



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 07:31 AM EDT

PDB ID : 5UAH
Title : Escherichia coli RNA polymerase and Rifampin complex, RpoB D516V mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

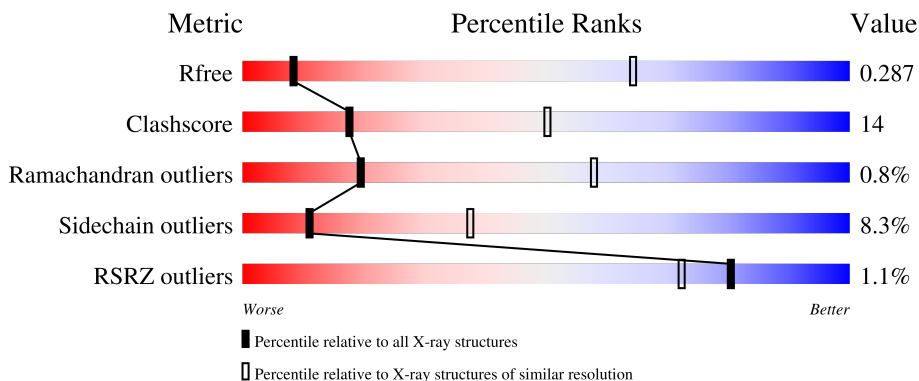
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	C	3002	-	-	-	X
7	MG	I	1401	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 55125 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
			Total	C	N	O	S			
1	A	233	Total	C	N	O	S	0	0	0
			1812	1127	323	356	6			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1340	Total	C	N	O	S	0	0	0
			10569	6632	1841	2053	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10565	6630	1840	2052	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2
I	516	VAL	ASP	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1167	Total	C	N	O	S	0	0	0
			9065	5700	1622	1697	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

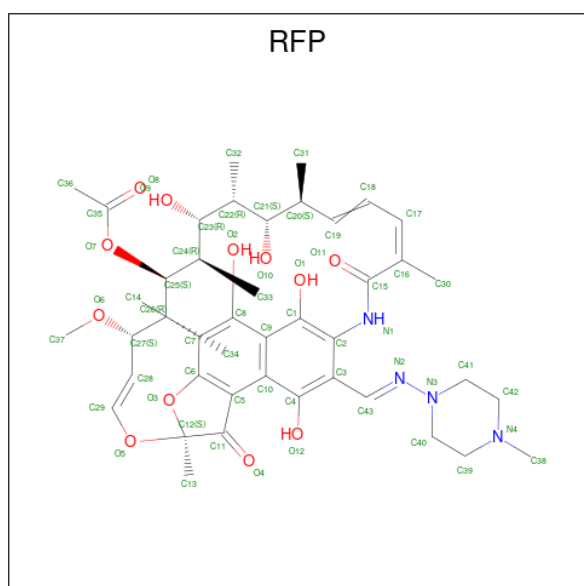
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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

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

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

- Molecule 6 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



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

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

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

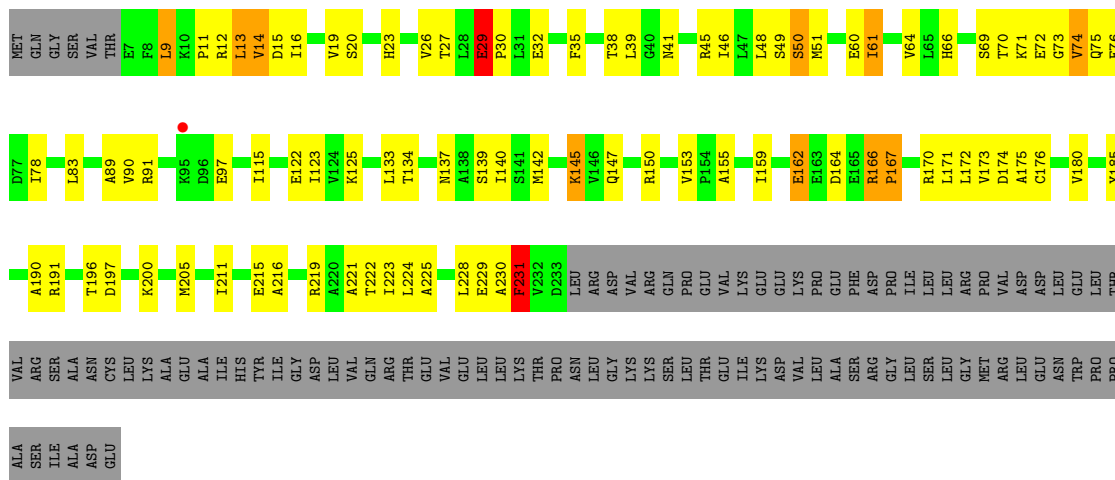
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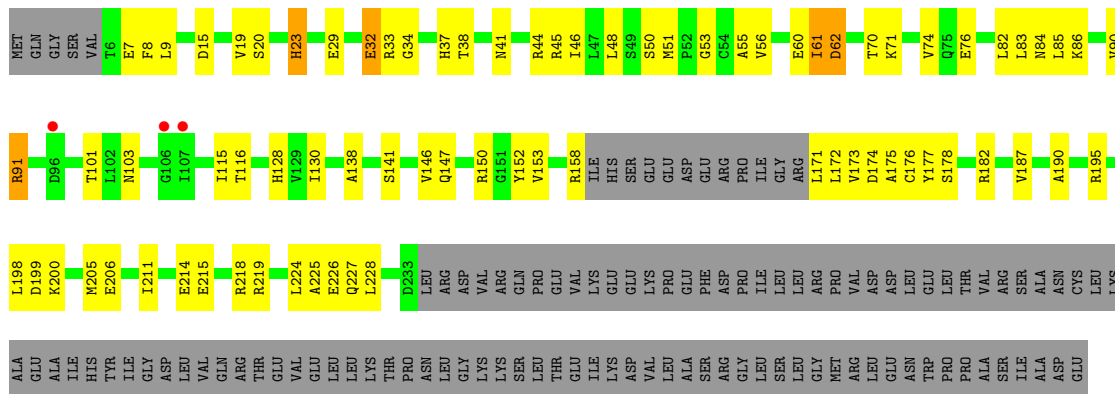
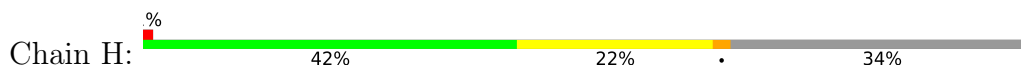
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total Mg 1 1	0	0
7	J	1	Total Mg 1 1	0	0

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

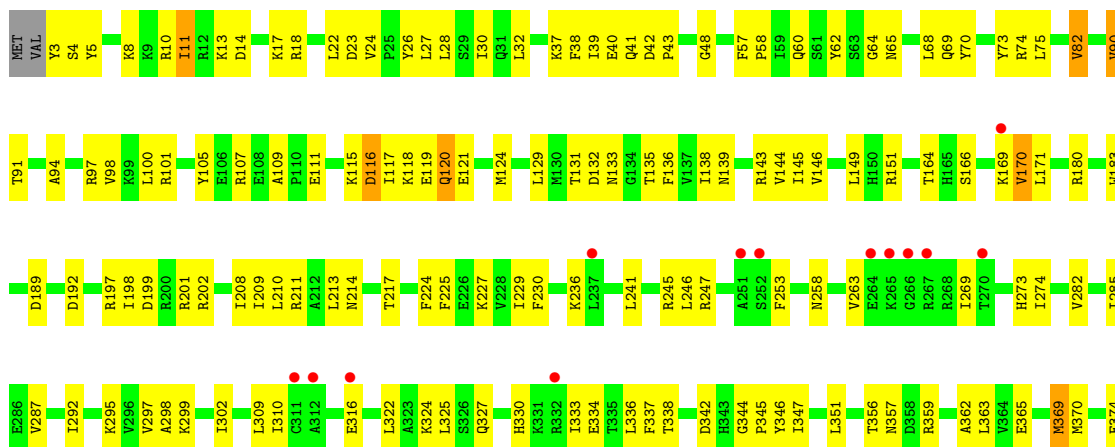
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	2	Total Zn 2 2	0	0
8	J	2	Total Zn 2 2	0	0

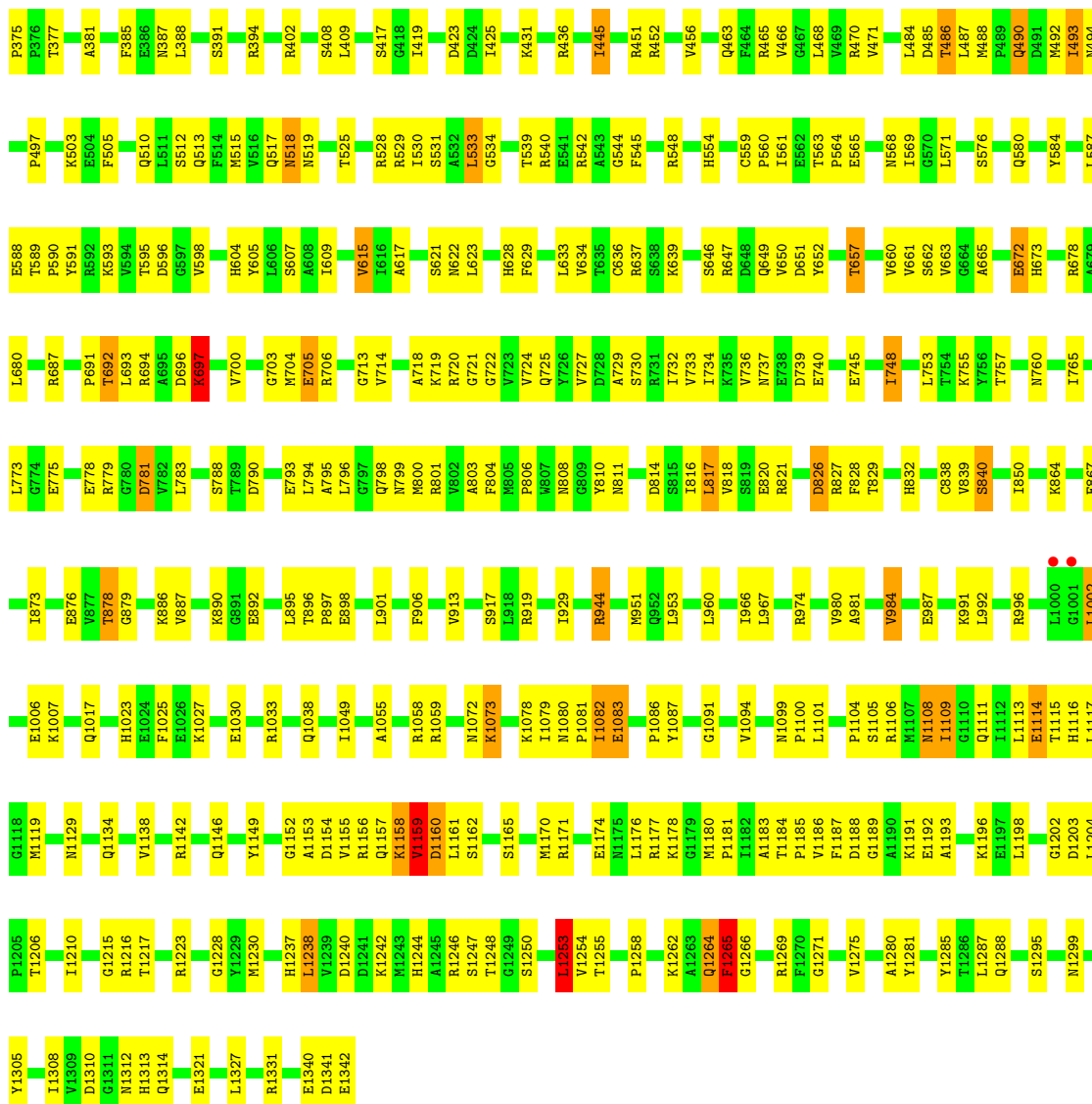


• Molecule 1: DNA-directed RNA polymerase subunit alpha

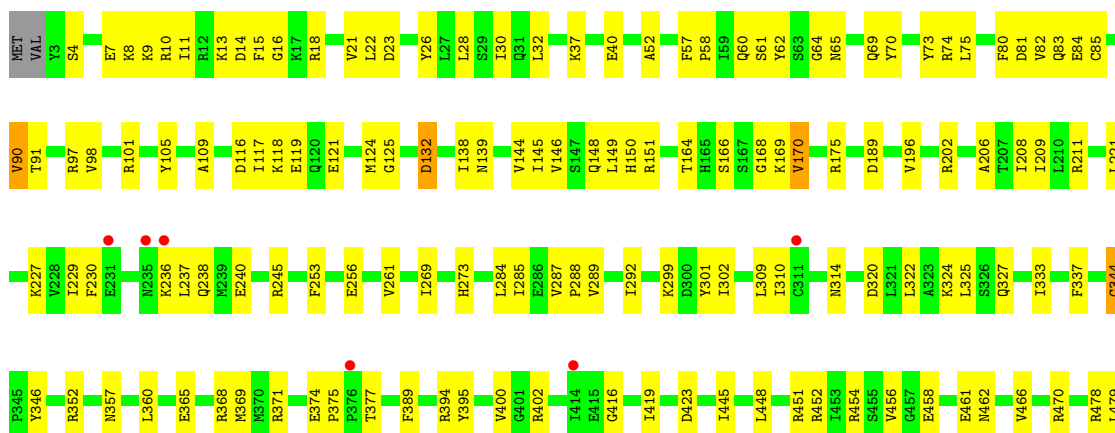


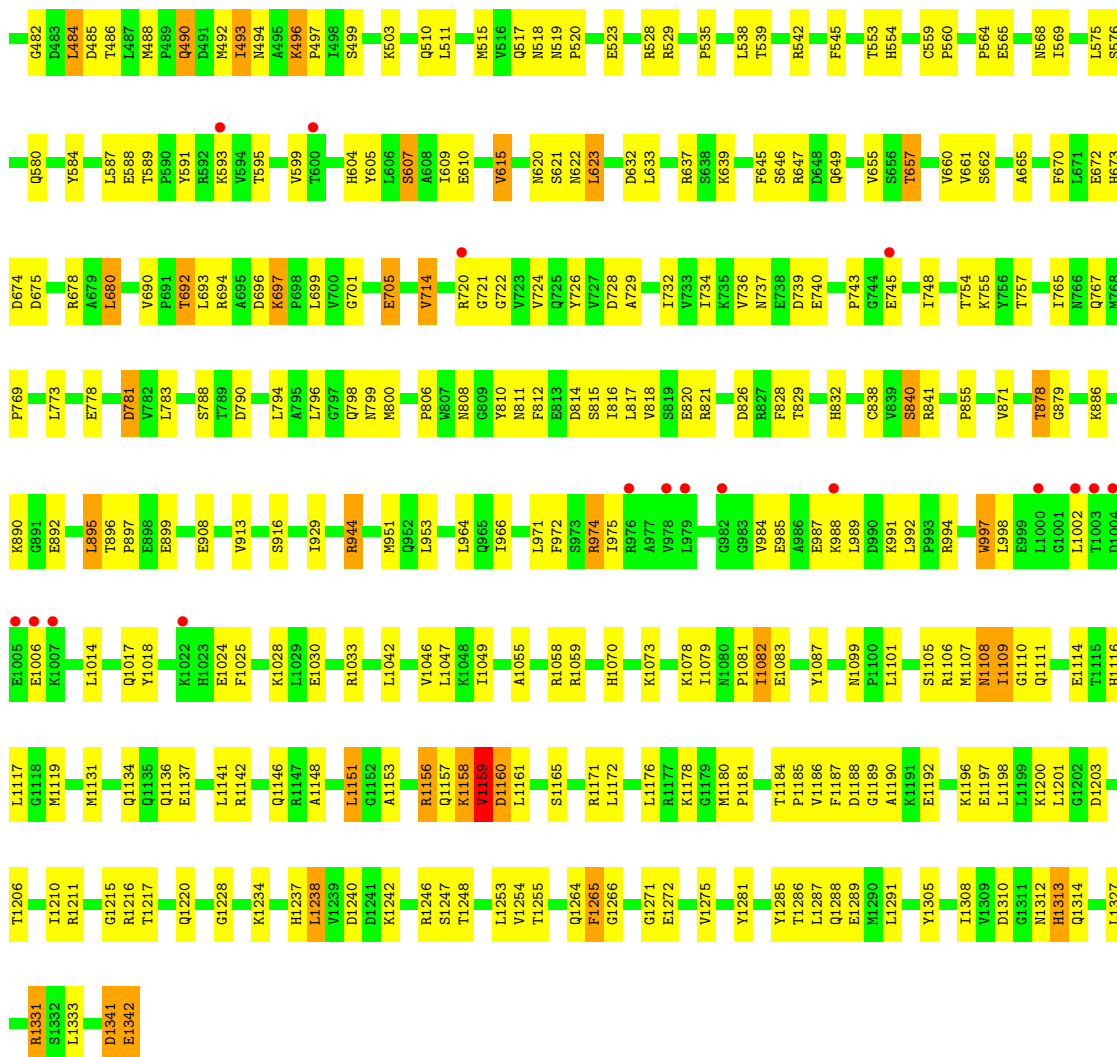
• Molecule 2: DNA-directed RNA polymerase subunit beta



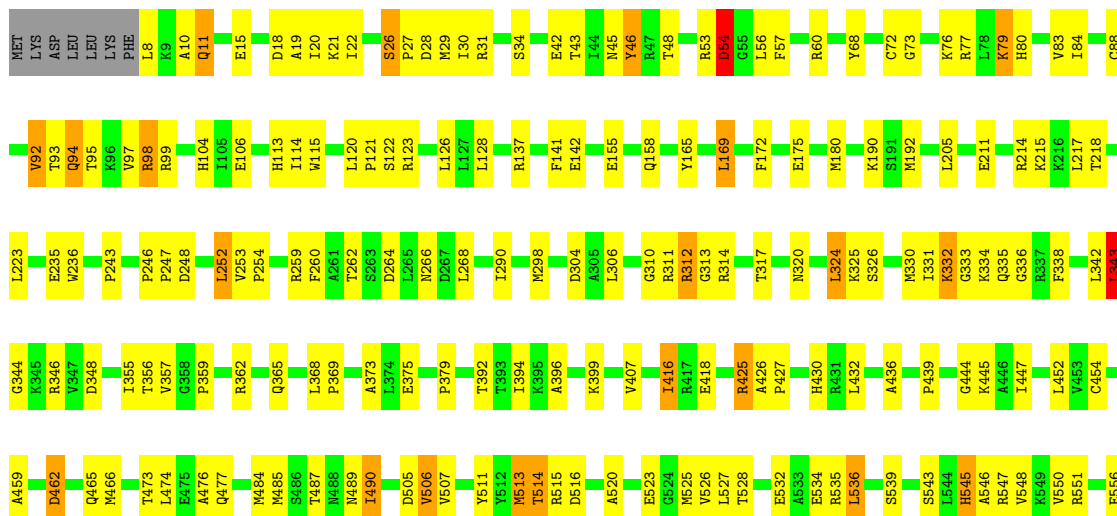


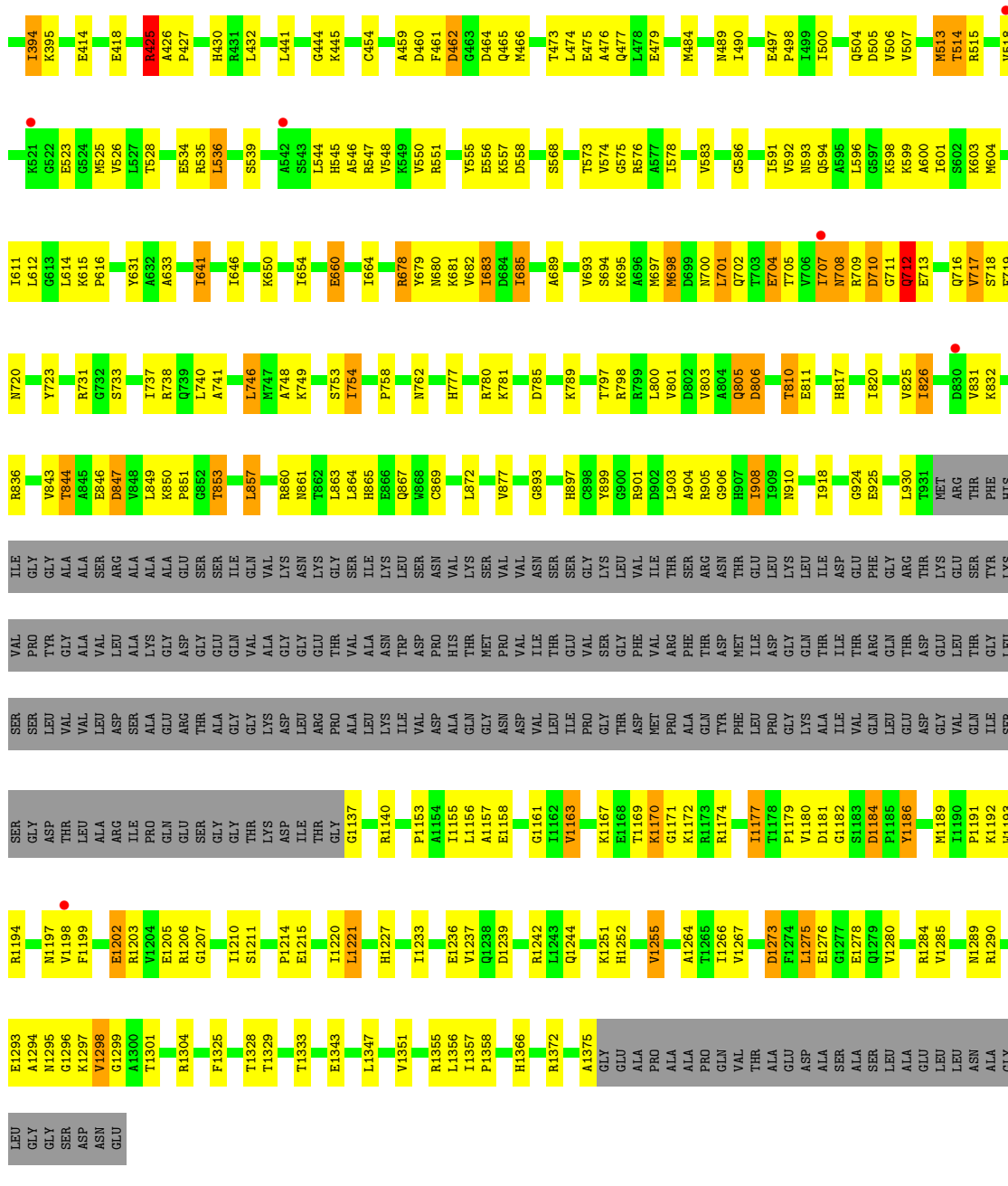
• Molecule 2: DNA-directed RNA polymerase subunit beta



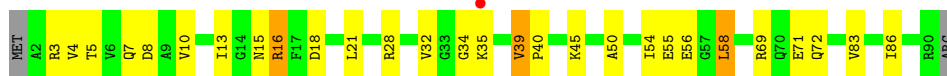


• Molecule 3: DNA-directed RNA polymerase subunit beta'



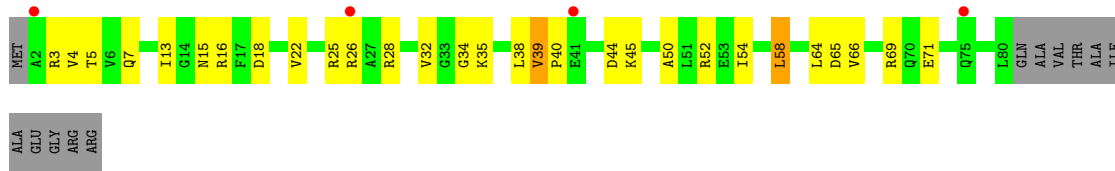


● Molecule 4: DNA-directed RNA polymerase subunit omega

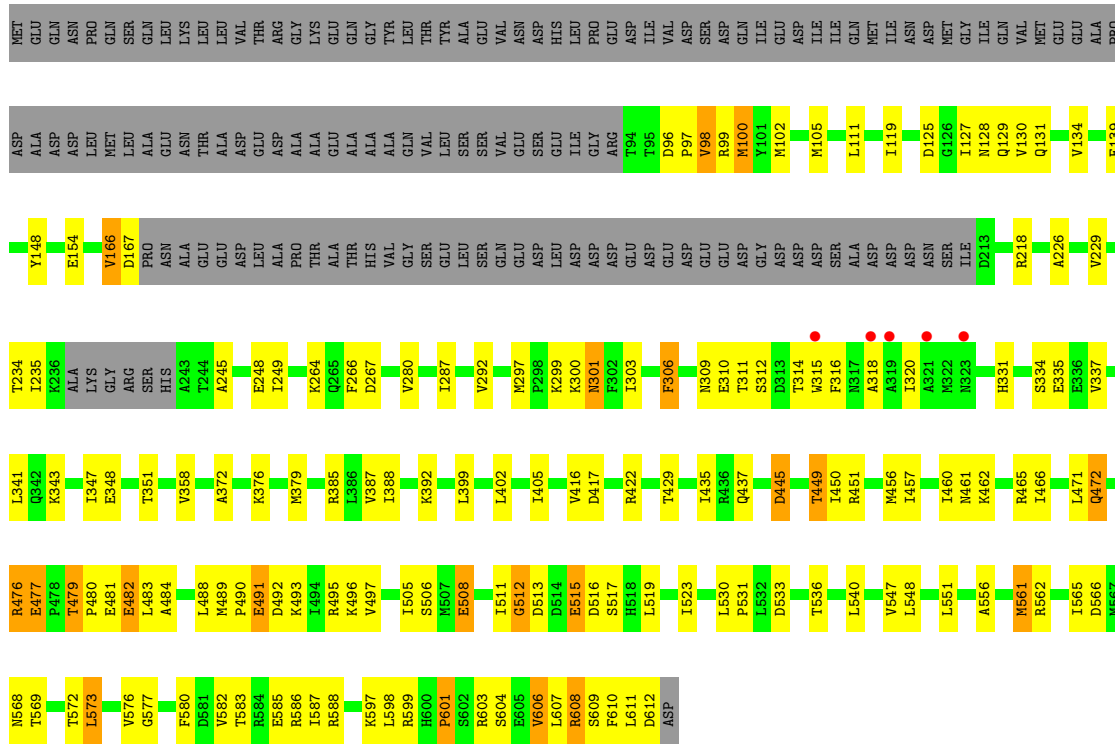


● Molecule 4: DNA-directed RNA polymerase subunit omega

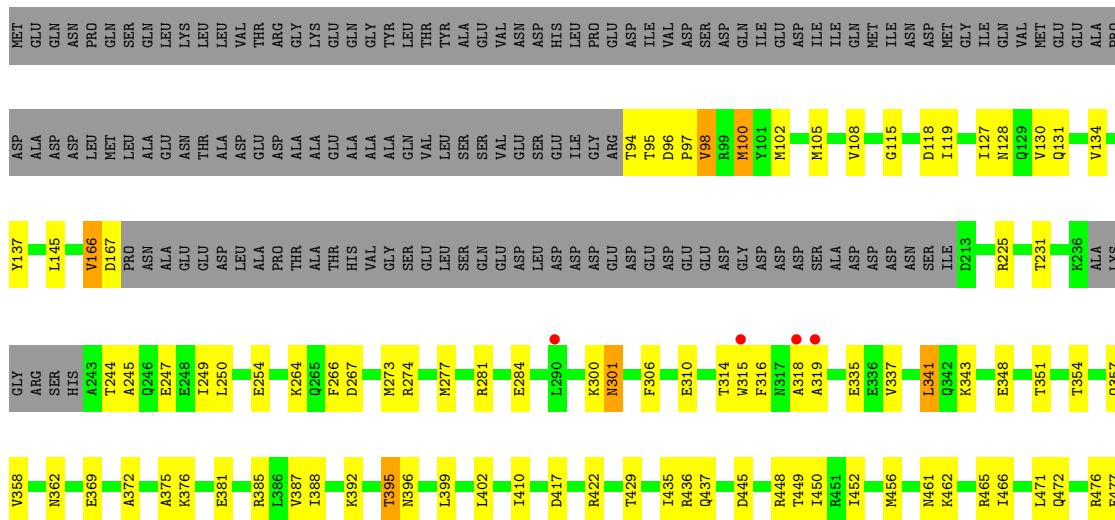


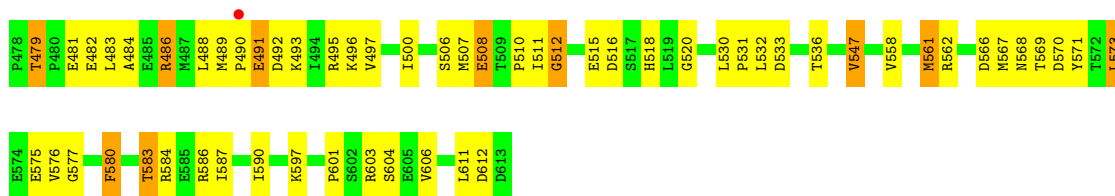


• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.81Å 206.67Å 310.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 4.10 29.74 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.74-4.10) 99.4 (29.74-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 4.11Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.243 , 0.287 0.243 , 0.287	Depositor DCC
R_{free} test set	1946 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	184.9	Xtrriage
Anisotropy	0.260	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 155.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55125	wwPDB-VP
Average B, all atoms (Å ²)	233.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: RFP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/1834	0.62	0/2485
1	B	0.34	0/1697	0.79	3/2300 (0.1%)
1	G	0.30	0/1777	0.63	1/2408 (0.0%)
1	H	0.34	0/1681	0.79	2/2278 (0.1%)
2	C	0.32	0/10738	0.62	5/14488 (0.0%)
2	I	0.31	2/10734 (0.0%)	0.62	2/14483 (0.0%)
3	D	0.29	0/9205	0.61	2/12430 (0.0%)
3	J	0.29	0/9140	0.64	4/12341 (0.0%)
4	E	0.26	0/693	0.53	0/935
4	K	0.32	0/629	0.55	0/847
5	F	0.28	0/3864	0.61	0/5194
5	L	0.29	0/3872	0.61	2/5205 (0.0%)
All	All	0.30	2/55864 (0.0%)	0.63	21/75394 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	3
2	I	0	3
3	D	0	2
3	J	0	3
5	F	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	344	GLY	C-N	-5.42	1.24	1.34
2	I	997	TRP	CB-CG	-5.04	1.41	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	425	ARG	NE-CZ-NH2	11.69	126.14	120.30
3	J	425	ARG	NE-CZ-NH1	-9.14	115.73	120.30
2	I	1137	GLU	CA-CB-CG	7.41	129.69	113.40
3	D	343	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	B	135	ASP	CB-CG-OD1	-6.66	112.30	118.30
3	J	343	LEU	CB-CG-CD1	-6.17	100.52	111.00
2	C	1265	PHE	CB-CG-CD1	-6.16	116.49	120.80
1	B	9	LEU	CA-CB-CG	6.02	129.15	115.30
3	J	54	ASP	N-CA-C	-5.93	94.98	111.00
2	C	1265	PHE	CB-CG-CD2	5.87	124.91	120.80
2	C	1264	GLN	N-CA-C	-5.78	95.40	111.00
1	B	68	TYR	CA-CB-CG	5.70	124.24	113.40
5	L	436	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	C	503	LYS	CB-CG-CD	5.52	125.95	111.60
1	G	29	GLU	N-CA-C	5.45	125.72	111.00
3	D	54	ASP	N-CA-C	-5.31	96.66	111.00
1	H	32	GLU	CG-CD-OE1	-5.26	107.78	118.30
1	H	32	GLU	CG-CD-OE2	5.22	128.74	118.30
2	C	1253	LEU	CA-CB-CG	5.21	127.29	115.30
2	I	1265	PHE	CB-CG-CD1	-5.12	117.21	120.80
5	L	583	THR	C-N-CA	5.12	134.51	121.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASN	Sidechain
1	B	135	ASP	Sidechain
2	C	107	ARG	Peptide
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	1153	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	1273	ASP	Mainchain
3	J	1296	GLY	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	1812	0	1839	73	0
1	B	1677	0	1703	93	0
1	G	1755	0	1773	73	0
1	H	1662	0	1687	68	0
2	C	10569	0	10587	326	0
2	I	10565	0	10581	267	0
3	D	9065	0	9210	297	0
3	J	9001	0	9165	277	0
4	E	691	0	695	17	0
4	K	627	0	634	18	0
5	F	3813	0	3880	103	0
5	L	3821	0	3884	95	0
6	C	59	0	56	6	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	I	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	55125	0	55694	1519	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 (1519) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.23	1.11
2:C:1269:ARG:HG2	3:D:343:LEU:HD12	1.36	1.07
5:L:97:PRO:HA	5:L:100:MET:HG3	1.45	0.97
2:C:18:ARG:NH1	2:C:621:SER:O	2.04	0.91
2:I:1271:GLY:HA2	3:J:343:LEU:HD11	1.51	0.90
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.52	0.88
1:B:75:GLN:HE22	1:B:132:HIS:HB2	1.37	0.88
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.56	0.87
2:C:1271:GLY:CA	3:D:343:LEU:HD21	2.03	0.87
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.38	0.87
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.59	0.85
3:J:54:ASP:OD2	3:J:60:ARG:NH1	2.08	0.85
3:D:54:ASP:OD2	3:D:60:ARG:NH1	2.09	0.85
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.59	0.84
1:A:45:ARG:HG2	1:B:38:THR:HB	1.59	0.84
1:H:32:GLU:HA	1:H:198:LEU:HD12	1.59	0.84
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.59	0.83
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.60	0.83
1:G:45:ARG:HG2	1:H:38:THR:HB	1.59	0.83
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.43	0.82
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.61	0.82
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.45	0.82
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.14	0.81
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.61	0.81
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.63	0.81
3:D:342:LEU:HA	3:D:343:LEU:HD23	1.61	0.81
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.61	0.81
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.63	0.80
1:G:228:LEU:O	1:G:230:ALA:N	2.13	0.80
2:I:560:PRO:O	3:J:780:ARG:NH2	2.14	0.80
2:I:821:ARG:HH21	2:I:1082:ILE:HG21	1.46	0.80
3:D:1206:ARG:NH2	3:J:1295:ASN:OD1	2.16	0.79
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.46	0.79
2:C:41:GLN:NE2	2:C:73:TYR:O	2.15	0.79
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.63	0.78
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.65	0.77
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.17	0.77
2:I:1271:GLY:CA	3:J:343:LEU:HD11	2.15	0.77
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.66	0.76
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.67	0.76
1:H:211:ILE:HD11	1:H:215:GLU:HG2	1.68	0.76
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.68	0.76
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.68	0.76
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.68	0.76
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.67	0.76
1:G:14:VAL:HG13	1:G:15:ASP:H	1.50	0.76
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.50	0.75
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.52	0.75
3:D:392:THR:HG21	5:F:606:VAL:HA	1.68	0.75
3:D:1298:VAL:N	3:D:1299:GLY:HA3	1.99	0.74
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.69	0.74
3:D:557:LYS:HB3	3:D:563:LEU:HD23	1.69	0.74
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.70	0.74
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.70	0.74
3:D:1155:ILE:HD13	3:D:1190:ILE:HD13	1.69	0.73
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.70	0.73
2:I:314:ASN:O	2:I:352:ARG:NH1	2.21	0.73
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.69	0.73
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.70	0.72
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.71	0.72
3:D:259:ARG:HD3	5:F:505:ILE:HD13	1.71	0.72
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.19	0.72
3:J:709:ARG:O	3:J:711:GLY:N	2.23	0.72
1:B:66:HIS:NE2	1:B:69:SER:OG	2.23	0.72
5:F:511:ILE:HG12	5:F:512:GLY:H	1.54	0.72
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.71	0.72
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.71	0.72
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.72	0.72
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.72	0.72
1:B:191:ARG:NH1	1:B:196:THR:O	2.22	0.71
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.71	0.71
3:J:343:LEU:HD12	3:J:344:GLY:HA3	1.72	0.71
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.72	0.71
1:B:134:THR:HG23	1:B:135:ASP:H	1.54	0.71
3:D:576:ARG:NH1	3:D:593:ASN:O	2.23	0.71
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.73	0.71
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.72	0.70
2:C:40:GLU:O	2:C:73:TYR:OH	2.07	0.70
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.73	0.70
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.39	0.70
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.71	0.70
1:A:11:PRO:HD3	1:B:227:GLN:OE1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.73	0.70
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.24	0.70
5:L:601:PRO:HA	5:L:604:SER:HB3	1.72	0.70
3:J:310:GLY:HA2	3:J:314:ARG:HG2	1.73	0.69
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.73	0.69
3:D:557:LYS:HA	3:D:563:LEU:HA	1.75	0.69
2:I:18:ARG:NH2	2:I:622:ASN:OD1	2.25	0.69
3:D:264:ASP:OD2	5:F:506:SER:OG	2.11	0.69
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.75	0.69
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.75	0.69
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.26	0.69
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.73	0.69
1:H:190:ALA:N	1:H:198:LEU:O	2.22	0.68
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.76	0.68
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.74	0.68
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.75	0.68
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.27	0.68
2:C:560:PRO:O	3:D:780:ARG:NH2	2.26	0.68
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.27	0.68
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.76	0.68
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.76	0.68
2:C:1223:ARG:NH1	3:D:721:SER:OG	2.20	0.68
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.76	0.67
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.58	0.67
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.27	0.67
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.59	0.67
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.77	0.67
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.23	0.67
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.76	0.67
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.76	0.67
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.28	0.66
5:L:476:ARG:NH1	5:L:477:GLU:O	2.28	0.66
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.44	0.66
3:D:416:ILE:HG23	3:D:439:PRO:HG2	1.78	0.66
5:F:461:ASN:O	5:F:465:ARG:HG2	1.95	0.66
2:C:821:ARG:HH21	2:C:1082:ILE:HG21	1.60	0.66
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.76	0.66
1:H:53:GLY:HA3	1:H:177:TYR:O	1.95	0.66
5:L:476:ARG:HD2	5:L:477:GLU:HG2	1.77	0.66
2:I:565:GLU:O	2:I:565:GLU:HG2	1.95	0.66
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.75	0.66
1:H:158:ARG:HB3	1:H:172:LEU:HD23	1.78	0.66
2:I:324:LYS:O	2:I:327:GLN:NE2	2.29	0.66
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.59	0.66
3:J:264:ASP:OD2	5:L:506:SER:OG	2.13	0.66
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.20	0.66
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.79	0.65
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.60	0.65
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.59	0.65
1:B:79:LEU:HD11	3:D:526:VAL:HG21	1.77	0.65
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.78	0.65
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.78	0.65
1:H:74:VAL:HG12	1:H:76:GLU:H	1.61	0.65
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.77	0.65
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.79	0.65
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.77	0.65
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.78	0.65
2:C:302:ILE:O	2:C:330:HIS:NE2	2.26	0.65
2:C:324:LYS:O	2:C:327:GLN:NE2	2.28	0.65
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.78	0.65
2:I:580:GLN:HB2	2:I:605:TYR:HE1	1.61	0.65
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.77	0.65
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.79	0.65
1:B:74:VAL:HG12	1:B:76:GLU:H	1.61	0.65
2:C:263:VAL:HG21	2:C:273:HIS:CD2	2.32	0.65
2:C:565:GLU:O	2:C:565:GLU:HG2	1.95	0.65
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.78	0.65
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.62	0.65
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.30	0.65
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.79	0.65
1:B:53:GLY:HA3	1:B:177:TYR:O	1.96	0.64
1:H:56:VAL:HG22	1:H:146:VAL:HG22	1.77	0.64
2:C:528:ARG:NH2	2:C:576:SER:O	2.30	0.64
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.12	0.64
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.26	0.64
1:G:71:LYS:HZ3	1:G:140:ILE:HG22	1.62	0.64
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.80	0.64
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.32	0.64
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.80	0.64
3:J:342:LEU:HA	3:J:343:LEU:HD13	1.79	0.64
2:C:30:ILE:HD12	2:C:30:ILE:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.79	0.64
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.80	0.64
5:F:573:LEU:H	5:F:573:LEU:HD23	1.63	0.64
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.79	0.64
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.78	0.64
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.80	0.64
3:J:901:ARG:HD2	3:J:906:GLY:O	1.98	0.64
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.63	0.64
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.79	0.64
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.12	0.63
1:B:75:GLN:NE2	1:B:132:HIS:HB2	2.11	0.63
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.32	0.63
3:D:1263:LYS:HE2	3:D:1279:GLN:NE2	2.12	0.63
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.44	0.63
3:D:342:LEU:HA	3:D:343:LEU:CD2	2.28	0.63
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.79	0.63
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.34	0.63
5:F:515:GLU:C	5:F:517:SER:H	2.00	0.63
2:I:722:GLY:HA2	2:I:737:ASN:OD1	1.99	0.63
1:B:55:ALA:HB1	1:B:176:CYS:SG	2.39	0.63
5:F:511:ILE:HG12	5:F:512:GLY:N	2.12	0.63
3:D:399:LYS:NZ	5:F:611:LEU:O	2.31	0.63
2:I:18:ARG:NH1	2:I:621:SER:O	2.32	0.63
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.81	0.63
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.80	0.63
2:C:201:ARG:NH2	2:C:370:MET:O	2.25	0.62
1:H:214:GLU:HG2	1:H:218:ARG:NH2	2.14	0.62
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.81	0.62
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.34	0.62
3:J:700:ASN:O	3:J:704:GLU:HB2	1.99	0.62
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.64	0.62
6:C:3001:RFP:O11	6:C:3001:RFP:O1	2.16	0.62
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.35	0.62
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.40	0.62
3:D:1301:THR:HA	3:J:1297:LYS:HE2	1.81	0.62
2:I:18:ARG:HH12	2:I:622:ASN:HA	1.65	0.62
2:I:30:ILE:HD12	2:I:30:ILE:H	1.64	0.62
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.64	0.62
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.64	0.61
1:H:195:ARG:HH21	1:H:198:LEU:HD11	1.64	0.61
2:I:721:GLY:N	2:I:740:GLU:OE1	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.81	0.61
3:J:34:SER:OG	3:J:104:HIS:ND1	2.33	0.61
3:J:576:ARG:NH1	3:J:593:ASN:O	2.33	0.61
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.64	0.61
1:H:147:GLN:OE1	1:H:158:ARG:NH2	2.33	0.61
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.32	0.61
2:I:81:ASP:OD1	2:I:83:GLN:HG3	2.00	0.61
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.97	0.61
2:C:197:ARG:NH1	2:C:201:ARG:O	2.28	0.61
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.83	0.61
5:L:461:ASN:O	5:L:465:ARG:HG2	2.01	0.61
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.82	0.61
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.82	0.61
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.83	0.60
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.83	0.60
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.81	0.60
3:D:45:ASN:HB3	3:D:48:THR:O	2.01	0.60
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.66	0.60
3:J:514:THR:HB	3:J:576:ARG:HG2	1.83	0.60
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.33	0.60
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.42	0.60
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.83	0.60
5:L:573:LEU:HD23	5:L:573:LEU:H	1.66	0.60
1:B:66:HIS:H	1:B:66:HIS:CD2	2.19	0.60
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.37	0.60
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.65	0.60
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.83	0.60
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.83	0.60
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.83	0.60
2:C:356:THR:HG21	2:C:362:ALA:HA	1.84	0.60
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.84	0.60
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.66	0.60
3:D:843:VAL:HG11	3:D:897:HIS:O	2.02	0.60
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.83	0.60
3:D:709:ARG:O	3:D:711:GLY:N	2.32	0.60
5:F:597:LYS:O	5:F:603:ARG:HG3	2.02	0.60
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.67	0.60
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.67	0.59
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.84	0.59
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.83	0.59
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:387:ASN:HA	2:C:391:SER:HB2	1.84	0.59
2:C:517:GLN:HE21	2:C:760:ASN:H	1.49	0.59
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.85	0.59
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.38	0.59
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.84	0.59
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.17	0.59
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.33	0.59
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.18	0.59
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.85	0.59
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.84	0.59
2:I:528:ARG:NH1	2:I:576:SER:O	2.36	0.59
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.84	0.59
1:G:12:ARG:H	1:G:30:PRO:HD2	1.68	0.59
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.35	0.59
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.84	0.59
3:D:211:GLU:OE2	3:D:214:ARG:NH1	2.35	0.59
3:D:336:GLY:HA3	3:D:1324:SER:O	2.02	0.59
5:F:235:ILE:HA	5:F:245:ALA:HB2	1.84	0.59
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.84	0.59
2:C:4:SER:OG	2:C:5:TYR:N	2.36	0.59
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.67	0.59
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.36	0.59
1:G:72:GLU:OE2	2:I:726:TYR:OH	2.16	0.59
3:J:45:ASN:HB3	3:J:48:THR:O	2.03	0.59
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.85	0.59
5:F:300:LYS:HE3	5:F:301:ASN:HD21	1.68	0.58
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.85	0.58
5:L:166:VAL:O	5:L:167:ASP:HB2	2.02	0.58
2:I:256:GLU:HB3	2:I:261:VAL:HG22	1.84	0.58
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.84	0.58
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.35	0.58
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.36	0.58
5:L:612:ASP:N	5:L:612:ASP:OD1	2.36	0.58
1:B:59:VAL:HG22	1:B:144:ILE:HG23	1.85	0.58
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.85	0.58
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.38	0.58
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.85	0.58
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.04	0.58
2:I:208:ILE:HD11	2:I:365:GLU:HB3	1.85	0.58
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.85	0.58
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:15:PHE:HE1	2:I:1151:LEU:HD12	1.68	0.58
1:B:56:VAL:HG22	1:B:146:VAL:HG22	1.84	0.58
2:C:1269:ARG:CG	3:D:343:LEU:HD12	2.23	0.58
3:D:317:THR:HB	3:D:324:LEU:HB3	1.85	0.58
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.85	0.58
1:A:158:ARG:HH22	1:A:172:LEU:HB3	1.68	0.58
2:C:210:LEU:HD11	2:C:224:PHE:HE2	1.68	0.58
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.84	0.58
1:G:219:ARG:O	1:G:223:ILE:HG13	2.03	0.58
2:I:452:ARG:NH1	2:I:584:TYR:O	2.36	0.58
1:B:27:THR:HG23	1:B:202:VAL:HG22	1.84	0.58
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.19	0.58
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.84	0.58
1:A:23:HIS:HE1	1:A:204:GLU:HG3	1.69	0.58
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.38	0.58
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.68	0.58
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.86	0.58
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.86	0.58
1:B:35:PHE:HA	1:B:38:THR:HG22	1.86	0.58
1:H:101:THR:HG22	1:H:116:THR:HG21	1.85	0.58
3:J:462:ASP:OD2	3:J:464:ASP:OD2	2.21	0.58
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.85	0.58
1:G:231:PHE:HB3	1:H:218:ARG:HB3	1.85	0.57
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.86	0.57
3:J:16:GLU:HG3	3:J:17:PHE:H	1.66	0.57
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.86	0.57
2:I:1272:GLU:N	3:J:343:LEU:HD11	2.19	0.57
1:B:175:ALA:HB1	1:B:177:TYR:CE1	2.40	0.57
3:D:901:ARG:HD2	3:D:906:GLY:O	2.05	0.57
1:H:7:GLU:HG2	1:H:8:PHE:H	1.70	0.57
2:I:15:PHE:CE1	2:I:1151:LEU:HD12	2.39	0.57
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.68	0.57
1:B:102:LEU:HD23	1:B:115:ILE:HA	1.86	0.57
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.70	0.57
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.86	0.57
3:D:598:LYS:N	3:D:728:SER:O	2.29	0.57
1:G:14:VAL:HG13	1:G:15:ASP:N	2.19	0.57
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.69	0.57
2:C:298:ALA:N	2:C:334:GLU:O	2.30	0.57
2:C:490:GLN:HG3	5:F:472:GLN:NE2	2.20	0.57
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.85	0.57
3:J:1169:THR:OG1	3:J:1192:LYS:HD3	2.04	0.57
5:F:388:ILE:O	5:F:392:LYS:HG3	2.05	0.57
2:I:1247:SER:HB3	3:J:375:GLU:O	2.05	0.57
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.86	0.57
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.86	0.57
5:L:343:LYS:H	5:L:343:LYS:HD2	1.69	0.57
1:A:14:VAL:HG22	1:A:15:ASP:H	1.70	0.57
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.87	0.57
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.87	0.56
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.85	0.56
2:C:615:VAL:HG13	2:C:651:ASP:H	1.70	0.56
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.05	0.56
1:G:45:ARG:NH1	1:H:34:GLY:O	2.38	0.56
1:G:225:ALA:HB2	1:H:228:LEU:HD13	1.86	0.56
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.87	0.56
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.86	0.56
2:I:150:HIS:CD2	2:I:454:ARG:HE	2.23	0.56
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.06	0.56
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.70	0.56
2:I:599:VAL:HG21	2:I:623:LEU:HD22	1.86	0.56
2:I:1271:GLY:HA2	3:J:343:LEU:CD1	2.32	0.56
2:C:533:LEU:HB2	6:C:3001:RFP:H143	1.86	0.56
3:J:473:THR:HG23	3:J:476:ALA:H	1.69	0.56
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.56
2:C:778:GLU:O	2:C:781:ASP:HB2	2.04	0.56
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.86	0.56
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.70	0.56
3:D:847:ASP:OD1	3:D:847:ASP:N	2.30	0.56
5:F:97:PRO:HA	5:F:100:MET:HG3	1.87	0.56
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.87	0.56
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.87	0.56
1:G:73:GLY:O	1:G:134:THR:HG22	2.06	0.56
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.87	0.56
3:D:56:LEU:HD12	3:D:56:LEU:H	1.72	0.56
1:H:19:VAL:O	1:H:20:SER:OG	2.19	0.56
1:A:23:HIS:HB2	1:A:206:GLU:HA	1.88	0.55
2:C:725:GLN:HE22	2:C:966:ILE:HG23	1.71	0.55
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.87	0.55
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.87	0.55
3:J:843:VAL:HG11	3:J:897:HIS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:94:THR:OG1	5:L:95:THR:N	2.39	0.55
2:C:705:GLU:HB2	2:C:794:LEU:H	1.72	0.55
2:I:40:GLU:O	2:I:73:TYR:OH	2.24	0.55
2:I:151:ARG:HH22	2:I:175:ARG:HD2	1.71	0.55
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.70	0.55
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.06	0.55
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.88	0.55
5:L:105:MET:HE3	5:L:385:ARG:HG2	1.88	0.55
2:C:510:GLN:OE1	2:C:534:GLY:HA2	2.05	0.55
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.41	0.55
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.89	0.55
2:I:705:GLU:HB2	2:I:794:LEU:H	1.71	0.55
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.88	0.55
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.87	0.55
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.89	0.55
5:F:148:TYR:OH	5:F:218:ARG:HA	2.06	0.55
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.06	0.55
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.21	0.55
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.88	0.55
5:L:395:THR:OG1	5:L:396:ASN:N	2.39	0.55
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.06	0.55
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.72	0.55
2:I:675:ASP:HB3	2:I:1107:MET:O	2.07	0.55
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.72	0.55
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.42	0.55
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.88	0.55
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.89	0.55
1:G:9:LEU:O	1:H:227:GLN:NE2	2.40	0.55
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.42	0.55
1:H:82:LEU:HD13	1:H:173:VAL:HG13	1.89	0.55
5:L:316:PHE:CZ	5:L:337:VAL:HB	2.42	0.55
1:A:191:ARG:NH1	1:A:198:LEU:O	2.40	0.55
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.88	0.55
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.89	0.55
3:D:19:ALA:O	3:D:20:ILE:HG13	2.07	0.54
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.88	0.54
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.07	0.54
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.87	0.54
5:L:372:ALA:O	5:L:376:LYS:HG3	2.06	0.54
1:A:150:ARG:NH1	1:B:7:GLU:O	2.40	0.54
5:F:314:THR:O	5:F:318:ALA:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.71	0.54
3:D:94:GLN:O	3:D:97:VAL:HG22	2.06	0.54
5:F:601:PRO:HA	5:F:604:SER:HB3	1.88	0.54
5:L:300:LYS:HE3	5:L:301:ASN:HD21	1.73	0.54
2:C:258:ASN:ND2	2:C:282:VAL:HG22	2.22	0.54
3:D:325:LYS:HE2	3:D:330:MET:HG2	1.90	0.54
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.72	0.54
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.90	0.54
2:I:1272:GLU:H	3:J:343:LEU:HD11	1.73	0.54
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.90	0.54
2:C:214:ASN:HB2	2:C:359:ARG:HD2	1.90	0.54
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.42	0.54
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.71	0.54
5:F:166:VAL:O	5:F:167:ASP:HB2	2.08	0.54
3:J:342:LEU:HA	3:J:343:LEU:CD1	2.37	0.54
2:C:211:ARG:NH1	2:C:357:ASN:O	2.40	0.54
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.07	0.54
3:J:901:ARG:HA	3:J:908:ILE:HA	1.90	0.54
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.88	0.54
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.72	0.54
1:H:62:ASP:OD1	1:H:62:ASP:N	2.37	0.54
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.42	0.54
3:J:847:ASP:OD2	3:J:860:ARG:HG2	2.08	0.54
2:C:292:ILE:HD12	2:C:322:LEU:HD11	1.90	0.54
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.73	0.54
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.81	0.54
5:F:316:PHE:CZ	5:F:334:SER:HA	2.43	0.54
1:H:61:ILE:HG22	1:H:62:ASP:OD1	2.08	0.54
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.40	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.88	0.54
3:J:460:ASP:HB2	3:J:462:ASP:OD1	2.07	0.54
2:C:617:ALA:HA	2:C:636:CYS:SG	2.48	0.54
3:D:514:THR:OG1	3:D:594:GLN:O	2.25	0.54
3:D:700:ASN:O	3:D:704:GLU:HB2	2.08	0.54
2:I:778:GLU:O	2:I:781:ASP:HB2	2.08	0.54
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.43	0.54
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.88	0.54
2:C:517:GLN:NE2	2:C:760:ASN:H	2.06	0.54
1:G:73:GLY:N	2:I:728:ASP:OD2	2.24	0.54
1:G:91:ARG:HH21	1:G:122:GLU:CD	2.12	0.54
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.41	0.54
3:J:19:ALA:O	3:J:20:ILE:HG13	2.08	0.54
1:B:14:VAL:HG23	1:B:27:THR:O	2.08	0.53
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.89	0.53
3:D:1273:ASP:N	3:D:1273:ASP:OD1	2.41	0.53
5:F:343:LYS:HD2	5:F:343:LYS:H	1.73	0.53
5:F:479:THR:HG23	5:F:481:GLU:H	1.72	0.53
1:H:153:VAL:O	1:H:175:ALA:N	2.28	0.53
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.90	0.53
5:L:511:ILE:HG13	5:L:512:GLY:H	1.73	0.53
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.44	0.53
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.38	0.53
6:C:3001:RFP:H10O	6:C:3001:RFP:HO9	1.52	0.53
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.40	0.53
5:F:562:ARG:HH21	5:F:573:LEU:HD22	1.72	0.53
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.90	0.53
1:G:74:VAL:HG22	1:G:76:GLU:H	1.73	0.53
1:H:51:MET:C	1:H:150:ARG:HG2	2.29	0.53
3:J:27:PRO:HB3	3:J:241:VAL:HG23	1.90	0.53
3:J:317:THR:HB	3:J:324:LEU:HB3	1.89	0.53
3:D:705:THR:OG1	3:D:718:SER:HA	2.08	0.53
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.39	0.53
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.41	0.53
1:A:158:ARG:NH2	1:A:172:LEU:HB3	2.23	0.53
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.91	0.53
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.89	0.53
2:C:730:SER:O	2:C:753:LEU:HB2	2.08	0.53
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.91	0.53
2:I:227:LYS:O	2:I:245:ARG:NH2	2.41	0.53
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.24	0.53
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.90	0.53
3:D:748:ALA:O	3:D:777:HIS:HD2	1.91	0.53
3:D:872:LEU:O	3:D:877:VAL:HG12	2.09	0.53
3:D:1273:ASP:O	3:D:1275:LEU:N	2.41	0.53
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.91	0.53
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.74	0.53
2:I:808:ASN:H	3:J:633:ALA:HB2	1.74	0.53
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.90	0.53
1:B:11:PRO:O	1:B:12:ARG:HG3	2.09	0.53
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.09	0.53
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.91	0.53
3:J:338:PHE:HA	3:J:342:LEU:O	2.09	0.53
2:C:540:ARG:NH2	6:C:3001:RFP:O12	2.42	0.53
4:E:10:VAL:HG13	4:E:16:ARG:HB2	1.91	0.53
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.74	0.53
1:B:118:ASP:H	1:B:121:VAL:HB	1.74	0.52
5:F:515:GLU:O	5:F:517:SER:N	2.42	0.52
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.74	0.52
2:C:721:GLY:N	2:C:740:GLU:OE1	2.32	0.52
5:F:462:LYS:O	5:F:466:ILE:HG13	2.09	0.52
1:G:155:ALA:HB2	1:G:173:VAL:C	2.29	0.52
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	2.08	0.52
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.07	0.52
3:J:430:HIS:HD2	3:J:432:LEU:H	1.57	0.52
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.42	0.52
2:C:513:GLN:HB2	6:C:3001:RFP:O9	2.09	0.52
2:I:206:ALA:O	2:I:209:ILE:HG22	2.08	0.52
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.74	0.52
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.91	0.52
3:J:394:ILE:HG23	5:L:536:THR:HG22	1.89	0.52
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.75	0.52
3:D:490:ILE:HD13	3:D:490:ILE:H	1.74	0.52
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.91	0.52
1:G:23:HIS:HB2	1:G:205:MET:O	2.09	0.52
2:I:674:ASP:OD1	2:I:1110:GLY:N	2.34	0.52
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.24	0.52
1:A:86:LYS:HD3	1:A:176:CYS:SG	2.49	0.52
1:B:66:HIS:CE1	1:B:69:SER:HG	2.23	0.52
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.92	0.52
3:J:195:GLU:O	3:J:199:GLU:HG3	2.09	0.52
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.90	0.52
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.25	0.52
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.90	0.52
3:D:416:ILE:HD12	3:D:439:PRO:HG3	1.90	0.52
1:G:90:VAL:HG22	1:G:91:ARG:H	1.75	0.52
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.90	0.52
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.40	0.52
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.92	0.52
1:G:155:ALA:N	1:G:174:ASP:OD1	2.39	0.52
2:I:148:GLN:NE2	2:I:535:PRO:O	2.36	0.52
3:J:56:LEU:HD12	3:J:56:LEU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.92	0.52
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.89	0.52
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.91	0.52
3:J:343:LEU:HD12	3:J:344:GLY:CA	2.39	0.52
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.23	0.52
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.43	0.52
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.92	0.52
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.74	0.52
3:J:701:LEU:HD13	3:J:723:TYR:HB2	1.91	0.52
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.09	0.52
5:F:551:LEU:HD11	5:F:598:LEU:HD21	1.92	0.51
1:H:23:HIS:ND1	1:H:205:MET:O	2.38	0.51
1:H:90:VAL:HG12	1:H:91:ARG:H	1.76	0.51
1:A:7:GLU:O	1:B:150:ARG:NH1	2.43	0.51
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.91	0.51
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.76	0.51
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.43	0.51
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.43	0.51
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.45	0.51
3:J:515:ARG:NH2	3:J:717:VAL:O	2.44	0.51
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.51	0.51
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.24	0.51
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.92	0.51
2:I:371:ARG:HB3	2:I:374:GLU:OE2	2.10	0.51
2:I:692:THR:OG1	2:I:693:LEU:N	2.43	0.51
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.92	0.51
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.75	0.51
3:D:73:GLY:O	3:D:76:LYS:NZ	2.25	0.51
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.91	0.51
1:B:6:THR:OG1	1:B:7:GLU:N	2.40	0.51
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.25	0.51
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.76	0.51
1:B:19:VAL:O	1:B:20:SER:OG	2.24	0.51
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.26	0.51
1:B:113:ALA:HB2	1:B:126:PRO:HB3	1.91	0.51
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.92	0.51
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.43	0.51
1:G:32:GLU:OE2	1:H:150:ARG:NH2	2.44	0.51
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.75	0.51
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.11	0.51
3:D:832:LYS:HD3	3:D:1242:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:316:PHE:HZ	5:F:334:SER:HA	1.75	0.51
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.93	0.51
2:I:490:GLN:HE21	5:L:472:GLN:NE2	2.08	0.51
5:L:483:LEU:HD12	5:L:483:LEU:H	1.76	0.51
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.76	0.51
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.92	0.51
2:I:98:VAL:O	2:I:121:GLU:HA	2.10	0.51
3:J:475:GLU:OE1	4:K:28:ARG:NH2	2.44	0.51
3:J:678:ARG:HG3	3:J:679:TYR:N	2.26	0.51
3:J:749:LYS:HG2	3:J:753:SER:O	2.11	0.51
4:K:32:VAL:O	4:K:34:GLY:N	2.43	0.51
5:F:292:VAL:HG11	5:F:299:LYS:HG3	1.93	0.51
1:G:191:ARG:NH1	1:G:197:ASP:HA	2.25	0.51
2:I:871:VAL:O	2:I:944:ARG:NH1	2.44	0.51
1:B:9:LEU:HD23	1:B:10:LYS:O	2.11	0.51
2:C:692:THR:OG1	2:C:693:LEU:N	2.43	0.51
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.92	0.51
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.25	0.51
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.09	0.51
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.93	0.51
5:F:343:LYS:O	5:F:347:ILE:HG13	2.11	0.50
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.45	0.50
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.27	0.50
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.75	0.50
2:C:529:ARG:NH1	6:C:3001:RFP:O11	2.45	0.50
2:C:901:LEU:HD22	5:F:565:ILE:HD11	1.92	0.50
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.45	0.50
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.42	0.50
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.93	0.50
3:J:290:ILE:H	3:J:290:ILE:HD12	1.76	0.50
5:L:314:THR:O	5:L:318:ALA:HB3	2.11	0.50
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.93	0.50
2:C:906:PHE:CE2	5:F:608:ARG:HD3	2.45	0.50
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.93	0.50
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.92	0.50
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.47	0.50
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.76	0.50
2:C:808:ASN:H	3:D:633:ALA:HB2	1.77	0.50
5:F:457:ILE:HA	5:F:460:ILE:HD12	1.94	0.50
3:D:27:PRO:HD3	3:D:236:TRP:CD1	2.47	0.50
1:G:97:GLU:OE2	1:G:145:LYS:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.93	0.50
3:J:127:LEU:O	3:J:220:ARG:NH2	2.45	0.50
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.94	0.50
2:C:980:VAL:HA	2:C:984:VAL:HA	1.94	0.50
1:G:9:LEU:HD13	1:G:32:GLU:HG2	1.92	0.50
2:I:564:PRO:HG2	2:I:568:ASN:O	2.12	0.50
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.11	0.50
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.93	0.50
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.94	0.50
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.77	0.50
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.12	0.50
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.93	0.50
2:I:21:VAL:HG13	2:I:655:VAL:HG13	1.93	0.50
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.94	0.50
2:C:247:ARG:NH2	2:C:274:ILE:HD12	2.26	0.50
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.47	0.50
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.44	0.50
1:G:75:GLN:HA	2:I:729:ALA:N	2.27	0.50
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.27	0.50
3:J:462:ASP:CG	3:J:464:ASP:OD2	2.50	0.50
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.94	0.49
5:F:612:ASP:OD1	5:F:612:ASP:N	2.44	0.49
1:G:150:ARG:NH1	1:H:7:GLU:O	2.44	0.49
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.93	0.49
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.27	0.49
3:J:322:ARG:NE	5:L:510:PRO:HG2	2.27	0.49
3:D:1273:ASP:HB2	3:D:1276:GLU:HB2	1.93	0.49
5:F:127:ILE:O	5:F:130:VAL:HG22	2.13	0.49
3:J:115:TRP:O	3:J:119:SER:HB3	2.13	0.49
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.26	0.49
3:D:259:ARG:CD	5:F:505:ILE:HD13	2.42	0.49
5:F:372:ALA:O	5:F:376:LYS:HG3	2.12	0.49
2:C:246:LEU:O	2:C:269:ILE:HB	2.13	0.49
5:F:515:GLU:C	5:F:517:SER:N	2.65	0.49
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.38	0.49
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.77	0.49
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.45	0.49
3:J:94:GLN:O	3:J:97:VAL:HG22	2.12	0.49
3:J:1158:GLU:O	3:J:1206:ARG:NH1	2.46	0.49
3:J:1174:ARG:HA	3:J:1189:MET:HA	1.94	0.49
5:L:511:ILE:HG13	5:L:512:GLY:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:O	1:B:175:ALA:N	2.28	0.49
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.26	0.49
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.13	0.49
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	1.95	0.49
5:L:486:ARG:HB2	5:L:486:ARG:CZ	2.42	0.49
1:A:158:ARG:HH12	1:A:172:LEU:HD23	1.77	0.49
5:F:139:GLU:HG2	5:F:351:THR:HA	1.95	0.49
1:G:228:LEU:HD23	1:H:225:ALA:HB2	1.94	0.49
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.47	0.49
3:J:1297:LYS:HG3	3:J:1299:GLY:H	1.78	0.49
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.47	0.49
3:D:436:ALA:HB3	3:D:485:MET:HA	1.94	0.49
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.16	0.49
5:L:515:GLU:HG2	5:L:516:ASP:N	2.28	0.49
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.77	0.49
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.13	0.49
2:C:13:LYS:O	2:C:1183:ALA:N	2.38	0.49
2:C:722:GLY:HA2	2:C:737:ASN:OD1	2.13	0.49
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.53	0.49
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.34	0.49
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.27	0.49
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.13	0.49
3:J:705:THR:OG1	3:J:718:SER:HA	2.13	0.49
3:D:396:ALA:HB2	5:F:609:SER:CB	2.43	0.49
5:F:585:GLU:HA	5:F:588:ARG:HD3	1.95	0.49
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.94	0.49
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.94	0.49
3:J:331:ILE:O	3:J:337:ARG:HA	2.13	0.49
3:J:1167:LYS:HZ1	3:J:1170:LYS:HB2	1.77	0.49
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.95	0.49
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.48	0.49
2:I:499:SER:O	2:I:503:LYS:HB2	2.13	0.49
1:B:66:HIS:H	1:B:66:HIS:HD2	1.59	0.48
1:B:107:ILE:HG12	1:B:134:THR:O	2.12	0.48
2:C:169:LYS:O	2:C:170:VAL:HG22	2.13	0.48
3:D:43:THR:OG1	5:F:449:THR:O	2.17	0.48
5:F:483:LEU:HD12	5:F:483:LEU:H	1.78	0.48
3:J:73:GLY:O	3:J:76:LYS:NZ	2.24	0.48
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.42	0.48
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.95	0.48
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.13	0.48
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.95	0.48
3:J:325:LYS:HE2	3:J:330:MET:HA	1.95	0.48
1:A:45:ARG:HG2	1:B:38:THR:CB	2.38	0.48
1:B:214:GLU:O	1:B:218:ARG:HG3	2.12	0.48
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.13	0.48
3:D:418:GLU:HG3	4:E:45:LYS:H	1.76	0.48
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.76	0.48
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.95	0.48
2:I:52:ALA:HB2	2:I:461:GLU:HG3	1.94	0.48
2:I:754:THR:N	2:I:767:GLN:OE1	2.42	0.48
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.78	0.48
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.13	0.48
5:L:569:THR:OG1	5:L:570:ASP:N	2.42	0.48
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.75	0.48
4:E:69:ARG:HA	4:E:72:GLN:OE1	2.13	0.48
5:L:448:ARG:NH2	5:L:500:ILE:O	2.45	0.48
1:A:118:ASP:H	1:A:121:VAL:HB	1.77	0.48
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.79	0.48
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.13	0.48
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.49	0.48
4:E:58:LEU:HD12	4:E:58:LEU:H	1.78	0.48
1:G:172:LEU:HD12	1:G:172:LEU:H	1.77	0.48
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.95	0.48
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.94	0.48
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.95	0.48
3:D:165:TYR:O	3:D:169:LEU:HB2	2.14	0.48
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.94	0.48
2:I:607:SER:N	2:I:610:GLU:HB2	2.28	0.48
3:J:683:ILE:HD11	3:J:754:ILE:HG23	1.96	0.48
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.94	0.48
2:C:229:ILE:HD13	2:C:334:GLU:HG2	1.95	0.48
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.94	0.48
3:D:546:ALA:O	3:D:573:THR:HA	2.13	0.48
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.95	0.48
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.49	0.48
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.95	0.48
3:J:525:MET:O	3:J:548:VAL:HG13	2.13	0.48
3:J:1184:ASP:O	3:J:1186:TYR:N	2.46	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.14	0.48
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.13	0.48
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.43	0.48
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.48	0.48
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.78	0.48
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.67	0.48
2:I:832:HIS:HE1	2:I:1238:LEU:HD22	1.79	0.48
5:L:137:TYR:HE1	5:L:351:THR:HB	1.78	0.48
5:L:145:LEU:HD13	5:L:225:ARG:NH2	2.29	0.48
2:C:115:LYS:HD3	2:C:116:ASP:H	1.79	0.48
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.46	0.48
3:D:290:ILE:HD12	3:D:290:ILE:H	1.79	0.48
3:D:487:THR:HG21	4:E:4:VAL:HG23	1.96	0.48
3:D:513:MET:HE3	3:D:513:MET:HB3	1.81	0.48
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.49	0.48
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.48	0.48
3:J:232:ASN:HA	3:J:236:TRP:HZ3	1.79	0.48
1:A:75:GLN:HA	2:C:729:ALA:N	2.29	0.47
2:C:878:THR:OG1	2:C:879:GLY:N	2.47	0.47
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.96	0.47
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.96	0.47
5:F:303:ILE:HA	5:F:306:PHE:HB2	1.96	0.47
3:J:528:THR:O	3:J:551:ARG:HB3	2.14	0.47
4:K:15:ASN:O	4:K:16:ARG:HB3	2.14	0.47
5:L:354:THR:O	5:L:358:VAL:HG23	2.14	0.47
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.96	0.47
3:D:53:ARG:NH2	3:D:60:ARG:HD2	2.29	0.47
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.80	0.47
3:D:259:ARG:HG2	3:D:260:PHE:H	1.79	0.47
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.95	0.47
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.79	0.47
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.29	0.47
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.95	0.47
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.75	0.47
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.14	0.47
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.49	0.47
3:D:416:ILE:HD12	3:D:439:PRO:CG	2.42	0.47
3:D:511:TYR:CG	3:D:728:SER:HB3	2.49	0.47
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.95	0.47
4:E:8:ASP:HB2	4:E:55:GLU:HG2	1.95	0.47
2:I:462:ASN:O	2:I:466:VAL:HG23	2.13	0.47
3:J:77:ARG:HG3	3:J:79:LYS:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.96	0.47
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.95	0.47
5:F:312:SER:O	5:F:315:TRP:NE1	2.47	0.47
5:F:577:GLY:C	5:F:583:THR:HG23	2.34	0.47
2:I:565:GLU:HB2	2:I:680:LEU:HD21	1.96	0.47
2:I:878:THR:OG1	2:I:879:GLY:N	2.46	0.47
3:J:418:GLU:HG3	4:K:45:LYS:H	1.80	0.47
3:J:748:ALA:O	3:J:777:HIS:HD2	1.97	0.47
3:D:252:LEU:HD23	3:D:262:THR:HB	1.97	0.47
5:F:105:MET:HE3	5:F:385:ARG:HG2	1.94	0.47
5:F:548:LEU:HD22	5:F:556:ALA:HA	1.95	0.47
2:I:74:ARG:HG2	2:I:75:LEU:N	2.28	0.47
3:J:205:LEU:CD2	3:J:214:ARG:HB2	2.45	0.47
3:J:682:VAL:O	3:J:685:ILE:HG12	2.14	0.47
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.95	0.47
1:A:11:PRO:HD2	1:B:227:GLN:O	2.15	0.47
2:I:985:GLU:HB3	2:I:988:LYS:HD2	1.96	0.47
3:J:356:THR:OG1	3:J:357:VAL:N	2.45	0.47
3:J:846:GLU:HA	3:J:860:ARG:HD2	1.96	0.47
5:L:532:LEU:HD12	5:L:532:LEU:H	1.80	0.47
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.29	0.47
2:C:593:LYS:HA	2:C:652:TYR:CD2	2.50	0.47
2:I:13:LYS:NZ	2:I:1148:ALA:O	2.48	0.47
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.97	0.47
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.96	0.47
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.96	0.47
5:L:96:ASP:O	5:L:98:VAL:N	2.48	0.47
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.50	0.47
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.30	0.47
1:G:14:VAL:CG1	1:G:15:ASP:H	2.25	0.47
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.96	0.47
2:I:151:ARG:NH2	2:I:175:ARG:HD2	2.30	0.47
3:J:165:TYR:O	3:J:169:LEU:HB2	2.14	0.47
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.97	0.47
3:D:1375:ALA:HB1	3:J:853:THR:HG21	1.97	0.47
3:J:79:LYS:HB2	5:L:569:THR:H	1.79	0.47
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.30	0.47
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.96	0.47
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.45	0.47
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.97	0.47
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.80	0.47
3:D:1299:GLY:HA2	3:D:1300:ALA:HA	1.71	0.47
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.97	0.47
2:I:4:SER:HB2	2:I:7:GLU:HG3	1.97	0.47
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.97	0.47
2:I:1042:LEU:HD22	2:I:1049:ILE:HD12	1.96	0.47
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.44	0.46
1:B:48:LEU:HD22	3:D:539:SER:HB3	1.96	0.46
1:B:66:HIS:CD2	1:B:69:SER:HG	2.29	0.46
1:B:190:ALA:N	1:B:198:LEU:O	2.40	0.46
2:C:488:MET:C	2:C:490:GLN:H	2.18	0.46
2:C:548:ARG:HB3	2:C:569:ILE:O	2.14	0.46
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.15	0.46
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.14	0.46
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.45	0.46
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.15	0.46
3:D:332:LYS:HG2	3:D:333:GLY:H	1.80	0.46
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.50	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.15	0.46
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.98	0.46
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.48	0.46
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.81	0.46
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.16	0.46
3:D:525:MET:O	3:D:548:VAL:HG13	2.15	0.46
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.44	0.46
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.97	0.46
3:J:705:THR:HG21	3:J:719:PHE:H	1.79	0.46
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.97	0.46
1:A:61:ILE:HG22	1:A:62:ASP:H	1.79	0.46
2:C:544:GLY:O	2:C:548:ARG:HG3	2.14	0.46
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.26	0.46
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.97	0.46
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.96	0.46
2:I:1286:THR:N	3:J:479:GLU:OE2	2.47	0.46
1:B:73:GLY:O	1:B:134:THR:HG22	2.15	0.46
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.97	0.46
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.98	0.46
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.60	0.46
5:F:96:ASP:O	5:F:98:VAL:N	2.48	0.46
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.98	0.46
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:122:SER:O	3:J:126:LEU:HG	2.15	0.46
3:J:1266:ILE:HG13	3:J:1276:GLU:O	2.15	0.46
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.80	0.46
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.80	0.46
3:D:334:LYS:HA	3:D:335:GLN:HA	1.54	0.46
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.30	0.46
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.38	0.46
3:J:352:ARG:HD2	3:J:465:GLN:HE21	1.81	0.46
3:J:600:ALA:O	3:J:603:LYS:HG2	2.15	0.46
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.96	0.46
3:J:797:THR:O	3:J:801:VAL:HG12	2.15	0.46
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.51	0.46
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.51	0.46
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.98	0.46
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.97	0.46
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.40	0.46
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.98	0.46
2:I:812:PHE:O	2:I:1099:ASN:ND2	2.49	0.46
2:C:593:LYS:HD3	2:C:652:TYR:CZ	2.51	0.46
2:C:886:LYS:H	2:C:917:SER:HB3	1.81	0.46
3:D:298:MET:SD	5:F:402:LEU:HB3	2.56	0.46
3:D:708:ASN:OD1	3:D:708:ASN:N	2.49	0.46
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.42	0.46
3:J:555:TYR:HB2	3:J:586:GLY:HA2	1.98	0.46
2:C:3:TYR:HD1	2:C:3:TYR:HA	1.58	0.46
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.97	0.46
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.98	0.46
4:E:15:ASN:O	4:E:16:ARG:HB3	2.16	0.46
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.97	0.46
1:H:60:GLU:HA	1:H:171:LEU:HD12	1.98	0.46
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.30	0.46
2:C:298:ALA:HB3	2:C:334:GLU:HB2	1.97	0.46
3:D:608:CYS:HG	3:D:620:PHE:HD2	1.62	0.46
1:G:46:ILE:HD11	1:H:38:THR:HG21	1.98	0.46
1:G:89:ALA:H	1:G:125:LYS:HD3	1.81	0.46
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.98	0.46
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.80	0.46
3:J:694:SER:OG	3:J:738:ARG:NE	2.48	0.46
5:L:244:THR:O	5:L:247:GLU:HG2	2.15	0.46
5:L:533:ASP:O	5:L:536:THR:N	2.48	0.46
1:B:140:ILE:HD11	1:B:142:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	2.15	0.46
3:D:42:GLU:OE1	3:D:42:GLU:N	2.46	0.46
3:D:122:SER:O	3:D:126:LEU:HG	2.17	0.46
3:D:609:TYR:HD1	3:D:610:ARG:HH11	1.64	0.46
3:D:701:LEU:HD12	3:D:723:TYR:HB2	1.98	0.46
3:D:1307:LEU:HB3	3:D:1312:ALA:HB2	1.98	0.46
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.98	0.46
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.98	0.46
3:J:338:PHE:O	3:J:340:GLN:N	2.48	0.46
5:L:337:VAL:HG12	5:L:341:LEU:HD12	1.98	0.46
2:C:138:ILE:HG22	2:C:139:ASN:N	2.30	0.45
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.97	0.45
2:C:1248:THR:HG21	5:F:531:PRO:CG	2.46	0.45
3:D:520:ALA:HB1	3:D:543:SER:HB3	1.98	0.45
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.97	0.45
3:D:1172:LYS:HB3	3:D:1189:MET:HB3	1.98	0.45
2:I:701:GLY:O	2:I:1184:THR:N	2.34	0.45
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.98	0.45
3:J:514:THR:CB	3:J:576:ARG:HG2	2.46	0.45
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.69	0.45
3:D:810:THR:HG23	3:D:811:GLU:H	1.81	0.45
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.98	0.45
2:I:1116:HIS:HE1	3:J:641:ILE:N	2.12	0.45
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.16	0.45
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.51	0.45
1:A:90:VAL:HG22	1:A:91:ARG:H	1.80	0.45
1:A:91:ARG:HD3	1:A:210:THR:O	2.17	0.45
1:A:172:LEU:HD12	1:A:172:LEU:H	1.80	0.45
1:B:203:ILE:HD13	1:B:203:ILE:N	2.31	0.45
2:C:703:GLY:N	2:C:705:GLU:OE2	2.41	0.45
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.80	0.45
3:D:343:LEU:HD22	3:D:343:LEU:HA	1.29	0.45
5:F:445:ASP:OD2	5:F:451:ARG:HD2	2.16	0.45
1:G:71:LYS:HB2	1:G:78:ILE:HD11	1.97	0.45
2:I:90:VAL:HG12	2:I:91:THR:H	1.82	0.45
2:I:211:ARG:NH1	2:I:357:ASN:O	2.49	0.45
2:I:739:ASP:OD1	2:I:739:ASP:N	2.47	0.45
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.97	0.45
4:K:50:ALA:O	4:K:54:ILE:HG12	2.17	0.45
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.98	0.45
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1282:TYR:O	3:D:1285:VAL:HG22	2.16	0.45
1:G:50:SER:O	1:G:51:MET:HG2	2.17	0.45
3:J:518:VAL:HG12	3:J:707:ILE:HD13	1.98	0.45
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.85	0.45
2:C:1109:ILE:HG23	2:C:1113:LEU:HD13	1.98	0.45
2:C:1258:PRO:O	3:D:346:ARG:HD3	2.17	0.45
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.97	0.45
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.98	0.45
5:F:476:ARG:HG3	5:F:477:GLU:N	2.30	0.45
1:G:13:LEU:H	1:G:13:LEU:HD23	1.82	0.45
2:I:23:ASP:OD1	2:I:23:ASP:N	2.50	0.45
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.51	0.45
2:I:138:ILE:HG22	2:I:139:ASN:N	2.32	0.45
2:I:672:GLU:HB3	2:I:1187:PHE:HD2	1.81	0.45
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.51	0.45
2:I:989:LEU:HG	2:I:997:TRP:CE2	2.51	0.45
2:C:202:ARG:HH11	2:C:369:MET:HG2	1.81	0.45
2:C:580:GLN:HB2	2:C:605:TYR:HE1	1.81	0.45
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.81	0.45
3:D:825:VAL:C	3:D:826:ILE:HG13	2.37	0.45
3:D:1184:ASP:O	3:D:1186:TYR:N	2.49	0.45
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.39	0.45
1:H:205:MET:HG2	1:H:206:GLU:H	1.82	0.45
2:I:400:VAL:HG21	2:I:452:ARG:NH1	2.32	0.45
3:J:689:ALA:O	3:J:693:VAL:HG23	2.16	0.45
1:A:228:LEU:O	1:A:232:VAL:HG23	2.17	0.45
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.51	0.45
2:C:136:PHE:O	2:C:143:ARG:N	2.34	0.45
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.57	0.45
3:D:741:ALA:O	3:D:762:ASN:ND2	2.49	0.45
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.99	0.45
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.47	0.45
1:G:166:ARG:O	1:G:167:PRO:C	2.55	0.45
1:H:41:ASN:O	1:H:45:ARG:HG3	2.16	0.45
2:I:148:GLN:NE2	2:I:511:LEU:HD11	2.32	0.45
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.98	0.45
5:L:462:LYS:O	5:L:466:ILE:HG13	2.17	0.45
5:L:479:THR:HG23	5:L:481:GLU:H	1.82	0.45
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.66	0.45
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.50	0.45
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:533:ASP:O	5:F:536:THR:N	2.48	0.45
1:G:49:SER:OG	1:G:50:SER:N	2.49	0.45
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.82	0.45
3:J:232:ASN:HA	3:J:236:TRP:CZ3	2.52	0.45
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.99	0.45
1:A:23:HIS:CE1	1:A:204:GLU:HG3	2.51	0.45
1:B:219:ARG:O	1:B:223:ILE:HG13	2.16	0.45
2:C:149:LEU:HD12	2:C:452:ARG:O	2.17	0.45
3:D:34:SER:HG	3:D:104:HIS:CG	2.29	0.45
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.99	0.45
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.52	0.45
1:A:158:ARG:NH1	1:A:172:LEU:HD23	2.31	0.45
2:C:1160:ASP:HA	2:C:1162:SER:H	1.81	0.45
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.98	0.45
1:H:172:LEU:HD12	1:H:172:LEU:H	1.82	0.45
2:I:1211:ARG:HE	2:I:1220:GLN:HE21	1.63	0.45
3:J:594:GLN:HG3	3:J:596:LEU:HD22	1.99	0.45
3:J:810:THR:HG23	3:J:811:GLU:H	1.82	0.45
1:A:182:ARG:HB3	1:A:206:GLU:HB3	1.99	0.44
2:C:452:ARG:NH1	2:C:584:TYR:O	2.50	0.44
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.19	0.44
3:D:259:ARG:HG2	3:D:260:PHE:N	2.32	0.44
3:D:515:ARG:O	3:D:545:HIS:HB3	2.18	0.44
5:F:519:LEU:HD23	5:F:523:ILE:HD11	1.99	0.44
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.51	0.44
2:I:607:SER:H	2:I:610:GLU:HB2	1.82	0.44
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.18	0.44
1:A:49:SER:OG	1:A:50:SER:N	2.51	0.44
1:B:20:SER:OG	1:B:22:THR:HG22	2.16	0.44
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.51	0.44
2:C:143:ARG:NH2	2:C:512:SER:O	2.50	0.44
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.98	0.44
2:C:896:THR:HB	2:C:897:PRO:HD2	1.99	0.44
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.99	0.44
3:D:362:ARG:H	3:D:365:GLN:NE2	2.15	0.44
3:D:416:ILE:HA	3:D:416:ILE:HD13	1.68	0.44
3:D:473:THR:HG23	3:D:476:ALA:H	1.81	0.44
3:D:797:THR:O	3:D:801:VAL:HG12	2.17	0.44
5:F:456:MET:CE	5:F:497:VAL:HG13	2.47	0.44
1:G:14:VAL:HG12	1:G:27:THR:O	2.16	0.44
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:ILE:HD11	2:C:75:LEU:HG	2.00	0.44
2:C:135:THR:HG21	2:C:515:MET:SD	2.58	0.44
2:C:1340:GLU:HG3	3:D:21:LYS:HB2	1.98	0.44
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.80	0.44
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.78	0.44
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.99	0.44
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.46	0.44
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.81	0.44
1:H:153:VAL:HB	1:H:175:ALA:CB	2.44	0.44
2:I:402:ARG:HG2	2:I:416:GLY:H	1.83	0.44
3:J:334:LYS:HA	3:J:335:GLN:HA	1.54	0.44
3:J:546:ALA:O	3:J:573:THR:HA	2.17	0.44
3:J:557:LYS:HE3	3:J:557:LYS:HB2	1.84	0.44
5:L:108:VAL:HG11	5:L:381:GLU:C	2.38	0.44
5:L:456:MET:CE	5:L:497:VAL:HG13	2.47	0.44
2:C:27:LEU:O	2:C:528:ARG:NH1	2.43	0.44
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.99	0.44
3:D:306:LEU:O	3:D:326:SER:HB2	2.18	0.44
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.53	0.44
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.51	0.44
1:A:167:PRO:HB2	1:A:170:ARG:HG3	1.99	0.44
1:B:53:GLY:O	1:B:177:TYR:HB3	2.18	0.44
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.48	0.44
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.99	0.44
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.99	0.44
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.47	0.44
1:G:73:GLY:C	1:G:134:THR:HG22	2.37	0.44
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.76	0.44
2:I:896:THR:HB	2:I:897:PRO:HD2	2.00	0.44
3:J:490:ILE:HG13	3:J:500:ILE:HG13	1.98	0.44
5:L:105:MET:CE	5:L:385:ARG:HG2	2.46	0.44
1:B:154:PRO:HA	1:B:174:ASP:HB3	1.99	0.44
3:D:1183:SER:OG	3:D:1185:PRO:HD3	2.16	0.44
5:F:226:ALA:O	5:F:229:VAL:HG22	2.17	0.44
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.86	0.44
3:J:325:LYS:HE2	3:J:330:MET:HG2	2.00	0.44
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	1.99	0.44
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.81	0.44
5:L:127:ILE:O	5:L:130:VAL:HG22	2.16	0.44
5:L:583:THR:HG22	5:L:584:ARG:H	1.82	0.44
1:B:177:TYR:O	1:B:178:SER:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:24:VAL:HG21	2:C:704:MET:SD	2.57	0.44
2:C:733:VAL:HG11	2:C:966:ILE:HG21	2.00	0.44
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.17	0.44
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	2.00	0.44
1:G:91:ARG:NH2	1:G:122:GLU:OE2	2.50	0.44
2:I:565:GLU:HA	2:I:569:ILE:HG12	1.98	0.44
5:L:507:MET:HG2	5:L:520:GLY:CA	2.48	0.44
2:C:718:ALA:HB2	2:C:783:LEU:HD23	2.00	0.44
2:C:719:LYS:O	2:C:779:ARG:HG3	2.18	0.44
2:C:1288:GLN:NE2	3:D:1355:ARG:HA	2.33	0.44
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.98	0.44
2:I:292:ILE:HB	2:I:322:LEU:HD11	2.00	0.44
5:L:493:LYS:HA	5:L:496:LYS:HE2	2.00	0.44
1:B:187:VAL:HG13	1:B:199:ASP:HB3	1.99	0.44
2:C:27:LEU:HD13	2:C:663:VAL:HG11	2.00	0.44
2:C:864:LYS:NZ	2:C:876:GLU:O	2.32	0.44
3:D:528:THR:O	3:D:551:ARG:HB3	2.17	0.44
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.99	0.44
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	2.00	0.44
5:F:540:LEU:HD12	5:F:610:PHE:CD1	2.53	0.44
5:F:588:ARG:H	5:F:588:ARG:HG3	1.49	0.44
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.33	0.44
3:J:583:VAL:HG21	3:J:592:VAL:HG11	2.00	0.44
5:L:250:LEU:O	5:L:254:GLU:HG2	2.18	0.44
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.28	0.44
1:A:184:ALA:O	1:A:204:GLU:N	2.44	0.43
1:B:79:LEU:HD21	3:D:526:VAL:HG21	2.00	0.43
1:B:118:ASP:HB2	1:B:121:VAL:CG2	2.48	0.43
2:C:734:ILE:HD11	2:C:783:LEU:HD11	2.00	0.43
2:I:237:LEU:HD23	2:I:289:VAL:HG23	2.00	0.43
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.82	0.43
2:I:528:ARG:NH1	2:I:575:LEU:HD23	2.32	0.43
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.83	0.43
3:J:598:LYS:O	3:J:601:ILE:HG22	2.18	0.43
1:A:9:LEU:HD12	1:A:32:GLU:HG2	1.99	0.43
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.99	0.43
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.63	0.43
2:C:57:PHE:HD1	2:C:58:PRO:HA	1.84	0.43
2:C:230:PHE:HB2	2:C:333:ILE:O	2.19	0.43
2:C:466:VAL:O	2:C:470:ARG:HG2	2.18	0.43
2:C:564:PRO:HG2	2:C:568:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:706:ARG:HG3	2:C:793:GLU:HG2	2.00	0.43
2:C:829:THR:HA	2:C:1059:ARG:HA	2.00	0.43
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.99	0.43
2:C:1138:VAL:HG12	2:C:1170:MET:SD	2.58	0.43
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.17	0.43
3:D:205:LEU:HD22	3:D:214:ARG:HB2	1.99	0.43
3:D:396:ALA:HB2	5:F:609:SER:HB2	2.00	0.43
5:F:515:GLU:O	5:F:515:GLU:HG2	2.18	0.43
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.53	0.43
1:G:211:ILE:HG21	1:G:216:ALA:HB2	1.99	0.43
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.99	0.43
2:I:237:LEU:HD13	2:I:237:LEU:HA	1.77	0.43
2:I:832:HIS:CE1	2:I:1238:LEU:HD22	2.54	0.43
2:I:994:ARG:HD2	2:I:997:TRP:CZ2	2.54	0.43
3:J:544:LEU:O	3:J:574:VAL:HB	2.18	0.43
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	2.00	0.43
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.00	0.43
5:L:316:PHE:CE1	5:L:337:VAL:HB	2.53	0.43
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.50	0.43
2:C:38:PHE:HA	2:C:48:GLY:HA2	1.99	0.43
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.43
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.99	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.00	0.43
2:I:855:PRO:HG3	2:I:913:VAL:CG1	2.47	0.43
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.54	0.43
2:C:68:LEU:HD11	2:C:100:LEU:HB3	2.01	0.43
2:C:225:PHE:CB	2:C:336:LEU:HD22	2.49	0.43
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.83	0.43
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.18	0.43
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.99	0.43
3:D:1171:GLY:O	3:D:1172:LYS:HG3	2.18	0.43
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.74	0.43
2:I:816:ILE:HG22	2:I:818:VAL:HG23	2.01	0.43
2:I:1197:GLU:O	2:I:1200:LYS:HB2	2.18	0.43
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.83	0.43
3:J:844:THR:HG23	3:J:864:LEU:HD11	2.00	0.43
5:L:315:TRP:O	5:L:319:ALA:HB3	2.18	0.43
1:B:90:VAL:HG12	1:B:91:ARG:H	1.84	0.43
1:B:182:ARG:NH1	3:D:581:MET:SD	2.91	0.43
2:C:1099:ASN:ND2	3:D:505:ASP:OD1	2.51	0.43
2:C:1244:HIS:HD2	2:C:1265:PHE:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1247:SER:HB3	3:D:375:GLU:O	2.18	0.43
3:D:356:THR:OG1	3:D:357:VAL:N	2.51	0.43
3:D:1181:ASP:HB3	3:J:202:ARG:HH11	1.83	0.43
1:G:166:ARG:N	1:G:167:PRO:HD2	2.34	0.43
1:G:185:TYR:HE1	2:I:1087:TYR:HH	1.66	0.43
2:I:80:PHE:HB3	2:I:84:GLU:HB2	1.99	0.43
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	2.01	0.43
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.54	0.43
3:J:785:ASP:O	3:J:789:LYS:HG3	2.19	0.43
3:J:836:ARG:HG3	3:J:869:CYS:HB3	2.01	0.43
2:C:82:VAL:HG11	2:C:131:THR:HG23	2.00	0.43
1:H:84:ASN:O	1:H:128:HIS:HE1	2.02	0.43
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.74	0.43
3:J:362:ARG:H	3:J:365:GLN:HE21	1.66	0.43
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.00	0.43
3:J:850:LYS:HG2	3:J:857:LEU:HD23	2.00	0.43
5:L:388:ILE:O	5:L:392:LYS:HG3	2.17	0.43
1:B:53:GLY:C	1:B:177:TYR:HB3	2.39	0.43
1:B:104:LYS:HG2	1:B:110:VAL:HG22	2.01	0.43
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.19	0.43
3:D:93:THR:HG22	3:D:94:GLN:H	1.83	0.43
2:I:168:GLY:C	2:I:170:VAL:H	2.21	0.43
2:I:169:LYS:O	2:I:170:VAL:HG22	2.19	0.43
2:I:253:PHE:CD1	2:I:288:PRO:HD3	2.54	0.43
2:I:975:ILE:HG13	2:I:1014:LEU:HD22	2.00	0.43
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.64	0.43
2:C:1285:TYR:CD2	3:D:1356:LEU:HD21	2.53	0.43
2:I:164:THR:C	2:I:166:SER:H	2.20	0.43
3:J:50:LYS:HD3	3:J:71:LEU:HD21	2.00	0.43
3:J:733:SER:O	3:J:737:ILE:HG12	2.18	0.43
1:B:67:GLU:N	1:B:67:GLU:OE1	2.52	0.43
2:C:292:ILE:HG23	2:C:295:LYS:HB2	2.00	0.43
2:C:840:SER:HB2	2:C:850:ILE:HD11	2.00	0.43
2:C:980:VAL:O	2:C:984:VAL:HB	2.18	0.43
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.54	0.43
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	2.00	0.43
3:D:369:PRO:HB3	3:D:444:GLY:O	2.18	0.43
3:D:514:THR:HB	3:D:576:ARG:HG2	2.01	0.43
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.18	0.43
2:I:545:PHE:CZ	3:J:781:LYS:HG3	2.54	0.43
2:I:588:GLU:HG3	2:I:605:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:369:PRO:HB3	3:J:444:GLY:O	2.18	0.43
4:K:38:LEU:HD23	4:K:58:LEU:HD13	2.01	0.43
5:L:515:GLU:HG2	5:L:516:ASP:H	1.83	0.43
1:B:66:HIS:CD2	1:B:66:HIS:N	2.81	0.43
1:B:185:TYR:HA	1:B:202:VAL:O	2.19	0.43
2:C:518:ASN:O	2:C:691:PRO:HD3	2.19	0.43
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.91	0.43
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.85	0.43
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	2.01	0.43
4:E:50:ALA:O	4:E:54:ILE:HG12	2.19	0.43
1:H:33:ARG:NH1	2:I:1081:PRO:HB3	2.34	0.43
2:I:14:ASP:OD2	2:I:1156:ARG:NE	2.51	0.43
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.84	0.43
2:I:132:ASP:OD1	2:I:132:ASP:N	2.39	0.43
3:J:513:MET:O	3:J:575:GLY:HA3	2.19	0.43
3:J:556:GLU:HG2	3:J:558:ASP:HB2	2.01	0.43
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.33	0.43
5:L:561:MET:HA	5:L:567:MET:HE1	1.99	0.43
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	2.00	0.42
1:A:99:ILE:HG12	1:A:145:LYS:HG2	2.01	0.42
2:C:209:ILE:HD13	2:C:425:ILE:HG21	2.00	0.42
2:C:402:ARG:NE	2:C:417:SER:O	2.48	0.42
1:G:35:PHE:CZ	1:H:46:ILE:HG23	2.54	0.42
2:I:732:ILE:HD11	2:I:769:PRO:HB3	2.00	0.42
1:A:83:LEU:HD23	2:C:694:ARG:HH21	1.83	0.42
2:C:8:LYS:HE3	2:C:1171:ARG:HH21	1.84	0.42
2:C:225:PHE:CZ	2:C:347:ILE:HB	2.54	0.42
2:C:316:GLU:CD	2:C:316:GLU:H	2.23	0.42
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.99	0.42
2:C:826:ASP:OD1	2:C:829:THR:OG1	2.32	0.42
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.01	0.42
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	2.01	0.42
5:F:456:MET:HE3	5:F:497:VAL:HG13	2.00	0.42
3:J:701:LEU:CD1	3:J:723:TYR:HB2	2.49	0.42
3:J:817:HIS:CD2	3:J:817:HIS:H	2.37	0.42
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	2.01	0.42
2:C:74:ARG:HG2	2:C:75:LEU:N	2.35	0.42
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	2.01	0.42
3:D:515:ARG:NH2	3:D:717:VAL:O	2.52	0.42
3:D:901:ARG:HA	3:D:908:ILE:HA	2.01	0.42
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1183:SER:OG	3:J:206:ASN:ND2	2.47	0.42
2:I:62:TYR:C	2:I:64:GLY:H	2.23	0.42
2:I:1285:TYR:CD2	3:J:1356:LEU:HD21	2.54	0.42
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	2.00	0.42
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.54	0.42
3:J:741:ALA:O	3:J:762:ASN:ND2	2.52	0.42
3:J:825:VAL:C	3:J:826:ILE:HG13	2.39	0.42
5:L:508:GLU:HG3	5:L:518:HIS:ND1	2.33	0.42
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.53	0.42
2:C:145:ILE:HB	2:C:456:VAL:HG22	2.01	0.42
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.54	0.42
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.89	0.42
3:D:430:HIS:HD2	3:D:432:LEU:H	1.66	0.42
1:H:90:VAL:HG12	1:H:91:ARG:N	2.35	0.42
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.84	0.42
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.91	0.42
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	2.01	0.42
1:A:45:ARG:NH1	1:B:34:GLY:O	2.51	0.42
1:B:59:VAL:HG13	1:B:144:ILE:HG12	2.01	0.42
2:C:40:GLU:HG2	2:C:41:GLN:N	2.34	0.42
2:C:297:VAL:HG23	2:C:333:ILE:HG23	2.02	0.42
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.74	0.42
2:C:832:HIS:ND1	2:C:1058:ARG:HD2	2.34	0.42
1:G:11:PRO:HD3	1:H:227:GLN:CD	2.40	0.42
1:H:23:HIS:HB2	1:H:205:MET:O	2.19	0.42
1:H:177:TYR:O	1:H:178:SER:C	2.57	0.42
2:I:269:ILE:HA	2:I:273:HIS:ND1	2.34	0.42
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.95	0.42
3:J:518:VAL:N	3:J:716:GLN:HE22	2.18	0.42
3:J:591:ILE:HG23	3:J:604:MET:HE2	2.01	0.42
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.76	0.42
1:B:182:ARG:HG3	3:D:534:GLU:OE1	2.19	0.42
2:C:133:ASN:OD1	2:C:713:GLY:HA3	2.18	0.42
2:C:887:VAL:HB	2:C:913:VAL:HG22	2.01	0.42
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.01	0.42
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.79	0.42
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.53	0.42
3:D:1162:ILE:O	3:D:1178:THR:N	2.49	0.42
2:I:9:LYS:HA	2:I:1171:ARG:HD2	2.00	0.42
2:I:520:PRO:HG3	2:I:714:VAL:HG11	2.00	0.42
3:J:425:ARG:HD2	3:J:459:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.01	0.42
3:J:1290:ARG:HH11	3:J:1294:ALA:CB	2.32	0.42
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.46	0.42
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.35	0.42
5:L:488:LEU:H	5:L:488:LEU:HD12	1.84	0.42
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.54	0.42
3:D:26:SER:HB2	3:D:236:TRP:CE2	2.55	0.42
4:E:83:VAL:O	4:E:86:ILE:HG12	2.20	0.42
5:L:245:ALA:O	5:L:249:ILE:HG13	2.20	0.42
1:A:61:ILE:HB	1:A:64:VAL:HG22	2.01	0.42
1:A:166:ARG:O	1:A:167:PRO:C	2.59	0.42
2:C:568:ASN:HB2	2:C:571:LEU:HB2	2.01	0.42
3:D:860:ARG:HB3	3:D:861:ASN:H	1.76	0.42
5:F:402:LEU:HA	5:F:405:ILE:HG12	2.01	0.42
1:G:19:VAL:HG13	1:G:20:SER:H	1.85	0.42
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.02	0.42
1:H:85:LEU:HD23	1:H:130:ILE:HG12	2.02	0.42
2:I:1024:GLU:HG2	2:I:1028:LYS:CD	2.50	0.42
3:J:46:TYR:CD1	5:L:452:ILE:HG22	2.54	0.42
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.55	0.42
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.20	0.42
3:J:903:LEU:HD12	3:J:903:LEU:HA	1.83	0.42
1:B:173:VAL:HG12	1:B:174:ASP:H	1.85	0.42
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.84	0.42
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.20	0.42
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.55	0.42
3:D:425:ARG:HG2	3:D:426:ALA:H	1.84	0.42
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.50	0.42
5:F:245:ALA:O	5:F:249:ILE:HG13	2.20	0.42
5:F:280:VAL:HG21	5:F:358:VAL:HG11	2.02	0.42
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.83	0.42
2:I:829:THR:HA	2:I:1059:ARG:HA	2.02	0.42
2:I:840:SER:O	2:I:1047:LEU:N	2.50	0.42
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.50	0.42
2:I:1178:LYS:HA	2:I:1178:LYS:HD3	1.87	0.42
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	2.01	0.42
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	2.19	0.42
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	2.01	0.42
5:L:300:LYS:HE2	5:L:300:LYS:HB3	1.88	0.42
2:C:408:SER:O	2:C:431:LYS:NZ	2.50	0.42
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:697:LYS:HA	2:C:795:ALA:HB2	2.02	0.42
4:E:32:VAL:O	4:E:34:GLY:N	2.53	0.42
1:H:71:LYS:HD2	1:H:71:LYS:HA	1.94	0.42
1:H:158:ARG:HB3	1:H:172:LEU:CD2	2.48	0.42
2:I:620:ASN:ND2	2:I:620:ASN:O	2.53	0.42
2:I:632:ASP:O	2:I:647:ARG:HB2	2.20	0.42
2:I:1142:ARG:HD3	2:I:1161:LEU:HD22	2.02	0.42
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.83	0.42
3:J:695:LYS:HA	3:J:698:MET:HB2	2.02	0.42
5:L:231:THR:HG23	5:L:249:ILE:HG12	2.00	0.42
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.55	0.42
1:A:66:HIS:HA	1:A:171:LEU:HD11	2.02	0.41
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.94	0.41
2:C:62:TYR:C	2:C:64:GLY:H	2.23	0.41
2:C:628:HIS:HB3	2:C:647:ARG:HH21	1.85	0.41
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.50	0.41
3:D:312:ARG:HB2	3:D:313:GLY:H	1.57	0.41
3:D:770:LEU:H	3:D:770:LEU:HD22	1.84	0.41
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.85	0.41
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.56	0.41
3:J:201:LEU:HD22	3:J:217:LEU:HD11	2.01	0.41
1:A:12:ARG:H	1:A:30:PRO:HD2	1.85	0.41
1:A:83:LEU:HD23	2:C:694:ARG:NE	2.33	0.41
1:B:142:MET:HG3	1:B:144:ILE:HG13	2.02	0.41
2:C:164:THR:C	2:C:166:SER:H	2.23	0.41
2:C:202:ARG:H	2:C:202:ARG:HG3	1.66	0.41
2:C:213:LEU:HD23	2:C:385:PHE:HE2	1.85	0.41
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.01	0.41
3:D:18:ASP:HB2	3:D:1373:ARG:NH2	2.35	0.41
3:D:26:SER:HA	3:D:236:TRP:CD1	2.55	0.41
3:D:842:ARG:NH2	3:D:1254:GLU:OE1	2.46	0.41
3:D:1167:LYS:HZ1	3:D:1170:LYS:HB2	1.85	0.41
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.20	0.41
3:D:1302:TYR:CE1	3:J:1297:LYS:HD3	2.54	0.41
1:H:175:ALA:HB1	1:H:177:TYR:CZ	2.55	0.41
1:H:182:ARG:HG3	3:J:534:GLU:OE1	2.20	0.41
5:L:348:GLU:HG2	5:L:354:THR:HA	2.01	0.41
2:C:90:VAL:HG12	2:C:91:THR:H	1.85	0.41
2:C:149:LEU:HB2	2:C:530:ILE:HG22	2.02	0.41
2:C:486:THR:HG23	2:C:487:LEU:H	1.85	0.41
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:867:GLU:H	2:C:867:GLU:HG3	1.60	0.41
5:F:292:VAL:HG13	5:F:297:MET:O	2.21	0.41
5:F:306:PHE:HE1	5:F:315:TRP:CD2	2.38	0.41
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.52	0.41
1:H:173:VAL:HG12	1:H:174:ASP:H	1.85	0.41
2:I:221:LEU:HD11	2:I:314:ASN:HB2	2.03	0.41
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.94	0.41
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.56	0.41
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.21	0.41
5:L:134:VAL:HA	5:L:273:MET:HE1	2.02	0.41
5:L:456:MET:HE3	5:L:497:VAL:HG13	2.02	0.41
2:C:198:ILE:HD13	2:C:388:LEU:HD13	2.02	0.41
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.41
3:D:214:ARG:HA	3:D:217:LEU:HB3	2.02	0.41
3:D:612:LEU:HB3	3:D:616:PRO:HG2	2.03	0.41
3:D:930:LEU:HB2	3:D:1138:LEU:HB2	2.02	0.41
4:E:21:LEU:HD12	4:E:21:LEU:HA	1.82	0.41
5:F:125:ASP:O	5:F:129:GLN:HG3	2.21	0.41
1:G:29:GLU:OE1	1:G:200:LYS:HE2	2.20	0.41
2:I:15:PHE:CG	2:I:1190:ALA:HB2	2.55	0.41
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.54	0.41
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.50	0.41
3:J:79:LYS:HG3	3:J:80:HIS:ND1	2.35	0.41
3:J:331:ILE:CG2	3:J:1328:THR:HG21	2.50	0.41
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.74	0.41
3:J:817:HIS:CD2	3:J:817:HIS:N	2.88	0.41
4:K:40:PRO:O	4:K:52:ARG:NH2	2.54	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.88	0.41
1:B:22:THR:HG23	1:B:23:HIS:N	2.35	0.41
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.55	0.41
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.55	0.41
2:C:1104:PRO:HG2	3:D:725:MET:SD	2.61	0.41
2:C:1295:SER:OG	3:D:346:ARG:O	2.29	0.41
3:D:658:GLU:O	3:D:661:VAL:HG22	2.20	0.41
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.36	0.41
2:I:895:LEU:HB2	2:I:899:GLU:HB2	2.02	0.41
2:I:1070:HIS:CD2	2:I:1111:GLN:HA	2.56	0.41
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	2.01	0.41
2:I:1333:LEU:HD22	3:J:307:LEU:HD22	2.01	0.41
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.51	0.41
1:A:166:ARG:N	1:A:167:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:VAL:O	2:C:121:GLU:HA	2.20	0.41
2:C:820:GLU:HA	2:C:1079:ILE:HD11	2.03	0.41
2:C:1038:GLN:O	2:C:1038:GLN:HG3	2.19	0.41
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	2.21	0.41
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.21	0.41
5:F:606:VAL:HG13	5:F:607:LEU:HD12	2.03	0.41
2:I:301:TYR:CE2	2:I:333:ILE:HA	2.55	0.41
2:I:448:LEU:HG	2:I:553:THR:OG1	2.21	0.41
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.82	0.41
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.54	0.41
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.56	0.41
3:J:342:LEU:HA	3:J:343:LEU:HA	1.68	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.68	0.41
1:A:47:LEU:HD23	1:A:51:MET:HE2	2.03	0.41
1:B:11:PRO:HG3	1:B:28:LEU:HD21	2.02	0.41
1:B:41:ASN:O	1:B:45:ARG:HG3	2.20	0.41
2:C:23:ASP:OD1	2:C:23:ASP:N	2.53	0.41
3:D:30:ILE:HD13	3:D:243:PRO:HD3	2.01	0.41
3:D:697:MET:O	3:D:701:LEU:HB2	2.20	0.41
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.51	0.41
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.01	0.41
5:F:489:MET:HE2	5:F:493:LYS:HD2	2.03	0.41
1:G:38:THR:OG1	1:H:45:ARG:HD3	2.21	0.41
1:H:187:VAL:HG13	1:H:199:ASP:HB3	2.03	0.41
1:H:224:LEU:HD12	1:H:224:LEU:HA	1.78	0.41
3:J:156:ARG:NH2	3:J:191:SER:OG	2.50	0.41
3:J:317:THR:HG23	3:J:320:ASN:HB3	2.03	0.41
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.78	0.41
2:C:217:THR:HG23	2:C:351:LEU:HD13	2.03	0.41
2:C:898:GLU:HB3	5:F:540:LEU:CD2	2.51	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.89	0.41
3:D:1171:GLY:HA2	3:D:1193:TRP:CH2	2.56	0.41
5:F:111:LEU:HD23	5:F:111:LEU:HA	1.86	0.41
5:F:561:MET:HG2	5:F:576:VAL:CG2	2.50	0.41
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.56	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.20	0.41
1:A:218:ARG:NH1	1:B:231:PHE:O	2.54	0.41
1:A:223:ILE:HD13	1:B:8:PHE:CZ	2.55	0.41
1:A:228:LEU:HD22	1:B:221:ALA:HB1	2.03	0.41
2:C:11:ILE:CG2	2:C:1149:TYR:HE1	2.34	0.41
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:ARG:HB2	2:C:274:ILE:HD11	2.02	0.41
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.02	0.41
2:C:724:VAL:HG23	2:C:775:GLU:O	2.21	0.41
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	2.03	0.41
2:C:829:THR:HG23	2:C:1059:ARG:HA	2.03	0.41
3:D:77:ARG:HG3	3:D:79:LYS:H	1.86	0.41
3:D:688:ALA:O	3:D:692:ARG:HG3	2.21	0.41
1:G:137:ASN:OD1	1:G:137:ASN:N	2.53	0.41
1:G:159:ILE:HG13	1:G:162:GLU:HG3	2.02	0.41
2:I:517:GLN:HG3	2:I:523:GLU:OE2	2.21	0.41
2:I:743:PRO:O	2:I:974:ARG:NH2	2.53	0.41
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.51	0.41
3:J:800:LEU:O	3:J:803:VAL:HG12	2.21	0.41
3:J:847:ASP:HA	3:J:860:ARG:H	1.85	0.41
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.20	0.41
2:C:409:LEU:HD23	2:C:409:LEU:HA	1.96	0.41
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	2.03	0.41
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.56	0.41
2:I:908:GLU:OE1	5:L:611:LEU:HD22	2.21	0.41
3:J:860:ARG:HB3	3:J:861:ASN:H	1.72	0.41
3:J:1264:ALA:O	3:J:1278:GLU:N	2.38	0.41
1:B:183:ILE:CD1	1:B:205:MET:HG3	2.50	0.40
1:B:190:ALA:O	1:B:198:LEU:HB2	2.21	0.40
2:C:94:ALA:HB2	2:C:129:LEU:HD11	2.02	0.40
2:C:588:GLU:HG3	2:C:605:TYR:HD1	1.86	0.40
2:C:739:ASP:OD1	2:C:739:ASP:N	2.52	0.40
3:D:215:LYS:O	3:D:218:THR:HG22	2.21	0.40
2:I:145:ILE:HB	2:I:456:VAL:HG22	2.02	0.40
2:I:202:ARG:H	2:I:202:ARG:HG3	1.65	0.40
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.61	0.40
3:J:798:ARG:HH12	3:J:1325:PHE:HB3	1.87	0.40
5:L:586:ARG:O	5:L:590:ILE:HG13	2.20	0.40
1:A:13:LEU:HD12	1:A:16:ILE:HD11	2.03	0.40
2:C:169:LYS:O	2:C:169:LYS:HG2	2.20	0.40
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.36	0.40
3:D:45:ASN:O	3:D:46:TYR:HD2	2.04	0.40
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.37	0.40
2:I:724:VAL:HA	2:I:734:ILE:HD13	2.02	0.40
3:J:810:THR:HG21	3:J:893:GLY:HA3	2.03	0.40
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.36	0.40
2:C:42:ASP:HA	2:C:43:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:545:PHE:CZ	3:D:781:LYS:HG3	2.56	0.40
2:C:748:ILE:HD11	2:C:967:LEU:HA	2.03	0.40
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.86	0.40
3:D:832:LYS:HD3	3:D:1242:ARG:HH12	1.86	0.40
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.40
1:H:41:ASN:ND2	2:I:1217:THR:O	2.54	0.40
1:H:48:LEU:HG	3:J:535:ARG:HG3	2.04	0.40
2:I:9:LYS:HD3	2:I:1171:ARG:HD3	2.04	0.40
2:I:564:PRO:O	2:I:569:ILE:HG12	2.20	0.40
3:J:708:ASN:OD1	3:J:708:ASN:N	2.54	0.40
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	2.01	0.40
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.55	0.40
2:C:1119:MET:HG3	2:C:1204:LEU:HD13	2.04	0.40
2:C:1312:ASN:OD1	2:C:1314:GLN:HG3	2.21	0.40
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.02	0.40
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.36	0.40
3:D:392:THR:CG2	5:F:606:VAL:HA	2.47	0.40
3:D:452:LEU:HD23	3:D:452:LEU:HA	1.87	0.40
5:F:465:ARG:HG2	5:F:465:ARG:H	1.57	0.40
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.57	0.40
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.96	0.40
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.22	0.40
3:J:712:GLN:HB2	3:J:713:GLU:H	1.63	0.40
5:L:357:GLN:H	5:L:357:GLN:HG3	1.72	0.40
5:L:511:ILE:O	5:L:512:GLY:O	2.39	0.40
1:A:92:VAL:HG23	1:A:148:ARG:NH1	2.37	0.40
1:A:236:ASP:HA	1:B:14:VAL:HG13	2.03	0.40
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.56	0.40
2:C:338:THR:CG2	2:C:345:PRO:HB3	2.51	0.40
2:C:1178:LYS:HD3	2:C:1178:LYS:HA	1.88	0.40
3:D:682:VAL:O	3:D:685:ILE:HG12	2.21	0.40
3:D:891:ASP:OD2	3:D:1285:VAL:HG12	2.22	0.40
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.55	0.40
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.86	0.40
3:J:297:ARG:HD2	5:L:97:PRO:HB3	2.04	0.40
3:J:801:VAL:O	3:J:805:GLN:HB2	2.22	0.40
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.21	0.40
3:J:1197:ASN:HB2	3:J:1211:SER:HA	2.03	0.40
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.51	0.40
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.55	0.40
5:L:281:ARG:HA	5:L:284:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:597:LYS:HB2	5:L:597:LYS:HE3	1.85	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	231/329 (70%)	198 (86%)	29 (13%)	4 (2%)	9	42
1	B	213/329 (65%)	187 (88%)	24 (11%)	2 (1%)	17	54
1	G	225/329 (68%)	191 (85%)	28 (12%)	6 (3%)	5	33
1	H	212/329 (64%)	187 (88%)	24 (11%)	1 (0%)	29	67
2	C	1338/1342 (100%)	1230 (92%)	102 (8%)	6 (0%)	34	71
2	I	1338/1342 (100%)	1230 (92%)	100 (8%)	8 (1%)	25	63
3	D	1163/1407 (83%)	1071 (92%)	83 (7%)	9 (1%)	19	58
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	14	50
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	421 (91%)	34 (7%)	7 (2%)	10	44
5	L	463/613 (76%)	424 (92%)	37 (8%)	2 (0%)	34	71
All	All	6960/8222 (85%)	6355 (91%)	547 (8%)	58 (1%)	19	58

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	170	VAL
2	C	484	LEU
2	C	1159	VAL

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Mol	Chain	Res	Type
3	D	10	ALA
3	D	1274	PHE
3	D	1294	ALA
5	F	512	GLY
1	G	229	GLU
1	G	231	PHE
2	I	170	VAL
2	I	484	LEU
2	I	1159	VAL
2	I	1203	ASP
3	J	332	LYS
5	L	512	GLY
1	A	167	PRO
1	A	232	VAL
1	B	20	SER
2	C	697	LYS
3	D	332	LYS
5	F	569	THR
1	G	162	GLU
1	G	167	PRO
2	I	697	LYS
3	J	334	LYS
3	J	339	ARG
3	J	341	ASN
1	B	138	ALA
2	C	1158	LYS
3	D	712	GLN
5	F	515	GLU
5	F	516	ASP
3	J	333	GLY
3	J	712	GLN
1	A	162	GLU
3	D	806	ASP
2	I	1136	GLN
2	I	1158	LYS
3	J	338	PHE
3	J	344	GLY
3	J	806	ASP
5	F	513	ASP
1	H	138	ALA
3	J	710	ASP
5	L	166	VAL

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Mol	Chain	Res	Type
1	A	62	ASP
3	D	1273	ASP
1	G	196	THR
3	D	831	VAL
3	J	831	VAL
5	F	477	GLU
2	I	1186	VAL
3	J	826	ILE
2	C	1186	VAL
3	D	826	ILE
1	G	14	VAL
3	J	1180	VAL
5	F	166	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/286 (70%)	190 (94%)	11 (6%)	21	50
1	B	186/286 (65%)	167 (90%)	19 (10%)	7	28
1	G	193/286 (68%)	178 (92%)	15 (8%)	12	39
1	H	183/286 (64%)	169 (92%)	14 (8%)	13	40
2	C	1155/1157 (100%)	1059 (92%)	96 (8%)	11	37
2	I	1154/1157 (100%)	1058 (92%)	96 (8%)	11	37
3	D	962/1168 (82%)	880 (92%)	82 (8%)	10	37
3	J	960/1168 (82%)	882 (92%)	78 (8%)	11	38
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	29
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	47
5	F	417/540 (77%)	379 (91%)	38 (9%)	9	33
5	L	418/540 (77%)	384 (92%)	34 (8%)	11	38
All	All	5968/7024 (85%)	5474 (92%)	494 (8%)	11	37

All (494) 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	23	HIS
1	A	61	ILE
1	A	115	ILE
1	A	133	LEU
1	A	145	LYS
1	A	176	CYS
1	A	219	ARG
1	A	231	PHE
1	B	7	GLU
1	B	23	HIS
1	B	50	SER
1	B	61	ILE
1	B	64	VAL
1	B	66	HIS
1	B	68	TYR
1	B	70	THR
1	B	90	VAL
1	B	103	ASN
1	B	115	ILE
1	B	133	LEU
1	B	135	ASP
1	B	173	VAL
1	B	176	CYS
1	B	198	LEU
1	B	203	ILE
1	B	219	ARG
1	B	226	GLU
2	C	11	ILE
2	C	22	LEU
2	C	60	GLN
2	C	70	TYR
2	C	82	VAL
2	C	90	VAL
2	C	116	ASP
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	132	ASP
2	C	189	ASP

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Mol	Chain	Res	Type
2	C	285	ILE
2	C	299	LYS
2	C	342	ASP
2	C	369	MET
2	C	377	THR
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	445	ILE
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	492	MET
2	C	493	ILE
2	C	518	ASN
2	C	531	SER
2	C	533	LEU
2	C	539	THR
2	C	542	ARG
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	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

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Mol	Chain	Res	Type
2	C	817	LEU
2	C	826	ASP
2	C	840	SER
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	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	1146	GLN
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1160	ASP
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1250	SER
2	C	1253	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1299	ASN
2	C	1310	ASP
2	C	1313	HIS
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU

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Mol	Chain	Res	Type
3	D	8	LEU
3	D	11	GLN
3	D	26	SER
3	D	29	MET
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	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	343	LEU
3	D	394	ILE
3	D	407	VAL
3	D	416	ILE
3	D	425	ARG
3	D	454	CYS
3	D	462	ASP
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	568	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
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	798	ARG
3	D	805	GLN
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	860	ARG
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
3	D	1272	SER
3	D	1273	ASP
3	D	1275	LEU
3	D	1333	THR
3	D	1343	GLU
4	E	3	ARG
4	E	5	THR

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Mol	Chain	Res	Type
4	E	13	ILE
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	154	GLU
5	F	264	LYS
5	F	267	ASP
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
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	476	ARG
5	F	479	THR
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	508	GLU
5	F	530	LEU
5	F	547	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	599	ARG
5	F	606	VAL

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Mol	Chain	Res	Type
5	F	608	ARG
1	G	9	LEU
1	G	13	LEU
1	G	29	GLU
1	G	50	SER
1	G	61	ILE
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	139	SER
1	G	145	LYS
1	G	164	ASP
1	G	166	ARG
1	G	176	CYS
1	G	215	GLU
1	G	231	PHE
1	H	9	LEU
1	H	15	ASP
1	H	23	HIS
1	H	50	SER
1	H	61	ILE
1	H	62	ASP
1	H	70	THR
1	H	91	ARG
1	H	103	ASN
1	H	115	ILE
1	H	141	SER
1	H	176	CYS
1	H	219	ARG
1	H	226	GLU
2	I	11	ILE
2	I	22	LEU
2	I	60	GLN
2	I	70	TYR
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	116	ASP
2	I	118	LYS
2	I	119	GLU
2	I	132	ASP
2	I	189	ASP

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Mol	Chain	Res	Type
2	I	285	ILE
2	I	299	LYS
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	445	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	490	GLN
2	I	492	MET
2	I	493	ILE
2	I	496	LYS
2	I	510	GLN
2	I	518	ASN
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
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	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET

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Mol	Chain	Res	Type
2	I	814	ASP
2	I	815	SER
2	I	817	LEU
2	I	826	ASP
2	I	828	PHE
2	I	840	SER
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	944	ARG
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	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1160	ASP
2	I	1198	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1238	LEU
2	I	1253	LEU
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1313	HIS
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP
2	I	1342	GLU

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Mol	Chain	Res	Type
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	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	454	CYS
3	J	462	ASP
3	J	506	VAL
3	J	507	VAL
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	568	SER
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
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

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Mol	Chain	Res	Type
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	805	GLN
3	J	810	THR
3	J	844	THR
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	908	ILE
3	J	918	ILE
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	1275	LEU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1298	VAL
3	J	1333	THR
3	J	1343	GLU
4	K	3	ARG
4	K	13	ILE
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	100	MET

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Mol	Chain	Res	Type
5	L	102	MET
5	L	264	LYS
5	L	266	PHE
5	L	267	ASP
5	L	301	ASN
5	L	306	PHE
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	395	THR
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	479	THR
5	L	482	GLU
5	L	486	ARG
5	L	491	GLU
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	573	LEU
5	L	580	PHE
5	L	587	ILE
5	L	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	517	GLN
2	C	659	GLN

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Mol	Chain	Res	Type
2	C	725	GLN
2	C	1116	HIS
2	C	1146	GLN
2	C	1220	GLN
2	C	1288	GLN
2	C	1314	GLN
3	D	94	GLN
3	D	200	GLN
3	D	294	ASN
3	D	365	GLN
3	D	450	HIS
3	D	477	GLN
3	D	594	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	907	HIS
3	D	910	ASN
3	D	929	GLN
5	F	131	GLN
5	F	147	GLN
5	F	227	GLN
5	F	301	ASN
5	F	309	ASN
5	F	383	ASN
5	F	446	GLN
5	F	455	HIS
5	F	469	GLN
1	H	128	HIS
2	I	69	GLN
2	I	139	ASN
2	I	165	HIS
2	I	494	ASN
2	I	568	ASN
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	1288	GLN

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Mol	Chain	Res	Type
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	206	ASN
3	J	294	ASN
3	J	365	GLN
3	J	424	ASN
3	J	465	GLN
3	J	702	GLN
3	J	716	GLN
3	J	817	HIS
3	J	910	ASN
3	J	929	GLN
3	J	1366	HIS
5	L	131	GLN
5	L	301	ASN
5	L	446	GLN
5	L	472	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 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	-	63,63,63	2.15	11 (17%)	94,94,94	2.00	22 (23%)

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	-	-	10/60/85/85	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	10.23	1.57	1.37
6	C	3001	RFP	C15-N1	6.63	1.49	1.35
6	C	3001	RFP	C12-C11	-4.41	1.37	1.54
6	C	3001	RFP	C3-C43	4.02	1.54	1.46
6	C	3001	RFP	C18-C17	3.69	1.54	1.43
6	C	3001	RFP	O7-C25	-3.65	1.39	1.44
6	C	3001	RFP	O7-C35	2.65	1.41	1.35
6	C	3001	RFP	C2-N1	2.63	1.48	1.43
6	C	3001	RFP	C43-N2	2.29	1.34	1.27
6	C	3001	RFP	C17-C16	2.19	1.41	1.34
6	C	3001	RFP	O6-C27	-2.05	1.38	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C2-C3-C43	-5.64	118.44	124.17
6	C	3001	RFP	C38-N4-C42	5.39	118.72	110.66
6	C	3001	RFP	O4-C11-C5	-5.06	122.15	131.81
6	C	3001	RFP	C41-N3-N2	4.97	139.53	113.86
6	C	3001	RFP	C38-N4-C39	4.93	118.03	110.66
6	C	3001	RFP	O7-C35-C36	4.70	119.73	111.09
6	C	3001	RFP	C12-C11-C5	4.69	116.48	107.30
6	C	3001	RFP	C25-O7-C35	3.69	123.43	117.72
6	C	3001	RFP	C4-C3-C43	3.49	120.69	116.52
6	C	3001	RFP	C32-C22-C23	-3.46	104.40	111.39
6	C	3001	RFP	C40-N3-N2	-3.02	98.28	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C3-C2-N1	-2.91	114.40	119.25
6	C	3001	RFP	C41-C42-N4	2.88	114.06	110.80
6	C	3001	RFP	C37-O6-C27	2.81	119.75	113.01
6	C	3001	RFP	C42-N4-C39	2.69	113.28	109.52
6	C	3001	RFP	C41-N3-C40	2.66	120.68	113.74
6	C	3001	RFP	C2-C3-C4	2.44	120.77	119.20
6	C	3001	RFP	C5-C10-C9	-2.41	115.27	119.66
6	C	3001	RFP	O9-C23-C22	-2.26	104.46	109.49
6	C	3001	RFP	C18-C17-C16	-2.19	120.16	126.61
6	C	3001	RFP	C12-O3-C6	-2.17	104.02	107.68
6	C	3001	RFP	C3-C43-N2	-2.10	118.48	121.54

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C2-C3-C43-N2
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C43-N2-N3-C40
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C43-N2-N3-C41
6	C	3001	RFP	C1-C2-N1-C15
6	C	3001	RFP	C30-C16-C17-C18
6	C	3001	RFP	C28-C27-O6-C37
6	C	3001	RFP	C17-C18-C19-C20
6	C	3001	RFP	C21-C22-C23-C24

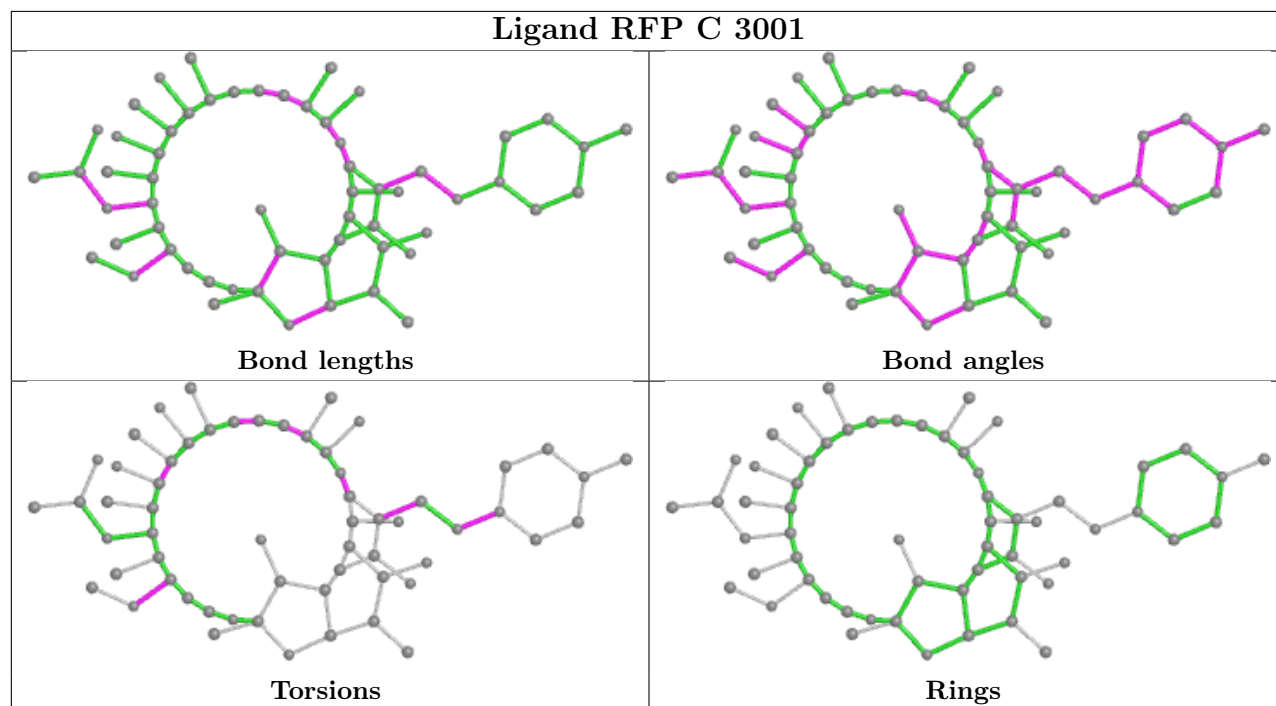
There are no ring outliers.

1 monomer is involved in 6 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	233/329 (70%)	-0.38	0 100 100	171, 206, 261, 301	0
1	B	217/329 (65%)	-0.12	3 (1%) 75 65	179, 243, 300, 333	0
1	G	227/329 (68%)	-0.26	1 (0%) 92 87	223, 269, 305, 330	0
1	H	216/329 (65%)	-0.13	3 (1%) 75 65	213, 288, 312, 327	0
2	C	1340/1342 (99%)	-0.30	15 (1%) 80 72	126, 197, 326, 418	0
2	I	1340/1342 (99%)	-0.08	23 (1%) 70 60	174, 254, 341, 465	0
3	D	1167/1407 (82%)	-0.29	2 (0%) 95 93	137, 186, 259, 335	0
3	J	1155/1407 (82%)	-0.20	12 (1%) 82 74	163, 218, 292, 350	0
4	E	89/91 (97%)	-0.34	1 (1%) 80 72	180, 221, 256, 264	0
4	K	79/91 (86%)	0.41	4 (5%) 28 24	244, 325, 377, 395	0
5	F	468/613 (76%)	-0.25	5 (1%) 80 72	185, 234, 373, 416	0
5	L	469/613 (76%)	-0.25	5 (1%) 80 72	219, 257, 379, 441	0
All	All	7000/8222 (85%)	-0.22	74 (1%) 80 72	126, 229, 321, 465	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	265	LYS	5.5
2	I	979	LEU	5.2
1	B	172	LEU	4.5
2	I	1000	LEU	4.5
2	C	316	GLU	3.9
5	F	319	ALA	3.8
2	C	1001	GLY	3.7
3	D	1203	ARG	3.6
2	I	1005	GLU	3.5
2	C	264	GLU	3.5
5	L	490	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	311	CYS	3.3
2	I	988	LYS	3.3
2	I	231	GLU	3.2
2	I	1004	ASP	3.2
2	C	251	ALA	3.1
1	H	96	ASP	3.1
2	C	266	GLY	3.1
5	F	315	TRP	3.1
3	J	521	LYS	3.1
4	K	2	ALA	3.0
2	C	267	ARG	3.0
2	I	376	PRO	3.0
1	H	107	ILE	2.9
1	H	106	GLY	2.9
3	D	1202	GLU	2.9
3	J	218	THR	2.9
4	K	75	GLN	2.8
2	I	978	VAL	2.8
3	J	707	ILE	2.8
2	I	982	GLY	2.7
3	J	208	THR	2.7
2	I	1022	LYS	2.7
5	L	315	TRP	2.6
2	I	1003	THR	2.6
2	C	332	ARG	2.5
2	C	312	ALA	2.4
2	I	236	LYS	2.4
2	I	414	ILE	2.4
2	I	593	LYS	2.4
2	I	1007	LYS	2.4
3	J	314	ARG	2.4
2	C	270	THR	2.3
4	E	35	LYS	2.3
3	J	1198	VAL	2.3
2	C	1000	LEU	2.3
3	J	830	ASP	2.3
2	I	235	ASN	2.2
2	I	976	ARG	2.2
3	J	207	GLU	2.2
2	C	252	SER	2.2
1	B	58	GLU	2.2
2	I	1006	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	J	209	ASN	2.2
5	L	319	ALA	2.1
3	J	149	GLY	2.1
4	K	26	ARG	2.1
5	F	323	ASN	2.1
1	G	95	LYS	2.1
1	B	145	LYS	2.1
2	C	237	LEU	2.1
5	F	321	ALA	2.1
2	I	745	GLU	2.1
5	F	318	ALA	2.1
2	I	311	CYS	2.1
5	L	318	ALA	2.1
3	J	542	ALA	2.1
5	L	290	LEU	2.1
2	I	1002	LEU	2.1
2	C	169	LYS	2.0
2	I	720	ARG	2.0
2	I	600	THR	2.0
4	K	41	GLU	2.0
3	J	518	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

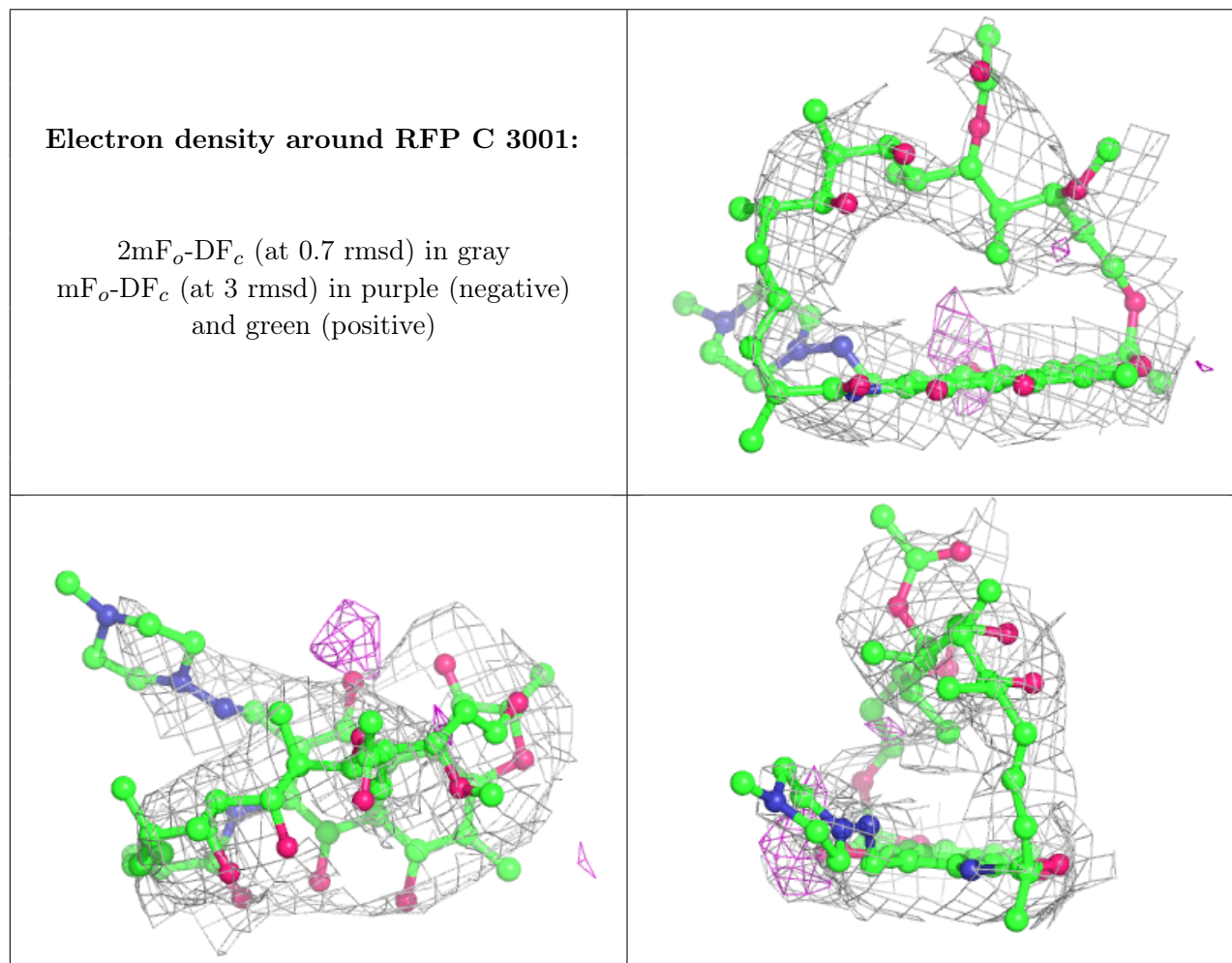
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	I	1401	1/1	0.23	0.47	216,216,216,216	0
7	MG	J	2001	1/1	0.46	0.21	216,216,216,216	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	C	3002	1/1	0.61	0.57	216,216,216,216	0
7	MG	D	2001	1/1	0.68	0.14	216,216,216,216	0
8	ZN	D	2002	1/1	0.83	0.15	216,216,216,216	0
8	ZN	J	2002	1/1	0.84	0.10	222,222,222,222	0
8	ZN	D	2003	1/1	0.88	0.33	216,216,216,216	0
6	RFP	C	3001	59/59	0.91	0.32	136,178,213,228	0
8	ZN	J	2003	1/1	0.91	0.29	216,216,216,216	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.