEU:HD12	2:C:796:LEU:N	2.25	0.50
2:C:799:ASN:HB3	2:C:1231:TYR:HA	1.93	0.50
2:C:876:GLU:HG2	2:C:927:THR:OG1	2.12	0.50
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.47	0.50
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.94	0.50
3:D:224:LEU:O	3:D:227:PHE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.93	0.50
1:G:45:ARG:NH2	1:H:37:HIS:HB3	2.26	0.50
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.94	0.50
2:I:553:THR:O	2:I:557:ARG:HD2	2.12	0.50
3:J:849:LEU:H	3:J:849:LEU:HD22	1.77	0.50
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.46	0.50
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.94	0.49
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.94	0.49
3:D:141:PHE:CD1	3:D:180:MET:HG3	2.39	0.49
5:F:106:GLY:HA2	5:F:385:ARG:HH22	1.77	0.49
1:H:51:MET:HB3	1:H:178:SER:HB2	1.94	0.49
2:I:465:ARG:O	2:I:469:VAL:HG13	2.12	0.49
2:I:466:VAL:O	2:I:469:VAL:HG22	2.12	0.49
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.93	0.49
3:J:266:ASN:O	3:J:270:ARG:HB2	2.12	0.49
5:L:287:ILE:HD13	5:L:315:TRP:CH2	2.47	0.49
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.27	0.49
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.27	0.49
2:C:119:GLU:HG3	2:C:489:PRO:HD2	1.94	0.49
2:C:131:THR:HB	2:C:133:ASN:H	1.77	0.49
2:C:540:ARG:HH11	2:C:540:ARG:HB2	1.77	0.49
2:C:5:TYR:O	2:C:8:LYS:HG2	2.11	0.49
3:D:144:TYR:HE2	3:D:162:GLU:HG2	1.77	0.49
3:D:347:VAL:HG12	3:D:348:ASP:O	2.11	0.49
3:D:60:ARG:HA	3:D:89:GLY:O	2.12	0.49
4:E:8:ASP:HB2	4:E:55:GLU:OE2	2.13	0.49
1:G:23:HIS:HB2	1:G:205:MET:O	2.12	0.49
1:A:195:ARG:HE	1:A:198:LEU:HD21	1.76	0.49
1:B:33:ARG:NH2	2:C:820:GLU:OE2	2.45	0.49
2:C:4:SER:OG	2:C:5:TYR:N	2.45	0.49
2:C:600:THR:HG22	2:C:601:ASP:H	1.77	0.49
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.41	0.49
1:H:11:PRO:O	1:H:12:ARG:HG3	2.13	0.49
2:I:1299:ASN:ND2	2:I:1303:LYS:HE2	2.27	0.49
5:L:134:VAL:HA	5:L:273:MET:CE	2.42	0.49
5:L:165:PHE:HD1	5:L:259:PHE:HA	1.77	0.49
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.94	0.49
3:D:749:LYS:HB2	3:D:750:PRO:CD	2.42	0.49
5:F:513:ASP:C	5:F:515:GLU:H	2.14	0.49
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.94	0.49
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.34	0.49
2:I:490:GLN:CG	5:L:472:GLN:HG3	2.42	0.49
5:L:515:GLU:HG2	5:L:516:ASP:H	1.77	0.49
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.95	0.49
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.46	0.49
2:I:32:LEU:HD23	2:I:130:MET:SD	2.52	0.49
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.95	0.49
2:I:9:LYS:HD2	2:I:791:LEU:HD21	1.93	0.49
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.95	0.49
3:J:647:PRO:HG3	3:J:697:MET:N	2.27	0.49
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.93	0.49
2:C:800:MET:HE1	2:C:822:VAL:HG13	1.95	0.49
3:D:1170:LYS:C	3:D:1172:LYS:H	2.15	0.49
3:D:218:THR:HA	3:D:221:ILE:HG22	1.94	0.49
3:D:825:VAL:HG22	3:D:833:GLU:N	2.26	0.49
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.12	0.49
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.95	0.49
2:I:117:ILE:HD12	2:I:488:MET:CG	2.43	0.49
2:I:143:ARG:NH2	2:I:512:SER:O	2.46	0.49
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.95	0.49
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.27	0.49
1:A:253:LEU:HA	1:A:278:ILE:HD11	1.93	0.49
1:A:7:GLU:O	1:B:150:ARG:NH1	2.45	0.49
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.48	0.49
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.27	0.49
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.95	0.49
2:I:1124:ILE:HG21	2:I:1180:MET:HE2	1.95	0.49
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.48	0.49
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.16	0.49
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.95	0.49
2:C:298:ALA:N	2:C:334:GLU:O	2.37	0.49
3:D:647:PRO:HG3	3:D:697:MET:CB	2.42	0.49
1:G:91:ARG:NH2	1:G:122:GLU:OE2	2.46	0.49
1:G:88:LEU:HD12	1:G:89:ALA:H	1.78	0.49
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.43	0.49
2:I:468:LEU:O	2:I:471:VAL:HG12	2.12	0.49
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.95	0.49
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.94	0.49
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.94	0.49
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.93	0.49
5:L:281:ARG:HG3	5:L:285:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.28	0.49
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.95	0.49
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.95	0.49
3:J:156:ARG:NH1	3:J:157:GLN:HE21	2.11	0.49
3:J:918:ILE:O	3:J:922:SER:OG	2.29	0.49
1:A:12:ARG:H	1:A:30:PRO:CD	2.25	0.49
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.94	0.49
2:C:93:SER:OG	2:C:126:GLU:OE1	2.19	0.49
2:C:619:ALA:HB1	2:C:657:THR:HA	1.95	0.49
2:C:79:VAL:HG23	2:C:80:PHE:H	1.78	0.49
2:C:836:LEU:HD12	2:C:836:LEU:N	2.27	0.49
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.27	0.49
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.47	0.49
5:F:363:ARG:O	5:F:367:ILE:HG13	2.12	0.49
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.95	0.49
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.77	0.49
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.94	0.49
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.95	0.49
5:L:148:TYR:OH	5:L:218:ARG:HA	2.13	0.49
1:A:224:LEU:O	1:A:228:LEU:HD12	2.12	0.48
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.94	0.48
2:C:323:ALA:O	2:C:327:GLN:HG3	2.12	0.48
2:C:209:ILE:HD13	2:C:425:ILE:HG21	1.93	0.48
1:G:167:PRO:HG2	1:G:170:ARG:HD2	1.95	0.48
1:G:12:ARG:N	1:G:30:PRO:HD2	2.18	0.48
1:H:98:VAL:HG21	1:H:121:VAL:HG23	1.95	0.48
1:H:60:GLU:HG3	1:H:143:ARG:O	2.12	0.48
2:I:151:ARG:NH2	2:I:175:ARG:HD2	2.21	0.48
2:C:104:ILE:O	2:C:113:THR:HA	2.13	0.48
2:C:162:GLY:O	2:C:164:THR:N	2.45	0.48
2:C:40:GLU:HG2	2:C:41:GLN:N	2.28	0.48
2:C:800:MET:HB3	2:C:800:MET:HE3	1.78	0.48
5:F:584:ARG:HH11	5:F:584:ARG:HA	1.78	0.48
1:H:18:GLN:HA	1:H:24:ALA:HA	1.95	0.48
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.26	0.48
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.13	0.48
5:L:262:VAL:HG11	5:L:264:LYS:HZ2	1.78	0.48
3:J:79:LYS:HB2	5:L:569:THR:H	1.79	0.48
1:B:195:ARG:CB	1:B:198:LEU:HD21	2.43	0.48
3:D:317:THR:HA	3:D:324:LEU:HD23	1.94	0.48
3:D:81:ARG:O	3:D:83:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:138:PRO:HD2	5:F:353:LEU:HD11	1.95	0.48
2:I:1060:ILE:HD11	2:I:1066:MET:HE1	1.96	0.48
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.28	0.48
3:J:98:ARG:O	3:J:248:ASP:HB2	2.13	0.48
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.96	0.48
2:C:1124:ILE:HG21	2:C:1180:MET:HE2	1.95	0.48
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.94	0.48
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.44	0.48
3:D:140:TYR:HB3	5:F:100:MET:SD	2.53	0.48
5:F:573:LEU:HD13	5:F:588:ARG:NE	2.29	0.48
1:H:98:VAL:O	1:H:146:VAL:HG22	2.12	0.48
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.96	0.48
2:I:580:GLN:HB2	2:I:605:TYR:HE1	1.78	0.48
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.34	0.48
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.95	0.48
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.48	0.48
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.95	0.48
5:F:227:GLN:HE22	5:F:251:LYS:NZ	2.11	0.48
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.77	0.48
5:L:338:HIS:CE1	5:L:341:LEU:HD13	2.48	0.48
1:A:156:SER:HB3	2:C:1059:ARG:HH22	1.78	0.48
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.95	0.48
1:G:195:ARG:HG3	1:G:198:LEU:HG	1.95	0.48
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.28	0.48
3:D:1301:THR:HG23	3:J:1301:THR:HG23	1.94	0.48
3:J:694:SER:O	3:J:698:MET:HB2	2.14	0.48
5:L:433:TRP:HE3	5:L:434:TRP:CD1	2.31	0.48
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.96	0.48
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.95	0.48
2:C:458:GLU:O	2:C:461:GLU:HB3	2.14	0.48
3:D:1166:GLY:O	3:D:1174:ARG:HB2	2.13	0.48
1:G:75:GLN:HG3	1:G:76:GLU:OE2	2.14	0.48
1:H:44:ARG:HG2	1:H:183:ILE:HD13	1.95	0.48
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.79	0.48
3:J:682:VAL:HG13	3:J:685:ILE:HD11	1.96	0.48
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.95	0.48
3:D:708:ASN:HB3	3:D:712:GLN:O	2.12	0.48
1:H:92:VAL:HG13	1:H:120:ASP:O	2.14	0.48
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.94	0.48
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.48	0.48
2:I:715:THR:OG1	2:I:782:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:116:PHE:O	3:J:123:ARG:HB2	2.14	0.48
5:L:139:GLU:HG2	5:L:351:THR:HA	1.96	0.48
5:L:230:VAL:O	5:L:234:THR:HG23	2.13	0.48
5:L:476:ARG:HH11	5:L:477:GLU:H	1.62	0.48
1:A:284:ARG:HG3	1:A:288:GLU:HG3	1.96	0.48
2:C:721:GLY:N	2:C:740:GLU:OE1	2.41	0.48
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.44	0.48
3:D:1283:SER:O	3:D:1286:LYS:N	2.46	0.48
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.96	0.48
1:G:39:LEU:HD21	1:H:224:LEU:HD11	1.96	0.48
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.14	0.48
2:I:871:VAL:O	2:I:944:ARG:NH1	2.46	0.48
2:I:1269:ARG:HA	3:J:346:ARG:HA	1.96	0.48
3:J:48:THR:C	3:J:50:LYS:H	2.12	0.48
3:J:691:ASP:O	3:J:695:LYS:HG2	2.14	0.48
1:A:321:TRP:CD2	1:A:322:PRO:HB3	2.49	0.48
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.48	0.48
2:C:462:ASN:O	2:C:466:VAL:HG23	2.14	0.48
3:D:1231:ARG:HA	3:D:1234:VAL:HG22	1.95	0.48
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.96	0.48
1:H:81:ILE:HG23	1:H:130:ILE:O	2.14	0.48
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.79	0.48
2:I:1284:ALA:N	3:J:479:GLU:OE1	2.47	0.48
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.78	0.48
5:L:470:MET:HA	5:L:473:GLU:HB3	1.96	0.48
1:A:118:ASP:O	1:A:120:ASP:N	2.47	0.47
2:C:1263:ALA:O	2:C:1265:PHE:HD1	1.97	0.47
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.95	0.47
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.49	0.47
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.43	0.47
3:D:244:VAL:HA	3:D:269:TYR:OH	2.13	0.47
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.46	0.47
3:D:744:ARG:HG3	3:D:744:ARG:O	2.14	0.47
1:H:76:GLU:N	1:H:76:GLU:OE1	2.47	0.47
1:H:67:GLU:O	1:H:78:ILE:HB	2.14	0.47
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.94	0.47
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.96	0.47
2:C:42:ASP:C	2:C:44:GLU:H	2.17	0.47
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.14	0.47
2:I:160:ASP:O	2:I:164:THR:OG1	2.30	0.47
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	1.95	0.47
2:C:1207:SER:C	2:C:1209:GLN:H	2.18	0.47
2:C:149:LEU:HG	2:C:451:ARG:HH11	1.79	0.47
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.15	0.47
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.46	0.47
2:I:1273:MET:HG2	2:I:1276:TRP:CZ3	2.49	0.47
2:I:521:LEU:O	2:I:525:THR:HB	2.15	0.47
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.44	0.47
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.97	0.47
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.28	0.47
3:J:88:CYS:O	3:J:90:VAL:N	2.47	0.47
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.45	0.47
2:C:1132:LEU:HD22	2:C:1177:ARG:CZ	2.44	0.47
3:D:291:ILE:HG23	5:F:406:GLN:HE22	1.79	0.47
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.97	0.47
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.14	0.47
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.79	0.47
2:I:310:ILE:HG21	2:I:325:LEU:HD23	1.97	0.47
3:J:398:LYS:HE2	5:L:532:LEU:HD23	1.96	0.47
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.71	0.47
2:C:106:GLU:HG3	2:C:107:ARG:N	2.29	0.47
2:C:1259:LEU:HD12	2:C:1260:GLY:H	1.79	0.47
3:D:342:LEU:HA	3:D:343:LEU:HA	1.64	0.47
5:F:468:ARG:HH11	5:F:469:GLN:NE2	2.12	0.47
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.97	0.47
2:I:972:PHE:HB3	2:I:994:ARG:HH21	1.79	0.47
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.44	0.47
3:J:1219:ASP:O	3:J:1222:ARG:N	2.48	0.47
3:J:214:ARG:O	3:J:218:THR:HB	2.15	0.47
3:J:826:ILE:HD12	3:J:826:ILE:O	2.15	0.47
4:K:6:VAL:O	4:K:10:VAL:HG23	2.15	0.47
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.47	0.47
2:C:565:GLU:HG2	2:C:565:GLU:O	2.14	0.47
2:C:1285:TYR:CE2	3:D:1356:LEU:HD11	2.49	0.47
3:D:239:LEU:HA	3:D:239:LEU:HD23	1.55	0.47
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.95	0.47
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.47
2:I:136:PHE:CE1	2:I:506:PHE:HE2	2.33	0.47
2:I:540:ARG:H	2:I:540:ARG:HD2	1.79	0.47
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.45	0.47
5:L:322:MET:HB3	5:L:324:LYS:HZ3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:101:TYR:CE2	5:L:405:ILE:HD11	2.49	0.47
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.80	0.47
5:L:561:MET:HA	5:L:567:MET:CE	2.43	0.47
1:B:223:ILE:O	1:B:226:GLU:HB2	2.14	0.47
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.23	0.47
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.96	0.47
2:C:826:ASP:O	2:C:829:THR:HB	2.14	0.47
3:D:298:MET:SD	5:F:402:LEU:HB3	2.55	0.47
5:F:448:ARG:HB3	5:F:448:ARG:HE	1.54	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.48	0.47
3:J:1270:GLY:HA2	3:J:1298:VAL:HG22	1.97	0.47
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.15	0.47
3:J:638:SER:OG	3:J:639:VAL:N	2.48	0.47
5:L:460:ILE:O	5:L:463:LEU:HB2	2.15	0.47
1:A:313:SER:OG	1:A:314:LEU:N	2.48	0.47
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.29	0.47
2:C:1247:SER:OG	2:C:1248:THR:N	2.47	0.47
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.97	0.47
3:D:292:VAL:O	3:D:296:LYS:HG3	2.14	0.47
3:D:705:THR:OG1	3:D:718:SER:HA	2.15	0.47
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	2.15	0.47
1:H:57:THR:HG22	1:H:58:GLU:OE1	2.15	0.47
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.79	0.47
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.80	0.47
2:I:238:GLN:OE1	2:I:284:LEU:HD21	2.14	0.47
3:J:1270:GLY:HA3	3:J:1298:VAL:O	2.15	0.47
3:J:198:CYS:O	3:J:202:ARG:HG3	2.15	0.47
3:J:342:LEU:HA	3:J:343:LEU:HA	1.69	0.47
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.97	0.47
3:J:511:TYR:CD2	3:J:728:SER:HB3	2.50	0.47
3:J:53:ARG:HA	3:J:54:ASP:HA	1.54	0.47
3:J:708:ASN:N	3:J:708:ASN:OD1	2.42	0.47
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.95	0.47
5:L:261:LEU:HD12	5:L:261:LEU:H	1.80	0.47
1:B:76:GLU:OE1	1:B:76:GLU:N	2.47	0.47
2:C:1124:ILE:O	2:C:1128:ILE:HG13	2.15	0.47
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.48	0.47
3:D:848:VAL:HG11	3:D:872:LEU:HD21	1.96	0.47
5:F:233:ASP:O	5:F:236:LYS:HE2	2.15	0.47
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.96	0.47
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:994:ARG:HD2	2:I:997:TRP:CZ2	2.50	0.47
3:J:1285:VAL:HG12	3:J:1286:LYS:HG2	1.96	0.47
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.14	0.47
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.50	0.47
3:J:356:THR:OG1	3:J:357:VAL:N	2.47	0.47
3:J:835:LEU:O	3:J:839:VAL:HG23	2.14	0.47
3:J:817:HIS:CE1	3:J:860:ARG:NH1	2.83	0.47
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.78	0.47
1:A:118:ASP:O	1:A:121:VAL:N	2.42	0.47
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.35	0.47
2:C:1131:MET:HE1	2:C:1141:LEU:HA	1.96	0.47
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.97	0.47
2:C:666:SER:OG	2:C:704:MET:HG3	2.15	0.47
3:D:805:GLN:O	3:D:807:LEU:N	2.48	0.47
5:F:163:THR:O	5:F:260:ARG:NH2	2.48	0.47
2:I:1204:LEU:HB3	2:I:1205:PRO:HD2	1.97	0.47
3:J:432:LEU:HD21	3:J:489:ASN:CB	2.45	0.47
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.15	0.47
2:C:107:ARG:HA	2:C:108:GLU:HA	1.43	0.47
5:F:562:ARG:HH21	5:F:573:LEU:HD23	1.79	0.47
1:G:65:LEU:O	1:G:169:GLY:HA2	2.14	0.47
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.48	0.47
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.97	0.47
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.97	0.46
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.50	0.46
1:B:228:LEU:C	1:B:230:ALA:H	2.18	0.46
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.80	0.46
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.42	0.46
5:F:585:GLU:HA	5:F:588:ARG:CD	2.46	0.46
1:H:151:GLY:O	1:H:177:TYR:HB2	2.16	0.46
2:I:131:THR:HG22	2:I:132:ASP:OD1	2.15	0.46
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.80	0.46
1:B:76:GLU:CD	1:B:132:HIS:H	2.19	0.46
2:C:883:LEU:HB3	2:C:1052:VAL:HG21	1.97	0.46
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.97	0.46
3:D:325:LYS:HE2	3:D:330:MET:HE2	1.98	0.46
3:D:668:PHE:HE1	3:D:675:ALA:HB2	1.80	0.46
3:D:695:LYS:HD3	3:D:695:LYS:HA	1.47	0.46
4:E:50:ALA:O	4:E:54:ILE:HG12	2.15	0.46
2:I:402:ARG:HG2	2:I:416:GLY:N	2.30	0.46
2:I:526:HIS:O	2:I:529:ARG:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:923:ILE:O	3:J:926:PRO:HD2	2.15	0.46
4:K:49:ILE:O	4:K:53:GLU:HG3	2.16	0.46
5:L:230:VAL:HG22	5:L:248:GLU:OE2	2.16	0.46
3:J:47:ARG:NH1	5:L:500:ILE:HD11	2.28	0.46
1:A:12:ARG:HG2	1:A:13:LEU:H	1.81	0.46
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.49	0.46
3:D:128:LEU:HD23	3:D:192:MET:CE	2.45	0.46
3:D:654:ILE:O	3:D:658:GLU:HB2	2.15	0.46
3:D:826:ILE:HD12	3:D:826:ILE:O	2.16	0.46
3:D:83:VAL:O	3:D:91:GLU:HA	2.15	0.46
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.58	0.46
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.40	0.46
5:L:482:GLU:O	5:L:486:ARG:NH2	2.49	0.46
2:C:854:ILE:O	2:C:857:VAL:HG22	2.16	0.46
3:D:518:VAL:N	3:D:716:GLN:HE22	2.13	0.46
3:D:741:ALA:O	3:D:762:ASN:ND2	2.47	0.46
3:D:918:ILE:O	3:D:922:SER:OG	2.25	0.46
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.50	0.46
2:I:1243:MET:HA	3:J:353:SER:HB3	1.97	0.46
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.97	0.46
2:I:810:TYR:CD1	2:I:1078:LYS:HD2	2.50	0.46
3:J:596:LEU:HD11	3:J:604:MET:HE3	1.98	0.46
3:J:620:PHE:CE2	3:J:624:ILE:HD11	2.50	0.46
3:J:667:GLN:O	3:J:671:GLY:N	2.49	0.46
5:L:225:ARG:O	5:L:229:VAL:HG13	2.16	0.46
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.50	0.46
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.29	0.46
2:C:1315:MET:CE	2:C:1317:PRO:HB3	2.45	0.46
3:D:1158:GLU:HB2	3:D:1177:ILE:HD11	1.98	0.46
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.98	0.46
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.96	0.46
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.45	0.46
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.96	0.46
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.98	0.46
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.97	0.46
4:K:44:ASP:HB3	4:K:48:VAL:HB	1.97	0.46
1:A:179:PRO:HA	1:A:208:ASN:ND2	2.30	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.96	0.46
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.97	0.46
3:D:793:SER:O	3:D:797:THR:HG23	2.16	0.46
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:402:ARG:HG2	2:I:416:GLY:H	1.81	0.46
2:I:462:ASN:O	2:I:466:VAL:HG23	2.14	0.46
2:I:975:ILE:HD13	2:I:998:LEU:HG	1.98	0.46
3:J:64:PRO:O	3:J:95:THR:OG1	2.29	0.46
5:L:253:SER:O	5:L:257:LYS:HG3	2.14	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.16	0.46
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.82	0.46
3:D:171:GLU:HB3	3:D:172:PHE:CD2	2.51	0.46
3:D:53:ARG:HA	3:D:54:ASP:HA	1.65	0.46
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.98	0.46
5:F:494:ILE:O	5:F:498:LEU:HB2	2.16	0.46
5:F:551:LEU:HA	5:F:551:LEU:HD23	1.68	0.46
1:G:140:ILE:O	1:G:140:ILE:HG13	2.15	0.46
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.79	0.46
1:G:150:ARG:NH1	1:H:7:GLU:O	2.35	0.46
2:I:241:LEU:HD11	2:I:246:LEU:HD11	1.96	0.46
2:I:891:GLY:O	2:I:892:GLU:HG3	2.15	0.46
3:J:401:VAL:HG12	3:J:408:VAL:HG11	1.98	0.46
3:J:514:THR:HG21	3:J:596:LEU:HG	1.97	0.46
1:A:97:GLU:HB3	1:A:147:GLN:HG2	1.97	0.46
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.81	0.46
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.98	0.46
2:C:1180:MET:HA	2:C:1181:PRO:HD3	1.70	0.46
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.81	0.46
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.80	0.46
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.82	0.46
3:D:325:LYS:HG2	3:D:330:MET:HE3	1.97	0.46
5:F:262:VAL:HG11	5:F:264:LYS:NZ	2.31	0.46
5:L:114:GLU:O	5:L:117:ILE:N	2.41	0.46
5:L:316:PHE:O	5:L:320:ILE:HG13	2.16	0.46
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.53	0.46
1:A:195:ARG:HD2	1:A:196:THR:H	1.80	0.46
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.16	0.46
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.60	0.46
1:A:83:LEU:HB3	2:C:694:ARG:HH21	1.81	0.46
3:D:1198:VAL:HB	3:D:1210:ILE:HG23	1.96	0.46
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.97	0.46
3:D:850:LYS:HB2	3:D:852:GLY:O	2.16	0.46
4:E:15:ASN:CB	4:E:18:ASP:HB2	2.45	0.46
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.81	0.46
3:J:81:ARG:C	3:J:83:VAL:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.98	0.46
5:L:300:LYS:HE3	5:L:301:ASN:HD21	1.81	0.46
5:L:363:ARG:O	5:L:367:ILE:HG13	2.15	0.46
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.96	0.46
1:B:88:LEU:HD12	1:B:89:ALA:H	1.81	0.46
1:B:98:VAL:O	1:B:146:VAL:HG13	2.16	0.46
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.51	0.46
2:C:1164:PHE:C	2:C:1166:ASP:H	2.19	0.46
2:C:980:VAL:HA	2:C:984:VAL:HA	1.97	0.46
3:D:710:ASP:OD1	3:D:711:GLY:N	2.49	0.46
1:G:197:ASP:O	1:G:198:LEU:HD23	2.15	0.46
1:H:22:THR:OG1	1:H:207:THR:O	2.34	0.46
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.78	0.46
2:I:607:SER:OG	2:I:609:ILE:HG13	2.16	0.46
3:J:156:ARG:HH12	3:J:157:GLN:NE2	2.14	0.46
3:J:288:PRO:O	3:J:292:VAL:HG13	2.16	0.46
3:J:650:LYS:NZ	3:J:762:ASN:HD22	2.13	0.46
5:L:483:LEU:HA	5:L:486:ARG:NH1	2.31	0.46
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.97	0.45
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.81	0.45
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.98	0.45
3:D:107:LEU:HD22	3:D:299:LEU:HD21	1.98	0.45
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.97	0.45
3:D:504:GLN:HG3	3:D:505:ASP:N	2.29	0.45
5:F:230:VAL:O	5:F:234:THR:HG23	2.16	0.45
1:G:23:HIS:HB2	1:G:206:GLU:HA	1.97	0.45
2:I:91:THR:HG21	2:I:503:LYS:HE3	1.98	0.45
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.82	0.45
3:J:500:ILE:O	3:J:500:ILE:HG22	2.16	0.45
3:J:548:VAL:CG1	3:J:550:VAL:HG13	2.46	0.45
3:J:796:LEU:HA	3:J:796:LEU:HD12	1.57	0.45
5:L:461:ASN:O	5:L:465:ARG:HG2	2.16	0.45
1:A:155:ALA:H	1:A:174:ASP:HA	1.81	0.45
1:B:118:ASP:HB2	1:B:121:VAL:HB	1.98	0.45
2:C:498:ILE:N	2:C:498:ILE:HD12	2.31	0.45
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.81	0.45
2:C:790:ASP:O	2:C:793:GLU:N	2.34	0.45
2:I:1082:ILE:H	2:I:1082:ILE:CD1	2.24	0.45
2:I:681:MET:O	2:I:685:MET:HE2	2.16	0.45
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.98	0.45
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.98	0.45
3:J:322:ARG:HG3	3:J:323:PRO:HD2	1.99	0.45
3:J:491:LEU:HD23	3:J:498:PRO:HA	1.98	0.45
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.98	0.45
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.31	0.45
2:C:1253:LEU:CD1	3:D:253:VAL:HG11	2.46	0.45
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.99	0.45
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.97	0.45
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.50	0.45
3:D:646:ILE:HG22	3:D:647:PRO:HD2	1.98	0.45
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.17	0.45
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.99	0.45
5:F:262:VAL:HG11	5:F:264:LYS:HZ2	1.80	0.45
1:G:154:PRO:HG2	1:G:157:THR:OG1	2.16	0.45
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.81	0.45
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.16	0.45
3:J:1170:LYS:C	3:J:1172:LYS:H	2.20	0.45
5:L:277:MET:SD	5:L:359:LYS:HG2	2.57	0.45
5:L:390:ILE:O	5:L:393:LYS:HB2	2.16	0.45
1:A:185:TYR:HB2	1:A:201:LEU:HD11	1.97	0.45
2:C:91:THR:HB	2:C:138:ILE:O	2.16	0.45
2:C:468:LEU:O	2:C:471:VAL:HG12	2.17	0.45
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.99	0.45
2:C:960:LEU:O	2:C:963:GLU:HB2	2.16	0.45
3:D:210:SER:HB2	3:D:213:LYS:CB	2.31	0.45
3:D:26:SER:O	3:D:29:MET:HB3	2.15	0.45
3:D:361:LEU:HD22	3:D:365:GLN:HG3	1.99	0.45
2:I:4:SER:OG	2:I:7:GLU:HG3	2.17	0.45
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.38	0.45
3:J:1285:VAL:O	3:J:1289:ASN:HB3	2.17	0.45
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.97	0.45
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.51	0.45
3:D:165:TYR:CE2	3:D:169:LEU:HG	2.52	0.45
3:D:362:ARG:H	3:D:365:GLN:HE21	1.64	0.45
3:D:587:LEU:HD23	3:D:591:ILE:HG21	1.99	0.45
3:D:827:GLU:O	3:D:829:GLY:N	2.43	0.45
3:D:908:ILE:HD13	3:D:909:ILE:N	2.30	0.45
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.64	0.45
2:I:1259:LEU:HD12	2:I:1260:GLY:N	2.32	0.45
2:I:194:LEU:HA	2:I:194:LEU:HD12	1.85	0.45
2:I:692:THR:OG1	2:I:827:ARG:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:202:ARG:HD3	3:J:1181:ASP:HA	1.99	0.45
3:J:1265:THR:HG22	3:J:1277:GLY:CA	2.45	0.45
3:J:474:LEU:HA	3:J:474:LEU:HD12	1.78	0.45
3:J:649:LYS:HA	3:J:649:LYS:HD3	1.66	0.45
5:L:399:LEU:HG	5:L:403:ASP:HB3	1.98	0.45
2:C:1083:GLU:HG3	2:C:1083:GLU:H	1.48	0.45
4:E:15:ASN:HB2	4:E:18:ASP:HB2	1.99	0.45
5:F:395:THR:OG1	5:F:396:ASN:N	2.49	0.45
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.71	0.45
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.31	0.45
2:I:730:SER:O	2:I:753:LEU:HB2	2.17	0.45
2:I:12:ARG:NE	2:I:793:GLU:OE1	2.35	0.45
3:J:1231:ARG:HA	3:J:1234:VAL:HG22	1.98	0.45
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.46	0.45
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.50	0.45
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.82	0.45
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.67	0.45
2:C:1236:ASN:HB2	2:C:1238:LEU:HD11	1.99	0.45
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.46	0.45
3:D:653:ILE:HG23	3:D:692:ARG:CZ	2.47	0.45
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.31	0.45
2:I:819:SER:HB3	2:I:1085:MET:SD	2.56	0.45
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.47	0.45
3:D:537:TYR:CE2	3:D:544:LEU:HD13	2.52	0.45
3:D:649:LYS:HA	3:D:649:LYS:HD3	1.77	0.45
5:F:557:LYS:O	5:F:561:MET:HB2	2.17	0.45
2:I:1180:MET:HA	2:I:1181:PRO:HD3	1.77	0.45
1:G:75:GLN:HA	2:I:729:ALA:H	1.81	0.45
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.17	0.45
2:I:1340:GLU:OE2	3:J:21:LYS:HD3	2.17	0.45
3:J:601:ILE:O	3:J:604:MET:HB3	2.17	0.45
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.81	0.45
1:A:8:PHE:CZ	1:B:150:ARG:HD2	2.52	0.45
1:B:151:GLY:O	1:B:177:TYR:HB2	2.17	0.45
2:C:193:ASN:ND2	2:C:353:VAL:HG21	2.31	0.45
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.98	0.45
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.31	0.45
3:D:416:ILE:HA	3:D:416:ILE:HD13	1.52	0.45
4:E:13:ILE:HD12	4:E:19:LEU:HA	1.99	0.45
5:F:143:TYR:CE2	5:F:147:GLN:HG3	2.52	0.45
1:G:108:GLY:O	1:G:133:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.46	0.45
2:I:593:LYS:HE3	2:I:595:THR:CG2	2.47	0.45
2:I:84:GLU:OE1	2:I:1035:LYS:HD2	2.17	0.45
3:J:47:ARG:NE	3:J:47:ARG:HA	2.31	0.45
3:J:99:ARG:HG3	3:J:249:LEU:HD21	1.98	0.45
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.77	0.45
2:C:744:GLY:O	2:C:746:ALA:N	2.47	0.45
3:D:501:VAL:HG22	3:D:502:PRO:O	2.17	0.45
3:D:903:LEU:HD22	3:D:909:ILE:HD12	1.98	0.45
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.98	0.45
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.90	0.45
1:A:180:VAL:HG12	1:A:183:ILE:HD13	1.99	0.44
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.98	0.44
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.17	0.44
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.32	0.44
2:C:487:LEU:H	2:C:487:LEU:HD23	1.82	0.44
2:C:681:MET:O	2:C:685:MET:HE2	2.17	0.44
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.17	0.44
3:D:1321:SER:O	3:D:1324:SER:HB2	2.16	0.44
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.46	0.44
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.99	0.44
4:E:15:ASN:C	4:E:17:PHE:H	2.20	0.44
2:I:672:GLU:HG2	2:I:1186:VAL:O	2.17	0.44
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.17	0.44
3:J:355:ILE:HG21	3:J:466:MET:HG3	2.00	0.44
3:J:694:SER:OG	3:J:738:ARG:NE	2.50	0.44
1:A:236:ASP:HA	1:B:14:VAL:O	2.17	0.44
1:B:62:ASP:OD2	1:B:140:ILE:HD12	2.17	0.44
2:C:1254:VAL:HG22	2:C:1255:THR:N	2.33	0.44
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.52	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.54	0.44
2:C:970:GLY:O	2:C:973:SER:OG	2.35	0.44
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.31	0.44
3:D:255:LEU:HA	3:D:255:LEU:HD13	1.62	0.44
2:I:151:ARG:HH12	2:I:175:ARG:HH11	1.64	0.44
2:I:360:LEU:O	2:I:364:VAL:HG23	2.17	0.44
3:J:619:ILE:O	3:J:623:GLN:HG2	2.16	0.44
2:C:218:GLU:HG3	2:C:299:LYS:HA	2.00	0.44
2:C:960:LEU:HA	2:C:960:LEU:HD13	1.81	0.44
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.98	0.44
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1301:THR:HG23	3:J:1301:THR:CG2	2.47	0.44
3:D:412:LEU:HD23	3:D:416:ILE:HG12	1.99	0.44
5:F:390:ILE:O	5:F:393:LYS:HB2	2.17	0.44
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.17	0.44
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.99	0.44
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.99	0.44
2:C:16:GLY:H	2:C:17:LYS:NZ	2.15	0.44
3:D:48:THR:C	3:D:50:LYS:N	2.68	0.44
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.17	0.44
1:G:134:THR:HG23	1:G:135:ASP:N	2.32	0.44
1:G:65:LEU:HA	1:G:65:LEU:HD13	1.71	0.44
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.16	0.44
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.32	0.44
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.64	0.44
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.98	0.44
3:J:804:ALA:O	3:J:806:ASP:N	2.50	0.44
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.99	0.44
1:B:205:MET:HE1	1:B:213:PRO:O	2.17	0.44
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.55	0.44
2:C:517:GLN:HG3	2:C:523:GLU:OE2	2.18	0.44
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.52	0.44
2:C:81:ASP:OD2	2:C:84:GLU:HG3	2.17	0.44
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.81	0.44
3:D:412:LEU:O	3:D:415:VAL:HG22	2.17	0.44
3:D:541:LEU:HA	3:D:541:LEU:HD23	1.72	0.44
3:D:514:THR:HG21	3:D:596:LEU:HB2	2.00	0.44
1:G:51:MET:HA	1:G:52:PRO:HD3	1.86	0.44
1:G:76:GLU:OE2	1:G:76:GLU:N	2.48	0.44
2:I:487:LEU:HD23	2:I:487:LEU:H	1.83	0.44
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	2.00	0.44
3:J:537:TYR:OH	3:J:634:ARG:NH2	2.50	0.44
3:J:748:ALA:HA	3:J:754:ILE:HA	2.00	0.44
5:L:134:VAL:HA	5:L:273:MET:HE1	1.99	0.44
5:L:503:GLU:OE1	5:L:504:PRO:HD2	2.18	0.44
1:B:16:ILE:HB	1:B:26:VAL:HG13	1.99	0.44
2:C:757:THR:O	2:C:765:ILE:HG23	2.17	0.44
3:D:1186:TYR:HE2	3:D:1188:GLU:HB2	1.82	0.44
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.32	0.44
5:F:343:LYS:O	5:F:347:ILE:HG13	2.18	0.44
5:F:530:LEU:HD11	5:F:533:ASP:OD2	2.17	0.44
1:G:187:VAL:HG13	1:G:201:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:THR:HG23	1:H:135:ASP:N	2.25	0.44
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.53	0.44
2:I:488:MET:O	2:I:490:GLN:N	2.48	0.44
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.99	0.44
3:J:1328:THR:O	3:J:1332:LEU:HD23	2.18	0.44
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.50	0.44
5:L:308:GLY:HA2	5:L:356:GLU:OE1	2.18	0.44
5:L:479:THR:HG23	5:L:481:GLU:H	1.83	0.44
1:B:178:SER:HA	1:B:179:PRO:HD3	1.74	0.44
1:A:45:ARG:CG	1:B:38:THR:HB	2.38	0.44
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.99	0.44
2:C:1134:GLN:C	2:C:1135:GLN:HG2	2.38	0.44
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.17	0.44
2:C:229:ILE:HB	2:C:240:GLU:CD	2.37	0.44
2:C:221:LEU:HD12	2:C:298:ALA:O	2.18	0.44
2:C:452:ARG:NH1	2:C:584:TYR:O	2.50	0.44
2:C:94:ALA:HA	2:C:95:PRO:HD3	1.66	0.44
3:D:749:LYS:HG3	3:D:751:ASP:HB2	1.99	0.44
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.51	0.44
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.47	0.44
2:I:800:MET:O	2:I:1229:TYR:HA	2.18	0.44
3:J:19:ALA:HB2	3:J:1373:ARG:NH2	2.33	0.44
3:J:30:ILE:HD13	3:J:243:PRO:HG3	1.99	0.44
5:L:137:TYR:CD1	5:L:138:PRO:HD2	2.52	0.44
5:L:346:GLN:HA	5:L:349:GLU:OE2	2.18	0.44
5:L:368:GLY:O	5:L:371:LYS:HB3	2.17	0.44
1:A:133:LEU:HD21	1:A:140:ILE:HG12	1.99	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
1:A:82:LEU:HD22	1:A:173:VAL:CG1	2.48	0.44
1:A:262:LEU:HD12	1:A:262:LEU:H	1.82	0.44
1:B:158:ARG:HB3	1:B:172:LEU:HD23	2.00	0.44
2:C:1142:ARG:CD	2:C:1161:LEU:HD22	2.47	0.44
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.81	0.44
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.00	0.44
3:D:48:THR:HB	3:D:50:LYS:HG3	2.00	0.44
3:D:490:ILE:N	3:D:490:ILE:HD13	2.26	0.44
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.80	0.44
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.98	0.44
3:J:1287:ILE:HG22	3:J:1300:ALA:H	1.82	0.44
3:J:203:GLU:O	3:J:207:GLU:HG2	2.18	0.44
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:O	1:A:167:PRO:C	2.56	0.44
2:C:95:PRO:CA	2:C:126:GLU:HG2	2.48	0.44
2:C:480:SER:HB3	2:C:481:LEU:HD22	1.99	0.44
2:C:534:GLY:HA3	2:C:535:PRO:HD2	1.83	0.44
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.50	0.44
2:C:878:THR:OG1	2:C:879:GLY:N	2.48	0.44
3:D:1184:ASP:O	3:D:1186:TYR:N	2.51	0.44
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.00	0.44
5:F:484:ALA:O	5:F:491:GLU:HB2	2.18	0.44
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.99	0.44
1:H:153:VAL:HG11	1:H:158:ARG:NH1	2.33	0.44
2:I:227:LYS:NZ	2:I:298:ALA:HB1	2.33	0.44
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.52	0.44
3:J:1162:ILE:HA	3:J:1203:ARG:HA	2.00	0.44
3:J:596:LEU:HD12	3:J:601:ILE:HG13	1.99	0.44
3:J:658:GLU:O	3:J:661:VAL:HG22	2.18	0.44
4:K:15:ASN:CB	4:K:18:ASP:HB2	2.48	0.44
5:L:280:VAL:O	5:L:284:GLU:HG3	2.18	0.44
3:D:660:GLU:O	3:D:664:ILE:HG12	2.17	0.43
5:F:230:VAL:HG13	5:F:231:THR:H	1.82	0.43
1:H:183:ILE:HG23	1:H:205:MET:HG3	1.99	0.43
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.52	0.43
2:I:672:GLU:HB3	2:I:1187:PHE:CD2	2.53	0.43
2:I:778:GLU:HB3	2:I:781:ASP:OD1	2.18	0.43
3:J:664:ILE:HG21	3:J:681:LYS:HB3	2.00	0.43
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.18	0.43
3:J:690:ASN:ND2	3:J:745:GLY:HA2	2.33	0.43
3:J:860:ARG:HB3	3:J:861:ASN:H	1.61	0.43
3:J:865:HIS:CE1	3:J:868:TRP:CD1	3.06	0.43
3:J:903:LEU:HD23	3:J:905:ARG:CG	2.48	0.43
4:K:42:GLU:O	4:K:43:ASN:HB2	2.17	0.43
1:A:179:PRO:HB3	1:A:208:ASN:HD21	1.84	0.43
2:C:70:TYR:HA	2:C:100:LEU:HD23	2.00	0.43
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.80	0.43
3:D:810:THR:HG21	3:D:893:GLY:HA3	2.00	0.43
5:F:310:GLU:O	5:F:344:LEU:HD21	2.18	0.43
1:H:62:ASP:HB3	1:H:141:SER:O	2.18	0.43
2:I:1239:VAL:C	2:I:1241:ASP:H	2.21	0.43
2:I:997:TRP:HA	2:I:1000:LEU:HD12	2.00	0.43
3:J:1314:LEU:HA	3:J:1326:GLN:NE2	2.34	0.43
3:J:429:LEU:HD13	3:J:429:LEU:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:442:ILE:HA	3:J:442:ILE:HD13	1.87	0.43
3:J:594:GLN:HB2	3:J:595:ALA:H	1.48	0.43
3:J:697:MET:O	3:J:701:LEU:N	2.32	0.43
2:C:38:PHE:HE1	2:C:461:GLU:HA	1.82	0.43
2:C:833:ILE:HA	2:C:1054:LEU:O	2.17	0.43
3:D:1285:VAL:O	3:D:1288:ALA:HB3	2.18	0.43
3:D:418:GLU:O	3:D:420:PRO:HD3	2.18	0.43
3:D:872:LEU:HD23	3:D:872:LEU:HA	1.80	0.43
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.18	0.43
5:F:372:ALA:O	5:F:376:LYS:HG3	2.18	0.43
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.53	0.43
1:G:166:ARG:N	1:G:167:PRO:HD2	2.32	0.43
1:G:191:ARG:NH1	1:G:197:ASP:HA	2.33	0.43
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.00	0.43
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.60	0.43
3:J:1257:VAL:HA	3:J:1260:MET:HG3	2.00	0.43
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.85	0.43
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.53	0.43
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.38	0.43
3:J:609:TYR:CE2	3:J:614:LEU:HD12	2.51	0.43
3:J:872:LEU:O	3:J:877:VAL:HG12	2.19	0.43
4:K:71:GLU:HA	4:K:74:GLU:HG3	2.00	0.43
5:L:458:GLU:O	5:L:462:LYS:HG3	2.19	0.43
2:C:4:SER:HB3	2:C:7:GLU:CG	2.45	0.43
3:D:1142:ALA:O	3:D:1146:GLU:N	2.48	0.43
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	2.00	0.43
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.01	0.43
4:E:3:ARG:HA	4:E:3:ARG:CZ	2.48	0.43
5:F:157:ARG:HB3	5:F:160:ASP:OD2	2.18	0.43
1:G:43:LEU:HD23	1:G:43:LEU:HA	1.66	0.43
1:H:78:ILE:O	1:H:82:LEU:HG	2.19	0.43
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.32	0.43
3:J:385:LEU:HA	3:J:385:LEU:HD23	1.79	0.43
3:J:58:CYS:SG	3:J:60:ARG:HB3	2.58	0.43
3:J:615:LYS:HE2	3:J:616:PRO:HD3	2.01	0.43
5:L:306:PHE:CE2	5:L:310:GLU:HG3	2.53	0.43
1:A:195:ARG:HD2	1:A:196:THR:N	2.33	0.43
1:B:195:ARG:HB2	1:B:198:LEU:HD21	2.01	0.43
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.99	0.43
2:C:268:ARG:HD2	2:C:270:THR:CG2	2.48	0.43
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.47	0.43
3:D:421:VAL:HG13	3:D:439:PRO:HG3	2.00	0.43
2:I:519:ASN:ND2	2:I:689:ALA:O	2.48	0.43
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.52	0.43
2:C:256:GLU:OE2	2:C:261:VAL:HG22	2.19	0.43
2:C:861:ALA:HB1	2:C:882:ILE:HD13	2.00	0.43
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.31	0.43
3:D:1343:GLU:HG2	3:D:1373:ARG:NH1	2.34	0.43
3:D:45:ASN:O	3:D:46:TYR:HB3	2.19	0.43
3:D:45:ASN:O	3:D:46:TYR:HD2	2.02	0.43
3:D:69:GLU:OE2	3:D:76:LYS:HD3	2.19	0.43
5:F:111:LEU:HD13	5:F:116:GLU:HA	2.01	0.43
5:F:142:THR:O	5:F:146:GLU:HG3	2.19	0.43
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.00	0.43
2:I:1081:PRO:HB3	2:I:1083:GLU:OE2	2.18	0.43
2:I:102:LEU:HB2	2:I:489:PRO:HG3	2.00	0.43
2:I:498:ILE:HD12	2:I:498:ILE:N	2.32	0.43
2:I:528:ARG:NH2	2:I:576:SER:O	2.52	0.43
2:I:930:ASP:OD2	2:I:931:VAL:N	2.51	0.43
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.34	0.43
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.83	0.43
2:C:53:PHE:CD1	2:C:468:LEU:HD11	2.53	0.43
2:C:782:VAL:HG21	2:C:792:GLY:HA3	2.00	0.43
3:D:147:ILE:HG22	3:D:188:LEU:HG	2.01	0.43
5:F:130:VAL:HB	5:F:365:MET:HG3	2.00	0.43
1:G:228:LEU:HG	1:H:221:ALA:HB1	2.00	0.43
2:I:1124:ILE:HG21	2:I:1180:MET:CE	2.49	0.43
2:I:55:SER:OG	2:I:56:VAL:N	2.51	0.43
3:J:186:GLN:HG3	3:J:238:ILE:HB	2.00	0.43
3:J:128:LEU:HD23	3:J:192:MET:HE1	2.00	0.43
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.49	0.43
5:L:453:PRO:O	5:L:456:MET:HB2	2.19	0.43
1:A:316:MET:SD	5:F:600:HIS:CE1	3.12	0.43
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.99	0.43
2:C:1009:ASN:O	2:C:1013:GLN:HG2	2.19	0.43
2:C:732:ILE:HG21	2:C:783:LEU:HD12	2.01	0.43
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.83	0.43
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.19	0.43
1:H:83:LEU:HA	1:H:86:LYS:HE2	2.01	0.43
2:I:590:PRO:HA	2:I:604:HIS:O	2.19	0.43
3:J:45:ASN:HB3	3:J:48:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:865:HIS:HE1	3:J:867:GLN:HB2	1.81	0.43
5:L:372:ALA:O	5:L:376:LYS:HG3	2.18	0.43
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.64	0.43
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	2.01	0.43
2:C:545:PHE:CZ	2:C:549:ASP:HB2	2.54	0.43
2:C:744:GLY:C	2:C:746:ALA:N	2.70	0.43
3:D:171:GLU:HB3	3:D:172:PHE:CE2	2.54	0.43
5:F:531:PRO:O	5:F:535:ALA:N	2.42	0.43
1:G:125:LYS:HE2	1:G:128:HIS:HB2	2.01	0.43
1:H:85:LEU:HD13	1:H:144:ILE:HD12	1.99	0.43
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	2.00	0.43
2:I:1134:GLN:O	2:I:1135:GLN:HG2	2.19	0.43
2:I:796:LEU:HD12	2:I:796:LEU:H	1.84	0.43
3:J:1184:ASP:O	3:J:1186:TYR:N	2.52	0.43
3:J:259:ARG:HD3	5:L:502:LYS:HD2	2.00	0.43
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.84	0.43
3:J:709:ARG:HD2	3:J:710:ASP:H	1.84	0.43
2:C:80:PHE:HB3	2:C:84:GLU:CB	2.49	0.43
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.01	0.43
3:D:597:GLY:O	3:D:601:ILE:HB	2.17	0.43
3:D:646:ILE:H	3:D:646:ILE:HG12	1.63	0.43
3:D:674:THR:N	3:D:677:GLU:OE1	2.42	0.43
5:F:228:TYR:HA	5:F:252:LEU:HD13	2.00	0.43
5:F:276:MET:O	5:F:280:VAL:HG23	2.19	0.43
1:G:155:ALA:HA	1:G:158:ARG:HD3	2.01	0.43
1:H:59:VAL:HG22	1:H:144:ILE:HG13	2.01	0.43
2:I:41:GLN:NE2	2:I:73:TYR:O	2.51	0.43
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.67	0.43
3:J:572:THR:HG21	3:J:589:TYR:OH	2.19	0.43
3:J:596:LEU:HD11	3:J:604:MET:CE	2.49	0.43
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.87	0.43
1:A:92:VAL:HA	1:A:120:ASP:O	2.19	0.42
1:B:73:GLY:O	1:B:133:LEU:HA	2.18	0.42
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	2.01	0.42
2:C:830:THR:HG23	2:C:832:HIS:NE2	2.33	0.42
2:C:968:GLU:O	2:C:971:LEU:N	2.52	0.42
3:D:1203:ARG:NH2	3:D:1205:GLU:OE2	2.52	0.42
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.65	0.42
5:F:384:LEU:HA	5:F:384:LEU:HD23	1.80	0.42
5:F:470:MET:O	5:F:478:PRO:HD3	2.18	0.42
1:H:107:ILE:HG23	1:H:134:THR:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:799:ASN:HB3	2:I:1231:TYR:HD1	1.84	0.42
2:I:593:LYS:HG3	2:I:595:THR:HG23	2.01	0.42
3:J:797:THR:HG22	3:J:924:GLY:CA	2.48	0.42
5:L:341:LEU:HD23	5:L:344:LEU:HD23	1.99	0.42
5:L:444:ALA:HB1	5:L:457:ILE:CD1	2.46	0.42
5:L:493:LYS:O	5:L:497:VAL:N	2.39	0.42
5:L:602:SER:OG	5:L:603:ARG:N	2.51	0.42
1:A:195:ARG:HG3	1:A:198:LEU:HD21	2.01	0.42
2:C:98:VAL:O	2:C:121:GLU:HA	2.18	0.42
2:C:748:ILE:HD11	2:C:967:LEU:HD12	2.00	0.42
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.35	0.42
3:D:712:GLN:HB2	3:D:713:GLU:H	1.59	0.42
1:H:89:ALA:HB1	1:H:210:THR:CG2	2.50	0.42
2:I:147:SER:HB2	2:I:529:ARG:O	2.19	0.42
2:I:646:SER:HB3	2:I:649:GLN:CD	2.39	0.42
3:J:122:SER:O	3:J:126:LEU:HG	2.19	0.42
3:J:57:PHE:CE1	3:J:252:LEU:HB2	2.54	0.42
1:A:253:LEU:HA	1:A:278:ILE:CD1	2.48	0.42
2:C:884:VAL:HG21	2:C:1050:VAL:HB	2.00	0.42
2:C:1066:MET:HE2	2:C:1076:ILE:HG22	2.01	0.42
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.54	0.42
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.42
2:C:943:LYS:HG2	2:C:947:GLU:OE1	2.19	0.42
3:D:1169:THR:CG2	3:D:1192:LYS:HD3	2.43	0.42
5:F:383:ASN:O	5:F:386:LEU:HB3	2.19	0.42
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.87	0.42
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.84	0.42
3:J:259:ARG:HG2	5:L:505:ILE:HD13	2.00	0.42
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.54	0.42
5:L:407:GLU:HG3	5:L:442:SER:OG	2.19	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.90	0.42
1:B:49:SER:O	1:B:151:GLY:HA2	2.19	0.42
3:D:491:LEU:HD23	3:D:498:PRO:HA	2.01	0.42
3:D:501:VAL:CG2	3:D:602:SER:HB2	2.48	0.42
3:D:884:SER:OG	3:D:886:VAL:HG12	2.20	0.42
5:F:585:GLU:O	5:F:589:GLN:HG3	2.19	0.42
3:J:120:LEU:HB3	3:J:121:PRO:HD3	2.01	0.42
3:J:416:ILE:HA	3:J:416:ILE:HD12	1.79	0.42
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.85	0.42
3:J:601:ILE:HG21	3:J:601:ILE:HD13	1.85	0.42
3:J:513:MET:SD	3:J:631:TYR:CD2	3.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:476:ARG:HD2	5:L:477:GLU:H	1.83	0.42
5:L:603:ARG:HD3	5:L:603:ARG:HA	1.76	0.42
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.90	0.42
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.20	0.42
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.51	0.42
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.78	0.42
3:D:99:ARG:HG3	3:D:249:LEU:HD21	2.00	0.42
3:D:358:GLY:N	3:D:359:PRO:HD3	2.35	0.42
3:D:859:PRO:HD2	3:D:862:THR:HG21	2.01	0.42
3:D:860:ARG:HB3	3:D:861:ASN:H	1.60	0.42
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.85	0.42
2:I:1131:MET:HE2	2:I:1136:GLN:HG3	2.02	0.42
2:I:745:GLU:HA	2:I:971:LEU:HD12	2.02	0.42
3:J:327:LEU:HA	3:J:327:LEU:HD23	1.82	0.42
3:J:758:PRO:O	3:J:760:THR:HG23	2.19	0.42
4:K:4:VAL:HG13	4:K:5:THR:HG23	2.00	0.42
5:L:611:LEU:HA	5:L:611:LEU:HD23	1.64	0.42
2:C:122:VAL:HG21	2:C:493:ILE:HG23	2.01	0.42
2:C:463:GLN:HA	2:C:463:GLN:OE1	2.19	0.42
2:C:119:GLU:CG	2:C:489:PRO:HD2	2.49	0.42
1:G:62:ASP:HB2	1:G:141:SER:O	2.19	0.42
1:G:228:LEU:HA	1:G:228:LEU:HD12	1.81	0.42
2:I:184:LEU:HD12	2:I:184:LEU:HA	1.86	0.42
2:I:616:ILE:HG22	2:I:617:ALA:O	2.20	0.42
2:I:803:ALA:CB	2:I:1094:VAL:HG21	2.50	0.42
2:I:850:ILE:O	2:I:850:ILE:HG22	2.19	0.42
3:J:131:PRO:O	3:J:135:ILE:HG13	2.20	0.42
3:J:159:ILE:O	3:J:159:ILE:HG13	2.18	0.42
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.34	0.42
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.34	0.42
5:L:493:LYS:HG2	5:L:496:LYS:HE2	2.01	0.42
1:A:162:GLU:HB3	1:A:163:GLU:H	1.68	0.42
1:B:86:LYS:HD3	1:B:174:ASP:HB2	2.01	0.42
2:C:1054:LEU:HD12	2:C:1054:LEU:HA	1.75	0.42
2:C:494:ASN:ND2	2:C:497:PRO:HD3	2.35	0.42
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.84	0.42
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.19	0.42
3:D:1156:LEU:HA	3:D:1208:ASP:O	2.19	0.42
3:D:148:GLU:H	3:D:156:ARG:HG3	1.85	0.42
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.01	0.42
3:D:77:ARG:HD2	3:D:77:ARG:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:822:MET:SD	3:D:838:ARG:HB3	2.60	0.42
4:E:38:LEU:HB2	4:E:53:GLU:OE1	2.19	0.42
1:G:59:VAL:HG21	1:G:85:LEU:CD1	2.49	0.42
2:I:1140:LYS:HD2	2:I:1140:LYS:HA	1.82	0.42
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	2.00	0.42
2:I:158:ASP:OD1	2:I:159:SER:N	2.46	0.42
2:I:800:MET:HB3	2:I:800:MET:HE3	1.86	0.42
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.34	0.42
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.83	0.42
3:J:743:MET:HB2	3:J:759:ILE:O	2.20	0.42
1:A:285:THR:HG23	1:A:288:GLU:HG2	2.01	0.42
2:C:48:GLY:N	2:C:461:GLU:OE1	2.53	0.42
2:C:582:ASN:O	2:C:585:GLY:N	2.52	0.42
3:D:926:PRO:CB	3:D:1246:VAL:HG11	2.50	0.42
3:D:594:GLN:HB2	3:D:595:ALA:H	1.72	0.42
1:H:147:GLN:HG3	1:H:148:ARG:H	1.84	0.42
2:I:1285:TYR:CD1	3:J:475:GLU:HG2	2.55	0.42
2:I:149:LEU:HD12	2:I:149:LEU:HA	1.67	0.42
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.73	0.42
2:I:715:THR:HG23	2:I:717:VAL:HG23	2.01	0.42
3:J:148:GLU:H	3:J:156:ARG:HG3	1.83	0.42
5:L:377:LYS:O	5:L:381:GLU:HG3	2.20	0.42
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.68	0.42
1:A:108:GLY:HA2	1:A:109:PRO:HD2	1.93	0.42
1:A:166:ARG:N	1:A:167:PRO:HD2	2.35	0.42
1:B:125:LYS:HE2	1:B:125:LYS:HB3	1.95	0.42
2:C:221:LEU:HD11	2:C:314:ASN:HB2	2.01	0.42
2:C:202:ARG:CZ	2:C:368:ARG:HH12	2.32	0.42
2:C:363:LEU:C	2:C:381:ALA:HB1	2.39	0.42
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.60	0.42
3:D:835:LEU:O	3:D:839:VAL:HG23	2.20	0.42
5:F:483:LEU:H	5:F:483:LEU:HD12	1.85	0.42
1:G:142:MET:SD	1:G:144:ILE:HD11	2.60	0.42
1:G:35:PHE:HA	1:G:35:PHE:HD1	1.70	0.42
2:I:497:PRO:HB2	2:I:498:ILE:HD12	2.02	0.42
2:I:61:SER:O	2:I:63:SER:N	2.53	0.42
4:K:71:GLU:O	4:K:75:GLN:HG3	2.19	0.42
1:A:195:ARG:HB3	1:A:198:LEU:HG	2.01	0.42
1:A:97:GLU:HA	1:A:146:VAL:O	2.20	0.42
2:C:1176:LEU:HD23	2:C:1176:LEU:HA	1.69	0.42
2:C:802:VAL:HG11	2:C:1230:MET:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.18	0.42
3:D:514:THR:HG23	3:D:596:LEU:HB2	2.02	0.42
3:D:901:ARG:HA	3:D:908:ILE:HA	2.02	0.42
5:F:536:THR:O	5:F:540:LEU:N	2.49	0.42
2:I:383:SER:O	2:I:387:ASN:HB2	2.20	0.42
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.54	0.42
3:J:116:PHE:O	3:J:124:ILE:HG13	2.20	0.42
3:J:650:LYS:O	3:J:654:ILE:HG13	2.20	0.42
3:J:844:THR:HG23	3:J:864:LEU:HD21	2.01	0.42
2:C:185:ASP:HB2	2:C:197:ARG:HG3	2.02	0.41
2:C:705:GLU:H	2:C:705:GLU:CD	2.24	0.41
2:C:775:GLU:HA	2:C:776:PRO:HD3	1.86	0.41
2:C:73:TYR:HB2	2:C:98:VAL:HG22	2.02	0.41
3:D:1158:GLU:HB3	3:D:1186:TYR:CE1	2.55	0.41
3:D:16:GLU:HA	3:D:16:GLU:OE2	2.20	0.41
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.50	0.41
1:G:91:ARG:HH21	1:G:122:GLU:CD	2.24	0.41
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.02	0.41
2:I:1086:PRO:O	2:I:1094:VAL:HG12	2.20	0.41
2:I:452:ARG:NH1	2:I:584:TYR:O	2.52	0.41
3:J:474:LEU:HD12	3:J:477:GLN:NE2	2.33	0.41
3:J:594:GLN:HG3	3:J:596:LEU:CD2	2.50	0.41
5:L:311:THR:HG21	5:L:348:GLU:CD	2.41	0.41
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.20	0.41
1:A:163:GLU:O	1:A:164:ASP:HB2	2.18	0.41
1:B:195:ARG:HB3	1:B:198:LEU:HD21	2.02	0.41
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.55	0.41
2:C:481:LEU:N	2:C:481:LEU:HD22	2.34	0.41
2:C:522:SER:O	2:C:525:THR:HG22	2.19	0.41
2:C:746:ALA:HB2	2:C:974:ARG:NE	2.35	0.41
2:C:886:LYS:HB3	2:C:917:SER:HA	2.01	0.41
3:D:11:GLN:HA	3:D:11:GLN:OE1	2.20	0.41
3:D:1372:ARG:HE	3:D:1372:ARG:HB2	1.63	0.41
3:D:215:LYS:O	3:D:219:LYS:HE3	2.20	0.41
3:D:349:TYR:CE1	3:D:472:LEU:HD11	2.56	0.41
3:D:537:TYR:OH	3:D:634:ARG:NH2	2.53	0.41
3:D:664:ILE:HG23	3:D:664:ILE:HD12	1.80	0.41
2:I:107:ARG:HA	2:I:108:GLU:HA	1.86	0.41
2:I:60:GLN:O	2:I:476:LYS:HE2	2.19	0.41
2:I:607:SER:H	2:I:610:GLU:HB2	1.85	0.41
3:J:57:PHE:CE2	3:J:252:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:504:GLN:HG3	3:J:505:ASP:H	1.85	0.41
1:H:83:LEU:HD11	3:J:526:VAL:HG23	2.01	0.41
3:J:901:ARG:HA	3:J:908:ILE:HA	2.01	0.41
1:A:211:ILE:HG21	1:A:216:ALA:HB2	2.01	0.41
1:A:46:ILE:CG2	1:A:223:ILE:HD12	2.50	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.75	0.41
2:C:1281:TYR:HD1	3:D:484:MET:HG2	1.86	0.41
3:D:57:PHE:N	3:D:57:PHE:CD2	2.88	0.41
3:D:733:SER:C	3:D:735:ALA:N	2.73	0.41
3:D:853:THR:O	3:D:854:ALA:HB3	2.20	0.41
3:D:902:ASP:OD1	3:D:903:LEU:N	2.53	0.41
5:F:414:LYS:HD3	5:F:434:TRP:CE3	2.55	0.41
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.02	0.41
1:H:178:SER:HA	1:H:179:PRO:HD3	1.82	0.41
2:I:1240:ASP:N	2:I:1240:ASP:OD1	2.40	0.41
2:I:30:ILE:H	2:I:30:ILE:CD1	2.25	0.41
2:I:470:ARG:HA	2:I:473:ARG:HD2	2.02	0.41
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.41
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.86	0.41
3:J:678:ARG:HG3	3:J:679:TYR:N	2.34	0.41
5:L:281:ARG:CG	5:L:285:ARG:HH11	2.30	0.41
2:C:629:PHE:HB2	2:C:647:ARG:HG3	2.02	0.41
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.50	0.41
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.51	0.41
3:D:411:ILE:O	3:D:414:GLU:HB2	2.21	0.41
3:D:8:LEU:HD23	3:D:9:LYS:N	2.35	0.41
5:F:412:LEU:HD13	5:F:435:ILE:HD11	2.01	0.41
2:C:490:GLN:HG3	5:F:472:GLN:HG3	2.03	0.41
1:G:187:VAL:CG1	1:G:201:LEU:HD13	2.50	0.41
1:G:218:ARG:HG3	1:H:231:PHE:O	2.21	0.41
1:G:45:ARG:HH22	1:H:37:HIS:CB	2.29	0.41
1:G:88:LEU:HD12	1:G:89:ALA:N	2.35	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
2:I:397:LEU:O	2:I:401:GLY:HA3	2.20	0.41
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.83	0.41
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.20	0.41
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.56	0.41
3:J:705:THR:OG1	3:J:718:SER:HA	2.21	0.41
5:L:299:LYS:HA	5:L:302:PHE:CB	2.49	0.41
1:A:13:LEU:O	1:A:13:LEU:HG	2.20	0.41
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:302:ILE:O	2:C:330:HIS:NE2	2.49	0.41
2:C:903:ARG:NE	2:C:910:ALA:HB2	2.35	0.41
3:D:121:PRO:HD2	3:D:123:ARG:NH2	2.35	0.41
3:D:184:ALA:O	3:D:187:ALA:HB3	2.21	0.41
3:D:532:GLU:HA	3:D:535:ARG:HB3	2.02	0.41
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.21	0.41
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.47	0.41
5:F:99:ARG:HG3	5:F:103:ARG:HH12	1.85	0.41
5:F:298:PRO:HD2	5:F:326:TRP:CG	2.56	0.41
1:G:168:ILE:H	1:G:168:ILE:HG12	1.57	0.41
1:G:59:VAL:HG21	1:G:85:LEU:HD13	2.01	0.41
2:I:1092:THR:HA	2:I:1093:PRO:HD3	1.82	0.41
2:I:234:ASP:OD1	2:I:235:ASN:N	2.53	0.41
2:I:888:THR:OG1	2:I:914:LYS:HB3	2.20	0.41
3:J:1163:VAL:HG11	3:J:1198:VAL:HG21	2.03	0.41
3:J:156:ARG:NH1	3:J:157:GLN:NE2	2.69	0.41
3:J:255:LEU:HD13	3:J:255:LEU:HA	1.76	0.41
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.89	0.41
1:B:113:ALA:HB2	1:B:126:PRO:HB3	2.01	0.41
1:B:196:THR:HG22	1:B:197:ASP:N	2.36	0.41
3:D:1282:TYR:HD2	3:D:1286:LYS:NZ	2.13	0.41
3:D:107:LEU:CD2	3:D:299:LEU:HD21	2.50	0.41
3:D:435:GLN:HB3	3:D:437:PHE:HE2	1.86	0.41
3:D:45:ASN:O	3:D:46:TYR:CD2	2.73	0.41
3:D:647:PRO:HG3	3:D:697:MET:N	2.36	0.41
3:D:863:LEU:HD11	3:D:901:ARG:HB3	2.02	0.41
5:F:465:ARG:HA	5:F:468:ARG:NH2	2.36	0.41
5:F:560:ARG:HA	5:F:565:ILE:HB	2.03	0.41
2:I:1117:LEU:HD21	2:I:1182:ILE:HD12	2.02	0.41
2:I:1234:LYS:CE	2:I:1238:LEU:HD23	2.50	0.41
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.48	0.41
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.55	0.41
2:I:42:ASP:O	2:I:44:GLU:N	2.48	0.41
3:J:1147:ALA:O	3:J:1218:HIS:NE2	2.54	0.41
3:J:650:LYS:HZ2	3:J:762:ASN:HD22	1.69	0.41
3:J:418:GLU:H	4:K:45:LYS:HZ3	1.68	0.41
1:B:109:PRO:HG3	1:B:132:HIS:CD2	2.55	0.41
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.41
3:D:1280:VAL:HG22	3:D:1284:ARG:HD2	2.02	0.41
3:D:24:LEU:HA	3:D:24:LEU:HD13	1.94	0.41
3:D:552:ILE:O	3:D:567:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:667:GLN:HG2	3:D:672:LEU:HD22	2.02	0.41
3:D:795:TYR:CE2	3:D:799:ARG:CZ	3.03	0.41
3:D:798:ARG:HH22	3:D:1325:PHE:HB3	1.84	0.41
3:D:81:ARG:C	3:D:83:VAL:N	2.74	0.41
5:F:562:ARG:NH2	5:F:573:LEU:HD23	2.36	0.41
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	2.03	0.41
2:I:1239:VAL:O	2:I:1242:LYS:N	2.50	0.41
2:I:93:SER:OG	2:I:126:GLU:OE1	2.22	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.77	0.41
2:I:237:LEU:HD13	2:I:237:LEU:HA	1.79	0.41
2:I:397:LEU:HB3	2:I:401:GLY:HA3	2.02	0.41
2:I:559:CYS:HB2	2:I:662:SER:HB3	2.01	0.41
3:J:316:ILE:HA	3:J:323:PRO:HA	2.02	0.41
3:J:723:TYR:CE1	3:J:727:ASP:HB2	2.56	0.41
3:J:735:ALA:O	3:J:739:GLN:HG3	2.21	0.41
3:J:843:VAL:HG13	3:J:883:ARG:HD3	2.02	0.41
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.50	0.41
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.61	0.41
1:A:106:GLY:HA2	1:A:136:GLU:O	2.21	0.41
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.94	0.41
2:C:358:ASP:OD2	2:C:361:SER:HB2	2.21	0.41
2:C:149:LEU:CD1	2:C:453:ILE:HG13	2.50	0.41
2:C:513:GLN:HE21	2:C:526:HIS:CE1	2.39	0.41
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	2.02	0.41
3:D:211:GLU:O	3:D:215:LYS:HB3	2.21	0.41
3:D:658:GLU:O	3:D:661:VAL:HG22	2.21	0.41
3:D:683:ILE:HD11	3:D:754:ILE:HG12	2.02	0.41
1:H:64:VAL:HG11	1:H:69:SER:HB2	2.03	0.41
2:I:596:ASP:CG	2:I:597:GLY:N	2.74	0.41
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.35	0.41
3:J:332:LYS:HA	3:J:337:ARG:H	1.85	0.41
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	2.03	0.41
5:L:405:ILE:HD13	5:L:405:ILE:HG21	1.79	0.41
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.20	0.41
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.84	0.41
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.54	0.41
1:B:75:GLN:HG2	1:B:76:GLU:OE1	2.21	0.41
2:C:145:ILE:HG21	2:C:456:VAL:HG13	2.03	0.41
2:C:481:LEU:H	2:C:481:LEU:HD22	1.86	0.41
2:C:533:LEU:HA	2:C:533:LEU:HD23	1.85	0.41
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.35	0.41
3:D:1278:GLU:OE1	3:D:1279:GLN:HG2	2.21	0.41
3:D:317:THR:HG23	3:D:320:ASN:CB	2.49	0.41
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.70	0.41
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.50	0.41
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.54	0.41
5:L:551:LEU:HD23	5:L:597:LYS:HD2	2.03	0.41
1:A:178:SER:HA	1:A:179:PRO:HD3	1.62	0.41
1:A:228:LEU:HA	1:A:231:PHE:HB2	2.03	0.41
1:A:53:GLY:O	1:A:148:ARG:HG3	2.21	0.41
2:C:1144:PHE:HE1	2:C:1201:LEU:HD11	1.86	0.41
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.56	0.41
2:C:248:GLY:O	2:C:249:GLU:HG3	2.21	0.41
2:C:42:ASP:O	2:C:44:GLU:N	2.51	0.41
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.02	0.41
2:C:55:SER:OG	2:C:56:VAL:N	2.54	0.41
3:D:1160:SER:HA	3:D:1204:VAL:O	2.21	0.41
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.85	0.41
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.23	0.41
3:D:501:VAL:HG23	3:D:602:SER:HB2	2.03	0.41
3:D:700:ASN:O	3:D:704:GLU:HB2	2.21	0.41
5:F:415:ALA:O	5:F:419:PHE:HB2	2.21	0.41
1:H:8:PHE:HB2	1:H:10:LYS:NZ	2.36	0.41
2:I:1255:THR:O	2:I:1257:GLN:N	2.54	0.41
2:I:519:ASN:HB3	2:I:522:SER:HB2	2.01	0.41
2:I:90:VAL:HG12	2:I:91:THR:N	2.36	0.41
3:J:1154:ALA:HB2	3:J:1213:GLY:O	2.21	0.41
3:J:1292:LEU:O	3:J:1293:GLU:HB2	2.21	0.41
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.21	0.41
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.03	0.41
3:J:702:GLN:HA	3:J:723:TYR:HE2	1.79	0.41
5:L:117:ILE:O	5:L:121:LYS:N	2.39	0.41
5:L:608:ARG:O	5:L:611:LEU:HB2	2.21	0.41
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.21	0.41
2:C:1131:MET:CE	2:C:1141:LEU:HD12	2.48	0.41
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	2.03	0.41
2:C:149:LEU:HD22	2:C:530:ILE:HG21	2.02	0.41
2:C:483:ASP:HB2	2:C:486:THR:HG22	2.01	0.41
3:D:1165:PHE:CD1	3:D:1165:PHE:N	2.88	0.41
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.86	0.41
3:D:504:GLN:CG	3:D:505:ASP:H	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:111:LEU:HD23	5:F:111:LEU:HA	1.78	0.41
5:F:269:LEU:HD23	5:F:269:LEU:HA	1.84	0.41
5:F:531:PRO:O	5:F:533:ASP:N	2.54	0.41
1:G:190:ALA:O	1:G:191:ARG:HD3	2.20	0.41
2:I:22:LEU:HB3	2:I:655:VAL:HG11	2.03	0.41
2:I:845:LEU:HG	2:I:845:LEU:H	1.56	0.41
3:J:1179:PRO:HG2	3:J:1183:SER:O	2.21	0.41
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.56	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
5:L:276:MET:O	5:L:280:VAL:HG23	2.20	0.41
5:L:343:LYS:H	5:L:343:LYS:HD2	1.85	0.41
5:L:547:VAL:HG13	5:L:598:LEU:HD22	2.03	0.41
1:A:92:VAL:HB	1:A:120:ASP:HB3	2.04	0.40
1:B:109:PRO:HB3	1:B:132:HIS:HD2	1.86	0.40
2:C:103:VAL:C	2:C:104:ILE:HD12	2.41	0.40
2:C:1233:LEU:HD13	2:C:1233:LEU:N	2.35	0.40
2:C:63:SER:C	2:C:65:ASN:H	2.25	0.40
2:C:879:GLY:HA2	2:C:920:VAL:HG12	2.03	0.40
3:D:123:ARG:NH1	3:D:1334:GLU:HG3	2.36	0.40
2:C:1272:GLU:H	3:D:342:LEU:CB	2.34	0.40
5:F:599:ARG:O	5:F:604:SER:HB2	2.21	0.40
2:I:5:TYR:CD1	2:I:8:LYS:HD3	2.42	0.40
3:J:1146:GLU:O	3:J:1147:ALA:HB3	2.20	0.40
3:J:712:GLN:HB2	3:J:713:GLU:H	1.65	0.40
5:L:482:GLU:HA	5:L:485:GLU:OE2	2.20	0.40
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.80	0.40
1:A:123:ILE:O	1:A:125:LYS:N	2.54	0.40
2:C:1111:GLN:HB2	2:C:1230:MET:HE2	2.04	0.40
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.22	0.40
2:C:139:ASN:HA	2:C:139:ASN:HD22	1.66	0.40
2:C:210:LEU:O	2:C:215:TYR:HB2	2.21	0.40
2:C:4:SER:O	2:C:8:LYS:HB3	2.21	0.40
2:C:500:ALA:O	2:C:504:GLU:HB2	2.21	0.40
3:D:122:SER:O	3:D:126:LEU:HG	2.22	0.40
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.20	0.40
3:D:1314:LEU:O	3:D:1326:GLN:NE2	2.52	0.40
3:D:252:LEU:HD23	3:D:252:LEU:HA	1.84	0.40
3:D:368:LEU:HD22	3:D:373:ALA:HB2	2.02	0.40
3:D:526:VAL:HA	3:D:549:LYS:O	2.21	0.40
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.86	0.40
5:F:540:LEU:HD23	5:F:544:THR:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:ARG:HD2	1:G:195:ARG:HA	1.85	0.40
1:G:224:LEU:O	1:G:228:LEU:HB2	2.21	0.40
1:G:32:GLU:HB2	1:G:35:PHE:CD2	2.56	0.40
2:I:13:LYS:NZ	2:I:1151:LEU:HB2	2.35	0.40
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.51	0.40
2:I:972:PHE:HD2	2:I:975:ILE:HD12	1.87	0.40
3:J:751:ASP:HB3	3:J:753:SER:H	1.86	0.40
3:J:819:GLY:HA3	3:J:882:VAL:O	2.21	0.40
5:L:394:TYR:OH	5:L:436:ARG:HD2	2.20	0.40
5:L:584:ARG:HD2	5:L:584:ARG:HA	1.84	0.40
2:C:159:SER:O	2:C:160:ASP:HB2	2.21	0.40
2:C:395:TYR:HB3	2:C:419:ILE:HG22	2.03	0.40
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.52	0.40
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.52	0.40
2:C:920:VAL:HA	2:C:921:PRO:HD3	1.70	0.40
3:D:54:ASP:HB2	3:D:61:ILE:HD11	2.03	0.40
5:F:124:GLU:O	5:F:127:ILE:HG13	2.21	0.40
5:F:280:VAL:O	5:F:284:GLU:HG3	2.22	0.40
1:G:47:LEU:HD13	1:G:183:ILE:HG12	2.04	0.40
1:G:79:LEU:O	1:G:79:LEU:HD13	2.20	0.40
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.37	0.40
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.52	0.40
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.51	0.40
2:I:553:THR:H	2:I:553:THR:HG1	1.52	0.40
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.89	0.40
3:J:526:VAL:HA	3:J:549:LYS:O	2.22	0.40
3:J:709:ARG:HD2	3:J:710:ASP:N	2.36	0.40
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.43	0.40
5:L:288:MET:CG	5:L:299:LYS:HE2	2.51	0.40
2:C:1062:PRO:HA	2:C:1076:ILE:HG13	2.03	0.40
2:C:1069:ARG:HH21	2:C:1114:GLU:CD	2.25	0.40
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.37	0.40
2:C:289:VAL:HG13	2:C:319:LEU:HD11	2.03	0.40
2:C:972:PHE:CB	2:C:994:ARG:HH21	2.34	0.40
3:D:1284:ARG:HH22	3:J:1292:LEU:HD11	1.87	0.40
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.02	0.40
5:F:493:LYS:HA	5:F:496:LYS:HG3	2.03	0.40
2:I:91:THR:HB	2:I:138:ILE:O	2.22	0.40
2:I:448:LEU:HD23	2:I:448:LEU:HA	1.83	0.40
2:I:888:THR:HG23	2:I:916:SER:OG	2.22	0.40
3:J:1287:ILE:H	3:J:1287:ILE:HG13	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:360:TYR:OH	3:J:442:ILE:HD11	2.21	0.40
3:J:650:LYS:HE2	3:J:654:ILE:HD11	2.03	0.40
1:A:88:LEU:HA	1:A:128:HIS:CD2	2.57	0.40
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.57	0.40
2:C:1252:SER:HB3	2:C:1255:THR:O	2.22	0.40
2:C:318:SER:OG	2:C:321:LEU:HB2	2.22	0.40
4:E:4:VAL:HG13	4:E:5:THR:HG23	2.02	0.40
3:D:392:THR:CG2	5:F:606:VAL:HA	2.51	0.40
1:G:77:ASP:O	1:G:81:ILE:HG13	2.22	0.40
1:H:195:ARG:HB3	1:H:198:LEU:HD21	2.04	0.40
2:I:1164:PHE:O	2:I:1166:ASP:N	2.55	0.40
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.25	0.40
2:I:534:GLY:HA3	2:I:535:PRO:HD2	1.78	0.40
2:I:582:ASN:HB3	2:I:586:PHE:N	2.33	0.40
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.03	0.40
3:J:104:HIS:HA	3:J:244:VAL:HG13	2.02	0.40
3:J:382:TYR:HE1	3:J:401:VAL:HG21	1.86	0.40
5:L:288:MET:HG2	5:L:299:LYS:HE2	2.03	0.40
5:L:320:ILE:O	5:L:327:SER:HB3	2.21	0.40
5:L:384:LEU:HA	5:L:384:LEU:HD23	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:712:GLN:NE2	2:I:862:LEU:O[4_545]	2.14	0.06

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	317/329 (96%)	246 (78%)	53 (17%)	18 (6%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/329 (65%)	193 (91%)	16 (8%)	4 (2%)	9	51
1	G	225/329 (68%)	198 (88%)	18 (8%)	9 (4%)	3	34
1	H	212/329 (64%)	196 (92%)	12 (6%)	4 (2%)	9	51
2	C	1338/1342 (100%)	1205 (90%)	112 (8%)	21 (2%)	11	54
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	11	54
3	D	1162/1407 (83%)	1030 (89%)	105 (9%)	27 (2%)	7	47
3	J	1151/1407 (82%)	1027 (89%)	98 (8%)	26 (2%)	7	47
4	E	87/91 (96%)	81 (93%)	5 (6%)	1 (1%)	17	61
4	K	77/91 (85%)	71 (92%)	3 (4%)	3 (4%)	3	34
5	F	462/613 (75%)	423 (92%)	32 (7%)	7 (2%)	12	55
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	11	53
All	All	7045/8222 (86%)	6292 (89%)	604 (9%)	149 (2%)	8	49

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO
1	A	242	VAL
1	A	320	ASN
1	B	193	GLU
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1153	ALA
2	C	1154	ASP
2	C	1159	VAL
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	89	GLY
3	D	426	ALA
3	D	496	GLY

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Mol	Chain	Res	Type
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	569	THR
1	G	162	GLU
1	G	167	PRO
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	496	GLY
3	J	710	ASP
3	J	712	GLN
3	J	805	GLN
3	J	850	LYS
3	J	1294	ALA
4	K	15	ASN
4	K	33	GLY
5	L	584	ARG
1	A	50	SER
1	A	119	GLY
1	A	164	ASP
1	A	232	VAL
1	A	315	GLY
1	B	13	LEU
2	C	121	GLU
3	D	805	GLN
3	D	1274	PHE

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Mol	Chain	Res	Type
5	F	566	ASP
5	F	584	ARG
1	G	168	ILE
1	H	138	ALA
2	I	1059	ARG
2	I	1165	SER
3	J	89	GLY
3	J	314	ARG
3	J	332	LYS
3	J	339	ARG
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
1	A	62	ASP
1	A	319	GLU
1	A	324	ALA
1	B	136	GLU
1	B	138	ALA
2	C	163	LYS
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY
3	D	314	ARG
3	D	417	ARG
3	D	1344	LEU
5	F	602	SER
1	G	229	GLU
1	H	193	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	417	ARG
3	J	745	GLY
4	K	14	GLY
2	C	62	TYR
2	C	813	GLU
2	C	1158	LYS
3	D	828	GLY

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Mol	Chain	Res	Type
3	D	1297	LYS
2	I	201	ARG
2	I	696	ASP
2	I	813	GLU
2	I	892	GLU
3	J	344	GLY
3	J	1344	LEU
5	L	585	GLU
1	A	318	LEU
2	C	1059	ARG
2	C	1256	GLN
3	D	46	TYR
3	D	345	LYS
1	H	20	SER
2	I	160	ASP
2	I	756	TYR
3	J	338	PHE
3	J	357	VAL
1	A	19	VAL
2	C	983	GLY
3	D	357	VAL
3	D	806	ASP
5	F	96	ASP
1	G	9	LEU
1	G	164	ASP
5	L	395	THR
3	D	120	LEU
3	J	173	GLY
3	J	333	GLY
3	J	639	VAL
3	D	82	GLY
3	D	826	ILE
5	F	361	ILE
1	G	166	ARG
3	J	336	GLY
5	L	475	GLY
3	D	831	VAL
2	I	1202	GLY
1	A	293	PRO
2	C	897	PRO
3	D	1184	ASP
1	G	14	VAL

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Mol	Chain	Res	Type
1	H	30	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	278/286 (97%)	227 (82%)	51 (18%)	2	13
1	B	186/286 (65%)	171 (92%)	15 (8%)	14	50
1	G	193/286 (68%)	164 (85%)	29 (15%)	3	23
1	H	183/286 (64%)	170 (93%)	13 (7%)	17	56
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	12	47
2	I	1154/1157 (100%)	1053 (91%)	101 (9%)	12	47
3	D	962/1168 (82%)	876 (91%)	86 (9%)	11	47
3	J	960/1168 (82%)	873 (91%)	87 (9%)	11	46
4	E	72/75 (96%)	63 (88%)	9 (12%)	5	31
4	K	67/75 (89%)	60 (90%)	7 (10%)	8	39
5	F	417/540 (77%)	385 (92%)	32 (8%)	15	52
5	L	418/540 (77%)	379 (91%)	39 (9%)	10	45
All	All	6045/7024 (86%)	5474 (91%)	571 (9%)	10	44

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	18	GLN
1	A	26	VAL
1	A	29	GLU
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	66	HIS

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Mol	Chain	Res	Type
1	A	70	THR
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL
1	A	99	ILE
1	A	105	SER
1	A	116	THR
1	A	125	LYS
1	A	133	LEU
1	A	139	SER
1	A	159	ILE
1	A	164	ASP
1	A	165	GLU
1	A	166	ARG
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL
1	A	195	ARG
1	A	207	THR
1	A	211	ILE
1	A	223	ILE
1	A	231	PHE
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	258	ASP
1	A	262	LEU
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU
1	A	302	GLU
1	A	306	VAL
1	A	316	MET
1	A	318	LEU
1	A	320	ASN

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Mol	Chain	Res	Type
1	B	9	LEU
1	B	16	ILE
1	B	27	THR
1	B	60	GLU
1	B	62	ASP
1	B	64	VAL
1	B	79	LEU
1	B	95	LYS
1	B	102	LEU
1	B	124	VAL
1	B	139	SER
1	B	183	ILE
1	B	191	ARG
1	B	196	THR
1	B	233	ASP
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	23	ASP
2	C	46	GLN
2	C	81	ASP
2	C	103	VAL
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR
2	C	135	THR
2	C	150	HIS
2	C	164	THR
2	C	201	ARG
2	C	208	ILE
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	377	THR
2	C	384	LEU
2	C	423	ASP
2	C	455	SER
2	C	471	VAL

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Mol	Chain	Res	Type
2	C	481	LEU
2	C	484	LEU
2	C	485	ASP
2	C	490	GLN
2	C	492	MET
2	C	518	ASN
2	C	525	THR
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	553	THR
2	C	561	ILE
2	C	575	LEU
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	663	VAL
2	C	672	GLU
2	C	694	ARG
2	C	697	LYS
2	C	714	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	778	GLU
2	C	781	ASP
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU

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Mol	Chain	Res	Type
2	C	1037	THR
2	C	1054	LEU
2	C	1059	ARG
2	C	1076	ILE
2	C	1082	ILE
2	C	1098	LEU
2	C	1134	GLN
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1233	LEU
2	C	1237	HIS
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1296	ASP
2	C	1310	ASP
2	C	1313	HIS
2	C	1327	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	11	GLN
3	D	12	THR
3	D	46	TYR
3	D	47	ARG
3	D	54	ASP
3	D	79	LYS
3	D	93	THR
3	D	95	THR
3	D	97	VAL

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Mol	Chain	Res	Type
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	248	ASP
3	D	252	LEU
3	D	259	ARG
3	D	292	VAL
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	374	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	413	ASP
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	490	ILE
3	D	505	ASP
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	560	ASN
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	639	VAL
3	D	641	ILE
3	D	678	ARG
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	753	SER
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	772	TYR
3	D	797	THR

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Mol	Chain	Res	Type
3	D	801	VAL
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG
3	D	890	THR
3	D	897	HIS
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	918	ILE
3	D	1135	THR
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1199	PHE
3	D	1221	LEU
3	D	1251	LYS
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1366	HIS
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL

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Mol	Chain	Res	Type
4	E	58	LEU
4	E	62	GLN
5	F	98	VAL
5	F	114	GLU
5	F	154	GLU
5	F	163	THR
5	F	261	LEU
5	F	277	MET
5	F	305	LEU
5	F	306	PHE
5	F	338	HIS
5	F	364	ARG
5	F	399	LEU
5	F	401	PHE
5	F	449	THR
5	F	471	LEU
5	F	472	GLN
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	516	ASP
5	F	526	THR
5	F	527	THR
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	569	THR
5	F	572	THR
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	33	ARG
1	G	50	SER
1	G	70	THR

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Mol	Chain	Res	Type
1	G	79	LEU
1	G	90	VAL
1	G	101	THR
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	145	LYS
1	G	156	SER
1	G	161	SER
1	G	163	GLU
1	G	166	ARG
1	G	168	ILE
1	G	171	LEU
1	G	178	SER
1	G	187	VAL
1	G	192	VAL
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	219	ARG
1	G	231	PHE
1	H	18	GLN
1	H	27	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	68	TYR
1	H	75	GLN
1	H	95	LYS
1	H	102	LEU
1	H	124	VAL
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	46	GLN
2	I	86	GLN
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE

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Mol	Chain	Res	Type
2	I	131	THR
2	I	132	ASP
2	I	138	ILE
2	I	156	PHE
2	I	164	THR
2	I	197	ARG
2	I	201	ARG
2	I	208	ILE
2	I	285	ILE
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	384	LEU
2	I	423	ASP
2	I	453	ILE
2	I	455	SER
2	I	471	VAL
2	I	481	LEU
2	I	484	LEU
2	I	485	ASP
2	I	490	GLN
2	I	492	MET
2	I	518	ASN
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	540	ARG
2	I	542	ARG
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	596	ASP
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	633	LEU
2	I	635	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU

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Mol	Chain	Res	Type
2	I	694	ARG
2	I	705	GLU
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	757	THR
2	I	764	CYS
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	828	PHE
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	919	ARG
2	I	922	ASN
2	I	951	MET
2	I	992	LEU
2	I	1005	GLU
2	I	1037	THR
2	I	1054	LEU
2	I	1082	ILE
2	I	1083	GLU
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1198	LEU
2	I	1210	ILE
2	I	1227	VAL
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER

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Mol	Chain	Res	Type
2	I	1254	VAL
2	I	1265	PHE
2	I	1287	LEU
2	I	1296	ASP
2	I	1299	ASN
2	I	1313	HIS
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	47	ARG
3	J	54	ASP
3	J	79	LYS
3	J	92	VAL
3	J	93	THR
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	206	ASN
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	259	ARG
3	J	292	VAL
3	J	324	LEU
3	J	343	LEU
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE
3	J	413	ASP
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG

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Mol	Chain	Res	Type
3	J	429	LEU
3	J	505	ASP
3	J	510	LEU
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	560	ASN
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	641	ILE
3	J	678	ARG
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	772	TYR
3	J	797	THR
3	J	801	VAL
3	J	810	THR
3	J	827	GLU
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	877	VAL
3	J	897	HIS
3	J	898	CYS
3	J	908	ILE
3	J	910	ASN
3	J	918	ILE
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1186	TYR
3	J	1194	ARG
3	J	1199	PHE

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Mol	Chain	Res	Type
3	J	1204	VAL
3	J	1221	LEU
3	J	1251	LYS
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1282	TYR
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	3	ARG
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	102	MET
5	L	114	GLU
5	L	154	GLU
5	L	261	LEU
5	L	266	PHE
5	L	277	MET
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	401	PHE
5	L	405	ILE
5	L	429	THR
5	L	445	ASP
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP

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Mol	Chain	Res	Type
5	L	526	THR
5	L	527	THR
5	L	552	THR
5	L	558	VAL
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
5	L	613	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	HIS
2	C	46	GLN
2	C	139	ASN
2	C	513	GLN
2	C	620	ASN
2	C	760	ASN
2	C	952	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1220	GLN
2	C	1236	ASN
2	C	1237	HIS
2	C	1299	ASN
2	C	1314	GLN
3	D	200	GLN
3	D	365	GLN
3	D	419	HIS
3	D	424	ASN
3	D	690	ASN
3	D	716	GLN
3	D	1366	HIS

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Mol	Chain	Res	Type
5	F	129	GLN
5	F	131	GLN
5	F	147	GLN
5	F	258	GLN
5	F	406	GLN
5	F	446	GLN
5	F	469	GLN
5	F	545	HIS
5	F	579	GLN
5	F	600	HIS
1	G	66	HIS
2	I	139	ASN
2	I	165	HIS
2	I	620	ASN
2	I	1038	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1220	GLN
2	I	1237	HIS
2	I	1299	ASN
3	J	200	GLN
3	J	206	ASN
3	J	294	ASN
3	J	365	GLN
3	J	424	ASN
3	J	430	HIS
3	J	435	GLN
3	J	450	HIS
3	J	477	GLN
3	J	690	ASN
3	J	716	GLN
3	J	817	HIS
3	J	929	GLN
3	J	1235	ASN
3	J	1295	ASN
3	J	1366	HIS
5	L	258	GLN
5	L	301	ASN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	319/329 (96%)	-0.36	1 (0%) 93 90	84, 129, 182, 196	0
1	B	217/329 (65%)	-0.18	5 (2%) 61 48	91, 164, 203, 214	0
1	G	227/329 (68%)	-0.28	1 (0%) 92 88	126, 154, 181, 218	0
1	H	216/329 (65%)	-0.10	3 (1%) 75 64	118, 174, 198, 207	0
2	C	1340/1342 (99%)	-0.38	19 (1%) 75 64	58, 114, 218, 253	0
2	I	1340/1342 (99%)	-0.19	44 (3%) 47 35	93, 148, 222, 378	0
3	D	1166/1407 (82%)	-0.39	2 (0%) 94 92	63, 107, 168, 218	0
3	J	1155/1407 (82%)	-0.27	14 (1%) 79 68	85, 128, 189, 228	0
4	E	89/91 (97%)	-0.59	0 100 100	67, 116, 140, 152	0
4	K	79/91 (86%)	-0.27	1 (1%) 77 65	99, 139, 205, 222	0
5	F	468/613 (76%)	-0.17	19 (4%) 38 27	93, 160, 273, 305	0
5	L	469/613 (76%)	-0.15	13 (2%) 53 41	114, 172, 279, 307	0
All	All	7085/8222 (86%)	-0.28	122 (1%) 70 58	58, 135, 209, 378	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	11.2
5	F	319	ALA	6.7
2	I	983	GLY	5.4
5	L	318	ALA	5.0
2	I	981	ALA	4.9
2	I	1004	ASP	4.9
2	I	998	LEU	4.8
2	I	979	LEU	4.7
5	F	325	PRO	4.6
2	I	1005	GLU	4.6
2	I	1003	THR	4.6

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Mol	Chain	Res	Type	RSRZ
5	L	315	TRP	4.4
3	J	208	THR	4.4
2	I	1007	LYS	4.4
2	I	1006	GLU	4.4
2	I	999	GLU	4.3
2	C	231	GLU	4.3
2	I	1002	LEU	4.0
5	F	318	ALA	3.9
2	I	1001	GLY	3.9
5	F	323	ASN	3.9
5	F	315	TRP	3.7
3	J	212	THR	3.6
2	I	1011	LEU	3.6
3	J	1297	LYS	3.5
3	J	521	LYS	3.5
2	I	1008	GLN	3.5
5	L	314	THR	3.4
2	C	332	ARG	3.4
5	F	337	VAL	3.4
2	C	333	ILE	3.3
5	L	167	ASP	3.3
1	G	193	GLU	3.2
5	F	313	ASP	3.2
3	J	1198	VAL	3.2
2	I	1000	LEU	3.1
5	F	321	ALA	3.1
2	I	1010	GLN	3.1
1	H	107	ILE	3.1
2	I	984	VAL	3.0
5	L	290	LEU	3.0
1	H	13	LEU	3.0
5	F	312	SER	3.0
2	C	373	GLY	2.9
3	J	857	LEU	2.9
2	I	601	ASP	2.9
5	L	321	ALA	2.9
2	I	978	VAL	2.9
3	J	830	ASP	2.9
5	L	322	MET	2.8
5	L	319	ALA	2.8
1	B	97	GLU	2.8
1	B	160	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	I	165	HIS	2.8
5	L	305	LEU	2.8
3	J	856	ILE	2.8
5	F	167	ASP	2.7
2	C	271	ALA	2.7
5	L	317	ASN	2.7
3	J	674	THR	2.7
2	I	985	GLU	2.7
5	L	111	LEU	2.7
2	C	265	LYS	2.7
5	F	322	MET	2.6
2	I	375	PRO	2.6
2	I	1009	ASN	2.6
1	B	98	VAL	2.6
2	C	1004	ASP	2.6
2	I	970	GLY	2.6
3	J	1375	ALA	2.6
2	C	251	ALA	2.6
3	J	209	ASN	2.6
2	I	413	GLU	2.6
5	F	314	THR	2.5
5	F	310	GLU	2.5
5	L	323	ASN	2.5
2	C	331	LYS	2.5
2	I	414	ILE	2.5
2	I	975	ILE	2.5
3	D	1202	GLU	2.5
2	C	1002	LEU	2.4
2	I	1020	GLU	2.4
5	L	490	PRO	2.4
2	C	267	ARG	2.4
2	I	111	GLU	2.4
2	C	338	THR	2.4
2	C	540	ARG	2.4
2	I	980	VAL	2.4
5	F	478	PRO	2.3
2	C	247	ARG	2.3
1	H	12	ARG	2.3
1	B	96	ASP	2.3
2	I	1025	PHE	2.3
2	I	1017	GLN	2.3
2	C	1003	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	972	PHE	2.2
5	F	307	THR	2.2
2	C	165	HIS	2.2
2	I	441	GLU	2.2
2	I	740	GLU	2.2
2	I	376	PRO	2.2
2	I	976	ARG	2.2
2	I	988	LYS	2.2
2	I	986	ALA	2.1
3	J	542	ALA	2.1
5	F	477	GLU	2.1
2	I	190	PRO	2.1
2	I	987	GLU	2.1
5	F	283	GLN	2.1
2	C	266	GLY	2.1
3	J	214	ARG	2.1
4	K	58	LEU	2.1
2	I	969	ALA	2.0
5	F	305	LEU	2.0
2	I	1012	GLU	2.0
1	A	241	GLU	2.0
3	J	708	ASN	2.0
1	B	65	LEU	2.0
2	C	270	THR	2.0
5	F	514	ASP	2.0
2	C	317	LEU	2.0
3	D	213	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
7	ZN	D	2003	1/1	0.99	0.17	-0.64	94,94,94,94	0
7	ZN	D	2002	1/1	0.99	0.09	-1.07	113,113,113,113	0
7	ZN	J	2003	1/1	0.98	0.11	-1.08	94,94,94,94	0
7	ZN	J	2002	1/1	0.97	0.05	-1.43	105,105,105,105	0
6	MG	J	2001	1/1	0.96	0.25	-	94,94,94,94	0
6	MG	C	1401	1/1	0.95	0.51	-	94,94,94,94	0
6	MG	I	1401	1/1	0.96	0.44	-	94,94,94,94	0
6	MG	D	2001	1/1	0.96	0.35	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.