



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2017 – 05:17 PM EST

PDB ID : 5UAL
Title : Escherichia coli RNA polymerase and Rifampin complex, RpoB S531L mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.89 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

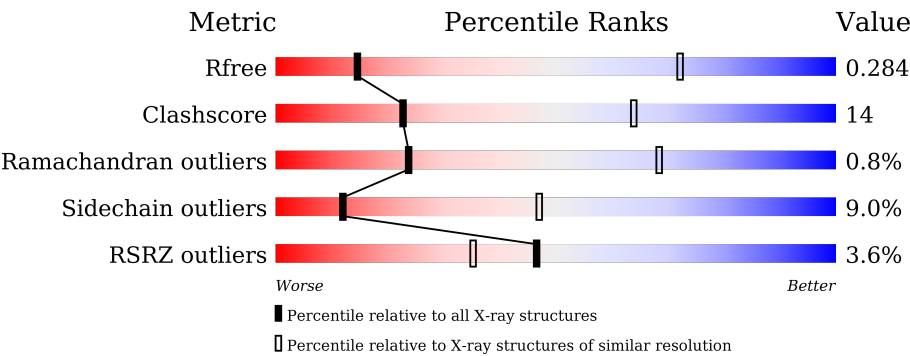
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (4.24-3.52)
Clashscore	102246	1026 (4.20-3.56)
Ramachandran outliers	100387	1003 (4.22-3.54)
Sidechain outliers	100360	1043 (4.24-3.52)
RSRZ outliers	91569	1009 (4.24-3.52)

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	<div><div>0.1%</div><div>44%</div><div>22%</div><div>•</div><div>31%</div></div>
1	B	329	<div><div>2%</div><div>39%</div><div>24%</div><div>•</div><div>35%</div></div>
1	G	329	<div><div>0.1%</div><div>41%</div><div>23%</div><div>•</div><div>32%</div></div>
1	H	329	<div><div>2%</div><div>37%</div><div>26%</div><div>•</div><div>35%</div></div>
2	C	1342	<div><div>5%</div><div>62%</div><div>34%</div><div>••</div></div>
2	I	1342	<div><div>5%</div><div>67%</div><div>29%</div><div>••</div></div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>52%27%•17%</div></div>
3	J	1407	<div><div><div></div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>53%25%•18%</div></div>
4	E	91	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>78%18%••</div></div>
4	K	91	<div><div><div></div><div></div><div></div><div></div></div><div>21%</div><div><div></div><div></div><div></div><div></div></div><div>56%27%•13%</div></div>
5	F	613	<div><div><div></div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>50%23%•24%</div></div>
5	L	613	<div><div><div></div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>53%21%•23%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54898 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	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1332	Total	C	N	O	S	0	0	0
			10514	6600	1827	2043	44			
2	I	1328	Total	C	N	O	S	0	0	0
			10486	6583	1822	2038	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	LEU	SER	engineered mutation	UNP P0A8V2
I	531	LEU	SER	engineered mutation	UNP P0A8V2

- 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
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

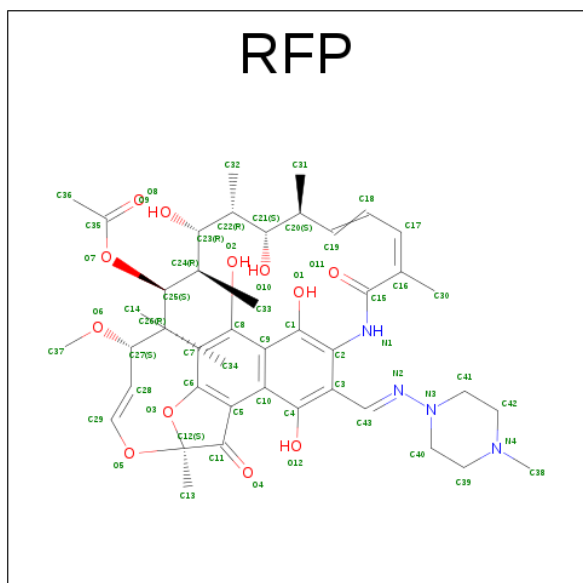
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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 RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



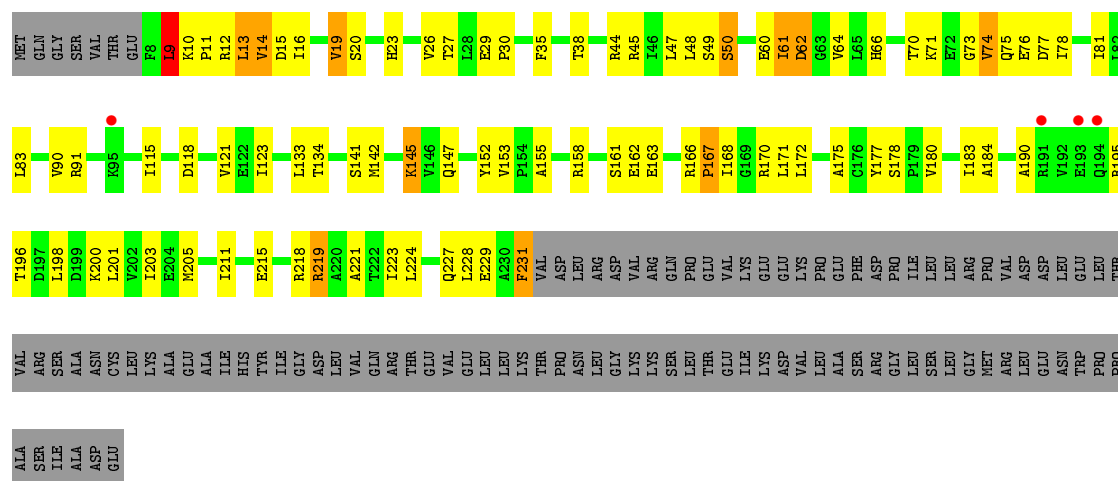
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

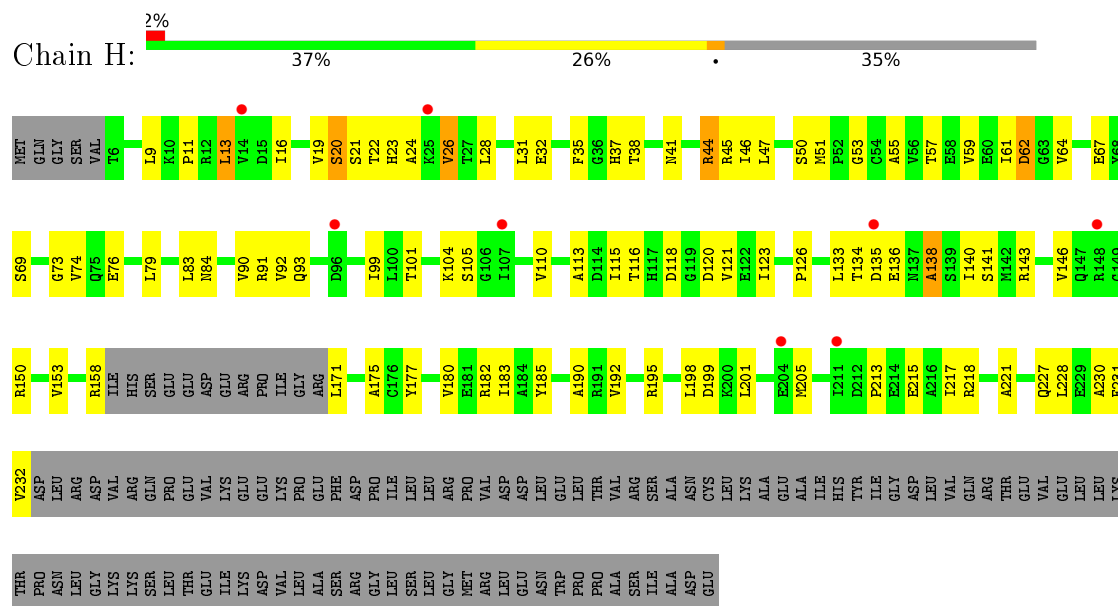
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

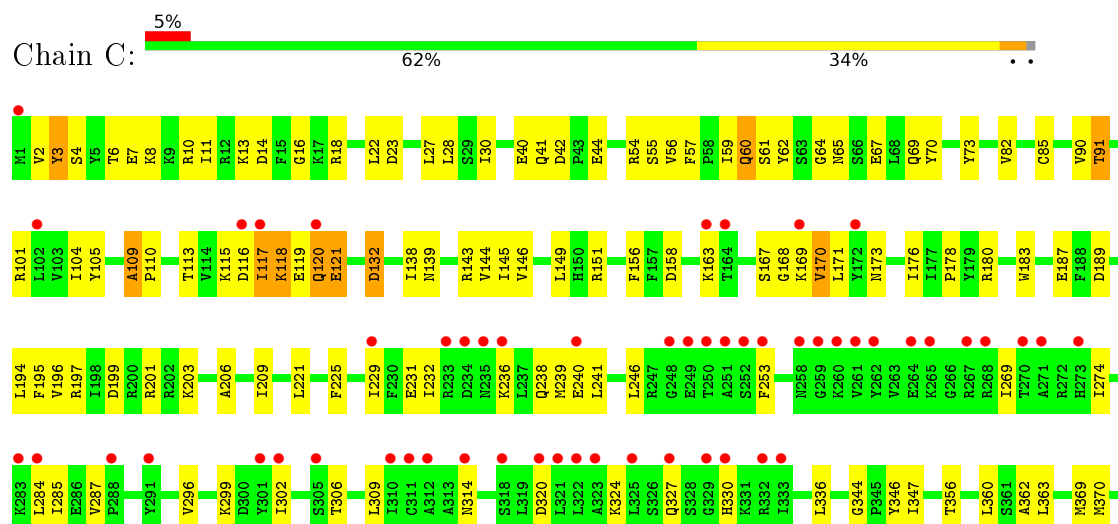
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total 2	Zn 2	0	0
8	D	2	Total 2	Zn 2	0	0

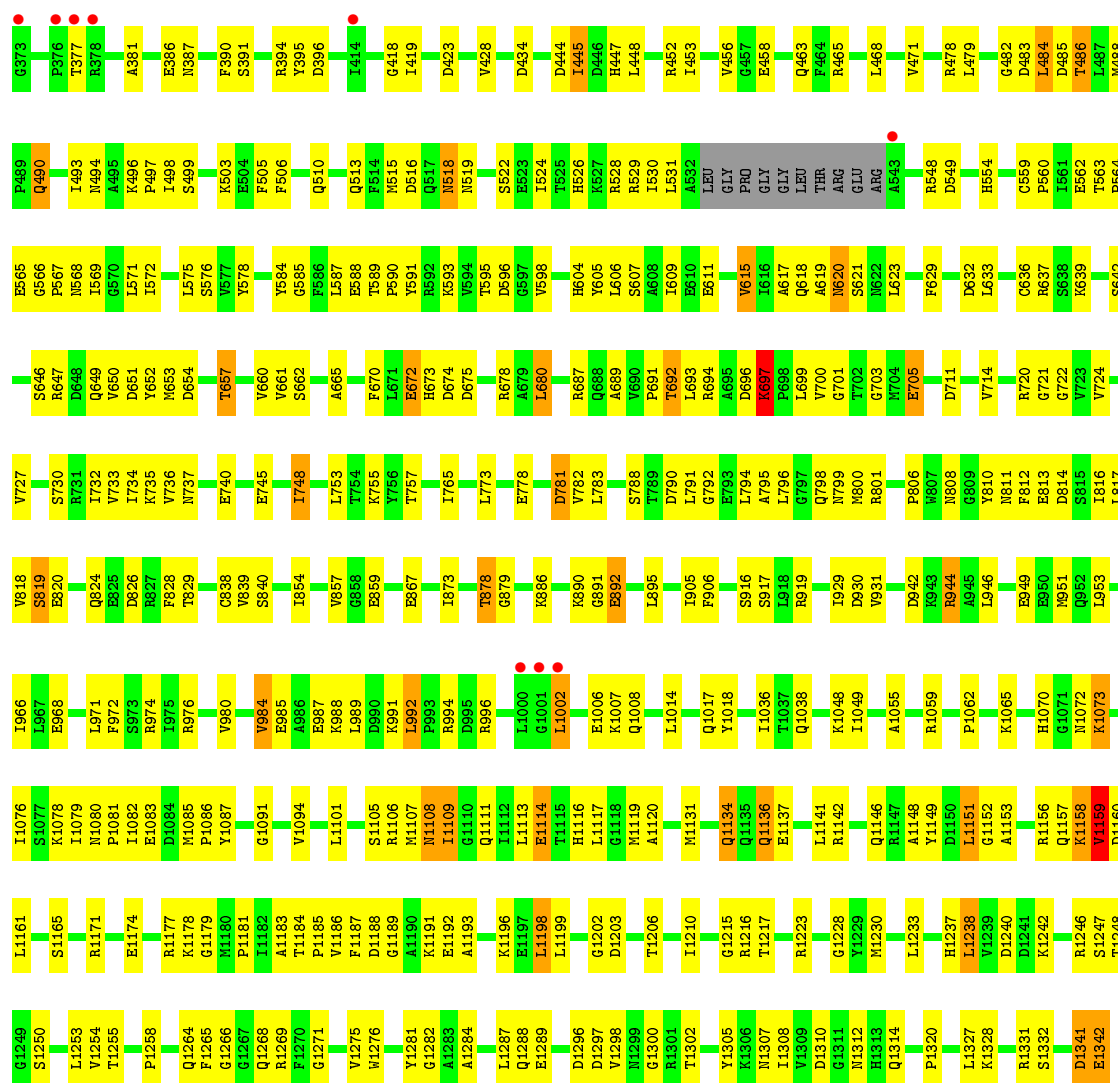


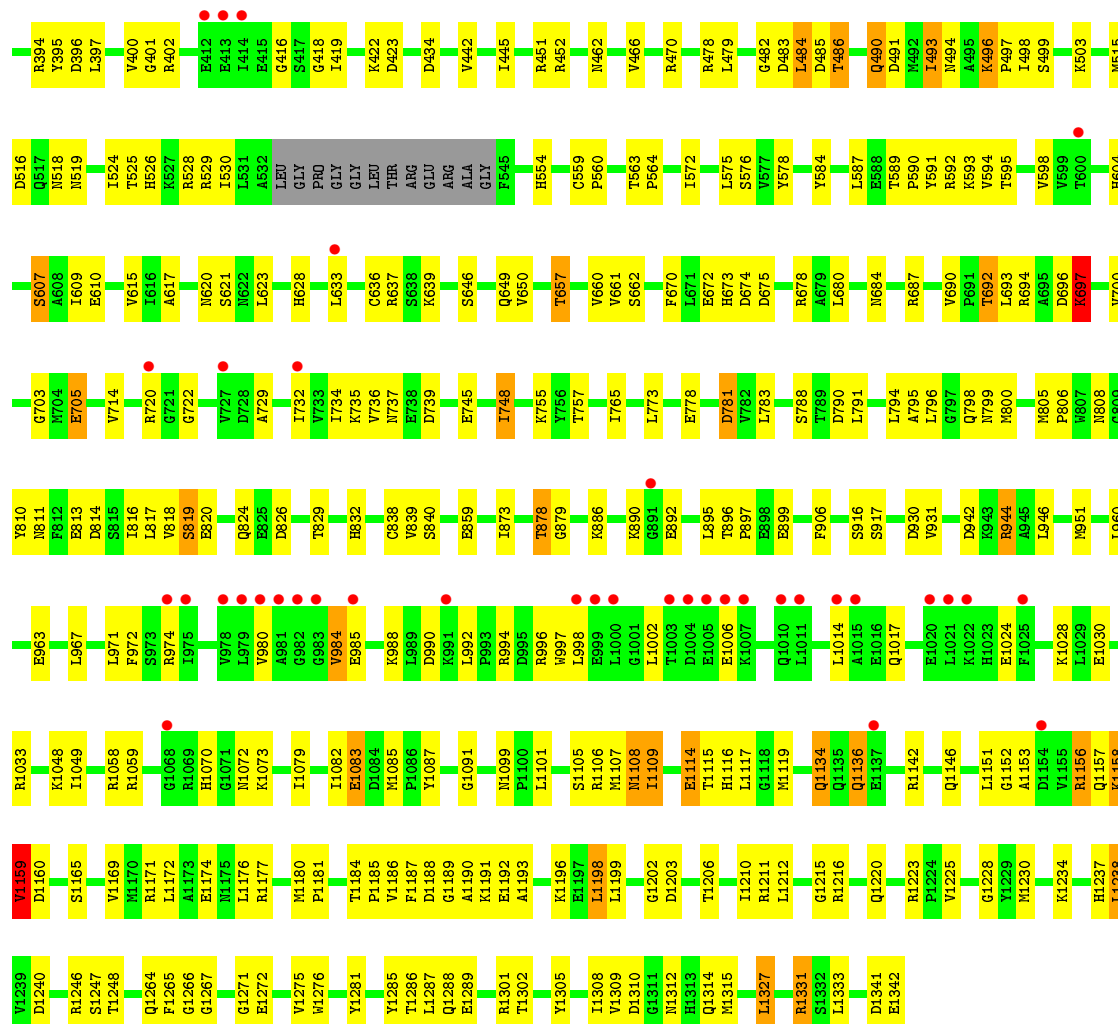
• Molecule 1: DNA-directed RNA polymerase subunit alpha



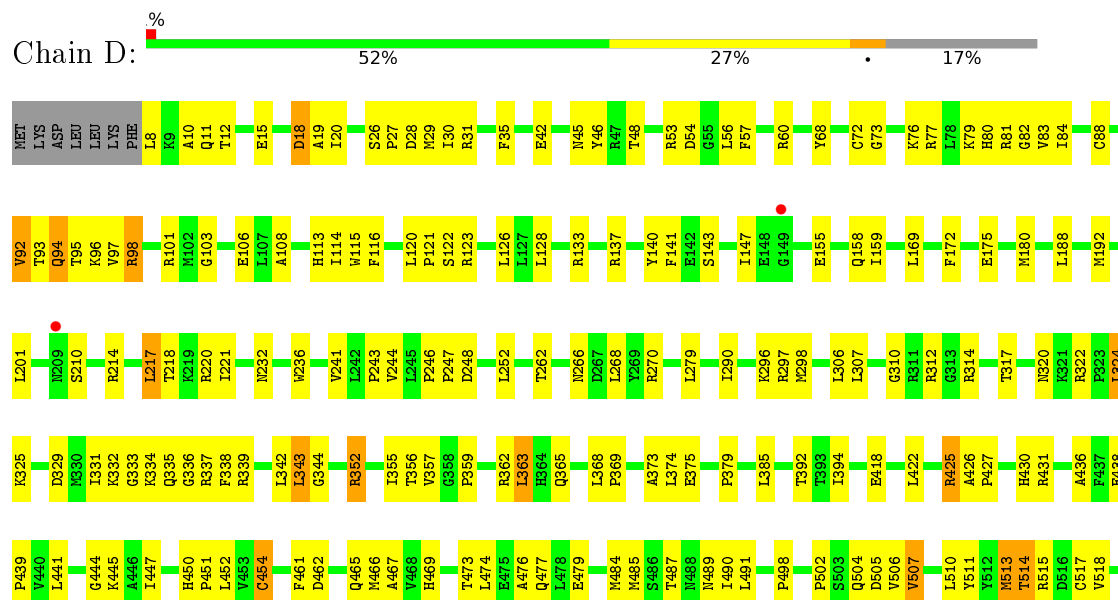
• Molecule 2: DNA-directed RNA polymerase subunit beta

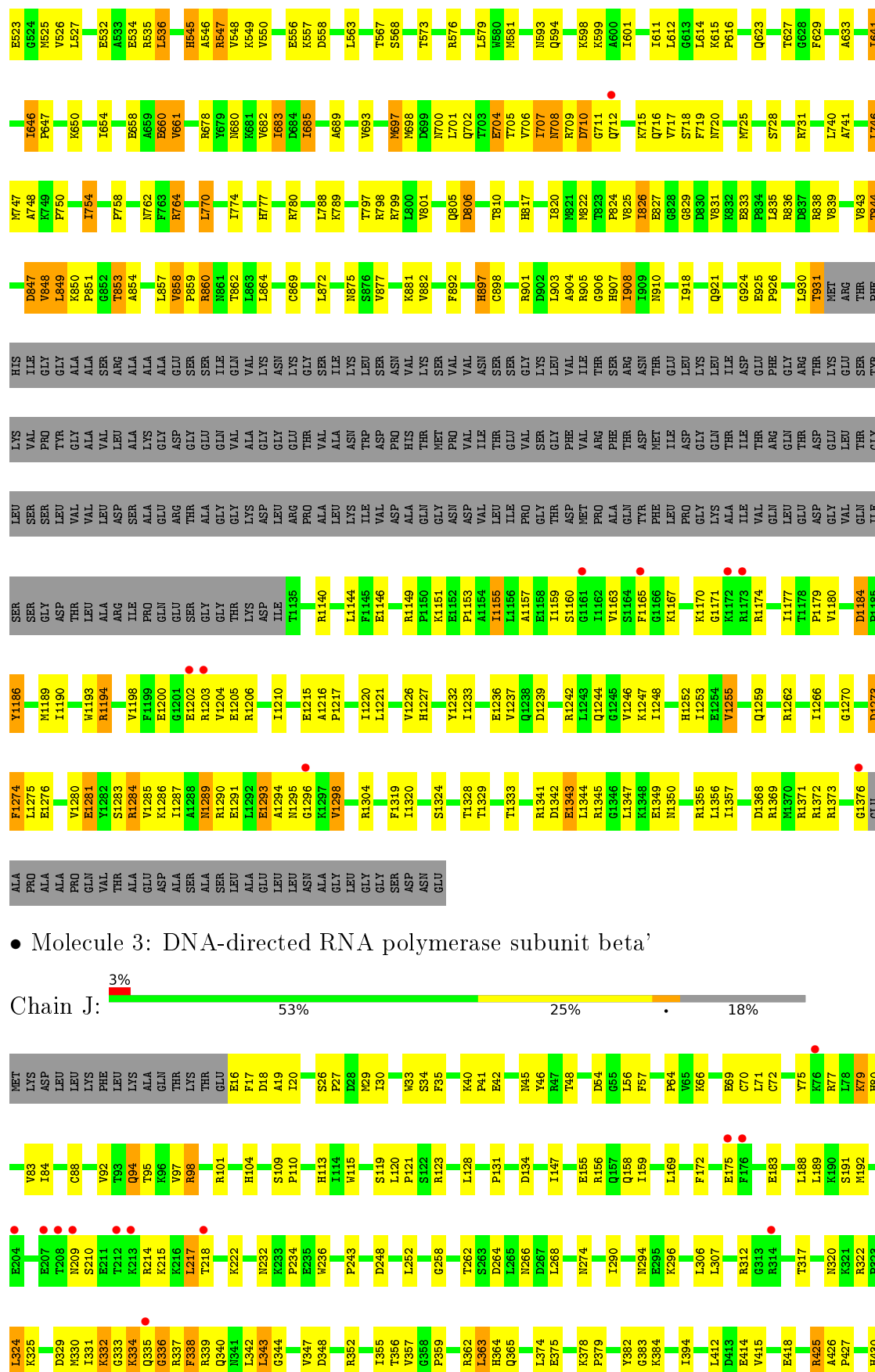


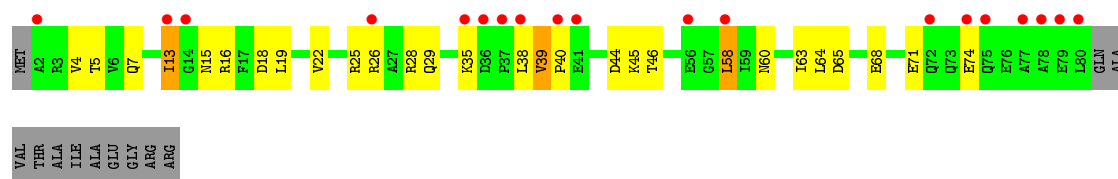




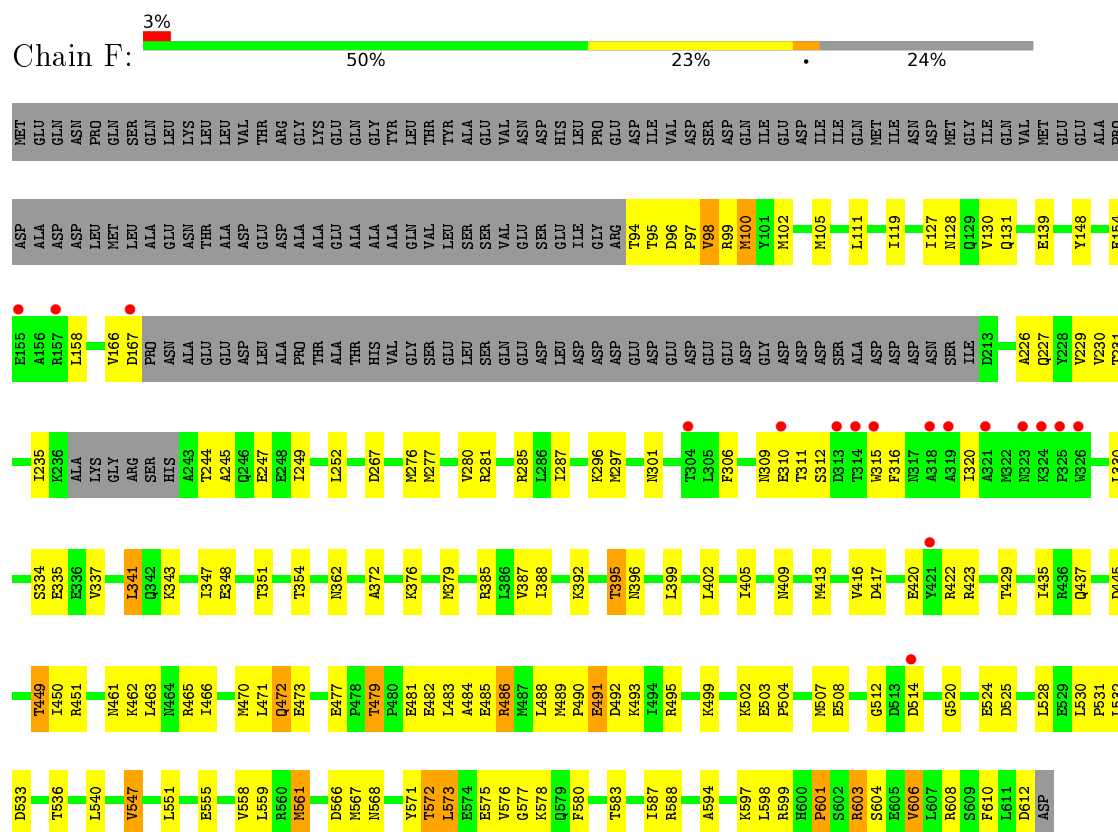
• Molecule 3: DNA-directed RNA polymerase subunit beta'



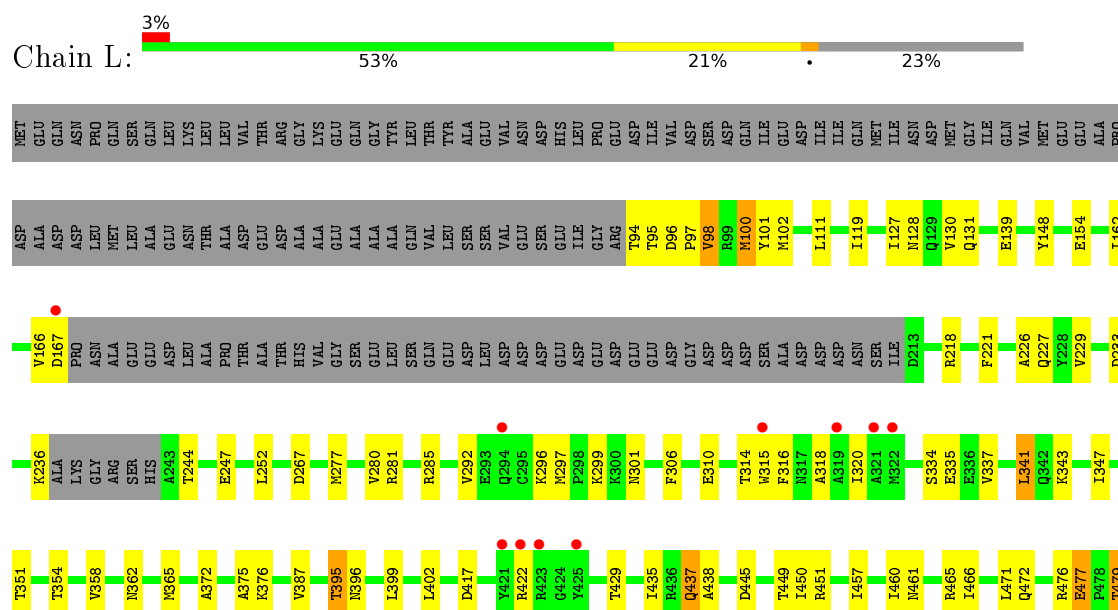


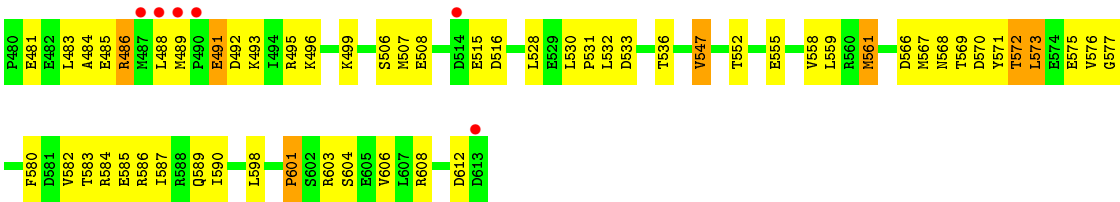


- Molecule 5: RNA polymerase sigma factor RpoD



- 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	187.37Å 205.95Å 309.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.89 29.94 – 3.89	Depositor EDS
% Data completeness (in resolution range)	82.9 (29.94-3.89) 82.9 (29.94-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.86Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.230 , 0.286 0.225 , 0.284	Depositor DCC
R_{free} test set	1975 reflections (2.16%)	DCC
Wilson B-factor (Å ²)	168.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 134.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54898	wwPDB-VP
Average B, all atoms (Å ²)	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, RFP, 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	0.42	1/1774 (0.1%)	0.57	0/2405
1	B	0.34	0/1668	0.71	2/2260 (0.1%)
1	G	0.36	1/1751 (0.1%)	0.55	1/2373 (0.0%)
1	H	0.29	0/1678	0.62	0/2274
2	C	0.37	0/10681	0.57	0/14410
2	I	0.30	0/10653	0.53	0/14373
3	D	0.39	1/9229 (0.0%)	0.61	0/12459
3	J	0.34	0/9140	0.58	2/12341 (0.0%)
4	E	0.29	0/693	0.51	0/935
4	K	0.26	0/629	0.47	0/847
5	F	0.30	0/3864	0.53	0/5194
5	L	0.28	0/3872	0.50	0/5205
All	All	0.34	3/55632 (0.0%)	0.57	5/75076 (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	2
5	F	0	1
5	L	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	C-N	10.64	1.54	1.34
1	G	29	GLU	C-N	9.19	1.51	1.34
3	D	898	CYS	CB-SG	-5.28	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	343	LEU	CA-CB-CG	12.07	143.06	115.30
1	B	9	LEU	C-N-CA	9.90	146.46	121.70
1	G	9	LEU	C-N-CA	5.58	135.64	121.70
3	J	857	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	13	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (10) 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	1296	GLY	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	601	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1780	64	0
1	B	1649	0	1673	71	0
1	G	1730	0	1756	66	0
1	H	1659	0	1692	72	0
2	C	10514	0	10531	335	0
2	I	10486	0	10496	268	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9089	0	9263	310	0
3	J	9001	0	9167	288	0
4	E	691	0	695	11	0
4	K	627	0	634	22	0
5	F	3813	0	3880	96	0
5	L	3821	0	3884	82	0
6	C	59	0	56	9	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	54898	0	55507	1505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1505) 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)
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.36	1.07
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.44	0.99
2:C:1269:ARG:HG3	3:D:343:LEU:HD12	1.49	0.94
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.50	0.91
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.52	0.91
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.54	0.89
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.53	0.89
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.55	0.88
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.40	0.85
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.56	0.85
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.57	0.85
3:D:342:LEU:HA	3:D:343:LEU:HD23	1.59	0.85
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.62	0.81
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.59	0.81
5:L:97:PRO:HA	5:L:100:MET:HG3	1.60	0.81
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.63	0.80
1:G:45:ARG:HG2	1:H:38:THR:HB	1.62	0.80
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.46	0.79
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.63	0.79
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.65	0.79
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.63	0.78
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ARG:HH11	1:H:232:VAL:HG22	1.48	0.78
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.66	0.78
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.67	0.77
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.67	0.77
1:B:29:GLU:OE1	1:B:200:LYS:HE2	1.84	0.77
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.18	0.77
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.50	0.77
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.66	0.76
2:I:560:PRO:O	3:J:780:ARG:NH2	2.18	0.76
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.67	0.76
2:C:1271:GLY:HA2	3:D:343:LEU:CD2	2.15	0.76
1:H:23:HIS:HB2	1:H:205:MET:O	1.86	0.76
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.19	0.75
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.68	0.75
2:C:1247:SER:HB3	3:D:375:GLU:O	1.87	0.75
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.69	0.74
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.20	0.74
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.68	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.53	0.74
3:D:576:ARG:NH1	3:D:593:ASN:O	2.20	0.74
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.69	0.74
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.21	0.73
5:F:598:LEU:O	5:F:604:SER:OG	2.06	0.73
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.69	0.73
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.70	0.73
3:J:665:GLN:HE22	3:J:678:ARG:HH21	1.36	0.72
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.54	0.72
3:J:156:ARG:NH2	3:J:191:SER:OG	2.21	0.72
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.71	0.72
2:I:324:LYS:O	2:I:327:GLN:NE2	2.22	0.72
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.23	0.72
3:J:436:ALA:HB3	3:J:485:MET:HA	1.72	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.22	0.71
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.72	0.71
3:D:700:ASN:O	3:D:704:GLU:HB2	1.89	0.71
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.22	0.71
2:I:18:ARG:NH1	2:I:621:SER:O	2.22	0.71
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.24	0.71
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.72	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.73	0.70
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:NH1	3:D:581:MET:SD	2.64	0.70
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.71	0.70
2:I:452:ARG:NH1	2:I:584:TYR:O	2.23	0.70
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.57	0.70
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.73	0.70
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.57	0.70
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.39	0.69
1:G:23:HIS:HB2	1:G:205:MET:O	1.92	0.69
1:G:12:ARG:H	1:G:30:PRO:HD2	1.56	0.69
3:J:700:ASN:O	3:J:704:GLU:HB2	1.91	0.69
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.92	0.69
5:F:97:PRO:HA	5:F:100:MET:HG3	1.73	0.69
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.75	0.69
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.74	0.69
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.73	0.69
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.73	0.69
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.74	0.69
1:A:45:ARG:HG2	1:B:38:THR:HB	1.74	0.69
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.74	0.69
5:F:316:PHE:HZ	5:F:334:SER:HA	1.56	0.69
1:A:23:HIS:HB2	1:A:205:MET:O	1.92	0.68
2:I:30:ILE:HD12	2:I:30:ILE:H	1.59	0.68
5:L:316:PHE:HZ	5:L:334:SER:HA	1.57	0.68
2:C:197:ARG:NH1	2:C:201:ARG:O	2.25	0.68
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.58	0.68
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.74	0.68
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.58	0.68
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.59	0.68
1:B:23:HIS:HB2	1:B:205:MET:O	1.94	0.67
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.76	0.67
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.76	0.67
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.42	0.67
1:A:12:ARG:H	1:A:30:PRO:HD2	1.58	0.67
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.76	0.67
3:D:392:THR:HG21	5:F:606:VAL:HA	1.76	0.67
1:H:101:THR:H	1:H:116:THR:HG22	1.60	0.67
1:A:14:VAL:HG22	1:A:15:ASP:H	1.60	0.67
1:B:102:LEU:HD11	1:B:110:VAL:HG11	1.75	0.67
2:C:615:VAL:HG13	2:C:651:ASP:H	1.60	0.67
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	1.94	0.67
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.25	0.67
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.09	0.67
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.77	0.66
3:J:848:VAL:HG11	3:J:880:VAL:HG22	1.76	0.66
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.26	0.66
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.76	0.66
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.77	0.66
1:B:32:GLU:OE2	1:B:195:ARG:NH2	2.29	0.66
2:C:30:ILE:H	2:C:30:ILE:HD12	1.61	0.66
3:J:901:ARG:HD2	3:J:906:GLY:O	1.95	0.66
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.26	0.66
1:G:14:VAL:HG22	1:G:15:ASP:H	1.61	0.66
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.76	0.66
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.61	0.66
3:J:576:ARG:NH1	3:J:593:ASN:O	2.28	0.66
2:C:40:GLU:O	2:C:73:TYR:OH	2.13	0.66
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.78	0.66
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.76	0.66
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.29	0.66
3:J:514:THR:HB	3:J:576:ARG:HG2	1.78	0.66
2:C:386:GLU:HA	2:C:390:PHE:HD2	1.61	0.65
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.94	0.65
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.26	0.65
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.77	0.65
2:C:721:GLY:N	2:C:740:GLU:OE1	2.29	0.65
2:C:531:LEU:HD13	6:C:3001:RFP:H141	1.78	0.65
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.76	0.65
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.28	0.65
6:C:3001:RFP:O1	6:C:3001:RFP:O11	2.14	0.65
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.79	0.65
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.30	0.65
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.11	0.65
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.79	0.65
2:I:499:SER:O	2:I:503:LYS:HB2	1.98	0.64
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.78	0.64
1:B:181:GLU:HA	3:D:535:ARG:HH21	1.60	0.64
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.62	0.64
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.79	0.64
2:I:109:ALA:HB1	2:I:110:PRO:C	2.17	0.64
2:I:27:LEU:O	2:I:528:ARG:NH1	2.30	0.64
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.79	0.64
3:J:418:GLU:HG3	4:K:45:LYS:H	1.62	0.64
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.62	0.64
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.79	0.64
2:I:155:VAL:HG23	2:I:176:ILE:HG12	1.80	0.64
5:L:601:PRO:HB3	5:L:608:ARG:HH22	1.62	0.64
2:C:109:ALA:HB1	2:C:110:PRO:C	2.19	0.64
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.31	0.64
1:H:67:GLU:OE1	1:H:67:GLU:N	2.31	0.64
2:I:40:GLU:O	2:I:73:TYR:OH	2.16	0.63
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.80	0.63
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.81	0.63
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.30	0.63
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.98	0.63
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.14	0.63
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.80	0.63
3:J:843:VAL:HG11	3:J:897:HIS:O	1.99	0.63
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.63	0.63
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.62	0.63
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.81	0.63
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.80	0.63
1:G:166:ARG:O	1:G:168:ILE:N	2.32	0.62
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.80	0.62
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.81	0.62
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.82	0.62
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.80	0.62
2:C:905:ILE:O	5:F:599:ARG:NH1	2.31	0.62
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.80	0.62
1:A:166:ARG:O	1:A:168:ILE:N	2.32	0.62
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.32	0.62
3:D:1155:ILE:HD13	3:D:1190:ILE:HD13	1.81	0.62
3:D:343:LEU:CD2	3:D:344:GLY:HA3	2.23	0.62
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.64	0.62
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.81	0.62
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.35	0.62
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.80	0.62
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.80	0.62
2:C:560:PRO:O	3:D:780:ARG:NH2	2.31	0.62
1:G:62:ASP:OD1	1:G:141:SER:OG	2.15	0.62
1:H:16:ILE:HG23	1:H:26:VAL:HG13	1.81	0.62
3:J:901:ARG:HA	3:J:908:ILE:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.35	0.62
1:H:53:GLY:HA3	1:H:177:TYR:O	2.00	0.62
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.82	0.62
2:C:6:THR:OG1	2:C:781:ASP:OD2	2.13	0.62
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.63	0.62
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.31	0.62
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.15	0.62
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.81	0.62
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.64	0.62
3:D:140:TYR:O	3:D:297:ARG:NH1	2.33	0.62
3:D:901:ARG:HA	3:D:908:ILE:HA	1.80	0.61
2:C:705:GLU:HB2	2:C:794:LEU:H	1.65	0.61
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.81	0.61
2:C:27:LEU:O	2:C:528:ARG:NH1	2.31	0.61
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.81	0.61
5:F:479:THR:HG23	5:F:481:GLU:H	1.66	0.61
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.81	0.61
5:L:601:PRO:HA	5:L:604:SER:HB2	1.82	0.61
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.82	0.61
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.83	0.61
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.82	0.61
2:I:1271:GLY:HA3	3:J:343:LEU:HD12	1.83	0.61
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.65	0.61
1:B:182:ARG:H	1:B:206:GLU:HB2	1.65	0.61
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.83	0.61
3:J:45:ASN:HB3	3:J:48:THR:O	2.01	0.61
2:C:588:GLU:HG3	2:C:605:TYR:HD1	1.66	0.61
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.36	0.61
1:H:32:GLU:OE2	1:H:195:ARG:NH2	2.33	0.61
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.66	0.61
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.82	0.60
5:F:573:LEU:H	5:F:573:LEU:HD23	1.64	0.60
3:D:1344:LEU:HB3	3:D:1350:ASN:HD21	1.65	0.60
5:L:533:ASP:O	5:L:536:THR:N	2.32	0.60
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.65	0.60
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.32	0.60
3:D:336:GLY:HA3	3:D:1324:SER:O	2.01	0.60
5:L:316:PHE:CZ	5:L:334:SER:HA	2.36	0.60
2:C:516:ASP:OD2	2:C:522:SER:OG	2.20	0.60
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.83	0.60
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.83	0.60
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.84	0.60
3:D:298:MET:SD	5:F:402:LEU:HB3	2.42	0.60
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.66	0.60
1:H:64:VAL:HG11	1:H:69:SER:OG	2.01	0.60
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.67	0.59
1:H:74:VAL:HG12	1:H:76:GLU:H	1.67	0.59
1:B:53:GLY:HA3	1:B:177:TYR:O	2.02	0.59
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.02	0.59
3:D:342:LEU:HA	3:D:343:LEU:CD2	2.31	0.59
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.36	0.59
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.84	0.59
2:C:528:ARG:NH2	2:C:576:SER:O	2.36	0.59
3:D:317:THR:HB	3:D:324:LEU:HB3	1.84	0.59
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.85	0.59
3:D:45:ASN:HB3	3:D:48:THR:O	2.02	0.59
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	2.03	0.59
3:D:847:ASP:OD1	3:D:847:ASP:N	2.33	0.59
3:J:115:TRP:O	3:J:119:SER:HB3	2.02	0.59
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.17	0.59
2:I:930:ASP:OD2	2:I:931:VAL:N	2.35	0.59
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.37	0.58
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.29	0.58
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.68	0.58
2:C:387:ASN:HA	2:C:391:SER:HB2	1.86	0.58
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.85	0.58
5:F:343:LYS:H	5:F:343:LYS:HD2	1.68	0.58
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.85	0.58
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.86	0.58
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.03	0.58
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.18	0.58
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.85	0.58
5:F:601:PRO:HA	5:F:604:SER:HB2	1.85	0.58
3:D:210:SER:O	3:D:214:ARG:HG2	2.03	0.58
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.86	0.58
1:G:161:SER:O	1:G:163:GLU:N	2.36	0.58
2:C:692:THR:OG1	2:C:693:LEU:N	2.36	0.58
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.67	0.58
2:C:930:ASP:OD2	2:C:931:VAL:N	2.36	0.58
3:D:436:ALA:HB3	3:D:485:MET:HA	1.85	0.58
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.84	0.58
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.67	0.58
3:J:683:ILE:HD11	3:J:754:ILE:HG23	1.86	0.58
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.85	0.58
2:C:2:VAL:O	2:C:3:TYR:HB2	2.03	0.58
2:C:529:ARG:NH1	6:C:3001:RFP:O11	2.36	0.58
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.84	0.58
3:D:56:LEU:HD12	3:D:56:LEU:H	1.69	0.58
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.69	0.58
3:D:525:MET:O	3:D:548:VAL:HG13	2.03	0.58
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.67	0.58
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.15	0.58
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.37	0.58
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.84	0.58
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.44	0.58
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.85	0.57
2:C:730:SER:O	2:C:753:LEU:HB2	2.04	0.57
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.19	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.85	0.57
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.66	0.57
3:J:709:ARG:O	3:J:711:GLY:N	2.38	0.57
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.85	0.57
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.85	0.57
1:A:13:LEU:H	1:A:13:LEU:HD23	1.70	0.57
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.87	0.57
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.86	0.57
2:C:617:ALA:HA	2:C:636:CYS:SG	2.43	0.57
3:D:425:ARG:HG2	3:D:426:ALA:H	1.68	0.57
2:I:607:SER:N	2:I:610:GLU:OE1	2.36	0.57
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.38	0.57
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.22	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.87	0.57
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.86	0.57
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.70	0.57
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.36	0.57
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.70	0.57
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.35	0.57
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.69	0.57
5:F:561:MET:HA	5:F:567:MET:HE1	1.87	0.57
3:J:1198:VAL:HB	3:J:1210:ILE:HA	1.87	0.57
5:L:479:THR:HG23	5:L:481:GLU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.85	0.57
3:D:1376:GLY:O	3:J:853:THR:OG1	2.21	0.57
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.70	0.57
1:A:161:SER:O	1:A:163:GLU:N	2.38	0.56
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.87	0.56
3:J:356:THR:OG1	3:J:357:VAL:N	2.38	0.56
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.85	0.56
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.87	0.56
1:H:190:ALA:N	1:H:198:LEU:O	2.33	0.56
2:I:208:ILE:HD11	2:I:365:GLU:HB3	1.85	0.56
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.38	0.56
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.56
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.56
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.86	0.56
1:B:55:ALA:O	1:B:146:VAL:HG13	2.04	0.56
1:B:6:THR:O	1:B:6:THR:OG1	2.16	0.56
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.85	0.56
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.87	0.56
5:F:540:LEU:HD12	5:F:610:PHE:CD1	2.39	0.56
3:D:1259:GLN:NE2	3:D:1262:ARG:HH12	2.03	0.56
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.88	0.56
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.86	0.56
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.87	0.56
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.52	0.56
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.88	0.56
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.87	0.56
1:G:49:SER:HB3	2:I:1083:GLU:HG2	1.88	0.56
2:I:684:ASN:OD1	2:I:687:ARG:NH1	2.39	0.56
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.87	0.56
2:C:201:ARG:NH2	2:C:370:MET:O	2.32	0.56
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.87	0.56
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.71	0.56
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.41	0.56
5:L:395:THR:OG1	5:L:396:ASN:N	2.36	0.56
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.88	0.56
5:F:348:GLU:HG2	5:F:354:THR:HA	1.86	0.56
5:L:601:PRO:HB3	5:L:608:ARG:NH2	2.21	0.56
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.87	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.06	0.56
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.88	0.55
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:362:ARG:H	3:J:365:GLN:NE2	2.04	0.55
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.88	0.55
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.89	0.55
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.89	0.55
3:D:843:VAL:HG11	3:D:897:HIS:O	2.06	0.55
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.86	0.55
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.07	0.55
5:F:533:ASP:O	5:F:536:THR:N	2.39	0.55
1:G:13:LEU:H	1:G:13:LEU:HD23	1.71	0.55
2:I:1271:GLY:CA	3:J:343:LEU:HD12	2.36	0.55
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.89	0.55
2:I:829:THR:HA	2:I:1059:ARG:HA	1.89	0.55
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.21	0.55
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.87	0.55
5:L:598:LEU:O	5:L:604:SER:OG	2.21	0.55
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.88	0.55
1:B:61:ILE:HG22	1:B:62:ASP:H	1.71	0.55
3:D:518:VAL:O	3:D:547:ARG:NH1	2.39	0.55
2:I:528:ARG:NH2	2:I:576:SER:O	2.40	0.55
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.87	0.55
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.89	0.55
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.89	0.55
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.41	0.55
2:I:692:THR:OG1	2:I:693:LEU:N	2.40	0.55
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.07	0.55
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.42	0.55
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.88	0.55
3:D:709:ARG:O	3:D:711:GLY:N	2.36	0.55
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.07	0.55
2:I:206:ALA:O	2:I:209:ILE:HG22	2.06	0.55
5:L:94:THR:OG1	5:L:95:THR:N	2.40	0.55
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.89	0.55
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.89	0.55
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.87	0.55
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.89	0.55
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.89	0.55
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.87	0.55
5:L:573:LEU:H	5:L:573:LEU:HD23	1.71	0.55
2:C:829:THR:HA	2:C:1059:ARG:HA	1.89	0.55
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.88	0.55
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.89	0.55
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.40	0.55
2:C:518:ASN:O	2:C:691:PRO:HD3	2.07	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.89	0.54
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.72	0.54
1:B:214:GLU:O	1:B:218:ARG:HG3	2.07	0.54
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.72	0.54
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.08	0.54
2:C:703:GLY:N	2:C:705:GLU:OE2	2.39	0.54
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.88	0.54
2:C:1296:ASP:HB3	2:C:1320:PRO:HB3	1.90	0.54
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.88	0.54
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.89	0.54
2:C:1131:MET:HE1	2:C:1141:LEU:HD12	1.89	0.54
2:C:91:THR:HG21	2:C:503:LYS:NZ	2.23	0.54
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.72	0.54
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.90	0.54
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.90	0.54
3:J:210:SER:O	3:J:214:ARG:HG2	2.08	0.54
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.73	0.54
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.90	0.54
4:E:80:LEU:O	4:E:84:THR:OG1	2.19	0.54
3:J:264:ASP:OD2	5:L:506:SER:OG	2.22	0.54
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.89	0.54
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.72	0.54
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.90	0.54
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.88	0.54
1:B:212:ASP:CG	1:B:215:GLU:HB2	2.28	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.88	0.54
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.90	0.54
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.54
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.43	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.89	0.54
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.43	0.53
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.90	0.53
2:C:562:GLU:OE2	2:C:662:SER:OG	2.17	0.53
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.48	0.53
3:J:338:PHE:HA	3:J:342:LEU:O	2.08	0.53
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.90	0.53
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:ALA:HB2	1:H:126:PRO:HB3	1.91	0.53
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.74	0.53
2:I:314:ASN:O	2:I:352:ARG:NH1	2.34	0.53
2:I:213:LEU:HB3	2:I:422:LYS:HD2	1.90	0.53
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.39	0.53
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.43	0.53
3:D:53:ARG:NH2	3:D:60:ARG:HD2	2.24	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.09	0.53
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.43	0.53
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.89	0.53
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.89	0.53
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.23	0.53
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.24	0.53
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.39	0.53
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.90	0.53
5:F:395:THR:OG1	5:F:396:ASN:N	2.40	0.53
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.90	0.53
2:I:819:SER:HB2	2:I:1085:MET:SD	2.49	0.53
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.89	0.53
2:C:819:SER:HB2	2:C:1085:MET:SD	2.47	0.53
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.73	0.53
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.91	0.53
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.49	0.53
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.91	0.53
1:H:182:ARG:HG3	3:J:534:GLU:OE1	2.09	0.53
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.73	0.53
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.08	0.53
2:C:471:VAL:HG21	2:C:498:ILE:HD11	1.90	0.53
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.91	0.53
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.90	0.53
2:I:598:VAL:HG22	2:I:628:HIS:HE1	1.74	0.53
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.08	0.53
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.90	0.53
1:B:195:ARG:HB2	1:B:198:LEU:HD21	1.91	0.53
2:C:548:ARG:NH2	2:C:567:PRO:O	2.42	0.53
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.73	0.53
1:H:59:VAL:O	1:H:171:LEU:N	2.41	0.53
3:J:1262:ARG:HD2	3:J:1279:GLN:OE1	2.09	0.53
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.90	0.53
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.09	0.53
5:L:130:VAL:HB	5:L:365:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.09	0.52
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.92	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.90	0.52
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.73	0.52
2:I:211:ARG:NH1	2:I:357:ASN:O	2.41	0.52
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.91	0.52
1:B:12:ARG:H	1:B:30:PRO:CD	2.22	0.52
2:C:886:LYS:H	2:C:917:SER:HB3	1.74	0.52
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.09	0.52
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.74	0.52
3:D:709:ARG:C	3:D:711:GLY:H	2.13	0.52
1:G:49:SER:OG	1:G:50:SER:N	2.40	0.52
1:H:55:ALA:O	1:H:146:VAL:HG13	2.08	0.52
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.92	0.52
1:A:45:ARG:HG2	1:B:38:THR:CB	2.38	0.52
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.92	0.52
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.73	0.52
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.91	0.52
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.91	0.52
3:D:654:ILE:O	3:D:658:GLU:HB2	2.10	0.52
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.90	0.52
2:C:490:GLN:HE21	5:F:472:GLN:NE2	2.07	0.52
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.92	0.52
5:F:483:LEU:H	5:F:483:LEU:HD12	1.74	0.52
1:H:35:PHE:HA	1:H:38:THR:HG22	1.92	0.52
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.92	0.52
3:J:847:ASP:N	3:J:847:ASP:OD1	2.35	0.52
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.09	0.52
1:H:59:VAL:N	1:H:171:LEU:O	2.32	0.52
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.91	0.52
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.74	0.52
2:I:878:THR:OG1	2:I:879:GLY:N	2.40	0.52
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.23	0.52
3:D:290:ILE:HD12	3:D:290:ILE:H	1.75	0.52
3:D:73:GLY:O	3:D:76:LYS:NZ	2.29	0.52
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.91	0.52
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.75	0.52
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.92	0.52
3:J:94:GLN:O	3:J:97:VAL:HG23	2.10	0.52
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.92	0.52
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1165:PHE:HE1	3:J:1200:GLU:HB3	1.75	0.52
2:I:1286:THR:N	3:J:479:GLU:OE2	2.39	0.52
4:K:25:ARG:NH2	4:K:68:GLU:OE1	2.43	0.52
3:J:1184:ASP:O	3:J:1186:TYR:N	2.42	0.52
3:J:709:ARG:C	3:J:711:GLY:H	2.13	0.52
5:L:314:THR:O	5:L:318:ALA:HB3	2.10	0.52
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.75	0.51
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.92	0.51
3:D:19:ALA:O	3:D:20:ILE:HG13	2.11	0.51
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.36	0.51
2:I:1247:SER:HB3	3:J:375:GLU:O	2.09	0.51
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.90	0.51
2:C:778:GLU:O	2:C:781:ASP:HB2	2.10	0.51
2:C:878:THR:OG1	2:C:879:GLY:N	2.42	0.51
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.92	0.51
2:I:462:ASN:O	2:I:466:VAL:HG23	2.09	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.10	0.51
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.92	0.51
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.75	0.51
2:I:170:VAL:HG23	2:I:171:LEU:N	2.25	0.51
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.09	0.51
4:K:13:ILE:HD12	4:K:19:LEU:HA	1.92	0.51
1:A:49:SER:OG	1:A:50:SER:N	2.43	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.46	0.51
2:C:516:ASP:HB2	6:C:3001:RFP:H20C	1.92	0.51
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.93	0.51
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.92	0.51
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.93	0.51
3:J:748:ALA:HA	3:J:754:ILE:HA	1.93	0.51
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.40	0.51
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.31	0.51
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.92	0.51
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.43	0.51
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.10	0.51
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.92	0.51
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.93	0.51
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.11	0.51
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.93	0.51
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.92	0.51
2:C:91:THR:HG21	2:C:503:LYS:HZ1	1.75	0.51
3:D:557:LYS:HA	3:D:563:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:789:LYS:NZ	3:D:931:THR:O	2.37	0.51
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.44	0.51
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.93	0.51
2:C:452:ARG:NH1	2:C:584:TYR:O	2.43	0.51
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.50	0.51
5:F:507:MET:HG2	5:F:520:GLY:CA	2.41	0.51
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.26	0.51
2:I:778:GLU:O	2:I:781:ASP:HB2	2.11	0.51
5:L:585:GLU:O	5:L:589:GLN:HG3	2.11	0.51
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.74	0.51
2:C:180:ARG:NH2	2:C:465:ARG:HH22	2.09	0.51
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.44	0.51
2:I:963:GLU:O	2:I:967:LEU:HB2	2.10	0.51
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.75	0.51
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.93	0.51
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.51	0.51
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.45	0.50
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.44	0.50
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.25	0.50
3:D:356:THR:OG1	3:D:357:VAL:N	2.44	0.50
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.93	0.50
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.77	0.50
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.60	0.50
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.93	0.50
2:C:170:VAL:HG23	2:C:171:LEU:N	2.26	0.50
3:D:103:GLY:CA	3:D:244:VAL:HG22	2.41	0.50
3:D:362:ARG:H	3:D:365:GLN:HE21	1.60	0.50
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.93	0.50
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.32	0.50
1:H:62:ASP:OD1	1:H:141:SER:OG	2.28	0.50
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.93	0.50
2:I:516:ASP:H	2:I:526:HIS:HD1	1.57	0.50
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.12	0.50
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.93	0.50
1:H:31:LEU:HB2	1:H:199:ASP:O	2.11	0.50
2:I:23:ASP:N	2:I:23:ASP:OD1	2.45	0.50
3:J:19:ALA:O	3:J:20:ILE:HG13	2.11	0.50
2:C:510:GLN:HE21	6:C:3001:RFP:H131	1.76	0.50
3:D:1295:ASN:OD1	3:J:1206:ARG:NH2	2.45	0.50
2:I:168:GLY:C	2:I:170:VAL:H	2.14	0.50
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:96:ASP:O	5:L:98:VAL:N	2.44	0.50
1:B:182:ARG:HG3	3:D:534:GLU:OE1	2.10	0.50
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.76	0.50
2:I:617:ALA:HA	2:I:636:CYS:SG	2.51	0.50
3:J:1165:PHE:CE1	3:J:1200:GLU:HB3	2.47	0.50
1:A:233:ASP:C	1:A:234:LEU:HD22	2.32	0.50
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	1.94	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.94	0.50
1:G:9:LEU:HD21	1:G:195:ARG:NH2	2.27	0.50
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.93	0.50
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.27	0.50
5:L:127:ILE:O	5:L:130:VAL:HG22	2.12	0.50
1:H:90:VAL:HG23	1:H:123:ILE:HD13	1.93	0.50
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.10	0.50
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.47	0.50
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.93	0.49
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.76	0.49
3:D:42:GLU:CG	5:F:451:ARG:HE	2.25	0.49
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.93	0.49
2:I:490:GLN:HG2	2:I:491:ASP:N	2.26	0.49
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.77	0.49
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.77	0.49
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.47	0.49
1:B:35:PHE:HA	1:B:38:THR:HG22	1.92	0.49
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.94	0.49
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.94	0.49
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.47	0.49
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.47	0.49
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.94	0.49
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.94	0.49
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.77	0.49
2:I:466:VAL:O	2:I:470:ARG:HG2	2.13	0.49
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.94	0.49
5:L:166:VAL:O	5:L:167:ASP:HB2	2.12	0.49
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	0.49
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.93	0.49
6:C:3001:RFP:O9	6:C:3001:RFP:O10	2.26	0.49
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.94	0.49
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.93	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.49
1:B:183:ILE:CD1	1:B:205:MET:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.47	0.49
2:C:529:ARG:HH12	6:C:3001:RFP:C18	2.26	0.49
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.27	0.49
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.94	0.49
3:D:473:THR:HG23	3:D:476:ALA:H	1.77	0.49
2:I:396:ASP:HA	2:I:418:GLY:O	2.13	0.49
3:D:11:GLN:HG2	3:D:15:GLU:HG2	1.95	0.49
3:D:363:LEU:HG	3:D:363:LEU:O	2.12	0.49
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.26	0.49
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.28	0.49
3:J:70:CYS:SG	3:J:71:LEU:N	2.85	0.49
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.49
1:A:73:GLY:O	1:A:134:THR:HG22	2.12	0.49
2:C:101:ARG:HG3	2:C:118:LYS:HD2	1.93	0.49
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.93	0.49
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.94	0.49
3:J:362:ARG:H	3:J:365:GLN:HE21	1.60	0.49
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.48	0.49
2:C:566:GLY:O	2:C:569:ILE:HG13	2.11	0.49
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.24	0.49
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.26	0.49
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.48	0.49
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.13	0.49
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.28	0.49
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.22	0.49
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.95	0.49
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.95	0.49
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.12	0.49
3:J:110:PRO:HG2	3:J:183:GLU:HG2	1.94	0.49
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.47	0.48
2:C:44:GLU:HA	2:C:54:ARG:NH1	2.28	0.48
3:D:514:THR:OG1	3:D:594:GLN:O	2.31	0.48
3:D:517:CYS:HA	3:D:716:GLN:NE2	2.28	0.48
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.95	0.48
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.28	0.48
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.93	0.48
2:I:262:TYR:HE1	2:I:280:ASP:OD2	1.96	0.48
3:J:914:ALA:O	3:J:918:ILE:HG23	2.13	0.48
1:A:185:TYR:HE1	2:C:1087:TYR:HH	1.59	0.48
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.94	0.48
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:94:GLN:O	3:D:97:VAL:HG23	2.12	0.48
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.94	0.48
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.28	0.48
3:J:290:ILE:HD12	3:J:290:ILE:H	1.77	0.48
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.95	0.48
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.48	0.48
3:J:838:ARG:NH1	3:J:1250:ASP:OD1	2.46	0.48
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.44	0.48
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.95	0.48
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.79	0.48
3:D:418:GLU:HG3	4:E:45:LYS:H	1.79	0.48
5:F:244:THR:O	5:F:247:GLU:HG2	2.11	0.48
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.95	0.48
3:J:209:ASN:HA	3:J:214:ARG:HE	1.77	0.48
1:H:83:LEU:HD11	3:J:526:VAL:CG2	2.43	0.48
2:C:513:GLN:OE1	6:C:3001:RFP:H343	2.14	0.48
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.95	0.48
3:D:214:ARG:HA	3:D:217:LEU:HB2	1.95	0.48
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.95	0.48
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.96	0.48
3:J:748:ALA:O	3:J:777:HIS:HD2	1.97	0.48
2:C:548:ARG:HB3	2:C:569:ILE:O	2.13	0.48
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.14	0.48
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.13	0.48
2:C:1281:TYR:OH	3:D:431:ARG:O	2.30	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.95	0.48
1:G:45:ARG:HG2	1:H:38:THR:CB	2.39	0.48
1:G:73:GLY:O	1:G:134:THR:HG22	2.13	0.48
2:I:138:ILE:HB	2:I:143:ARG:HD3	1.95	0.48
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.32	0.48
5:L:483:LEU:H	5:L:483:LEU:HD12	1.76	0.48
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.94	0.48
2:C:490:GLN:HE21	5:F:472:GLN:HE21	1.60	0.48
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.95	0.48
3:J:525:MET:O	3:J:548:VAL:HG13	2.12	0.48
1:H:182:ARG:NH1	3:J:581:MET:SD	2.87	0.48
1:B:153:VAL:H	1:B:175:ALA:HB3	1.78	0.48
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	1.95	0.48
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.77	0.48
2:I:1285:TYR:CD2	3:J:1356:LEU:HD21	2.48	0.48
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.96	0.48
1:B:57:THR:HG21	1:B:158:ARG:HE	1.78	0.48
1:B:47:LEU:O	1:B:180:VAL:HG21	2.13	0.48
3:D:827:GLU:O	3:D:829:GLY:N	2.37	0.48
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.43	0.48
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.78	0.48
4:K:60:ASN:H	4:K:63:ILE:HB	1.79	0.48
1:A:9:LEU:HD21	1:A:195:ARG:HH21	1.79	0.48
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.95	0.48
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.44	0.48
5:L:354:THR:O	5:L:358:VAL:HG23	2.14	0.48
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.95	0.48
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.96	0.48
5:F:571:TYR:CD1	5:F:575:GLU:HG2	2.48	0.48
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.95	0.48
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.96	0.48
2:I:886:LYS:H	2:I:917:SER:HB3	1.78	0.48
3:J:1154:ALA:N	3:J:1214:PRO:O	2.43	0.48
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.29	0.47
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.96	0.47
1:H:13:LEU:HD23	1:H:13:LEU:H	1.78	0.47
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.78	0.47
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.95	0.47
3:J:317:THR:HB	3:J:324:LEU:HB3	1.95	0.47
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.96	0.47
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.95	0.47
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.95	0.47
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.95	0.47
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.96	0.47
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.95	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.96	0.47
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.13	0.47
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.14	0.47
3:J:518:VAL:N	3:J:716:GLN:HE22	2.12	0.47
3:D:1174:ARG:HG2	3:D:1189:MET:SD	2.54	0.47
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.49	0.47
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.47	0.47
4:E:10:VAL:HG13	4:E:16:ARG:HB2	1.96	0.47
5:F:470:MET:HA	5:F:473:GLU:HB3	1.96	0.47
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.97	0.47
1:H:51:MET:O	1:H:150:ARG:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1307:LEU:HB3	3:J:1312:ALA:HB2	1.97	0.47
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.95	0.47
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.96	0.47
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.49	0.47
2:C:42:ASP:OD2	2:C:44:GLU:HG2	2.14	0.47
3:D:11:GLN:HG3	3:D:12:THR:H	1.79	0.47
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.78	0.47
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.44	0.47
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.95	0.47
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.96	0.47
3:D:748:ALA:O	3:D:777:HIS:HD2	1.98	0.47
5:F:388:ILE:O	5:F:392:LYS:HG3	2.14	0.47
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.96	0.47
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.49	0.47
5:L:532:LEU:HD12	5:L:532:LEU:H	1.79	0.47
2:C:231:GLU:O	2:C:238:GLN:N	2.46	0.47
2:C:632:ASP:O	2:C:647:ARG:HB2	2.14	0.47
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.49	0.47
5:F:499:LYS:HA	5:F:502:LYS:HE2	1.96	0.47
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.97	0.47
1:B:113:ALA:HB2	1:B:126:PRO:HB3	1.97	0.47
2:I:739:ASP:N	2:I:739:ASP:OD1	2.47	0.47
2:I:1272:GLU:H	3:J:343:LEU:HD12	1.79	0.47
3:J:35:PHE:HD1	3:J:101:ARG:HB3	1.80	0.47
4:K:29:GLN:CD	4:K:35:LYS:HE2	2.35	0.47
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.62	0.47
2:C:468:LEU:O	2:C:471:VAL:HG12	2.15	0.47
3:D:741:ALA:O	3:D:762:ASN:ND2	2.48	0.47
1:H:19:VAL:HG23	1:H:24:ALA:HA	1.96	0.47
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.80	0.47
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.96	0.47
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.14	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.96	0.47
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	1.97	0.47
3:D:513:MET:HE3	3:D:579:LEU:HD22	1.97	0.47
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.97	0.47
1:H:20:SER:OG	1:H:21:SER:N	2.48	0.47
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.49	0.47
5:L:148:TYR:OH	5:L:218:ARG:HA	2.15	0.47
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.80	0.47
2:C:18:ARG:NH1	2:C:621:SER:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	1.96	0.47
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.47
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.96	0.47
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.29	0.47
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.97	0.47
3:J:262:THR:C	5:L:507:MET:HB2	2.36	0.47
1:B:125:LYS:HG3	1:B:128:HIS:HB2	1.96	0.46
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.97	0.46
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.50	0.46
2:C:891:GLY:O	2:C:892:GLU:HG3	2.15	0.46
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.44	0.46
3:D:121:PRO:HG2	3:D:123:ARG:HH21	1.80	0.46
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.15	0.46
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.96	0.46
3:J:338:PHE:C	3:J:340:GLN:H	2.18	0.46
3:J:544:LEU:O	3:J:574:VAL:HB	2.15	0.46
3:J:587:LEU:HD23	3:J:591:ILE:HG21	1.95	0.46
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.96	0.46
1:A:90:VAL:HG22	1:A:91:ARG:H	1.80	0.46
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.46
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.49	0.46
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.50	0.46
3:J:425:ARG:HG2	3:J:426:ALA:H	1.80	0.46
2:C:13:LYS:O	2:C:1183:ALA:N	2.42	0.46
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.18	0.46
3:D:334:LYS:HA	3:D:335:GLN:HA	1.57	0.46
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.98	0.46
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.46	0.46
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.97	0.46
3:D:1227:HIS:CB	3:J:1293:GLU:HG2	2.44	0.46
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.98	0.46
1:A:39:LEU:O	1:A:43:LEU:N	2.40	0.46
1:B:190:ALA:N	1:B:198:LEU:O	2.40	0.46
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.80	0.46
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.97	0.46
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.16	0.46
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.96	0.46
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.45	0.46
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.61	0.46
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.49	0.46
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.96	0.46
3:D:515:ARG:O	3:D:545:HIS:HB3	2.15	0.46
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.81	0.46
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.97	0.46
2:I:4:SER:HB2	2:I:7:GLU:HG3	1.97	0.46
3:J:338:PHE:O	3:J:340:GLN:N	2.48	0.46
3:J:34:SER:HG	3:J:104:HIS:CG	2.27	0.46
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.98	0.46
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.98	0.46
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.16	0.46
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.97	0.46
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.51	0.46
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	1.97	0.46
3:D:598:LYS:O	3:D:601:ILE:HG22	2.16	0.46
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.98	0.46
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.16	0.46
2:I:387:ASN:HA	2:I:391:SER:HB2	1.96	0.46
3:J:733:SER:O	3:J:737:ILE:HG12	2.14	0.46
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.46
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.97	0.46
3:J:451:PRO:O	3:J:454:CYS:HB2	2.15	0.46
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.97	0.46
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.98	0.46
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.80	0.46
2:C:149:LEU:HD12	2:C:452:ARG:O	2.15	0.46
2:C:60:GLN:HA	2:C:67:GLU:HA	1.98	0.46
5:F:343:LYS:O	5:F:347:ILE:HG13	2.16	0.46
1:H:213:PRO:O	1:H:217:ILE:HG13	2.16	0.46
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.51	0.46
2:I:169:LYS:O	2:I:170:VAL:HG22	2.15	0.46
3:J:121:PRO:HG2	3:J:123:ARG:HH21	1.80	0.46
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.98	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.97	0.46
1:B:74:VAL:HG22	1:B:133:LEU:HD12	1.96	0.46
1:B:19:VAL:O	1:B:20:SER:HB3	2.15	0.46
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.50	0.46
2:C:1298:VAL:HG11	3:D:96:LYS:HE3	1.98	0.46
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.16	0.46
3:D:658:GLU:O	3:D:661:VAL:HG13	2.16	0.46
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:MET:SD	3:D:741:ALA:HB3	2.56	0.46
5:F:575:GLU:OE2	5:F:578:LYS:NZ	2.43	0.46
1:G:118:ASP:H	1:G:121:VAL:HB	1.81	0.46
2:I:132:ASP:N	2:I:132:ASP:OD1	2.38	0.46
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.48	0.46
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.15	0.46
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.96	0.46
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.96	0.46
3:D:133:ARG:HD2	3:D:133:ARG:HA	1.77	0.46
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.98	0.46
3:D:748:ALA:O	3:D:777:HIS:CD2	2.69	0.46
1:H:101:THR:H	1:H:116:THR:CG2	2.28	0.46
1:H:118:ASP:H	1:H:121:VAL:HB	1.81	0.46
2:I:1211:ARG:HE	2:I:1220:GLN:HE21	1.63	0.46
3:J:473:THR:HG23	3:J:476:ALA:H	1.81	0.46
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.50	0.45
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.98	0.45
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.51	0.45
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.98	0.45
3:D:1165:PHE:CE1	3:D:1200:GLU:HB3	2.52	0.45
5:F:127:ILE:O	5:F:130:VAL:HG22	2.15	0.45
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.51	0.45
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.97	0.45
5:L:316:PHE:CZ	5:L:337:VAL:HB	2.50	0.45
1:A:56:VAL:HG11	1:A:85:LEU:HB3	1.99	0.45
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.97	0.45
1:G:19:VAL:HG13	1:G:20:SER:H	1.80	0.45
1:G:77:ASP:O	1:G:81:ILE:HG13	2.16	0.45
1:H:183:ILE:HG13	1:H:205:MET:HG3	1.96	0.45
1:H:41:ASN:O	1:H:45:ARG:HG3	2.15	0.45
2:I:138:ILE:HG22	2:I:139:ASN:N	2.31	0.45
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.30	0.45
3:J:336:GLY:O	3:J:337:ARG:HB2	2.16	0.45
1:A:172:LEU:H	1:A:172:LEU:HD12	1.81	0.45
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.98	0.45
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.30	0.45
2:C:138:ILE:HG22	2:C:139:ASN:N	2.30	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.16	0.45
3:D:122:SER:O	3:D:126:LEU:HG	2.16	0.45
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.63	0.45
2:C:1248:THR:HG21	5:F:531:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:VAL:HG22	1:G:91:ARG:H	1.81	0.45
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.97	0.45
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.31	0.45
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.17	0.45
2:C:195:PHE:CG	2:C:203:LYS:HD3	2.51	0.45
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.36	0.45
3:D:489:ASN:HA	3:D:904:ALA:CB	2.46	0.45
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.97	0.45
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.73	0.45
3:J:215:LYS:O	3:J:218:THR:HG22	2.17	0.45
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.17	0.45
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.99	0.45
3:D:797:THR:O	3:D:801:VAL:HG13	2.16	0.45
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.50	0.45
1:H:105:SER:HA	1:H:138:ALA:O	2.17	0.45
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.97	0.45
3:J:222:LYS:HE2	3:J:1276:GLU:OE1	2.16	0.45
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.98	0.45
2:C:239:MET:O	2:C:284:LEU:HD12	2.17	0.45
2:C:498:ILE:HD12	2:C:498:ILE:H	1.81	0.45
2:C:499:SER:O	2:C:503:LYS:HB2	2.17	0.45
2:C:675:ASP:HB3	2:C:1107:MET:O	2.15	0.45
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	1.99	0.45
3:D:331:ILE:CG2	3:D:1328:THR:HG21	2.47	0.45
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.98	0.45
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.97	0.45
2:I:180:ARG:NH2	2:I:396:ASP:HB2	2.32	0.45
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.99	0.45
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.32	0.45
1:A:62:ASP:OD1	1:A:141:SER:OG	2.29	0.45
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.49	0.45
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.83	0.45
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.72	0.45
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.98	0.45
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.52	0.45
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.99	0.45
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.99	0.45
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.17	0.45
3:J:56:LEU:H	3:J:56:LEU:HD12	1.82	0.45
3:J:905:ARG:HH21	3:J:907:HIS:CB	2.30	0.45
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.99	0.45
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.46	0.45
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.82	0.45
2:C:701:GLY:O	2:C:1184:THR:N	2.37	0.45
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.50	0.45
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.82	0.45
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.81	0.45
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.99	0.45
3:J:77:ARG:HG3	3:J:79:LYS:H	1.81	0.45
2:C:132:ASP:OD1	2:C:132:ASP:N	2.37	0.45
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.99	0.45
2:I:15:PHE:CG	2:I:1190:ALA:HB2	2.52	0.45
3:J:364:HIS:CD2	4:K:4:VAL:HG23	2.52	0.45
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.98	0.45
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.32	0.45
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.52	0.45
2:I:1099:ASN:HD21	3:J:505:ASP:CG	2.20	0.45
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.52	0.45
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.17	0.45
2:I:27:LEU:HB2	2:I:524:ILE:HD11	1.98	0.45
2:I:703:GLY:N	2:I:705:GLU:OE2	2.43	0.45
3:J:432:LEU:HD13	3:J:499:ILE:HG21	1.98	0.45
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.80	0.45
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.52	0.44
1:B:57:THR:O	1:B:173:VAL:HG22	2.17	0.44
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.44
3:D:343:LEU:HD22	3:D:343:LEU:HA	1.42	0.44
1:H:73:GLY:C	1:H:134:THR:HG22	2.38	0.44
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.99	0.44
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.52	0.44
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.82	0.44
3:J:746:LEU:HB2	3:J:754:ILE:HD11	2.00	0.44
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.32	0.44
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.32	0.44
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.44
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.83	0.44
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.51	0.44
3:J:759:ILE:HG23	3:J:771:GLN:HB3	1.98	0.44
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.50	0.44
5:L:515:GLU:HG2	5:L:516:ASP:N	2.32	0.44
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLN:HB2	1:B:120:ASP:OD1	2.16	0.44
1:B:194:GLN:O	1:B:195:ARG:HG2	2.18	0.44
1:B:74:VAL:HG12	1:B:76:GLU:H	1.82	0.44
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.99	0.44
2:C:867:GLU:H	2:C:867:GLU:HG3	1.52	0.44
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.82	0.44
1:H:13:LEU:HD12	1:H:16:ILE:HD11	1.98	0.44
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.52	0.44
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.18	0.44
3:J:849:LEU:HD13	3:J:849:LEU:H	1.82	0.44
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.82	0.44
5:L:372:ALA:O	5:L:376:LYS:HG3	2.17	0.44
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.45	0.44
2:C:168:GLY:C	2:C:170:VAL:H	2.20	0.44
2:C:494:ASN:HB3	2:C:497:PRO:HD2	2.00	0.44
2:C:782:VAL:HG11	2:C:792:GLY:HA2	1.99	0.44
3:D:113:HIS:HB3	3:D:116:PHE:HD2	1.82	0.44
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.99	0.44
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.98	0.44
3:D:903:LEU:HD23	3:D:905:ARG:HD3	1.99	0.44
5:F:555:GLU:OE2	5:F:597:LYS:NZ	2.46	0.44
1:H:84:ASN:OD1	3:J:551:ARG:NH2	2.51	0.44
2:I:1288:GLN:HG2	2:I:1315:MET:HE1	1.99	0.44
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.99	0.44
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.99	0.44
2:I:1272:GLU:H	3:J:343:LEU:CD1	2.30	0.44
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.98	0.44
3:J:79:LYS:HG3	3:J:80:HIS:N	2.32	0.44
5:L:139:GLU:HG2	5:L:351:THR:HA	2.00	0.44
1:A:90:VAL:HG23	1:A:123:ILE:HD13	2.00	0.44
3:D:646:ILE:H	3:D:646:ILE:HG12	1.57	0.44
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.50	0.44
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.47	0.44
2:I:98:VAL:C	2:I:121:GLU:HA	2.38	0.44
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.99	0.44
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.99	0.44
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.99	0.44
2:C:62:TYR:C	2:C:64:GLY:H	2.21	0.44
2:C:980:VAL:O	2:C:984:VAL:HB	2.17	0.44
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.98	0.44
3:D:892:PHE:CE1	3:D:1281:GLU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LYS:HG2	1:H:110:VAL:HG22	2.00	0.44
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.52	0.44
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.18	0.44
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.17	0.44
5:L:226:ALA:O	5:L:229:VAL:HG22	2.18	0.44
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.32	0.44
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	2.00	0.44
2:C:356:THR:HG21	2:C:362:ALA:HA	2.00	0.44
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.83	0.44
3:D:612:LEU:HB3	3:D:616:PRO:HG2	2.00	0.44
2:I:91:THR:HG21	2:I:503:LYS:HZ1	1.82	0.44
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.17	0.44
1:B:12:ARG:H	1:B:30:PRO:HD2	1.81	0.44
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.17	0.44
2:C:23:ASP:OD1	2:C:23:ASP:N	2.48	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
3:D:903:LEU:HA	3:D:903:LEU:HD12	1.91	0.44
5:F:281:ARG:O	5:F:285:ARG:HG3	2.18	0.44
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.00	0.44
1:H:90:VAL:HG22	1:H:91:ARG:H	1.82	0.44
2:I:90:VAL:HG12	2:I:91:THR:H	1.81	0.44
3:J:232:ASN:HA	3:J:236:TRP:HZ3	1.83	0.44
4:K:26:ARG:HH22	4:K:38:LEU:HD13	1.83	0.44
2:C:732:ILE:HG21	2:C:783:LEU:HD12	2.00	0.44
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.29	0.44
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.99	0.44
3:D:441:LEU:HA	3:D:441:LEU:HD13	1.87	0.44
5:F:94:THR:O	5:F:95:THR:OG1	2.27	0.44
1:G:9:LEU:H	1:G:9:LEU:HD23	1.83	0.44
2:I:225:PHE:CE2	2:I:347:ILE:HB	2.52	0.44
2:I:808:ASN:H	3:J:633:ALA:HB2	1.83	0.44
5:L:528:LEU:HD23	5:L:528:LEU:HA	1.85	0.44
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.31	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.77	0.43
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.00	0.43
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.00	0.43
2:I:1072:ASN:N	2:I:1072:ASN:OD1	2.36	0.43
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.73	0.43
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.72	0.43
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.82	0.43
1:G:75:GLN:HA	2:I:729:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1333:LEU:HD22	3:J:307:LEU:HD22	2.00	0.43
3:J:334:LYS:HA	3:J:335:GLN:HA	1.54	0.43
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.82	0.43
1:B:20:SER:OG	1:B:21:SER:N	2.51	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.98	0.43
2:C:104:ILE:O	2:C:113:THR:HA	2.18	0.43
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.00	0.43
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.48	0.43
5:F:507:MET:HG2	5:F:520:GLY:HA3	2.00	0.43
1:G:12:ARG:HA	1:H:230:ALA:HB2	1.99	0.43
1:G:74:VAL:HG22	1:G:76:GLU:H	1.82	0.43
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.19	0.43
2:I:896:THR:HB	2:I:897:PRO:HD2	1.99	0.43
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.87	0.43
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.30	0.43
3:J:514:THR:CB	3:J:576:ARG:HG2	2.47	0.43
3:J:801:VAL:O	3:J:805:GLN:HB2	2.18	0.43
1:A:118:ASP:H	1:A:121:VAL:HB	1.83	0.43
1:A:83:LEU:HD23	2:C:694:ARG:NH2	2.33	0.43
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.89	0.43
2:I:559:CYS:CB	2:I:662:SER:HB3	2.47	0.43
5:L:569:THR:OG1	5:L:570:ASP:N	2.48	0.43
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.00	0.43
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.54	0.43
2:C:806:PRO:HB3	3:D:505:ASP:OD1	2.18	0.43
3:D:1344:LEU:HB3	3:D:1350:ASN:ND2	2.30	0.43
3:D:708:ASN:N	3:D:708:ASN:OD1	2.49	0.43
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.99	0.43
1:H:93:GLN:H	1:H:120:ASP:HB3	1.83	0.43
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.88	0.43
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.99	0.43
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.54	0.43
2:I:757:THR:HG23	2:I:765:ILE:HG23	2.00	0.43
3:J:682:VAL:O	3:J:685:ILE:HG12	2.17	0.43
4:K:58:LEU:O	4:K:63:ILE:HG21	2.18	0.43
5:L:461:ASN:O	5:L:465:ARG:HG2	2.19	0.43
1:B:153:VAL:O	1:B:175:ALA:N	2.28	0.43
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.18	0.43
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.99	0.43
2:C:642:SER:HB2	3:D:770:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:931:THR:OG1	3:D:931:THR:O	2.36	0.43
5:F:99:ARG:HD3	5:F:99:ARG:HA	1.68	0.43
1:G:73:GLY:C	1:G:134:THR:HG22	2.39	0.43
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.53	0.43
2:I:316:GLU:CD	2:I:316:GLU:H	2.22	0.43
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.54	0.43
5:L:227:GLN:HG2	5:L:252:LEU:HA	2.00	0.43
1:A:47:LEU:O	1:A:180:VAL:HG21	2.19	0.43
2:C:120:GLN:HB2	2:C:120:GLN:HE21	1.49	0.43
2:C:696:ASP:O	2:C:697:LYS:HB3	2.18	0.43
2:C:972:PHE:HD1	2:C:994:ARG:HH21	1.65	0.43
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.86	0.43
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.83	0.43
3:J:1246:VAL:HG12	3:J:1248:ILE:HG13	2.01	0.43
3:J:800:LEU:O	3:J:803:VAL:HG12	2.19	0.43
5:L:316:PHE:O	5:L:320:ILE:HG13	2.18	0.43
2:C:660:VAL:HG13	2:C:661:VAL:HG13	2.00	0.43
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.00	0.43
5:F:512:GLY:O	5:F:514:ASP:N	2.52	0.43
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.84	0.43
2:I:159:SER:HB2	2:I:442:VAL:HG21	2.01	0.43
2:I:62:TYR:C	2:I:64:GLY:H	2.22	0.43
3:J:546:ALA:O	3:J:573:THR:HA	2.18	0.43
3:J:698:MET:O	3:J:702:GLN:HB3	2.18	0.43
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.84	0.43
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.48	0.43
2:C:687:ARG:HH22	6:C:3001:RFP:H301	1.83	0.43
3:D:822:MET:SD	3:D:838:ARG:HB3	2.58	0.43
5:F:499:LYS:HE3	5:F:499:LYS:HB2	1.77	0.43
2:I:10:ARG:HA	2:I:1172:LEU:HD23	2.00	0.43
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.74	0.43
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.43
5:L:486:ARG:HB2	5:L:486:ARG:CZ	2.49	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.84	0.43
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.63	0.43
2:C:735:LYS:HA	2:C:748:ILE:HG22	2.00	0.43
3:D:1237:VAL:HG11	3:D:1253:ILE:HG21	2.01	0.43
3:D:513:MET:HE1	3:D:579:LEU:HD13	2.01	0.43
5:F:227:GLN:HG2	5:F:252:LEU:HA	2.01	0.43
2:C:1250:SER:OG	5:F:524:GLU:OE1	2.37	0.43
2:I:101:ARG:HG3	2:I:118:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.58	0.43
2:I:149:LEU:HD11	2:I:451:ARG:HB3	2.00	0.43
2:I:69:GLN:HG3	2:I:101:ARG:HB3	2.00	0.43
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.18	0.43
3:J:661:VAL:HB	3:J:682:VAL:HG13	2.01	0.43
2:C:463:GLN:HG3	2:C:505:PHE:HB2	2.01	0.43
2:C:619:ALA:HB1	2:C:657:THR:HA	2.00	0.43
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.41	0.43
2:C:992:LEU:HD23	2:C:992:LEU:H	1.84	0.43
3:D:1184:ASP:O	3:D:1186:TYR:N	2.52	0.43
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.32	0.43
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.81	0.43
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.51	0.43
3:D:546:ALA:O	3:D:573:THR:HA	2.18	0.43
3:D:689:ALA:O	3:D:693:VAL:HG23	2.19	0.43
3:D:647:PRO:CG	3:D:697:MET:HB3	2.46	0.43
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.54	0.43
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.49	0.42
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.54	0.42
2:C:565:GLU:HB2	2:C:680:LEU:HD21	1.99	0.42
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.84	0.42
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.84	0.42
5:F:559:LEU:HD22	5:F:594:ALA:HB1	2.01	0.42
1:G:90:VAL:HG23	1:G:123:ILE:HD13	2.00	0.42
3:J:536:LEU:HD12	3:J:542:ALA:HB2	2.00	0.42
3:J:64:PRO:HB3	3:J:69:GLU:O	2.19	0.42
3:J:708:ASN:N	3:J:708:ASN:OD1	2.51	0.42
3:J:793:SER:O	3:J:797:THR:HG23	2.18	0.42
1:B:41:ASN:OD1	2:C:1217:THR:HG22	2.19	0.42
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.19	0.42
5:F:96:ASP:O	5:F:98:VAL:N	2.52	0.42
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.01	0.42
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	2.00	0.42
2:I:498:ILE:H	2:I:498:ILE:HD12	1.83	0.42
2:I:816:ILE:HG22	2:I:818:VAL:HG23	2.01	0.42
1:A:177:TYR:O	1:A:178:SER:HB2	2.19	0.42
1:B:154:PRO:HA	1:B:174:ASP:HB3	2.01	0.42
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.23	0.42
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.61	0.42
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.91	0.42
5:F:532:LEU:H	5:F:532:LEU:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.31	0.42
2:I:980:VAL:O	2:I:984:VAL:HB	2.19	0.42
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.02	0.42
1:A:19:VAL:HG13	1:A:20:SER:H	1.84	0.42
1:A:219:ARG:O	1:A:223:ILE:HG13	2.19	0.42
1:A:228:LEU:HD23	1:A:231:PHE:HD2	1.83	0.42
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.84	0.42
2:C:221:LEU:HD11	2:C:314:ASN:HB2	2.01	0.42
2:C:488:MET:O	2:C:490:GLN:N	2.46	0.42
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.34	0.42
3:D:218:THR:HA	3:D:221:ILE:HG22	2.01	0.42
3:D:824:PRO:HD3	3:D:835:LEU:HB2	2.01	0.42
3:D:93:THR:HG22	3:D:94:GLN:H	1.83	0.42
5:F:462:LYS:O	5:F:466:ILE:HG13	2.18	0.42
5:F:512:GLY:C	5:F:514:ASP:H	2.23	0.42
1:G:38:THR:HG23	1:H:45:ARG:HB2	2.02	0.42
1:G:47:LEU:O	1:G:180:VAL:HG21	2.20	0.42
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.80	0.42
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.85	0.42
5:L:292:VAL:HG21	5:L:299:LYS:HG2	2.00	0.42
2:C:618:GLN:HG3	2:C:620:ASN:H	1.83	0.42
3:D:137:ARG:HD3	3:D:143:SER:OG	2.19	0.42
3:D:114:ILE:HG22	3:D:307:LEU:HD12	2.01	0.42
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.19	0.42
4:K:15:ASN:HB3	4:K:18:ASP:HB2	2.01	0.42
5:L:561:MET:HA	5:L:567:MET:HE1	2.01	0.42
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.55	0.42
2:C:516:ASP:H	2:C:526:HIS:HD1	1.68	0.42
2:C:593:LYS:HA	2:C:652:TYR:CD2	2.55	0.42
2:C:854:ILE:O	2:C:857:VAL:HG22	2.18	0.42
3:D:1283:SER:O	3:D:1286:LYS:N	2.52	0.42
3:D:598:LYS:N	3:D:728:SER:O	2.41	0.42
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.02	0.42
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.35	0.42
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.78	0.42
3:J:42:GLU:HG3	5:L:451:ARG:HE	1.83	0.42
1:A:38:THR:OG1	1:B:45:ARG:HG2	2.20	0.42
1:B:155:ALA:HB2	1:B:173:VAL:C	2.39	0.42
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.48	0.42
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.20	0.42
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:VAL:HG12	2:C:206:ALA:HA	2.00	0.42
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.54	0.42
2:C:324:LYS:O	2:C:327:GLN:NE2	2.51	0.42
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.84	0.42
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.84	0.42
5:F:409:ASN:O	5:F:413:MET:HG3	2.20	0.42
1:G:71:LYS:HB2	1:G:78:ILE:HD11	2.01	0.42
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.84	0.42
3:J:806:ASP:HA	3:J:1347:LEU:HD13	2.01	0.42
2:C:615:VAL:HG13	2:C:651:ASP:N	2.33	0.42
3:D:27:PRO:HB3	3:D:241:VAL:HG23	2.00	0.42
5:F:98:VAL:HB	5:F:402:LEU:HD11	2.02	0.42
1:H:192:VAL:HG21	1:H:198:LEU:HD12	2.02	0.42
2:I:1174:GLU:OE2	2:I:1177:ARG:NH1	2.51	0.42
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	2.01	0.42
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.55	0.42
2:I:194:LEU:HA	2:I:194:LEU:HD12	1.77	0.42
2:I:402:ARG:HG2	2:I:416:GLY:N	2.35	0.42
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.85	0.42
3:J:342:LEU:HA	3:J:343:LEU:HA	1.57	0.42
3:J:598:LYS:O	3:J:601:ILE:HG22	2.19	0.42
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.35	0.42
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	2.02	0.42
5:L:552:THR:OG1	5:L:555:GLU:HG3	2.20	0.42
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.49	0.42
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.83	0.42
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.19	0.42
2:C:985:GLU:HB3	2:C:988:LYS:HB2	2.02	0.42
2:C:810:TYR:CD2	3:D:359:PRO:HG2	2.55	0.42
3:D:623:GLN:O	3:D:627:THR:HG22	2.19	0.42
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.33	0.42
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.50	0.42
3:J:825:VAL:C	3:J:826:ILE:HG13	2.39	0.42
1:B:177:TYR:O	1:B:178:SER:C	2.58	0.42
3:D:682:VAL:O	3:D:685:ILE:HG12	2.20	0.42
3:D:825:VAL:C	3:D:826:ILE:HG13	2.39	0.42
2:I:1114:GLU:OE1	2:I:1230:MET:HA	2.20	0.42
2:I:1314:GLN:HG2	4:K:28:ARG:NE	2.35	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.50	0.42
2:I:61:SER:HB3	2:I:479:LEU:HB3	2.02	0.42
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.85	0.42
5:L:493:LYS:HA	5:L:496:LYS:HE2	2.02	0.42
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.23	0.41
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.85	0.41
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.85	0.41
3:D:526:VAL:HA	3:D:549:LYS:O	2.19	0.41
2:C:808:ASN:H	3:D:633:ALA:HB2	1.85	0.41
3:D:641:ILE:HD13	3:D:641:ILE:O	2.20	0.41
3:D:849:LEU:HB3	3:D:853:THR:HG23	2.01	0.41
5:F:276:MET:O	5:F:280:VAL:HG23	2.20	0.41
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.20	0.41
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.49	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.01	0.41
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.20	0.41
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.85	0.41
5:L:476:ARG:HG3	5:L:477:GLU:N	2.35	0.41
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.49	0.41
5:L:603:ARG:H	5:L:603:ARG:HG2	1.65	0.41
1:B:212:ASP:OD1	1:B:215:GLU:HB2	2.20	0.41
2:C:169:LYS:O	2:C:169:LYS:HG2	2.19	0.41
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.77	0.41
2:C:722:GLY:HA2	2:C:737:ASN:OD1	2.20	0.41
2:C:953:LEU:HA	2:C:953:LEU:HD12	1.85	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.84	0.41
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.35	0.41
3:D:875:ASN:OD1	3:D:875:ASN:N	2.54	0.41
1:G:211:ILE:HA	1:G:211:ILE:HD13	1.95	0.41
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.84	0.41
2:I:593:LYS:HE3	2:I:595:THR:HG22	2.02	0.41
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.35	0.41
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.01	0.41
3:J:850:LYS:HG2	3:J:857:LEU:HD23	2.02	0.41
1:A:228:LEU:HD11	1:B:224:LEU:HD22	2.01	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:B:35:PHE:O	1:B:38:THR:HG22	2.20	0.41
2:C:1328:LYS:O	2:C:1332:SER:N	2.52	0.41
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.38	0.41
2:C:41:GLN:NE2	2:C:73:TYR:O	2.54	0.41
3:D:859:PRO:HG2	3:D:862:THR:HG21	2.01	0.41
5:F:316:PHE:CZ	5:F:334:SER:HA	2.45	0.41
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:985:GLU:HB3	2:I:988:LYS:HB2	2.00	0.41
3:J:19:ALA:CB	3:J:1373:ARG:HH22	2.33	0.41
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.91	0.41
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.35	0.41
2:C:1038:GLN:HG3	2:C:1038:GLN:O	2.20	0.41
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.85	0.41
2:C:796:LEU:O	2:C:1233:LEU:HD12	2.20	0.41
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.81	0.41
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.20	0.41
3:D:451:PRO:O	3:D:454:CYS:HB2	2.19	0.41
2:I:86:GLN:HA	2:I:140:GLY:HA2	2.02	0.41
2:I:705:GLU:HB2	2:I:794:LEU:H	1.86	0.41
3:J:214:ARG:HA	3:J:217:LEU:HB2	2.02	0.41
3:J:332:LYS:HE3	3:J:332:LYS:HB2	1.82	0.41
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.28	0.41
3:J:689:ALA:O	3:J:693:VAL:HG23	2.21	0.41
3:J:810:THR:HG23	3:J:811:GLU:H	1.86	0.41
3:J:860:ARG:HB3	3:J:861:ASN:H	1.73	0.41
5:L:457:ILE:HA	5:L:460:ILE:HD12	2.02	0.41
5:L:586:ARG:O	5:L:590:ILE:HG13	2.21	0.41
1:A:167:PRO:HB2	1:A:170:ARG:HB2	2.02	0.41
1:A:181:GLU:HB3	1:A:206:GLU:HG3	2.02	0.41
1:B:118:ASP:H	1:B:121:VAL:HB	1.84	0.41
1:B:201:LEU:HG	1:B:203:ILE:HG13	2.02	0.41
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.02	0.41
2:C:590:PRO:HG3	2:C:605:TYR:OH	2.21	0.41
2:C:791:LEU:HA	2:C:791:LEU:HD23	1.79	0.41
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.87	0.41
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.51	0.41
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.86	0.41
1:G:227:GLN:HE21	1:H:35:PHE:HD2	1.68	0.41
3:J:461:PHE:HD2	3:J:461:PHE:HA	1.72	0.41
3:J:818:GLU:HB3	3:J:887:SER:HB2	2.03	0.41
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.55	0.41
2:C:396:ASP:HA	2:C:418:GLY:O	2.20	0.41
2:C:519:ASN:ND2	2:C:796:LEU:HD23	2.34	0.41
3:D:30:ILE:HD13	3:D:243:PRO:HD3	2.03	0.41
3:D:317:THR:HG22	3:D:322:ARG:O	2.20	0.41
3:D:362:ARG:H	3:D:365:GLN:NE2	2.17	0.41
1:B:79:LEU:HD11	3:D:526:VAL:HG21	2.03	0.41
2:I:98:VAL:O	2:I:121:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:607:SER:N	2:I:610:GLU:HB2	2.35	0.41
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.02	0.41
5:L:584:ARG:HA	5:L:584:ARG:HH11	1.86	0.41
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.53	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.02	0.41
1:A:83:LEU:HD23	2:C:694:ARG:HH21	1.85	0.41
2:C:980:VAL:HA	2:C:984:VAL:HA	2.03	0.41
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.36	0.41
5:F:226:ALA:O	5:F:229:VAL:HG22	2.20	0.41
1:G:35:PHE:CE1	1:H:46:ILE:HG23	2.55	0.41
1:H:47:LEU:HA	1:H:47:LEU:HD23	1.70	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
3:J:1174:ARG:HG2	3:J:1189:MET:SD	2.60	0.41
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.20	0.41
5:L:233:ASP:O	5:L:236:LYS:HE2	2.21	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.68	0.41
2:C:206:ALA:O	2:C:209:ILE:HG22	2.21	0.41
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.55	0.41
3:D:18:ASP:HB2	3:D:1373:ARG:CZ	2.50	0.41
3:D:422:LEU:HB2	3:D:469:HIS:HB2	2.03	0.41
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.41
1:G:27:THR:HA	1:G:201:LEU:O	2.21	0.41
1:G:38:THR:HA	1:H:45:ARG:HD3	2.03	0.41
2:I:1198:LEU:HA	2:I:1198:LEU:HD22	1.84	0.41
2:I:299:LYS:HB3	2:I:299:LYS:HE2	1.91	0.41
2:I:202:ARG:NH2	2:I:368:ARG:HH12	2.19	0.41
1:G:83:LEU:HD23	2:I:694:ARG:HH21	1.85	0.41
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.20	0.41
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	2.03	0.41
2:I:1309:VAL:HA	3:J:383:GLY:HA3	2.01	0.41
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.41
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.21	0.41
2:C:149:LEU:HD13	2:C:453:ILE:HG12	2.01	0.41
3:D:839:VAL:HG13	3:D:882:VAL:HG21	2.01	0.41
5:F:230:VAL:HG13	5:F:231:THR:H	1.83	0.41
5:F:320:ILE:HG12	5:F:330:LEU:HD12	2.02	0.41
1:H:57:THR:HG21	1:H:158:ARG:NH2	2.35	0.41
2:I:675:ASP:HB3	2:I:1107:MET:O	2.21	0.41
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.56	0.41
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.54	0.41
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.41
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.56	0.41
3:J:325:LYS:HG3	3:J:329:ASP:HB2	2.02	0.41
3:J:600:ALA:O	3:J:603:LYS:HG2	2.21	0.41
1:B:82:LEU:HD13	1:B:173:VAL:HG12	2.02	0.41
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.56	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.21	0.41
3:D:844:THR:HG23	3:D:864:LEU:HD11	2.03	0.41
5:F:572:THR:O	5:F:576:VAL:HG23	2.20	0.41
5:F:588:ARG:H	5:F:588:ARG:HG3	1.58	0.41
1:G:61:ILE:HB	1:G:64:VAL:CG2	2.51	0.41
2:I:163:LYS:HB3	2:I:163:LYS:HE3	1.88	0.41
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.86	0.41
2:I:805:MET:HE2	2:I:805:MET:HB2	1.92	0.41
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.55	0.41
3:J:363:LEU:HG	3:J:363:LEU:O	2.21	0.41
3:J:701:LEU:CD1	3:J:723:TYR:HB2	2.51	0.41
1:A:137:ASN:OD1	1:A:137:ASN:N	2.53	0.41
2:C:269:ILE:HG22	2:C:274:ILE:HG13	2.03	0.41
2:C:57:PHE:CD1	2:C:59:ILE:HG13	2.55	0.41
3:D:11:GLN:NE2	3:D:15:GLU:OE2	2.54	0.41
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.20	0.41
3:D:647:PRO:HG3	3:D:697:MET:CB	2.47	0.41
4:E:15:ASN:O	4:E:16:ARG:HB3	2.20	0.41
1:H:198:LEU:HA	1:H:198:LEU:HD23	1.86	0.41
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.21	0.41
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.56	0.41
3:J:809:VAL:HA	3:J:894:VAL:O	2.21	0.41
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.80	0.40
1:A:73:GLY:C	1:A:134:THR:HG22	2.42	0.40
2:C:1178:LYS:HA	2:C:1178:LYS:HD3	1.96	0.40
2:C:187:GLU:OE2	2:C:203:LYS:HE2	2.21	0.40
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	2.02	0.40
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.40	0.40
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.95	0.40
3:D:369:PRO:HB3	3:D:444:GLY:O	2.21	0.40
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.51	0.40
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.56	0.40
2:I:94:ALA:HB2	2:I:129:LEU:HD11	2.02	0.40
5:L:281:ARG:HG2	5:L:285:ARG:HD2	2.03	0.40
5:L:296:LYS:HA	5:L:296:LYS:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:653:MET:HG2	2:C:654:ASP:N	2.37	0.40
3:D:339:ARG:O	3:D:344:GLY:HA2	2.21	0.40
1:G:177:TYR:O	1:G:178:SER:HB2	2.21	0.40
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.03	0.40
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.03	0.40
3:J:189:LEU:HD22	3:J:234:PRO:HB3	2.01	0.40
3:J:526:VAL:HA	3:J:549:LYS:O	2.21	0.40
3:J:77:ARG:HD2	3:J:77:ARG:HA	1.85	0.40
4:K:15:ASN:O	4:K:16:ARG:HB3	2.22	0.40
1:A:233:ASP:N	1:A:233:ASP:OD2	2.55	0.40
2:C:232:ILE:HD12	2:C:330:HIS:O	2.20	0.40
2:C:62:TYR:O	2:C:64:GLY:N	2.54	0.40
2:C:646:SER:HB3	2:C:649:GLN:HG3	2.02	0.40
2:C:819:SER:HB2	2:C:1085:MET:CG	2.51	0.40
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.84	0.40
3:D:901:ARG:HD2	3:D:906:GLY:O	2.22	0.40
5:F:372:ALA:O	5:F:376:LYS:HG3	2.21	0.40
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.04	0.40
1:H:92:VAL:HA	1:H:120:ASP:O	2.21	0.40
2:I:496:LYS:HB3	2:I:497:PRO:HD3	2.02	0.40
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	2.21	0.40
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.22	0.40
3:J:294:ASN:HB2	5:L:101:TYR:CD1	2.56	0.40
3:J:785:ASP:O	3:J:789:LYS:HG3	2.21	0.40
5:L:437:GLN:HG3	5:L:438:ALA:N	2.35	0.40
5:L:547:VAL:CG2	5:L:603:ARG:HB3	2.51	0.40
2:C:678:ARG:HD3	2:C:678:ARG:HA	1.92	0.40
2:C:27:LEU:HG	2:C:711:ASP:OD2	2.21	0.40
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	2.03	0.40
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.19	0.40
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.92	0.40
5:F:105:MET:HE1	5:F:385:ARG:HG2	2.02	0.40
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.21	0.40
1:B:211:ILE:HD13	1:B:211:ILE:HA	1.90	0.40
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.57	0.40
2:C:1131:MET:CE	2:C:1141:LEU:HD12	2.51	0.40
2:C:444:ASP:OD1	2:C:447:HIS:HB2	2.22	0.40
2:C:606:LEU:HD23	2:C:611:GLU:HA	2.03	0.40
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.36	0.40
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.52	0.40
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:705:THR:OG1	3:D:718:SER:HA	2.21	0.40
5:F:235:ILE:HA	5:F:245:ALA:HB2	2.04	0.40
1:G:219:ARG:O	1:G:223:ILE:HG13	2.22	0.40
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.36	0.40
2:I:564:PRO:HG3	2:I:572:ILE:HG13	2.04	0.40
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.21	0.40
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	195 (87%)	26 (12%)	4 (2%)	11	54
1	B	210/329 (64%)	180 (86%)	25 (12%)	5 (2%)	7	49
1	G	222/329 (68%)	192 (86%)	24 (11%)	6 (3%)	6	46
1	H	211/329 (64%)	185 (88%)	21 (10%)	5 (2%)	7	49
2	C	1328/1342 (99%)	1220 (92%)	101 (8%)	7 (0%)	34	76
2	I	1324/1342 (99%)	1220 (92%)	97 (7%)	7 (0%)	34	76
3	D	1162/1407 (83%)	1070 (92%)	85 (7%)	7 (1%)	30	73
3	J	1151/1407 (82%)	1059 (92%)	80 (7%)	12 (1%)	19	64
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
5	F	462/613 (75%)	424 (92%)	37 (8%)	1 (0%)	52	86
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	52	86
All	All	6922/8222 (84%)	6328 (91%)	539 (8%)	55 (1%)	24	68

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	B	13	LEU
2	C	3	TYR
2	C	1159	VAL
3	D	10	ALA
3	D	332	LYS
2	I	1159	VAL
1	A	167	PRO
1	B	136	GLU
2	C	170	VAL
2	C	697	LYS
1	G	162	GLU
1	G	167	PRO
1	H	20	SER
1	H	135	ASP
2	I	170	VAL
2	I	697	LYS
3	J	332	LYS
3	J	334	LYS
3	J	339	ARG
1	B	20	SER
1	H	136	GLU
1	A	14	VAL
2	C	484	LEU
2	C	1158	LYS
3	D	710	ASP
3	D	806	ASP
2	I	484	LEU
2	I	1158	LYS
3	J	333	GLY
3	J	338	PHE
3	J	710	ASP
1	A	62	ASP
1	G	14	VAL
1	G	62	ASP
1	G	229	GLU
1	H	138	ALA
3	J	344	GLY
3	J	806	ASP
1	B	14	VAL
1	B	62	ASP
3	D	831	VAL
1	G	196	THR

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Mol	Chain	Res	Type
1	H	62	ASP
2	I	63	SER
3	J	831	VAL
5	F	477	GLU
2	I	1186	VAL
2	C	1186	VAL
3	D	826	ILE
3	D	1180	VAL
3	J	826	ILE
3	J	1180	VAL
5	L	477	GLU
3	J	336	GLY

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	194/286 (68%)	181 (93%)	13 (7%)	20	59
1	B	182/286 (64%)	172 (94%)	10 (6%)	27	66
1	G	191/286 (67%)	179 (94%)	12 (6%)	22	61
1	H	184/286 (64%)	175 (95%)	9 (5%)	31	68
2	C	1150/1157 (99%)	1050 (91%)	100 (9%)	13	48
2	I	1147/1157 (99%)	1045 (91%)	102 (9%)	12	47
3	D	970/1168 (83%)	871 (90%)	99 (10%)	9	40
3	J	960/1168 (82%)	864 (90%)	96 (10%)	9	41
4	E	72/75 (96%)	65 (90%)	7 (10%)	10	43
4	K	67/75 (89%)	63 (94%)	4 (6%)	24	63
5	F	417/540 (77%)	376 (90%)	41 (10%)	10	42
5	L	418/540 (77%)	378 (90%)	40 (10%)	10	43
All	All	5952/7024 (85%)	5419 (91%)	533 (9%)	12	47

All (533) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	19	VAL
1	A	50	SER
1	A	61	ILE
1	A	74	VAL
1	A	115	ILE
1	A	133	LEU
1	A	145	LYS
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	A	233	ASP
1	B	6	THR
1	B	7	GLU
1	B	8	PHE
1	B	13	LEU
1	B	44	ARG
1	B	50	SER
1	B	61	ILE
1	B	115	ILE
1	B	133	LEU
1	B	215	GLU
2	C	11	ILE
2	C	22	LEU
2	C	60	GLN
2	C	70	TYR
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	189	ASP
2	C	285	ILE
2	C	299	LYS

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Mol	Chain	Res	Type
2	C	306	THR
2	C	320	ASP
2	C	360	LEU
2	C	369	MET
2	C	377	THR
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	518	ASN
2	C	554	HIS
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	800	MET
2	C	814	ASP
2	C	819	SER
2	C	826	ASP

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Mol	Chain	Res	Type
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	944	ARG
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1073	LYS
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	18	ASP
3	D	26	SER
3	D	29	MET

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Mol	Chain	Res	Type
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	98	ARG
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	217	LEU
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	343	LEU
3	D	352	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	425	ARG
3	D	454	CYS
3	D	490	ILE
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE

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Mol	Chain	Res	Type
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	704	GLU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	805	GLN
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL

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Mol	Chain	Res	Type
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1333	THR
3	D	1343	GLU
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	154	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	422	ARG
5	F	429	THR
5	F	437	GLN
5	F	445	ASP
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	485	GLU
5	F	486	ARG

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Mol	Chain	Res	Type
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	587	ILE
5	F	603	ARG
5	F	606	VAL
5	F	612	ASP
1	G	9	LEU
1	G	13	LEU
1	G	19	VAL
1	G	50	SER
1	G	61	ILE
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	9	LEU
1	H	13	LEU
1	H	22	THR
1	H	26	VAL
1	H	44	ARG
1	H	50	SER
1	H	61	ILE
1	H	115	ILE
1	H	215	GLU
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN

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Mol	Chain	Res	Type
2	I	70	TYR
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	124	MET
2	I	132	ASP
2	I	167	SER
2	I	189	ASP
2	I	285	ILE
2	I	299	LYS
2	I	306	THR
2	I	320	ASP
2	I	360	LEU
2	I	369	MET
2	I	377	THR
2	I	394	ARG
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	518	ASN
2	I	554	HIS
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU

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Mol	Chain	Res	Type
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	817	LEU
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	944	ARG
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	984	VAL
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1073	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN

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Mol	Chain	Res	Type
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1198	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1238	LEU
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	26	SER
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	98	ARG
3	J	159	ILE
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	217	LEU
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	352	ARG
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	454	CYS
3	J	490	ILE
3	J	506	VAL
3	J	507	VAL

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Mol	Chain	Res	Type
3	J	513	MET
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	704	GLU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	770	LEU
3	J	798	ARG
3	J	805	GLN
3	J	810	THR
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG

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Mol	Chain	Res	Type
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	931	THR
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	154	GLU
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	306	PHE
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	395	THR

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Mol	Chain	Res	Type
5	L	417	ASP
5	L	422	ARG
5	L	429	THR
5	L	437	GLN
5	L	445	ASP
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	587	ILE
5	L	606	VAL
5	L	612	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	66	HIS
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	510	GLN
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1288	GLN

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Mol	Chain	Res	Type
2	C	1314	GLN
3	D	11	GLN
3	D	94	GLN
3	D	200	GLN
3	D	365	GLN
3	D	419	HIS
3	D	450	HIS
3	D	469	HIS
3	D	594	GLN
3	D	665	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1259	GLN
5	F	131	GLN
5	F	246	GLN
5	F	309	ASN
5	F	383	ASN
5	F	446	GLN
5	F	472	GLN
5	F	518	HIS
1	H	186	ASN
2	I	69	GLN
2	I	139	ASN
2	I	343	HIS
2	I	494	ASN
2	I	513	GLN
2	I	628	HIS
2	I	688	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	206	ASN
3	J	365	GLN
3	J	665	GLN

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Mol	Chain	Res	Type
3	J	702	GLN
3	J	716	GLN
3	J	777	HIS
3	J	910	ASN
3	J	929	GLN
3	J	1259	GLN
3	J	1366	HIS
5	L	131	GLN
5	L	246	GLN
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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	RFP	C	3001	-	62,63,63	2.47	13 (20%)	76,94,94	2.02	22 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RFP	C	3001	-	-	0/60/85/85	0/1/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	C12-C11	-6.54	1.36	1.54
6	C	3001	RFP	O7-C25	-4.93	1.37	1.44
6	C	3001	RFP	O6-C27	-2.87	1.37	1.43
6	C	3001	RFP	C6-C7	-2.41	1.35	1.39
6	C	3001	RFP	C26-C25	-2.16	1.49	1.53
6	C	3001	RFP	C24-C23	-2.02	1.49	1.54
6	C	3001	RFP	C2-N1	2.23	1.47	1.43
6	C	3001	RFP	C17-C16	2.78	1.41	1.34
6	C	3001	RFP	C43-N2	2.78	1.34	1.27
6	C	3001	RFP	C18-C17	3.96	1.55	1.43
6	C	3001	RFP	C3-C43	4.32	1.54	1.46
6	C	3001	RFP	C15-N1	6.48	1.49	1.35
6	C	3001	RFP	O3-C6	11.84	1.56	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C24-C23-C22	-4.78	108.47	115.46
6	C	3001	RFP	O4-C11-C5	-4.61	122.23	131.67
6	C	3001	RFP	C12-O3-C6	-3.90	103.36	107.86
6	C	3001	RFP	C20-C19-C18	-3.37	118.62	126.06
6	C	3001	RFP	C18-C17-C16	-3.14	118.11	127.02
6	C	3001	RFP	C2-C3-C43	-3.04	119.06	123.33
6	C	3001	RFP	C17-C16-C15	-3.00	113.07	121.52
6	C	3001	RFP	C40-N3-N2	-2.86	99.28	113.51
6	C	3001	RFP	C5-C10-C9	-2.75	114.11	119.83
6	C	3001	RFP	C13-C12-C11	-2.61	108.11	113.94
6	C	3001	RFP	C20-C21-C22	-2.23	110.84	114.30
6	C	3001	RFP	O7-C35-O8	-2.12	118.61	122.92
6	C	3001	RFP	C41-N3-C40	2.06	120.01	114.22
6	C	3001	RFP	C41-C42-N4	2.78	113.79	110.76
6	C	3001	RFP	C37-O6-C27	2.81	118.57	113.33
6	C	3001	RFP	C40-C39-N4	2.99	114.02	110.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	O5-C12-C13	3.13	112.24	106.92
6	C	3001	RFP	C42-N4-C39	3.20	113.86	109.50
6	C	3001	RFP	O7-C35-C36	3.95	118.61	111.09
6	C	3001	RFP	C38-N4-C39	4.06	117.16	110.68
6	C	3001	RFP	C38-N4-C42	4.27	117.50	110.68
6	C	3001	RFP	C41-N3-N2	5.11	138.90	113.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/329 (68%)	-0.30	3 (1%) 79 70	134, 178, 241, 363	0
1	B	214/329 (65%)	0.05	8 (3%) 45 34	141, 222, 328, 396	0
1	G	224/329 (68%)	-0.10	4 (1%) 71 61	175, 225, 285, 364	0
1	H	215/329 (65%)	0.20	8 (3%) 45 34	179, 247, 312, 401	0
2	C	1332/1342 (99%)	-0.10	64 (4%) 34 25	101, 169, 396, 542	0
2	I	1328/1342 (98%)	0.06	62 (4%) 35 26	139, 219, 353, 523	0
3	D	1166/1407 (82%)	-0.25	11 (0%) 85 79	93, 151, 275, 441	0
3	J	1155/1407 (82%)	-0.09	40 (3%) 48 36	128, 181, 311, 455	0
4	E	89/91 (97%)	-0.14	1 (1%) 82 74	144, 205, 237, 275	0
4	K	79/91 (86%)	0.92	19 (24%) 1 1	255, 318, 411, 416	0
5	F	468/613 (76%)	-0.15	17 (3%) 46 35	139, 222, 362, 481	0
5	L	469/613 (76%)	-0.15	16 (3%) 49 37	161, 231, 357, 487	0
All	All	6966/8222 (84%)	-0.08	253 (3%) 46 35	93, 196, 346, 542	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	311	CYS	14.1
2	C	252	SER	11.6
2	I	981	ALA	8.1
2	I	982	GLY	7.9
2	C	283	LYS	7.6
2	I	1000	LEU	7.6
2	C	323	ALA	7.2
2	C	376	PRO	7.0
2	I	978	VAL	6.9
2	C	1	MET	6.6
2	C	258	ASN	6.4

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Mol	Chain	Res	Type	RSRZ
2	I	979	LEU	6.3
1	H	96	ASP	6.1
2	I	1011	LEU	5.9
2	C	284	LEU	5.6
5	L	490	PRO	5.2
2	C	377	THR	5.2
2	C	234	ASP	5.1
2	I	1004	ASP	4.7
2	I	975	ILE	4.7
2	C	236	LYS	4.6
2	C	265	LYS	4.6
2	C	120	GLN	4.6
2	I	983	GLY	4.5
2	C	322	LEU	4.4
5	F	314	THR	4.4
2	I	999	GLU	4.4
2	C	378	ARG	4.4
2	C	312	ALA	4.4
2	I	998	LEU	4.3
2	I	311	CYS	4.3
2	C	235	ASN	4.3
5	F	167	ASP	4.3
2	I	1006	GLU	4.2
3	J	542	ALA	4.2
5	F	319	ALA	4.2
5	F	318	ALA	4.2
5	F	325	PRO	4.1
1	B	147	GLN	4.1
2	C	330	HIS	4.1
1	G	95	LYS	4.1
3	J	712	GLN	4.1
2	I	1005	GLU	4.0
1	B	172	LEU	4.0
2	C	329	GLY	4.0
2	C	301	TYR	3.9
3	D	1203	ARG	3.9
4	K	37	PRO	3.8
2	C	288	PRO	3.8
3	J	518	VAL	3.7
2	C	314	ASN	3.7
2	C	240	GLU	3.7
2	I	413	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	I	980	VAL	3.7
3	J	218	THR	3.6
3	J	175	GLU	3.5
3	J	1202	GLU	3.5
4	K	41	GLU	3.4
4	K	38	LEU	3.4
2	I	1010	GLN	3.4
5	F	324	LYS	3.4
3	J	827	GLU	3.4
1	H	148	ARG	3.4
2	C	310	ILE	3.4
3	D	1202	GLU	3.4
4	K	14	GLY	3.4
3	J	212	THR	3.3
1	H	135	ASP	3.3
2	C	251	ALA	3.3
2	I	727	VAL	3.3
3	J	1204	VAL	3.3
5	L	488	LEU	3.3
3	J	1203	ARG	3.3
2	I	376	PRO	3.2
5	L	315	TRP	3.2
1	H	107	ILE	3.2
3	J	209	ASN	3.2
2	C	229	ILE	3.2
2	C	262	TYR	3.2
4	K	77	ALA	3.2
2	C	1000	LEU	3.2
2	I	247	ARG	3.2
3	J	857	LEU	3.2
2	I	412	GLU	3.2
2	I	163	LYS	3.2
4	K	75	GLN	3.2
3	J	208	THR	3.2
2	I	1014	LEU	3.1
4	K	78	ALA	3.1
2	I	374	GLU	3.1
4	K	79	GLU	3.1
4	K	36	ASP	3.1
1	H	14	VAL	3.1
5	F	313	ASP	3.1
5	F	315	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	248	GLY	3.1
2	C	259	GLY	3.1
2	I	185	ASP	3.1
2	C	250	THR	3.1
5	L	322	MET	3.1
3	J	176	PHE	3.1
2	C	1001	GLY	3.0
5	L	487	MET	3.0
2	C	169	LYS	3.0
2	I	1020	GLU	3.0
2	C	267	ARG	3.0
3	J	207	GLU	3.0
2	I	375	PRO	2.9
2	I	985	GLU	2.9
3	J	830	ASP	2.9
2	I	891	GLY	2.9
2	I	234	ASP	2.9
1	B	158	ARG	2.9
2	C	325	LEU	2.8
2	I	110	PRO	2.8
4	K	13	ILE	2.8
3	D	1173	ARG	2.8
2	C	273	HIS	2.8
5	L	319	ALA	2.8
3	J	677	GLU	2.8
4	K	40	PRO	2.8
3	J	931	THR	2.8
4	E	2	ALA	2.8
5	L	321	ALA	2.8
2	C	264	GLU	2.8
5	F	421	TYR	2.8
2	I	112	GLY	2.8
3	D	1161	GLY	2.7
2	I	233	ARG	2.7
2	C	305	SER	2.7
2	C	260	LYS	2.7
2	C	327	GLN	2.7
1	A	194	GLN	2.6
2	I	373	GLY	2.6
3	D	1172	LYS	2.6
5	F	321	ALA	2.6
3	J	708	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	1022	LYS	2.6
4	K	56	GLU	2.6
2	I	258	ASN	2.6
2	I	1068	GLY	2.6
4	K	35	LYS	2.6
3	J	204	GLU	2.6
5	F	155	GLU	2.6
2	I	974	ARG	2.6
2	I	600	THR	2.6
3	J	828	GLY	2.6
4	K	26	ARG	2.5
2	C	333	ILE	2.5
2	C	332	ARG	2.5
2	I	414	ILE	2.5
4	K	74	GLU	2.5
2	C	318	SER	2.5
2	C	321	LEU	2.5
3	J	675	ALA	2.5
2	I	302	ILE	2.5
2	C	543	ALA	2.5
2	I	231	GLU	2.5
2	I	174	ALA	2.5
3	J	1148	ARG	2.5
2	I	1025	PHE	2.5
2	C	249	GLU	2.4
2	I	66	SER	2.4
3	J	566	LYS	2.4
3	J	1250	ASP	2.4
4	K	2	ALA	2.4
2	I	1007	LYS	2.4
2	C	268	ARG	2.4
3	J	930	LEU	2.4
5	L	423	ARG	2.4
1	B	41	ASN	2.4
5	F	326	TRP	2.4
2	I	1154	ASP	2.4
3	J	707	ILE	2.4
3	J	213	LYS	2.4
3	J	1166	GLY	2.4
5	F	157	ARG	2.4
2	I	190	PRO	2.4
1	A	162	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	1137	GLU	2.3
3	J	849	LEU	2.3
2	I	254	ASP	2.3
5	L	294	GLN	2.3
1	B	146	VAL	2.3
1	G	193	GLU	2.3
1	H	204	GLU	2.3
3	D	209	ASN	2.3
1	B	143	ARG	2.3
2	C	261	VAL	2.3
1	G	194	GLN	2.3
5	L	167	ASP	2.3
5	L	489	MET	2.3
2	C	116	ASP	2.3
2	C	117	ILE	2.3
1	A	41	ASN	2.3
2	I	1003	THR	2.3
3	J	715	LYS	2.3
5	L	613	ASP	2.3
2	C	320	ASP	2.2
3	J	1198	VAL	2.2
2	C	253	PHE	2.2
2	C	164	THR	2.2
2	C	373	GLY	2.2
2	I	633	LEU	2.2
2	I	1015	ALA	2.2
5	L	422	ARG	2.2
2	C	414	ILE	2.2
2	C	270	THR	2.2
4	K	72	GLN	2.2
2	I	117	ILE	2.2
3	J	831	VAL	2.2
1	G	191	ARG	2.2
2	C	271	ALA	2.2
2	C	302	ILE	2.2
3	J	76	LYS	2.2
3	J	1375	ALA	2.2
2	I	107	ARG	2.2
4	K	80	LEU	2.2
3	D	1165	PHE	2.2
3	J	714	GLU	2.2
2	C	1002	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
5	L	421	TYR	2.2
2	I	991	LYS	2.2
4	K	58	LEU	2.2
1	B	135	ASP	2.1
3	J	335	GLN	2.1
3	J	471	PRO	2.1
5	F	310	GLU	2.1
5	F	514	ASP	2.1
1	H	211	ILE	2.1
2	I	108	GLU	2.1
3	J	314	ARG	2.1
1	B	66	HIS	2.1
3	J	1249	ASN	2.1
1	H	25	LYS	2.1
2	C	102	LEU	2.1
2	C	233	ARG	2.1
5	L	514	ASP	2.1
2	I	1021	LEU	2.1
3	D	712	GLN	2.1
5	F	323	ASN	2.1
2	I	732	ILE	2.1
3	D	149	GLY	2.1
2	I	269	ILE	2.1
2	C	163	LYS	2.0
2	I	720	ARG	2.0
3	D	1296	GLY	2.0
5	L	425	TYR	2.0
2	I	267	ARG	2.0
2	C	291	TYR	2.0
5	F	304	THR	2.0
2	C	172	TYR	2.0
3	D	1376	GLY	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

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(Å ²)	Q<0.9
6	RFP	C	3001	59/59	0.95	0.21	-0.19	91,139,195,202	0
8	ZN	J	1503	1/1	0.98	0.14	-0.24	126,126,126,126	0
8	ZN	D	1502	1/1	0.97	0.07	-1.13	150,150,150,150	0
8	ZN	D	1503	1/1	0.99	0.12	-1.41	82,82,82,82	0
8	ZN	J	1502	1/1	0.96	0.05	-1.42	174,174,174,174	0
7	MG	J	1501	1/1	0.95	0.42	-	121,121,121,121	0
7	MG	D	1501	1/1	0.94	0.39	-	77,77,77,77	0

6.5 Other polymers

There are no such residues in this entry.