



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:38 PM UTC

PDB ID : 5W1T / pdb_00005w1t
Title : X-ray crystal structure of Escherichia coli RNA polymerase and DksA complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-06-04
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

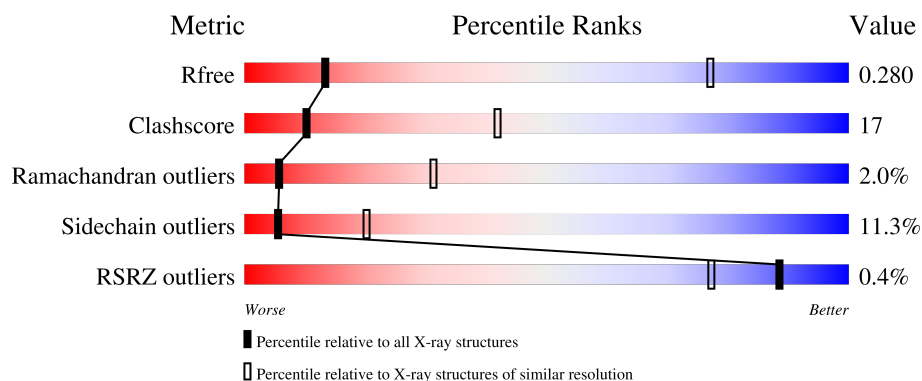
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

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



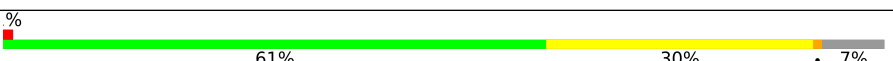
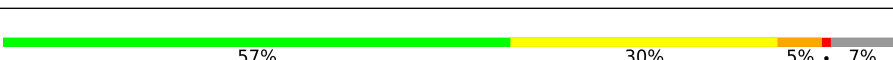
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	44% 41% 12% ••
1	B	329	41% 22% • 34%
1	G	329	% 40% 24% 5% 31%
1	H	329	43% 21% • 34%
2	C	1342	57% 37% 5%

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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	
6	M	151	
6	N	151	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58066 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1171	Total	C	N	O	S	0	0	0
			9085	5712	1626	1701	46			
3	J	1159	Total	C	N	O	S	0	0	0
			9021	5671	1616	1688	46			

- Molecule 4 is a protein called RpoZ.

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

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

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

- Molecule 6 is a protein called RNA polymerase-binding transcription factor DksA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			
6	N	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

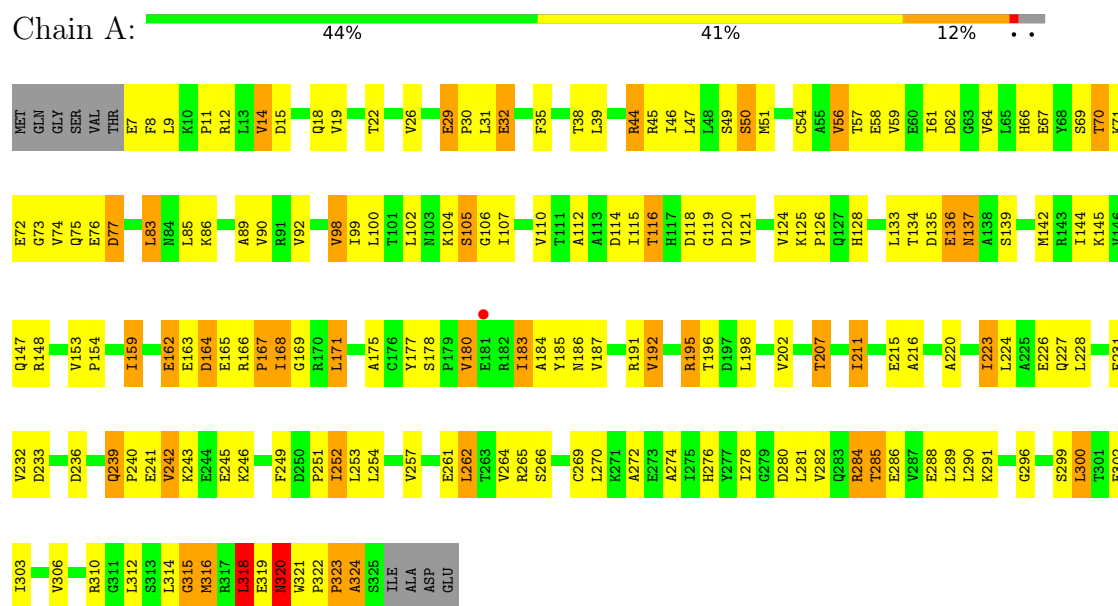
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	J	2	Total	Zn	0	0
			2	2		
8	M	1	Total	Zn	0	0
			1	1		
8	N	1	Total	Zn	0	0
			1	1		

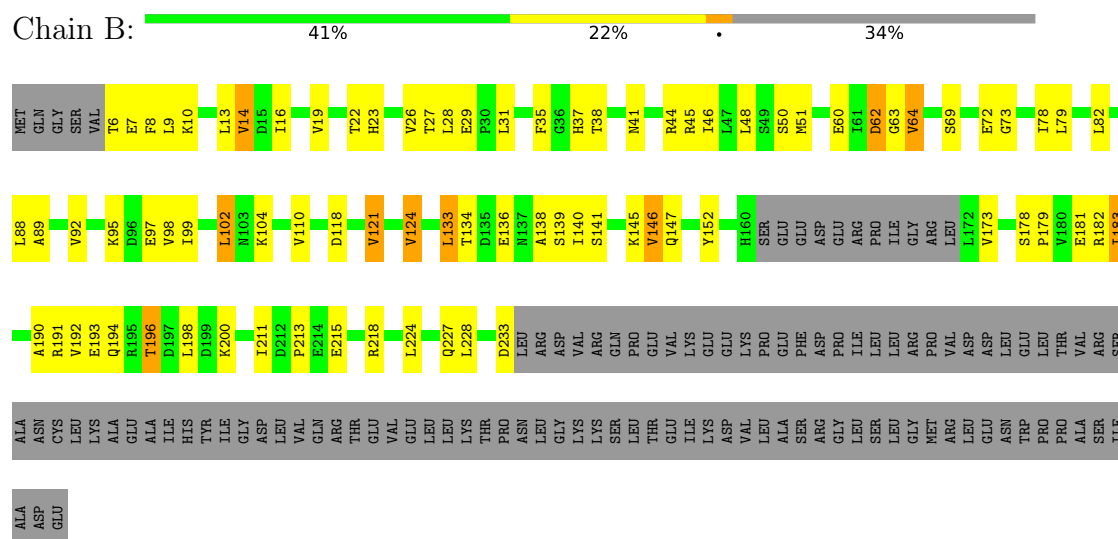
3 Residue-property plots

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

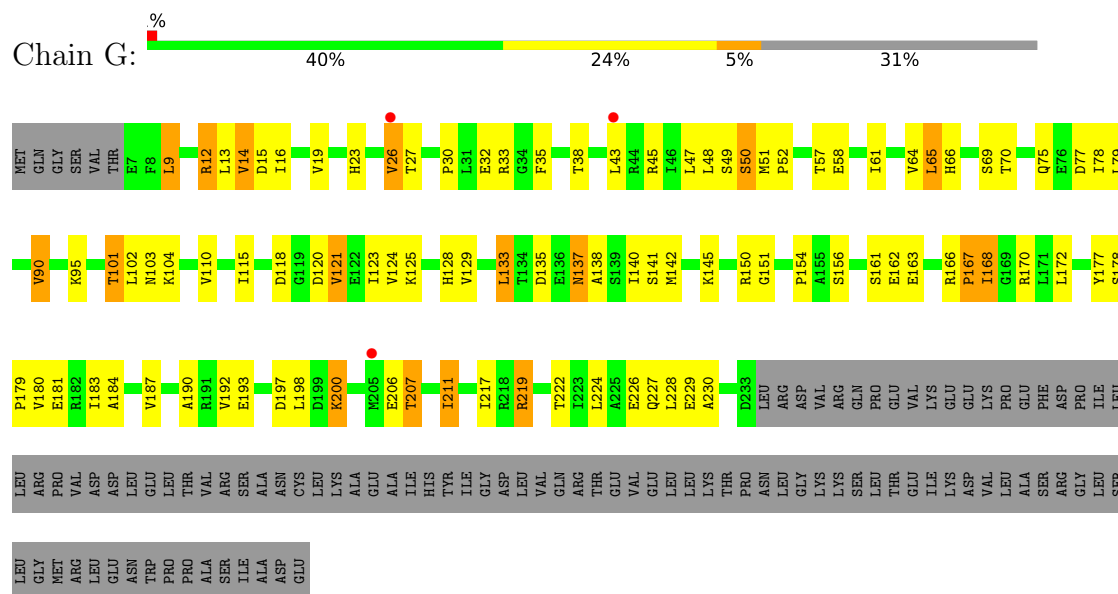
• Molecule 1: DNA-directed RNA polymerase subunit alpha



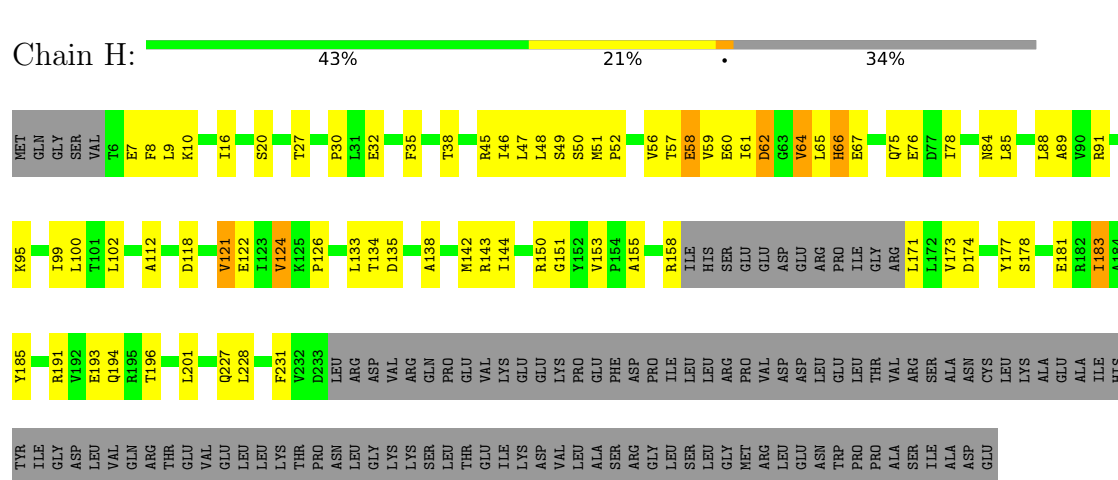
• Molecule 1: DNA-directed RNA polymerase subunit alpha



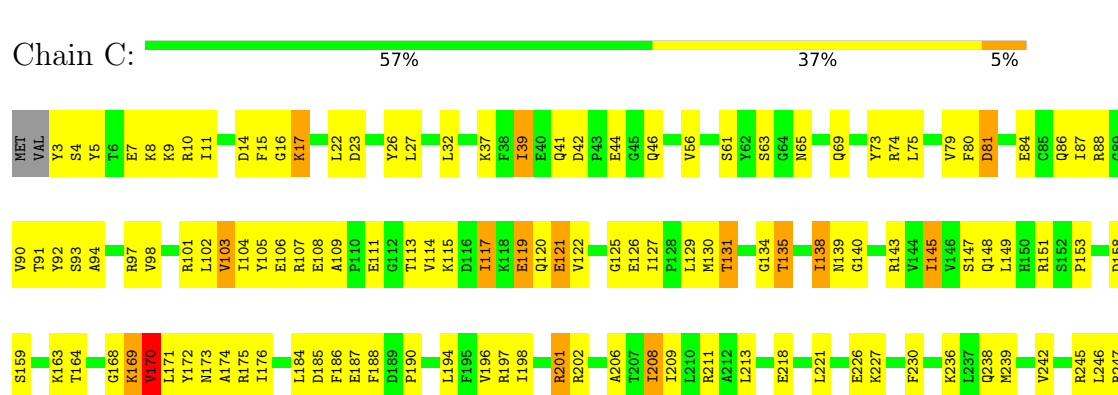
- Molecule 1: DNA-directed RNA polymerase subunit alpha

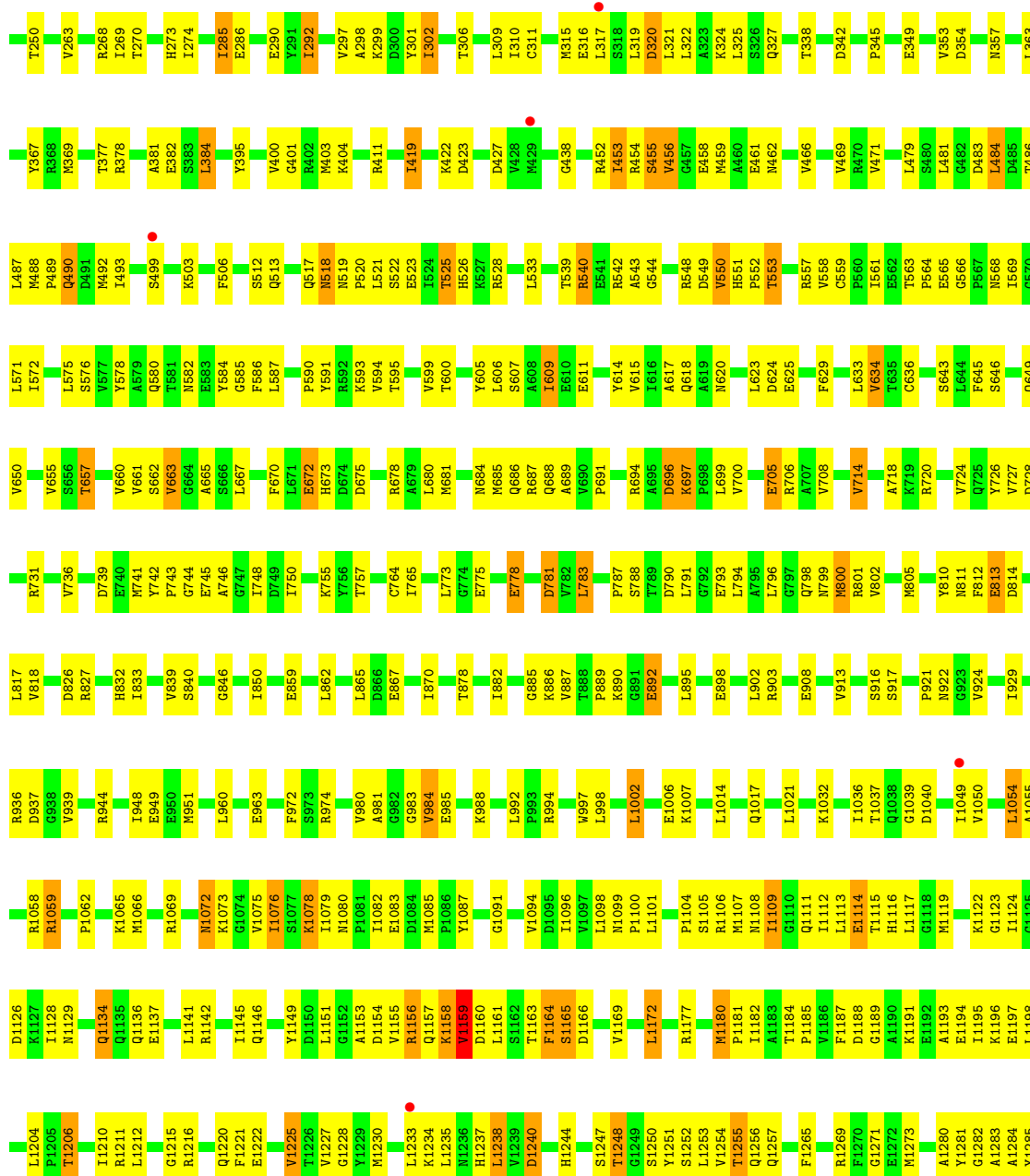


- Molecule 1: DNA-directed RNA polymerase subunit alpha



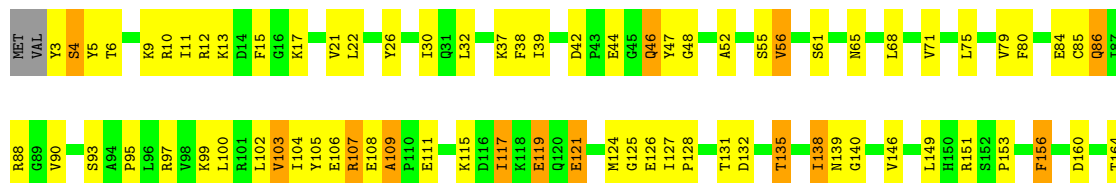
- Molecule 2: DNA-directed RNA polymerase subunit beta

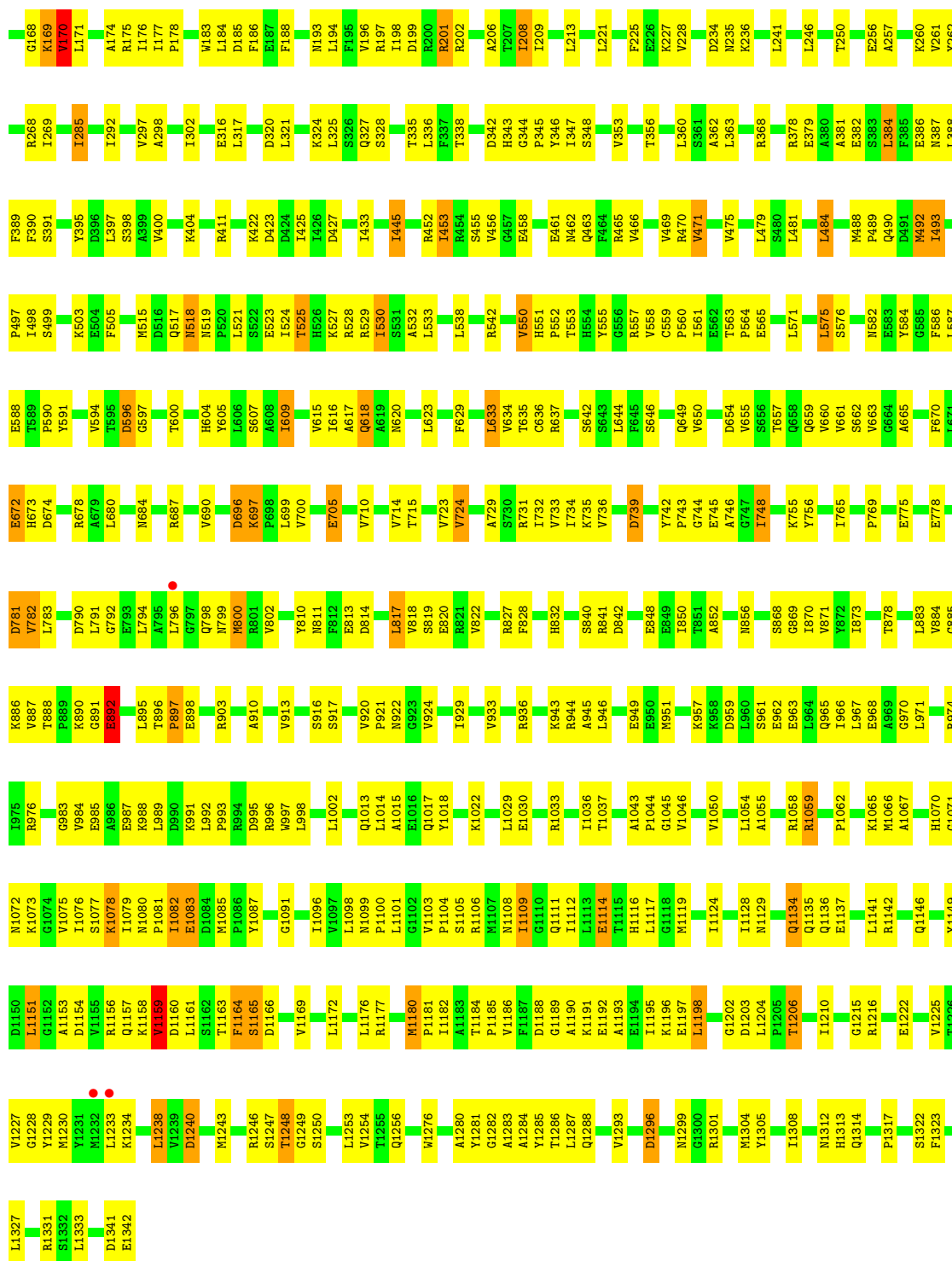




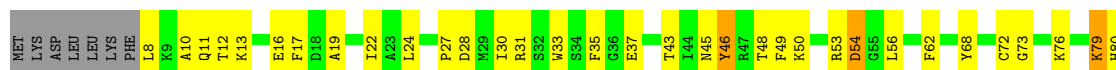
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 58% 37% 5%





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

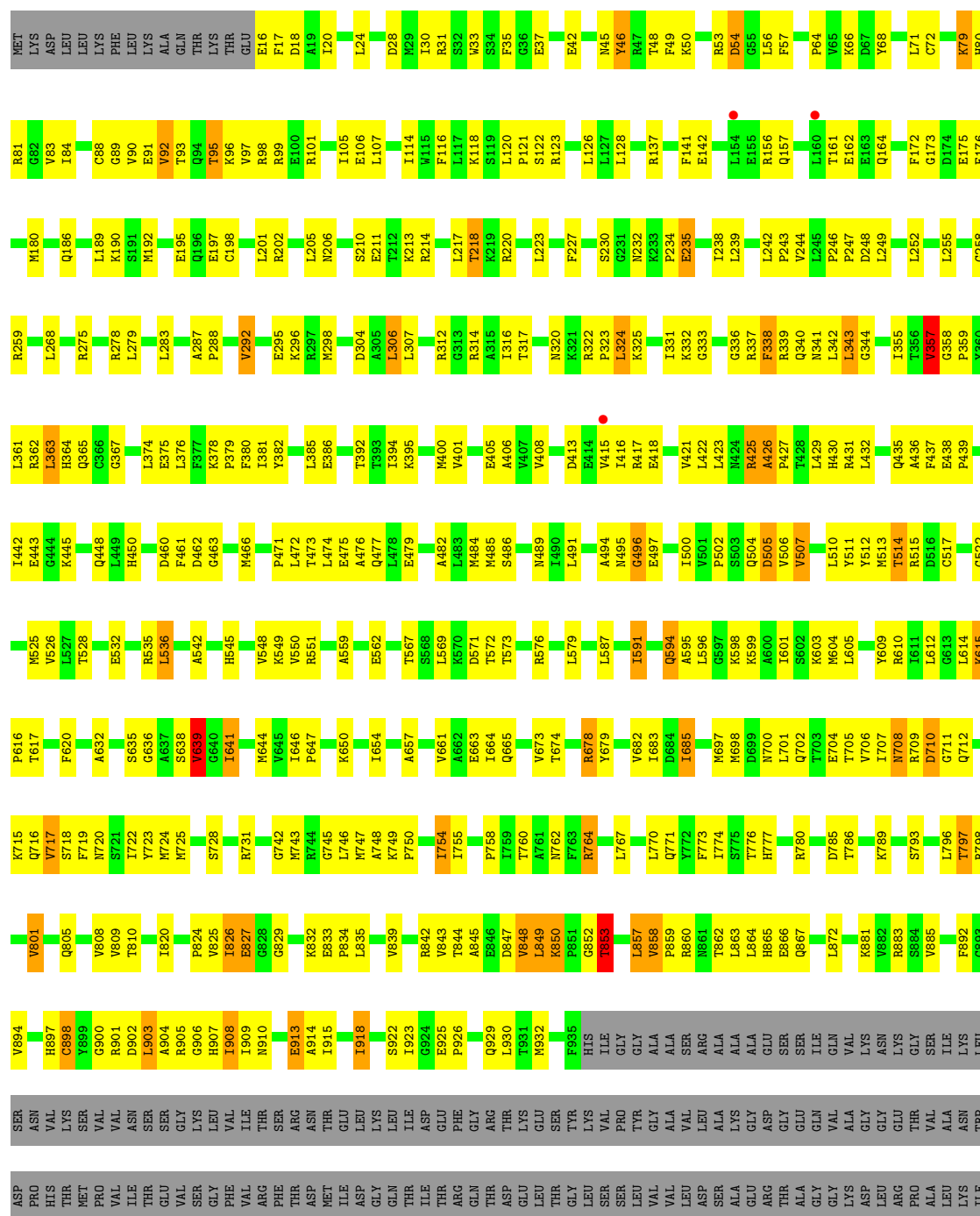


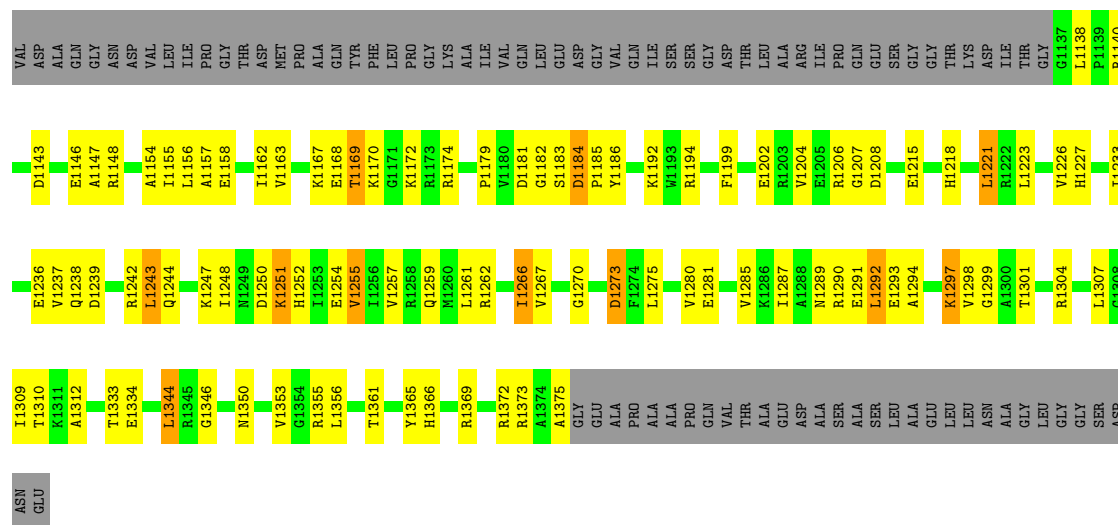
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T1230	I1155	ASP	VAL	VAL	R883	V809	D710	K599	V507	P427	K345	V253	T161	G82
Y1231	L1156	LEU	THR	ASN	S884	T810	G711	A600	L508	T428	R346	P254	Q164	V83
I1233	A1157	ILE	GLU	SER	V885	E811	Q712	I601	G509	L429	V347	L255	I184	I84
E1236	E1158	PRO	VAL	GLY	T890	D812	Q716	M604	L510	R430	D348	G258	F172	C88
V1237	I1159	GLY	SER	LYS	G893	D813	V717	Y609	Y512	H431	G173	R259	G173	G89
Q1238	G1161	THR	ASP	PHE	V894	H817	S718	L614	M513	L432	D174	T262	D174	V90
	V1162	MET	VAL	ILE				P616	R515	I434	E175	T262	F176	E91
	V1163	PRO	ARG	THR	R901	I820	S721		R518	Q435	G358	N266	G176	V92
	S1164	ALA	PHE	SER	D902	R821	T722		V518	F437	P359	N266	E183	T93
V1246	L1165	GLN	THR	ARG	I903	R822	Y723	R634	M525	E438		L268	T95	T95
K1247	G1166	TYR	ASP	ARG	A904	T823	W724		V526	L363	K362	T269	K96	K96
I1248	K1167	PHE	MET	THR	R905	R824	W725	S638	L527	H964	L188	R270	V97	V97
	E1168	ILE	GLU	THR	G906	V825		V639	T528	Q365	L189		K190	R98
K1251	T1169	PRO	ASP	LEU	H907	R826	R731	I641	G529	E443	G367	R275	L194	R99
H1252	K1170	GLY	GLY	LYS	I908	G828	G732		G529	G444	G276	N276	E100	E100
	G1171	LYS	GLN	LEU	E913	G829	S733		E532	K445	R277	N277	R101	R101
V1255	H1172	ALA	THR	ILE		D830		P647	A533	Q448	K372	R276	E197	M102
I1256	R1173	ILE	ILE	ASP		V831	Q736		A534	L374	A373	L279	G103	G103
V1257	R1174	VAL	THR	GLU	T918	R832	T737	K650	E534	H450	L374	K280	H104	H104
	L1175	GLN	ARG	PHE					R535		E375	R202		
M1260	V1176	LEU	GLN	GLY	E925	R833	Q738	A659	L536		F377	V292	L107	L107
R1262	I1177	GLY	THR	ARG	P926	E834	L740	E660	L541	A459	K378	E295	P110	P110
A1263	T1178	ASP	ASP	THR		L835		E660	A542	D460	K378	K296	T111	T111
A1264		GLY	GLY	LYS	Q929	V839	M743	E663	S543	F461	P379	K296	A112	A112
I1265	D1181	VAL	LEU	GLU	L930		R744	E663	R543	D462	R297	K296	H113	H113
I1266	S1183	GLN	THR	SER	F935	R842	G745	Q665	R551	Q463	L381	W298	R213	R213
	D1184	ILE	GLY	TYR		V843	L746	Q667	H545	L472	Y382	D304	R214	R214
P1185	P1185	SER	LEU	LYS	HIS	T844	W747	Q667	V548	T473	E386	D304	K215	K215
Y1186	E1187	GLY	SER	VAL	ILE		A748	F668	K549	T474		A305	K216	F116
E1188	E1188	ASP	LEU	PRO	GLY	D847	K749	Q669	R551	A475	T392	L306	L217	L117
		THR	VAL	GLY	ALA	V848	P750			E476	T393	L307	T218	K118
E1276		LEU	VAL	ALA	ALA	L849		L672	Y555	Q477	I394	D308	I221	L120
G1277	K1192	ALA	VAL	SER	SER	K850	I754	V673		L478	K395	N309	L223	P121
E1278	V1193	ARG	LEU	ARG	ARG	P851		T674	A559	E479	M400	G310	L224	S122
Q1279	R1194	ILE	LEU	LEU	ALA	G852	P758	A675	A562		V407	R312	L240	R123
V1280		PRO	SER	ALA	ALA	T853		G676	E562	A482	V408	G313	S230	R133
E1281	V1198	GLN	ALA	LYS	ALA	A854	N762	E677	L579	L483	R403	R321	P234	R137
R1284	F1199	GLU	ARG	ASP	GLU	D855	F763	R678	M580	E404	E404	R322	E235	Y140
V1285	E1200	SER	THR	GLY	GLU	T856	R764	Y679	M581	M484	E405	P323	F141	F141
K1286	G1201	GLY	THR	GLY	SER	L857		K680	G569	M485	A406	K325	E142	E142
I1287	E1202	GLY	GLY	GLN	ILE	V858	L770	K681	D571		V407	M330	V241	I147
I1288		THR	GLY	VAL	VAL	P859	T776	V682	T572	G496	I416	R330	L242	L242
M1289	G1207	ASP	ASP	GLY	GLN	N861	H777	I685	L579	E497	E418	K335	P243	P243
		LYS	LYS	GLY	LYS	T862	T766	N690	M587		E418	K335	V244	N153
L1292	I1210	ARG	GLY	GLY	ASN	L863			G586	I500	V421	Q335	L239	L239
E1293	E1215	PRO	ARG	THR	GLY	L864		M697	M587	P502	L422	R337	T240	T240
A1294		ALA	VAL	VAL	ILE		K789	M698	G587	P502	L422	R337	V246	P246
	D1219	LEU	ALA	VAL	THR	E866	T790		L587	Q503	L423	R337	P247	P247
K1297	P1139	LYS	LYS	ASN	LYS	L872	S793	L701	Y588	Q504	N424	K337	D248	D248
V1298	I1221	ILE	TRP	LEU	LEU				Y589					
G1299	L1221	VAL	TRP	LEU	SER									
A1300	R1222	ASP	ASP	SER	ASN	V877	T797	T705						
T1301		VAL	PRO	SER	ASN	D878		V705	Q594					
	H1227	ALA	GLN	THR	LYS	A879	V801	I707						
R1304	A1228	GLY	MET	THR	SER			N708	L596	D505	R425			I159



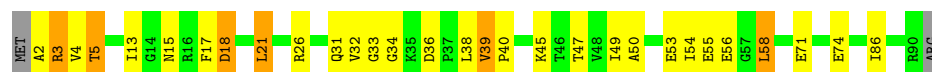
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 46% 32% 18%

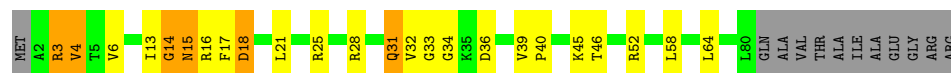




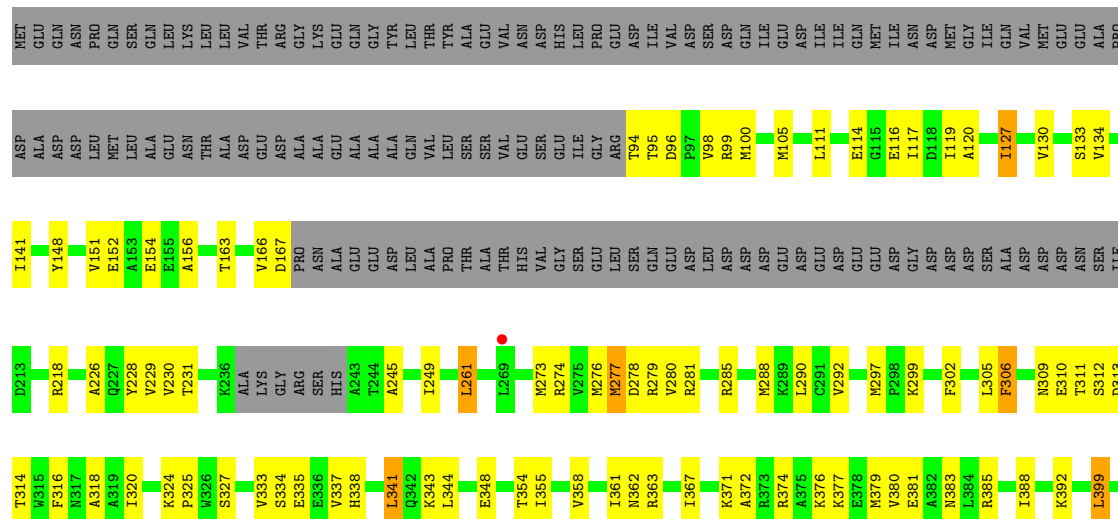
• Molecule 4: RpoZ

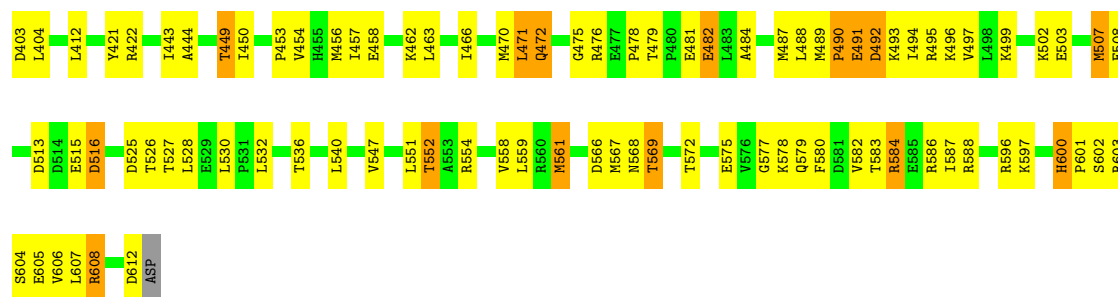


• Molecule 4: RpoZ



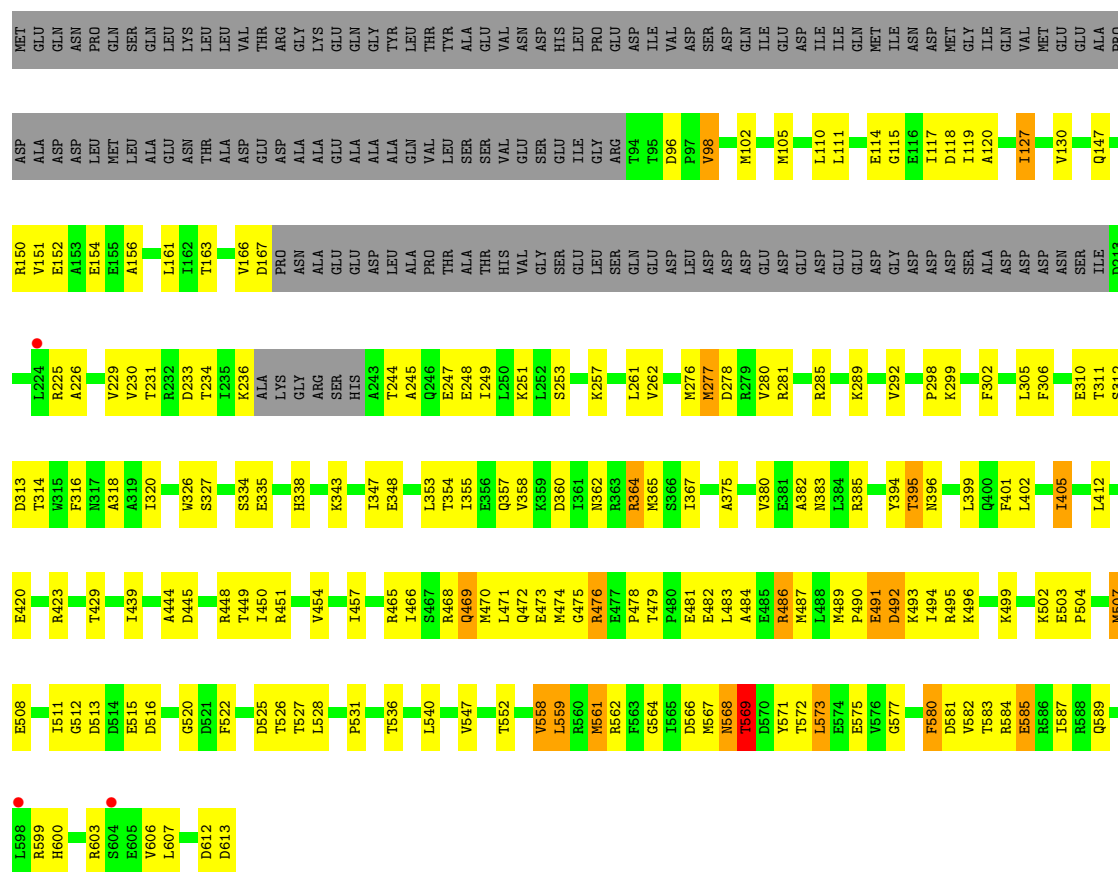
• Molecule 5: RNA polymerase sigma factor RpoD





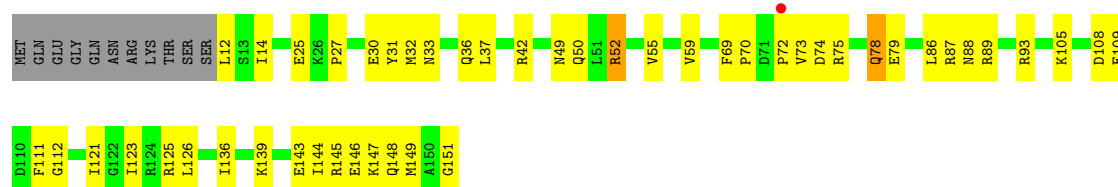
• Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 46% 27% 23%



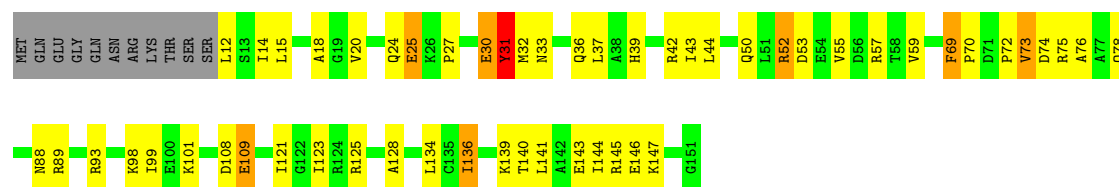
• Molecule 6: RNA polymerase-binding transcription factor DksA

Chain M: 61% 30% 7%



• Molecule 6: RNA polymerase-binding transcription factor DksA

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.00Å 204.89Å 314.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.08 – 4.50 47.08 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.08-4.50) 88.5 (47.08-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.220 , 0.276 0.225 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	198.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 272.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	58066	wwPDB-VP
Average B, all atoms (Å ²)	291.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	0/2524	0.77	2/3421 (0.1%)
1	B	0.27	0/1697	0.73	1/2300 (0.0%)
1	G	0.26	0/1777	0.64	0/2408
1	H	0.23	0/1681	0.66	0/2278
2	C	0.30	0/10739	0.69	0/14489
2	I	0.26	0/10735	0.64	2/14484 (0.0%)
3	D	0.34	0/9225	0.76	1/12458 (0.0%)
3	J	0.30	0/9160	0.71	0/12369
4	E	0.29	0/693	0.64	0/935
4	K	0.21	0/629	0.62	0/847
5	F	0.28	0/3864	0.67	0/5194
5	L	0.25	0/3872	0.62	0/5205
6	M	0.27	0/1155	0.80	2/1549 (0.1%)
6	N	0.28	0/1155	0.90	4/1549 (0.3%)
All	All	0.29	0/58906	0.70	12/79486 (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	H	0	1
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
4	K	0	1
All	All	0	10

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	PRO	CA-C-N	5.43	131.48	121.70
1	A	323	PRO	C-N-CA	5.43	131.48	121.70
6	N	109	GLU	CA-C-N	5.42	131.90	121.54
6	N	109	GLU	C-N-CA	5.42	131.90	121.54
6	M	31	TYR	CA-C-N	-5.26	114.19	122.76
6	M	31	TYR	C-N-CA	-5.26	114.19	122.76
6	N	31	TYR	CA-C-N	-5.22	114.63	122.47
6	N	31	TYR	C-N-CA	-5.22	114.63	122.47
2	I	1136	GLN	CA-C-N	5.16	131.40	121.54
2	I	1136	GLN	C-N-CA	5.16	131.40	121.54
1	B	63	GLY	N-CA-C	5.12	125.30	113.18
3	D	672	LEU	N-CA-C	-5.01	102.97	110.23

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
1	H	171	LEU	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	853	THR	Peptide
4	K	3	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2542	120	0
1	B	1677	0	1703	53	1
1	G	1755	0	1773	62	1
1	H	1662	0	1687	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10570	0	10582	401	2
2	I	10566	0	10576	384	0
3	D	9085	0	9218	397	1
3	J	9021	0	9175	391	0
4	E	691	0	695	21	0
4	K	627	0	634	16	0
5	F	3813	0	3880	124	1
5	L	3821	0	3884	116	0
6	M	1140	0	1119	36	0
6	N	1140	0	1119	55	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	58066	0	58587	1996	3

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 17.

All (1996) 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:525:THR:HG21	2:C:687:ARG:HD2	1.39	1.04
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.45	0.98
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.43	0.97
1:A:45:ARG:HG2	1:B:38:THR:HB	1.48	0.95
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.49	0.94
6:N:30:GLU:HG3	6:N:31:TYR:H	1.31	0.93
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.51	0.92
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.17	0.91
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.52	0.91
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.52	0.90
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.38	0.89
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.39	0.86
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.35	0.86
2:C:1101:LEU:HB3	3:D:731:ARG:HD3	1.56	0.85
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.58	0.85
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.39	0.85
2:I:1105:SER:OG	6:N:74:ASP:OD2	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.59	0.84
3:D:362:ARG:H	3:D:365:GLN:HE21	1.25	0.84
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.59	0.84
2:C:324:LYS:O	2:C:327:GLN:NE2	2.11	0.83
3:J:418:GLU:HG3	4:K:45:LYS:H	1.43	0.83
6:N:33:ASN:ND2	6:N:36:GLN:OE1	2.11	0.83
1:G:12:ARG:H	1:G:30:PRO:HD2	1.41	0.83
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.14	0.83
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.44	0.83
3:J:258:GLY:HA3	5:L:499:LYS:HE2	1.62	0.82
6:N:20:VAL:HG21	6:N:43:ILE:HG12	1.62	0.82
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.61	0.81
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	1.63	0.81
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.62	0.81
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.14	0.81
3:D:668:PHE:HB2	3:D:678:ARG:HG3	1.63	0.81
1:A:296:GLY:H	1:A:299:SER:HB2	1.44	0.81
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.63	0.80
3:D:460:ASP:OD1	3:D:462:ASP:OD1	1.98	0.80
3:D:660:GLU:HB3	3:D:685:ILE:HD13	1.61	0.80
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.61	0.80
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.45	0.80
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.22	0.80
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.64	0.79
1:A:191:ARG:NH1	1:A:198:LEU:O	2.15	0.79
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.62	0.79
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.16	0.79
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.15	0.79
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.64	0.79
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.64	0.79
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.65	0.78
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.65	0.78
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.65	0.78
4:K:14:GLY:O	4:K:16:ARG:N	2.15	0.78
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.66	0.78
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.66	0.78
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.49	0.78
5:L:573:LEU:HD23	5:L:573:LEU:H	1.49	0.78
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.66	0.78
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.65	0.77
1:A:47:LEU:HD23	1:A:51:MET:HE2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.17	0.77
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.65	0.77
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.48	0.77
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.67	0.77
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.65	0.77
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.65	0.77
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.67	0.76
3:J:259:ARG:HD3	5:L:502:LYS:HD2	1.68	0.76
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	1.65	0.76
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.66	0.75
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.68	0.75
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.67	0.75
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.51	0.75
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.69	0.75
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.66	0.75
2:I:1101:LEU:HB3	3:J:731:ARG:HD3	1.66	0.75
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.17	0.75
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.20	0.75
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.51	0.75
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.70	0.74
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.20	0.74
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.67	0.74
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.20	0.74
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.69	0.74
3:J:79:LYS:HB2	5:L:569:THR:H	1.51	0.74
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.70	0.73
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.69	0.73
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.70	0.73
3:D:490:ILE:H	3:D:490:ILE:HD13	1.52	0.73
2:C:168:GLY:O	2:C:170:VAL:N	2.17	0.73
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.70	0.73
5:F:292:VAL:HG11	5:F:299:LYS:HG3	1.69	0.73
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.70	0.73
6:M:121:ILE:HG23	6:M:125:ARG:HH11	1.53	0.73
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.20	0.73
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.71	0.73
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.05	0.73
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.71	0.73
3:J:48:THR:O	3:J:50:LYS:N	2.21	0.73
6:N:20:VAL:HG11	6:N:43:ILE:HD11	1.71	0.73
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.71	0.72
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.71	0.72
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.53	0.72
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.71	0.72
3:D:664:ILE:HD11	3:D:685:ILE:HD12	1.71	0.72
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.70	0.72
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.54	0.72
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.20	0.72
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.70	0.72
3:D:664:ILE:HD13	3:D:681:LYS:HG2	1.72	0.72
2:I:528:ARG:NH2	2:I:576:SER:O	2.22	0.72
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.55	0.72
2:I:30:ILE:HD12	2:I:30:ILE:H	1.53	0.72
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.71	0.72
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.72	0.72
6:N:121:ILE:HG23	6:N:125:ARG:HH11	1.53	0.71
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.24	0.71
3:D:473:THR:HG23	3:D:476:ALA:H	1.55	0.71
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.70	0.71
2:I:724:VAL:HG23	2:I:775:GLU:H	1.54	0.71
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.26	0.71
2:I:892:GLU:OE2	3:J:66:LYS:NZ	2.24	0.71
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.23	0.71
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.73	0.71
2:I:1106:ARG:HH21	6:N:73:VAL:HG21	1.56	0.71
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.73	0.70
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.57	0.70
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.74	0.70
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.71	0.70
3:D:495:ASN:O	3:D:497:GLU:N	2.25	0.70
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.56	0.70
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.74	0.70
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.26	0.70
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.72	0.70
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.73	0.70
3:J:42:GLU:OE2	5:L:451:ARG:NE	2.22	0.70
3:J:495:ASN:O	3:J:497:GLU:N	2.24	0.70
1:H:134:THR:HG23	1:H:135:ASP:H	1.56	0.69
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.73	0.69
3:J:709:ARG:O	3:J:711:GLY:N	2.24	0.69
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.75	0.69
3:J:596:LEU:HD11	3:J:604:MET:HE1	1.75	0.69
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.73	0.69
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.75	0.69
2:I:168:GLY:O	2:I:170:VAL:N	2.26	0.69
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.75	0.68
3:D:674:THR:HG21	6:M:139:LYS:HG3	1.75	0.68
3:D:709:ARG:O	3:D:711:GLY:N	2.25	0.68
3:J:107:LEU:HD11	3:J:242:LEU:HB2	1.74	0.68
3:J:473:THR:HG23	3:J:476:ALA:H	1.58	0.68
2:C:175:ARG:HG3	2:C:185:ASP:OD1	1.93	0.68
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.76	0.68
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.75	0.68
5:F:479:THR:HG23	5:F:481:GLU:H	1.59	0.68
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.59	0.68
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.59	0.68
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.75	0.68
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.57	0.68
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.27	0.68
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.76	0.68
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.76	0.68
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.76	0.68
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.22	0.68
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.75	0.68
3:D:935:PHE:O	6:M:87:ARG:NH2	2.28	0.68
1:A:47:LEU:O	1:A:180:VAL:HG21	1.94	0.67
1:A:77:ASP:OD1	1:A:77:ASP:N	2.27	0.67
2:C:617:ALA:HA	2:C:636:CYS:SG	2.34	0.67
4:E:4:VAL:HG13	4:E:5:THR:H	1.59	0.67
4:E:32:VAL:O	4:E:34:GLY:N	2.26	0.67
1:G:45:ARG:HG2	1:H:38:THR:HB	1.76	0.67
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.24	0.67
1:A:14:VAL:HG22	1:A:15:ASP:H	1.59	0.67
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.76	0.67
3:D:1181:ASP:HB3	3:J:202:ARG:HH11	1.59	0.67
2:I:596:ASP:CG	2:I:597:GLY:H	2.02	0.67
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.75	0.67
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.28	0.67
3:D:48:THR:O	3:D:50:LYS:N	2.28	0.67
2:I:324:LYS:O	2:I:327:GLN:NE2	2.28	0.67
3:J:722:ILE:HA	3:J:725:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.27	0.67
1:H:52:PRO:HG3	1:H:150:ARG:HG2	1.77	0.66
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.76	0.66
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.76	0.66
3:J:460:ASP:OD1	3:J:462:ASP:OD1	2.13	0.66
6:M:121:ILE:HG23	6:M:125:ARG:NH1	2.10	0.66
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.77	0.66
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.78	0.66
6:N:139:LYS:NZ	6:N:143:GLU:OE2	2.28	0.66
3:J:700:ASN:O	3:J:704:GLU:HB2	1.95	0.66
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	1.77	0.66
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.77	0.66
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.78	0.66
2:I:723:VAL:O	2:I:735:LYS:N	2.25	0.66
3:J:661:VAL:HG13	3:J:682:VAL:HG11	1.78	0.66
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.78	0.66
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.28	0.66
3:J:357:VAL:HG22	3:J:461:PHE:HE1	1.60	0.66
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.78	0.66
6:M:105:LYS:HB3	6:M:111:PHE:HB2	1.78	0.66
3:D:258:GLY:HA3	5:F:499:LYS:HE2	1.77	0.65
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.77	0.65
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.79	0.65
5:F:134:VAL:HA	5:F:273:MET:HE1	1.77	0.65
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.28	0.65
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.78	0.65
4:K:32:VAL:O	4:K:34:GLY:N	2.29	0.65
4:K:25:ARG:HD3	4:K:64:LEU:HD13	1.76	0.65
1:B:118:ASP:HB2	1:B:121:VAL:HB	1.76	0.65
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.78	0.65
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.26	0.65
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.27	0.65
1:H:181:GLU:HA	3:J:535:ARG:HH21	1.61	0.65
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.36	0.65
3:J:705:THR:HG21	3:J:719:PHE:H	1.61	0.65
3:D:491:LEU:HD22	3:D:496:GLY:O	1.96	0.65
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.78	0.65
3:D:793:SER:O	3:D:797:THR:HG23	1.97	0.65
1:A:236:ASP:HA	1:B:14:VAL:O	1.96	0.65
2:C:1066:MET:HG2	2:C:1234:LYS:HA	1.77	0.65
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:O	3:D:545:HIS:HB3	1.97	0.65
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.79	0.65
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.78	0.65
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.79	0.65
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.11	0.65
5:F:316:PHE:HE1	5:F:337:VAL:HB	1.62	0.64
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.79	0.64
2:I:206:ALA:O	2:I:209:ILE:HG22	1.97	0.64
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.79	0.64
3:J:786:THR:HG21	6:N:76:ALA:HB2	1.79	0.64
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.79	0.64
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.78	0.64
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.78	0.64
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.79	0.64
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.79	0.64
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.78	0.64
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.77	0.64
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.62	0.64
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.78	0.64
3:D:202:ARG:HD3	3:J:1181:ASP:HA	1.80	0.64
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.32	0.64
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.80	0.64
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	1.78	0.64
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.26	0.64
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.06	0.64
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.78	0.64
2:C:591:TYR:OH	2:C:611:GLU:OE1	2.07	0.64
3:J:128:LEU:HA	3:J:192:MET:HE1	1.78	0.64
3:J:425:ARG:HG2	3:J:426:ALA:H	1.63	0.64
3:D:731:ARG:HH22	6:M:73:VAL:HG11	1.63	0.64
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.80	0.64
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.33	0.63
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.80	0.63
6:N:20:VAL:HG21	6:N:43:ILE:CG1	2.28	0.63
2:C:93:SER:OG	2:C:126:GLU:OE1	2.15	0.63
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.81	0.63
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.79	0.63
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.63	0.63
2:I:1247:SER:HB3	3:J:375:GLU:O	1.96	0.63
2:C:802:VAL:HG11	2:C:1230:MET:HB3	1.80	0.63
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:LYS:HD2	2:I:791:LEU:HD21	1.80	0.63
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.81	0.63
3:J:650:LYS:NZ	3:J:762:ASN:HD22	1.97	0.63
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.64	0.63
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.28	0.62
2:I:168:GLY:C	2:I:170:VAL:H	2.07	0.62
1:A:22:THR:O	1:A:207:THR:N	2.30	0.62
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.63	0.62
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.00	0.62
2:I:37:LYS:HD2	2:I:46:GLN:HE21	1.65	0.62
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.80	0.62
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.62
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.28	0.62
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.34	0.62
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.81	0.62
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.80	0.62
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.82	0.62
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.34	0.62
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.80	0.62
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.80	0.62
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.81	0.62
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.65	0.62
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.63	0.62
2:I:739:ASP:OD1	2:I:739:ASP:N	2.28	0.62
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.82	0.62
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.81	0.62
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.81	0.62
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.80	0.62
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.82	0.62
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.28	0.62
3:D:722:ILE:HA	3:D:725:MET:HE3	1.81	0.62
1:H:51:MET:HB3	1:H:178:SER:HB2	1.82	0.62
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.80	0.62
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.12	0.62
1:B:102:LEU:O	1:B:141:SER:HA	2.00	0.62
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.81	0.62
2:C:239:MET:N	2:C:285:ILE:O	2.28	0.61
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.80	0.61
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.14	0.61
2:C:1282:GLY:O	2:C:1284:ALA:N	2.33	0.61
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.82	0.61
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.15	0.61
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.81	0.61
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.35	0.61
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.83	0.61
3:J:663:GLU:HB3	6:N:12:LEU:HD22	1.81	0.61
2:C:125:GLY:HA3	2:C:499:SER:HB2	1.81	0.61
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.25	0.61
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.81	0.61
3:D:43:THR:OG1	5:F:449:THR:O	2.15	0.61
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.83	0.61
3:J:702:GLN:HA	3:J:723:TYR:HE2	1.64	0.61
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.83	0.61
1:G:14:VAL:HG13	1:G:15:ASP:H	1.64	0.61
2:C:1073:LYS:CE	3:D:462:ASP:HB2	2.26	0.61
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.34	0.61
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.32	0.61
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.83	0.61
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.83	0.61
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.83	0.60
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.64	0.60
6:M:32:MET:SD	6:M:37:LEU:HD21	2.41	0.60
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.22	0.60
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.82	0.60
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.83	0.60
3:D:1178:THR:HG23	3:D:1184:ASP:HB3	1.84	0.60
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.84	0.60
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.15	0.60
3:D:460:ASP:CG	3:D:462:ASP:OD1	2.45	0.60
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.29	0.60
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.37	0.60
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.82	0.60
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.83	0.60
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.37	0.60
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.83	0.60
3:J:844:THR:OG1	3:J:860:ARG:O	2.14	0.60
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.83	0.60
3:D:504:GLN:HG3	3:D:505:ASP:H	1.67	0.60
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.82	0.60
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.17	0.60
2:I:873:ILE:HG13	2:I:944:ARG:NH2	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:59:VAL:HG22	6:N:89:ARG:HD2	1.83	0.60
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.84	0.60
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.84	0.60
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.83	0.60
3:D:418:GLU:HG3	4:E:45:LYS:H	1.67	0.60
6:N:30:GLU:HG3	6:N:31:TYR:N	2.12	0.60
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.37	0.60
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.82	0.60
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.84	0.60
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.66	0.60
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.84	0.59
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.84	0.59
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.84	0.59
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.83	0.59
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.83	0.59
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.84	0.59
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.82	0.59
1:H:151:GLY:O	1:H:177:TYR:HB2	2.03	0.59
2:I:1106:ARG:NH2	6:N:73:VAL:HG21	2.16	0.59
3:J:1143:ASP:HA	3:J:1148:ARG:HH11	1.67	0.59
6:M:52:ARG:HB2	6:M:52:ARG:HH11	1.67	0.59
3:D:252:LEU:HD23	3:D:262:THR:HB	1.85	0.59
3:D:849:LEU:H	3:D:849:LEU:HD22	1.66	0.59
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.85	0.59
3:J:793:SER:O	3:J:797:THR:HG23	2.01	0.59
5:L:487:MET:HE2	5:L:487:MET:HA	1.84	0.59
3:J:436:ALA:HB3	3:J:485:MET:HA	1.83	0.59
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.84	0.59
1:B:62:ASP:OD1	1:B:62:ASP:N	2.29	0.59
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.03	0.59
3:J:16:GLU:HG3	3:J:17:PHE:H	1.66	0.59
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.83	0.59
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.35	0.59
1:G:161:SER:O	1:G:163:GLU:N	2.35	0.59
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.85	0.59
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.83	0.59
3:J:128:LEU:HB3	3:J:157:GLN:HE22	1.66	0.59
6:M:108:ASP:CG	6:M:109:GLU:H	2.10	0.59
2:C:563:THR:HG22	2:C:680:LEU:HD11	1.84	0.59
3:D:1157:ALA:HB3	3:D:1207:GLY:H	1.67	0.59
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.85	0.59
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.84	0.59
2:I:633:LEU:HB2	2:I:644:LEU:HD12	1.84	0.59
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.84	0.59
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.84	0.59
2:C:488:MET:O	2:C:490:GLN:N	2.30	0.59
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.03	0.59
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.85	0.59
2:I:38:PHE:HA	2:I:48:GLY:HA2	1.85	0.59
2:I:471:VAL:HG21	2:I:498:ILE:HD11	1.85	0.59
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.68	0.59
4:E:49:ILE:O	4:E:53:GLU:HG3	2.02	0.58
2:I:4:SER:OG	2:I:5:TYR:N	2.34	0.58
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.68	0.58
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.85	0.58
1:A:135:ASP:O	1:A:137:ASN:N	2.36	0.58
2:C:557:ARG:HD3	2:C:587:LEU:HB3	1.84	0.58
2:I:452:ARG:NH1	2:I:584:TYR:O	2.36	0.58
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.38	0.58
3:J:720:ASN:OD1	3:J:722:ILE:HG22	2.03	0.58
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.37	0.58
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.85	0.58
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.85	0.58
3:D:650:LYS:NZ	3:D:762:ASN:HD22	2.01	0.58
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.86	0.58
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.38	0.58
3:D:708:ASN:OD1	3:D:708:ASN:N	2.36	0.58
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.84	0.58
3:J:598:LYS:O	3:J:601:ILE:HG22	2.03	0.58
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.84	0.58
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.85	0.58
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.69	0.58
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.16	0.58
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.68	0.58
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.68	0.58
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.29	0.58
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.84	0.58
2:C:80:PHE:HB3	2:C:84:GLU:HB2	1.84	0.58
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.68	0.58
3:D:510:LEU:HA	3:D:513:MET:HE2	1.86	0.58
3:D:731:ARG:NH1	6:M:73:VAL:HG21	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:HB3	1:A:303:ILE:HD11	1.85	0.58
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.38	0.58
2:C:936:ARG:HD2	2:C:939:VAL:HG23	1.86	0.58
5:F:348:GLU:HG2	5:F:354:THR:HA	1.84	0.58
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.84	0.58
2:I:138:ILE:O	2:I:139:ASN:ND2	2.37	0.58
3:J:83:VAL:O	3:J:91:GLU:HA	2.04	0.58
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.66	0.58
3:D:1165:PHE:HE1	3:D:1200:GLU:HB2	1.68	0.58
3:J:789:LYS:NZ	3:J:932:MET:H	2.02	0.58
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.04	0.58
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.86	0.57
3:D:81:ARG:C	3:D:83:VAL:H	2.12	0.57
3:D:926:PRO:HB3	3:D:1246:VAL:HG11	1.86	0.57
2:I:1276:TRP:HH2	3:J:798:ARG:HG3	1.69	0.57
3:J:211:GLU:OE2	3:J:214:ARG:NH1	2.37	0.57
1:A:159:ILE:HG13	1:A:162:GLU:HG3	1.84	0.57
3:D:676:GLY:HA2	3:D:679:TYR:HD2	1.69	0.57
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.28	0.57
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.18	0.57
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.70	0.57
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.86	0.57
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.86	0.57
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.86	0.57
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.37	0.57
5:L:380:VAL:HG13	5:L:412:LEU:HD23	1.86	0.57
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.86	0.57
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.86	0.57
3:J:664:ILE:HG12	6:N:12:LEU:HD11	1.87	0.57
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.05	0.57
1:A:318:LEU:O	1:A:320:ASN:N	2.36	0.57
5:F:487:MET:HA	5:F:487:MET:HE2	1.85	0.57
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.39	0.57
2:I:961:SER:O	2:I:965:GLN:N	2.36	0.57
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.05	0.57
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.03	0.57
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.53	0.57
2:C:1164:PHE:O	2:C:1166:ASP:N	2.38	0.57
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.87	0.57
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.40	0.57
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.87	0.56
2:C:41:GLN:NE2	2:C:73:TYR:O	2.38	0.56
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.86	0.56
3:D:357:VAL:HG22	3:D:461:PHE:HE1	1.70	0.56
2:I:347:ILE:HD11	2:I:433:ILE:HD11	1.86	0.56
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.70	0.56
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.87	0.56
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.20	0.56
1:A:115:ILE:HG22	1:A:116:THR:H	1.70	0.56
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.34	0.56
2:C:1124:ILE:HG21	2:C:1180:MET:HE2	1.87	0.56
2:C:1244:HIS:HD2	2:C:1265:PHE:HB2	1.70	0.56
2:C:1296:ASP:CG	2:C:1322:SER:HB3	2.30	0.56
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.87	0.56
2:I:52:ALA:HB2	2:I:461:GLU:HG3	1.87	0.56
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.39	0.56
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.87	0.56
3:J:908:ILE:HG12	3:J:909:ILE:N	2.20	0.56
1:A:39:LEU:HD21	1:B:224:LEU:HD11	1.87	0.56
2:C:452:ARG:NH1	2:C:584:TYR:O	2.37	0.56
1:H:191:ARG:NH1	3:J:413:ASP:OD2	2.38	0.56
2:I:582:ASN:HB3	2:I:586:PHE:H	1.71	0.56
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.87	0.56
3:J:842:ARG:NH2	3:J:1254:GLU:OE1	2.36	0.56
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.04	0.56
6:N:44:LEU:HD22	6:N:99:ILE:HG23	1.87	0.56
1:A:270:LEU:HD11	1:A:281:LEU:HD22	1.88	0.56
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.87	0.56
2:C:1247:SER:HB3	3:D:375:GLU:O	2.05	0.56
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.38	0.56
4:E:2:ALA:HB2	4:E:55:GLU:CD	2.31	0.56
2:I:588:GLU:HB3	2:I:607:SER:HA	1.85	0.56
1:A:12:ARG:H	1:A:30:PRO:HD2	1.70	0.56
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.88	0.56
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.30	0.56
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.88	0.56
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.05	0.56
3:J:708:ASN:OD1	3:J:708:ASN:N	2.36	0.56
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.41	0.56
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.31	0.56
1:A:137:ASN:N	1:A:137:ASN:OD1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.21	0.56
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.87	0.56
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.88	0.56
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.70	0.56
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.87	0.56
3:J:1344:LEU:O	3:J:1346:GLY:N	2.36	0.56
5:L:316:PHE:HZ	5:L:334:SER:HA	1.71	0.56
3:D:672:LEU:O	3:D:673:VAL:HG22	2.05	0.56
5:F:561:MET:HA	5:F:567:MET:HE1	1.87	0.56
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.88	0.56
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.41	0.56
2:I:842:ASP:N	2:I:1045:GLY:O	2.39	0.56
3:J:460:ASP:CG	3:J:462:ASP:OD1	2.48	0.56
3:J:786:THR:HG21	6:N:76:ALA:CB	2.35	0.56
6:N:52:ARG:HH11	6:N:52:ARG:HB2	1.71	0.56
1:A:192:VAL:HG12	1:A:195:ARG:HB2	1.88	0.56
3:D:227:PHE:O	3:D:230:SER:HB3	2.04	0.56
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.88	0.56
3:D:674:THR:HB	6:M:139:LYS:HD2	1.88	0.56
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.71	0.56
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.41	0.55
2:C:1285:TYR:CZ	3:D:1356:LEU:HD11	2.41	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.40	0.55
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.40	0.55
3:J:632:ALA:O	3:J:635:SER:OG	2.21	0.55
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.87	0.55
2:I:560:PRO:O	3:J:780:ARG:NH2	2.35	0.55
1:G:103:ASN:OD1	1:G:141:SER:HB2	2.05	0.55
1:G:227:GLN:NE2	1:H:9:LEU:O	2.34	0.55
6:N:59:VAL:HG22	6:N:89:ARG:HH11	1.71	0.55
2:I:378:ARG:NH1	2:I:382:GLU:OE2	2.40	0.55
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.88	0.55
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.89	0.55
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.87	0.55
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.40	0.55
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	1.87	0.55
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.24	0.55
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.37	0.55
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.37	0.55
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.89	0.55
3:J:786:THR:HA	3:J:789:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.42	0.55
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.70	0.55
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.37	0.55
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.36	0.55
1:A:257:VAL:HG13	1:A:276:HIS:O	2.06	0.55
2:C:9:LYS:NZ	2:C:775:GLU:OE2	2.38	0.55
2:C:1269:ARG:HB3	3:D:343:LEU:HG	1.89	0.55
3:D:425:ARG:HG2	3:D:426:ALA:H	1.71	0.55
5:F:601:PRO:HA	5:F:604:SER:HB3	1.89	0.55
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.89	0.55
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.88	0.55
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.07	0.55
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.89	0.55
4:K:40:PRO:O	4:K:52:ARG:NH2	2.39	0.55
1:A:45:ARG:HG3	1:A:46:ILE:HD13	1.89	0.55
1:A:310:ARG:O	5:F:608:ARG:NH2	2.40	0.55
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.89	0.55
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.07	0.55
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.21	0.55
1:B:104:LYS:HG2	1:B:110:VAL:HG13	1.88	0.54
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.54	0.54
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.89	0.54
3:J:664:ILE:CG1	6:N:12:LEU:HD11	2.37	0.54
3:J:770:LEU:H	3:J:770:LEU:HD22	1.71	0.54
3:J:785:ASP:HB3	3:J:789:LYS:HE2	1.88	0.54
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.40	0.54
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.88	0.54
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.88	0.54
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.37	0.54
3:J:362:ARG:H	3:J:365:GLN:HE21	1.54	0.54
5:L:292:VAL:HG11	5:L:299:LYS:HE3	1.89	0.54
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.07	0.54
3:D:48:THR:C	3:D:50:LYS:H	2.15	0.54
5:F:312:SER:OG	5:F:313:ASP:N	2.41	0.54
2:I:106:GLU:O	2:I:109:ALA:HB2	2.06	0.54
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.22	0.54
2:C:1282:GLY:H	3:D:483:LEU:HD13	1.71	0.54
3:D:201:LEU:HB2	3:D:221:ILE:HD13	1.88	0.54
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.38	0.54
3:D:1160:SER:N	3:D:1206:ARG:HB3	2.23	0.54
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:438:GLU:OE1	4:K:3:ARG:NH2	2.41	0.54
2:I:174:ALA:N	2:I:186:PHE:O	2.40	0.54
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.90	0.54
5:L:312:SER:OG	5:L:313:ASP:N	2.41	0.54
2:C:1248:THR:HG22	2:C:1251:TYR:OH	2.07	0.54
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.90	0.54
3:D:1181:ASP:HB3	3:J:202:ARG:NH1	2.22	0.54
3:J:650:LYS:HZ3	3:J:762:ASN:HD22	1.53	0.54
5:L:489:MET:HE2	5:L:493:LYS:HB2	1.88	0.54
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.43	0.54
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.22	0.54
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.88	0.54
2:I:963:GLU:O	2:I:967:LEU:HB2	2.07	0.54
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.41	0.54
2:C:174:ALA:N	2:C:186:PHE:O	2.36	0.54
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.89	0.54
2:C:778:GLU:O	2:C:781:ASP:HB2	2.08	0.54
5:F:261:LEU:H	5:F:261:LEU:HD12	1.72	0.54
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.90	0.54
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.43	0.54
3:J:797:THR:O	3:J:801:VAL:HG12	2.08	0.54
1:A:49:SER:O	1:A:51:MET:N	2.39	0.54
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.89	0.54
2:I:563:THR:HG22	2:I:680:LEU:HD11	1.90	0.54
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.08	0.54
2:I:1081:PRO:HB3	2:I:1083:GLU:OE2	2.08	0.54
3:J:56:LEU:HD12	3:J:56:LEU:H	1.73	0.54
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.40	0.54
2:C:130:MET:SD	2:C:134:GLY:HA2	2.48	0.54
2:C:250:THR:HA	2:C:268:ARG:HA	1.90	0.54
2:C:582:ASN:HB3	2:C:586:PHE:H	1.73	0.54
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.42	0.54
3:D:596:LEU:HD12	3:D:601:ILE:HG13	1.89	0.54
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.41	0.54
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.23	0.54
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.89	0.54
2:I:411:ARG:NH2	2:I:427:ASP:OD2	2.41	0.54
3:J:278:ARG:HD2	3:J:295:GLU:CD	2.33	0.54
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.90	0.54
1:H:76:GLU:OE1	1:H:76:GLU:N	2.40	0.53
3:J:1239:ASP:O	3:J:1243:LEU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:452:ARG:NH2	2:C:458:GLU:OE2	2.40	0.53
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.72	0.53
3:J:48:THR:C	3:J:50:LYS:H	2.15	0.53
3:J:64:PRO:O	3:J:95:THR:OG1	2.22	0.53
1:A:241:GLU:HG3	1:A:242:VAL:H	1.72	0.53
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.08	0.53
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.24	0.53
2:I:260:LYS:HE3	2:I:262:TYR:CE1	2.43	0.53
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.72	0.53
2:I:868:SER:HB2	2:I:943:LYS:HB3	1.91	0.53
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.90	0.53
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	1.89	0.53
3:D:24:LEU:HD11	3:D:116:PHE:CZ	2.44	0.53
1:G:102:LEU:HD11	1:G:110:VAL:HG11	1.89	0.53
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.90	0.53
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.43	0.53
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.23	0.53
2:C:1105:SER:OG	6:M:74:ASP:OD1	2.25	0.53
1:G:184:ALA:HB2	2:I:1091:GLY:CA	2.39	0.53
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.89	0.53
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.89	0.53
3:J:674:THR:HG22	6:N:136:ILE:HD12	1.91	0.53
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.91	0.53
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.73	0.53
3:D:22:ILE:HG23	3:D:1336:ALA:HA	1.91	0.53
3:D:848:VAL:HG13	3:D:857:LEU:HB2	1.90	0.53
2:C:885:GLY:HA2	2:C:917:SER:HB3	1.90	0.53
3:D:659:ALA:O	3:D:663:GLU:HG2	2.09	0.53
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.73	0.53
3:J:99:ARG:HG3	3:J:249:LEU:HD21	1.90	0.53
3:J:425:ARG:HG2	3:J:426:ALA:N	2.22	0.53
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.90	0.53
2:I:1296:ASP:CG	2:I:1322:SER:HB3	2.34	0.53
5:L:343:LYS:O	5:L:347:ILE:HG13	2.08	0.53
1:A:211:ILE:HG21	1:A:216:ALA:HB2	1.91	0.53
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.91	0.53
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.91	0.53
3:D:54:ASP:OD1	3:D:54:ASP:N	2.41	0.53
5:F:127:ILE:O	5:F:130:VAL:HG22	2.09	0.53
5:F:612:ASP:OD1	5:F:612:ASP:N	2.42	0.53
2:I:387:ASN:HA	2:I:391:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:518:ASN:OD1	2:I:518:ASN:N	2.41	0.53
3:J:504:GLN:HG3	3:J:505:ASP:H	1.73	0.53
5:L:245:ALA:O	5:L:249:ILE:HG13	2.08	0.53
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.53
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.91	0.53
3:D:666:GLU:O	3:D:669:GLN:HG3	2.09	0.53
5:F:281:ARG:O	5:F:285:ARG:HG3	2.09	0.53
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.90	0.53
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.91	0.53
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.90	0.53
3:J:705:THR:OG1	3:J:718:SER:HA	2.08	0.53
2:C:813:GLU:HG3	3:D:460:ASP:HA	1.91	0.52
2:I:871:VAL:O	2:I:944:ARG:NH1	2.42	0.52
3:J:405:GLU:O	3:J:408:VAL:HG22	2.09	0.52
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.45	0.52
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.91	0.52
3:D:362:ARG:H	3:D:365:GLN:NE2	2.00	0.52
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.39	0.52
2:I:800:MET:O	2:I:1229:TYR:HA	2.08	0.52
6:N:108:ASP:OD1	6:N:109:GLU:N	2.33	0.52
1:B:192:VAL:O	1:B:194:GLN:N	2.43	0.52
2:C:519:ASN:HB3	2:C:522:SER:CB	2.39	0.52
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.09	0.52
3:D:930:LEU:HB2	3:D:1138:LEU:HB2	1.91	0.52
5:F:316:PHE:CZ	5:F:338:HIS:HB2	2.45	0.52
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.73	0.52
2:I:1284:ALA:HB3	3:J:1361:THR:HB	1.90	0.52
3:J:79:LYS:HD3	5:L:568:ASN:HB3	1.90	0.52
5:L:127:ILE:O	5:L:130:VAL:HG22	2.09	0.52
5:L:479:THR:HG23	5:L:481:GLU:H	1.74	0.52
6:N:141:LEU:O	6:N:145:ARG:HG3	2.09	0.52
2:C:540:ARG:HB2	2:C:540:ARG:HH11	1.75	0.52
2:C:705:GLU:HB2	2:C:794:LEU:H	1.75	0.52
5:F:245:ALA:O	5:F:249:ILE:HG13	2.10	0.52
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.92	0.52
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.90	0.52
2:C:1211:ARG:HE	2:C:1220:GLN:NE2	2.07	0.52
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.39	0.52
3:J:495:ASN:C	3:J:497:GLU:H	2.17	0.52
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.91	0.52
2:C:1165:SER:HA	2:C:1169:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:317:THR:HG22	3:D:322:ARG:O	2.08	0.52
3:D:664:ILE:HG12	3:D:681:LYS:HE2	1.91	0.52
1:B:35:PHE:HA	1:B:38:THR:HG22	1.91	0.52
1:B:98:VAL:O	1:B:146:VAL:HG13	2.09	0.52
3:D:667:GLN:O	3:D:672:LEU:HB2	2.08	0.52
5:F:148:TYR:OH	5:F:218:ARG:HA	2.10	0.52
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.45	0.52
1:G:133:LEU:HD21	1:G:140:ILE:HG12	1.91	0.52
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.91	0.52
6:N:20:VAL:HG13	6:N:39:HIS:NE2	2.24	0.52
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.91	0.52
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.90	0.52
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.91	0.52
2:I:1164:PHE:O	2:I:1166:ASP:N	2.43	0.52
3:J:755:ILE:HD12	3:J:774:ILE:HG23	1.90	0.52
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.92	0.52
2:C:1062:PRO:HA	2:C:1076:ILE:HG13	1.91	0.52
3:D:214:ARG:HA	3:D:217:LEU:HB3	1.92	0.52
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.42	0.52
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.75	0.52
1:G:140:ILE:HG13	1:G:140:ILE:O	2.10	0.52
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.45	0.52
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.52
3:J:825:VAL:C	3:J:826:ILE:HG13	2.35	0.52
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.92	0.52
1:A:35:PHE:HE1	1:B:46:ILE:HG12	1.75	0.52
1:H:112:ALA:HB3	1:H:126:PRO:HA	1.92	0.52
2:I:169:LYS:O	2:I:170:VAL:HG22	2.10	0.52
3:J:845:ALA:HB3	3:J:881:LYS:HB3	1.92	0.52
5:L:470:MET:O	5:L:478:PRO:HD3	2.10	0.52
6:N:108:ASP:CG	6:N:109:GLU:H	2.13	0.52
3:D:1198:VAL:HB	3:D:1210:ILE:HG23	1.91	0.51
1:G:166:ARG:O	1:G:168:ILE:N	2.43	0.51
2:I:596:ASP:CG	2:I:597:GLY:N	2.68	0.51
1:A:211:ILE:HD12	1:A:215:GLU:HG2	1.92	0.51
1:A:252:ILE:HG21	1:A:312:LEU:HD11	1.92	0.51
2:C:238:GLN:HA	2:C:286:GLU:HA	1.91	0.51
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.45	0.51
5:F:292:VAL:HG13	5:F:297:MET:O	2.10	0.51
1:G:58:GLU:OE2	1:G:170:ARG:HD3	2.09	0.51
6:N:121:ILE:HG23	6:N:125:ARG:NH1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.93	0.51
3:D:709:ARG:HD2	3:D:710:ASP:H	1.74	0.51
3:D:1273:ASP:HB2	3:D:1276:GLU:HB3	1.91	0.51
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.91	0.51
2:I:1066:MET:HG2	2:I:1234:LYS:HA	1.92	0.51
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.46	0.51
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.46	0.51
5:L:612:ASP:OD1	5:L:612:ASP:N	2.43	0.51
3:D:133:ARG:O	3:D:137:ARG:HB2	2.11	0.51
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.11	0.51
3:J:37:GLU:HG3	3:J:105:ILE:HA	1.91	0.51
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.75	0.51
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.93	0.51
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.25	0.51
4:K:15:ASN:C	4:K:17:PHE:H	2.18	0.51
5:L:244:THR:O	5:L:247:GLU:HG2	2.09	0.51
5:L:281:ARG:O	5:L:285:ARG:HG3	2.10	0.51
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.91	0.51
2:C:818:VAL:O	2:C:1079:ILE:HD12	2.10	0.51
2:C:1107:MET:HG2	3:D:740:LEU:HD11	1.93	0.51
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.93	0.51
3:J:760:THR:H	3:J:771:GLN:HE21	1.58	0.51
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.51	0.51
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.40	0.51
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.91	0.51
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.92	0.51
1:G:47:LEU:O	1:G:51:MET:HG3	2.11	0.51
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.93	0.51
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.92	0.51
3:D:820:ILE:HD11	3:D:822:MET:HE2	1.91	0.51
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	1.93	0.51
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.93	0.51
5:L:253:SER:O	5:L:257:LYS:HG3	2.11	0.51
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.46	0.51
1:A:56:VAL:HG11	1:A:85:LEU:HB3	1.93	0.51
1:A:316:MET:SD	5:F:600:HIS:CE1	3.04	0.51
2:C:17:LYS:NZ	2:C:1194:GLU:OE1	2.44	0.51
3:D:205:LEU:HD22	3:D:214:ARG:HB2	1.92	0.51
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.75	0.51
2:C:455:SER:HA	2:C:459:MET:HE2	1.93	0.51
3:D:1181:ASP:CA	3:J:202:ARG:HD3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1356:LEU:HD13	3:D:1362:GLY:HA2	1.93	0.51
1:H:194:GLN:NE2	3:J:406:ALA:HB2	2.26	0.51
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.26	0.51
3:J:673:VAL:HG13	6:N:128:ALA:HB1	1.93	0.51
1:A:49:SER:HB3	2:C:1083:GLU:CD	2.37	0.50
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.92	0.50
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.93	0.50
3:D:107:LEU:HD11	3:D:242:LEU:HB2	1.92	0.50
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.92	0.50
3:J:709:ARG:HD2	3:J:710:ASP:H	1.75	0.50
5:L:316:PHE:CZ	5:L:334:SER:HA	2.45	0.50
2:C:198:ILE:O	2:C:201:ARG:HB2	2.11	0.50
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.12	0.50
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.93	0.50
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.93	0.50
5:L:465:ARG:HD2	5:L:468:ARG:HH22	1.76	0.50
2:C:624:ASP:OD1	2:C:625:GLU:N	2.42	0.50
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.40	0.50
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.93	0.50
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.92	0.50
5:F:117:ILE:HA	5:F:120:ALA:HB3	1.93	0.50
5:F:575:GLU:O	5:F:579:GLN:HG2	2.11	0.50
1:G:166:ARG:N	1:G:167:PRO:HD2	2.26	0.50
2:I:1085:MET:HE2	2:I:1085:MET:HA	1.93	0.50
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.11	0.50
6:M:112:GLY:HA2	6:M:126:LEU:HD11	1.92	0.50
2:C:1101:LEU:HB3	3:D:731:ARG:CD	2.38	0.50
2:C:1255:THR:O	2:C:1257:GLN:N	2.44	0.50
3:D:425:ARG:HG2	3:D:426:ALA:N	2.27	0.50
1:H:51:MET:HB3	1:H:178:SER:CB	2.41	0.50
2:I:499:SER:O	2:I:503:LYS:HB2	2.12	0.50
3:J:709:ARG:HD2	3:J:710:ASP:N	2.26	0.50
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.94	0.50
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.26	0.50
2:C:172:TYR:OH	6:M:148:GLN:O	2.30	0.50
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.50
3:D:30:ILE:HD13	3:D:243:PRO:HG3	1.92	0.50
3:D:833:GLU:OE1	3:D:1242:ARG:HD3	2.11	0.50
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.11	0.50
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.45	0.50
3:J:494:ALA:HB2	3:J:922:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:GLU:OE2	2:C:490:GLN:HB3	2.12	0.50
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.92	0.50
3:D:709:ARG:HD2	3:D:710:ASP:N	2.25	0.50
3:D:825:VAL:C	3:D:826:ILE:HG13	2.36	0.50
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.94	0.50
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.76	0.50
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	1.92	0.50
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	1.92	0.50
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.93	0.50
5:L:507:MET:HE3	5:L:520:GLY:HA3	1.94	0.50
6:N:93:ARG:HG2	6:N:93:ARG:HH11	1.77	0.50
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.93	0.50
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.42	0.50
3:D:903:LEU:HD21	3:D:913:GLU:OE1	2.12	0.50
3:D:1264:ALA:O	3:D:1277:GLY:HA2	2.11	0.50
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.21	0.50
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.92	0.50
1:G:197:ASP:O	1:G:198:LEU:HD23	2.12	0.50
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.92	0.50
2:I:1103:VAL:HG11	2:I:1112:ILE:HG13	1.94	0.50
2:I:1124:ILE:O	2:I:1128:ILE:HG13	2.11	0.50
3:J:268:LEU:HD11	3:J:324:LEU:HD13	1.93	0.50
6:N:53:ASP:O	6:N:57:ARG:HG3	2.11	0.50
1:A:45:ARG:HG2	1:B:38:THR:CB	2.33	0.50
1:A:134:THR:HG21	2:C:727:VAL:O	2.11	0.50
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.47	0.50
3:D:56:LEU:H	3:D:56:LEU:HD12	1.77	0.50
5:F:489:MET:O	5:F:491:GLU:N	2.44	0.50
2:I:213:LEU:HB3	2:I:422:LYS:HD2	1.93	0.50
5:L:525:ASP:CG	5:L:528:LEU:HG	2.36	0.50
2:C:138:ILE:O	2:C:139:ASN:ND2	2.44	0.50
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.47	0.50
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.41	0.50
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.93	0.50
2:I:13:LYS:HD2	2:I:1157:GLN:OE1	2.12	0.50
3:J:122:SER:O	3:J:126:LEU:HG	2.11	0.50
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.93	0.50
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.12	0.49
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.94	0.49
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.94	0.49
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:297:VAL:HB	2:I:317:LEU:HD21	1.94	0.49
3:J:664:ILE:HD12	3:J:682:VAL:HG22	1.94	0.49
6:M:59:VAL:HG22	6:M:89:ARG:HD2	1.94	0.49
2:C:1087:TYR:CE1	2:C:1215:GLY:HA2	2.41	0.49
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.95	0.49
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	1.94	0.49
5:F:372:ALA:O	5:F:376:LYS:HG3	2.11	0.49
2:I:209:ILE:HD11	2:I:425:ILE:HD13	1.93	0.49
3:J:362:ARG:H	3:J:365:GLN:NE2	2.10	0.49
3:J:598:LYS:N	3:J:728:SER:O	2.30	0.49
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.94	0.49
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.93	0.49
3:D:88:CYS:O	3:D:90:VAL:N	2.44	0.49
2:I:802:VAL:HG11	2:I:1230:MET:HB3	1.95	0.49
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.42	0.49
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.27	0.49
6:M:93:ARG:HG2	6:M:93:ARG:HH11	1.77	0.49
6:N:139:LYS:HZ2	6:N:143:GLU:CD	2.20	0.49
2:C:812:PHE:CZ	3:D:503:SER:HB2	2.48	0.49
2:C:833:ILE:HA	2:C:1054:LEU:O	2.12	0.49
1:G:13:LEU:HD23	1:G:13:LEU:H	1.77	0.49
1:G:50:SER:HG	1:H:35:PHE:HE1	1.58	0.49
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.52	0.49
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.94	0.49
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.78	0.49
3:J:18:ASP:HB2	3:J:1373:ARG:NH2	2.27	0.49
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.44	0.49
3:J:1350:ASN:OD1	3:J:1355:ARG:HD2	2.13	0.49
2:C:61:SER:O	2:C:63:SER:N	2.46	0.49
2:C:1107:MET:HG2	3:D:740:LEU:CD1	2.42	0.49
3:D:292:VAL:O	3:D:296:LYS:HG3	2.11	0.49
1:G:95:LYS:HE3	1:G:120:ASP:OD1	2.12	0.49
2:I:198:ILE:O	2:I:201:ARG:HB2	2.12	0.49
2:I:257:ALA:HB2	2:I:285:ILE:HA	1.94	0.49
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.94	0.49
1:A:83:LEU:HB3	2:C:694:ARG:HH21	1.78	0.49
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.95	0.49
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.47	0.49
2:I:149:LEU:O	2:I:532:ALA:HA	2.13	0.49
2:I:617:ALA:HA	2:I:636:CYS:SG	2.51	0.49
5:L:483:LEU:HD12	5:L:483:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:561:MET:HA	5:L:567:MET:HE1	1.95	0.49
2:C:549:ASP:OD1	3:D:750:PRO:HG3	2.12	0.49
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.95	0.49
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.78	0.49
3:D:405:GLU:O	3:D:408:VAL:HG22	2.12	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.76	0.49
1:G:150:ARG:NH2	1:H:32:GLU:OE1	2.45	0.49
2:I:93:SER:HA	2:I:128:PRO:HA	1.95	0.49
2:I:564:PRO:HA	2:I:684:ASN:HD21	1.77	0.49
2:I:672:GLU:HG2	2:I:1186:VAL:O	2.12	0.49
5:L:511:ILE:HG21	5:L:522:PHE:HE2	1.77	0.49
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.93	0.49
2:I:462:ASN:O	2:I:466:VAL:HG23	2.13	0.49
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.27	0.49
3:J:258:GLY:HA3	5:L:499:LYS:CE	2.38	0.49
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.28	0.49
1:B:6:THR:OG1	1:B:7:GLU:N	2.44	0.49
3:D:667:GLN:OE1	3:D:681:LYS:NZ	2.23	0.49
3:D:901:ARG:HA	3:D:908:ILE:HA	1.94	0.49
3:D:1232:TYR:HD2	3:D:1233:ILE:HD12	1.77	0.49
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.78	0.49
2:I:778:GLU:O	2:I:781:ASP:HB2	2.13	0.49
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.78	0.49
6:M:139:LYS:HZ2	6:M:143:GLU:CD	2.20	0.49
1:A:195:ARG:HD2	1:A:196:THR:H	1.78	0.49
1:A:285:THR:OG1	1:A:286:GLU:N	2.46	0.49
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.95	0.49
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.95	0.49
2:I:517:GLN:HG3	2:I:523:GLU:OE2	2.12	0.49
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.95	0.49
2:I:976:ARG:HB2	2:I:997:TRP:CZ3	2.48	0.49
4:K:3:ARG:O	4:K:3:ARG:HG3	2.12	0.49
2:C:145:ILE:HG21	2:C:456:VAL:HG13	1.95	0.48
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.48	0.48
2:C:1164:PHE:C	2:C:1166:ASP:H	2.21	0.48
5:F:314:THR:O	5:F:318:ALA:HB3	2.13	0.48
1:G:219:ARG:HE	1:G:219:ARG:HB2	1.34	0.48
2:I:817:LEU:HD11	2:I:1085:MET:HE1	1.94	0.48
3:J:161:THR:H	3:J:164:GLN:HB2	1.77	0.48
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.48	0.48
3:D:861:ASN:HD22	3:D:883:ARG:NH1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.95	0.48
4:E:15:ASN:C	4:E:17:PHE:H	2.21	0.48
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.95	0.48
1:A:265:ARG:O	1:A:269:CYS:HB2	2.14	0.48
3:D:53:ARG:HA	3:D:54:ASP:HA	1.60	0.48
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.94	0.48
2:I:42:ASP:O	2:I:44:GLU:N	2.42	0.48
2:I:620:ASN:O	2:I:620:ASN:ND2	2.46	0.48
2:I:700:VAL:HG21	2:I:1114:GLU:HG2	1.94	0.48
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.95	0.48
3:J:88:CYS:O	3:J:90:VAL:N	2.46	0.48
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.37	0.48
5:L:515:GLU:HG2	5:L:516:ASP:N	2.28	0.48
6:M:139:LYS:NZ	6:M:143:GLU:OE2	2.45	0.48
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.49	0.48
2:C:796:LEU:H	2:C:796:LEU:HD12	1.78	0.48
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.48	0.48
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.54	0.48
3:J:674:THR:CG2	6:N:125:ARG:HH21	2.27	0.48
1:A:289:LEU:HD11	1:A:314:LEU:HD21	1.95	0.48
1:B:211:ILE:HD11	1:B:215:GLU:CD	2.39	0.48
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.95	0.48
3:D:83:VAL:O	3:D:91:GLU:HA	2.13	0.48
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.95	0.48
3:D:797:THR:O	3:D:801:VAL:HG12	2.13	0.48
5:F:288:MET:HG2	5:F:299:LYS:HE2	1.94	0.48
5:F:453:PRO:O	5:F:456:MET:HB2	2.13	0.48
1:G:13:LEU:HD22	1:H:231:PHE:CD1	2.48	0.48
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.49	0.48
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.95	0.48
1:B:97:GLU:OE1	1:B:147:GLN:NE2	2.47	0.48
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.49	0.48
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.96	0.48
2:I:117:ILE:HD12	2:I:488:MET:CG	2.43	0.48
3:J:515:ARG:NH2	3:J:717:VAL:O	2.47	0.48
5:L:226:ALA:O	5:L:229:VAL:HG22	2.13	0.48
3:D:197:GLU:O	3:D:201:LEU:HG	2.14	0.48
2:I:241:LEU:HD11	2:I:246:LEU:HD11	1.96	0.48
3:J:141:PHE:HA	3:J:180:MET:HE2	1.96	0.48
3:J:365:GLN:O	3:J:437:PHE:HD1	1.97	0.48
3:J:572:THR:OG1	3:J:576:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:230:VAL:O	5:L:234:THR:HG23	2.14	0.48
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.95	0.48
5:L:449:THR:OG1	5:L:503:GLU:OE1	2.25	0.48
2:C:862:LEU:HA	2:C:865:LEU:HB2	1.96	0.48
2:C:1106:ARG:O	2:C:1108:ASN:N	2.45	0.48
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.79	0.48
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.49	0.48
3:J:1270:GLY:HA3	3:J:1298:VAL:O	2.13	0.48
5:L:314:THR:O	5:L:318:ALA:HB3	2.14	0.48
6:N:20:VAL:HG13	6:N:39:HIS:CE1	2.49	0.48
3:D:827:GLU:O	3:D:829:GLY:N	2.45	0.48
1:G:32:GLU:HB2	1:G:35:PHE:CD2	2.48	0.48
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.14	0.48
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.14	0.48
3:J:317:THR:HG22	3:J:322:ARG:O	2.14	0.48
3:J:929:GLN:HA	6:N:75:ARG:HD2	1.96	0.48
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.96	0.48
2:C:691:PRO:HA	2:C:788:SER:OG	2.14	0.48
3:D:850:LYS:HE2	3:D:855:ASP:HB3	1.95	0.48
4:E:4:VAL:HG13	4:E:5:THR:N	2.28	0.48
5:F:151:VAL:HG22	5:F:156:ALA:HB3	1.95	0.48
1:G:172:LEU:HD12	1:G:172:LEU:H	1.79	0.48
5:L:573:LEU:H	5:L:573:LEU:CD2	2.21	0.48
3:D:103:GLY:C	3:D:244:VAL:HG22	2.39	0.47
5:F:561:MET:HE2	5:F:567:MET:SD	2.54	0.47
1:H:62:ASP:OD1	1:H:62:ASP:N	2.33	0.47
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.95	0.47
1:A:166:ARG:O	1:A:168:ILE:N	2.47	0.47
2:C:902:LEU:HD12	5:F:607:LEU:HD23	1.95	0.47
3:D:461:PHE:C	3:D:463:GLY:H	2.22	0.47
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.96	0.47
1:G:49:SER:HB3	2:I:1083:GLU:CD	2.39	0.47
1:G:137:ASN:OD1	1:G:137:ASN:N	2.47	0.47
1:G:228:LEU:O	1:G:230:ALA:N	2.47	0.47
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.95	0.47
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.62	0.47
3:J:665:GLN:CG	3:J:678:ARG:HH21	2.27	0.47
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.29	0.47
2:C:490:GLN:HG3	5:F:472:GLN:OE1	2.14	0.47
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.80	0.47
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:LYS:HG3	1:G:128:HIS:HB2	1.96	0.47
2:I:616:ILE:HG22	2:I:617:ALA:O	2.14	0.47
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.96	0.47
3:J:650:LYS:HZ2	3:J:742:GLY:HA2	1.79	0.47
3:J:1184:ASP:O	3:J:1186:TYR:N	2.48	0.47
5:L:478:PRO:HG2	5:L:483:LEU:HD11	1.96	0.47
6:M:55:VAL:O	6:M:59:VAL:HG23	2.13	0.47
1:A:14:VAL:HG22	1:A:15:ASP:N	2.26	0.47
1:A:223:ILE:HD13	1:B:8:PHE:CZ	2.48	0.47
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.44	0.47
3:D:518:VAL:N	3:D:716:GLN:HE22	2.13	0.47
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.29	0.47
3:D:1199:PHE:HB2	3:D:1202:GLU:CB	2.42	0.47
5:F:515:GLU:HG2	5:F:516:ASP:N	2.29	0.47
2:I:168:GLY:C	2:I:170:VAL:N	2.72	0.47
2:I:733:VAL:HG21	2:I:966:ILE:HD13	1.95	0.47
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.96	0.47
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.97	0.47
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.49	0.47
5:L:395:THR:OG1	5:L:396:ASN:N	2.45	0.47
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.47	0.47
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.97	0.47
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.44	0.47
3:D:1167:LYS:HZ2	3:D:1168:GLU:H	1.60	0.47
5:F:276:MET:SD	5:F:279:ARG:NH1	2.87	0.47
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.48	0.47
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.79	0.47
3:J:901:ARG:HA	3:J:908:ILE:HA	1.95	0.47
4:K:15:ASN:HB3	4:K:18:ASP:H	1.80	0.47
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.30	0.47
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.96	0.47
3:D:748:ALA:O	3:D:777:HIS:CD2	2.68	0.47
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.96	0.47
3:D:1273:ASP:O	3:D:1275:LEU:N	2.41	0.47
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.60	0.47
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.95	0.47
2:I:1246:ARG:NH2	2:I:1249:GLY:H	2.13	0.47
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.96	0.47
5:L:489:MET:O	5:L:491:GLU:N	2.47	0.47
1:A:73:GLY:O	1:A:134:THR:HG22	2.15	0.47
1:A:272:ALA:C	1:A:274:ALA:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.44	0.47
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.97	0.47
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.50	0.47
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.30	0.47
2:C:607:SER:OG	2:C:609:ILE:HG13	2.15	0.47
2:C:728:ASP:HB3	2:C:731:ARG:H	1.79	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.97	0.47
3:D:770:LEU:H	3:D:770:LEU:HD22	1.79	0.47
5:F:399:LEU:HG	5:F:403:ASP:HB3	1.97	0.47
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.96	0.47
2:I:710:VAL:HA	2:I:715:THR:HG21	1.95	0.47
2:I:782:VAL:HG11	2:I:792:GLY:HA2	1.96	0.47
2:I:1119:MET:HE3	2:I:1204:LEU:HD22	1.96	0.47
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.80	0.47
3:J:198:CYS:O	3:J:202:ARG:HG3	2.14	0.47
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.95	0.47
3:J:849:LEU:H	3:J:849:LEU:HD22	1.80	0.47
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.79	0.47
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.47	0.47
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.97	0.47
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.96	0.47
2:I:1022:LYS:HD2	2:I:1022:LYS:HA	1.73	0.47
2:I:1243:MET:SD	3:J:445:LYS:HD3	2.54	0.47
3:J:292:VAL:O	3:J:296:LYS:HG3	2.15	0.47
1:A:32:GLU:HB2	1:A:35:PHE:CD2	2.50	0.47
1:A:261:GLU:OE2	2:C:859:GLU:HB2	2.15	0.47
3:D:489:ASN:HA	3:D:904:ALA:CB	2.45	0.47
5:F:379:MET:O	5:F:383:ASN:ND2	2.48	0.47
2:I:959:ASP:O	2:I:963:GLU:HG2	2.14	0.47
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.48	0.47
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.97	0.47
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.97	0.47
2:C:487:LEU:HD23	2:C:487:LEU:H	1.80	0.47
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.97	0.47
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.80	0.47
5:F:94:THR:C	5:F:95:THR:HG1	2.21	0.47
5:F:226:ALA:O	5:F:229:VAL:HG22	2.15	0.47
2:I:17:LYS:NZ	2:I:1154:ASP:OD1	2.38	0.47
2:I:452:ARG:HH21	2:I:458:GLU:CD	2.23	0.47
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.80	0.47
3:J:587:LEU:HD23	3:J:591:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.97	0.47
2:C:104:ILE:O	2:C:113:THR:HA	2.14	0.46
2:C:176:ILE:HB	2:C:184:LEU:HB3	1.97	0.46
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.55	0.46
2:C:566:GLY:O	2:C:569:ILE:HG13	2.14	0.46
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.96	0.46
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.15	0.46
5:F:551:LEU:CD2	5:F:597:LYS:HD2	2.44	0.46
2:I:557:ARG:HD3	2:I:587:LEU:HB3	1.97	0.46
2:I:565:GLU:HG2	2:I:565:GLU:O	2.15	0.46
2:I:1282:GLY:O	2:I:1284:ALA:N	2.48	0.46
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.47	0.46
3:J:900:GLY:HA3	3:J:1251:LYS:HD3	1.98	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.30	0.46
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.79	0.46
1:B:44:ARG:HG3	1:B:183:ILE:HD13	1.98	0.46
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.80	0.46
2:C:147:SER:OG	2:C:455:SER:HB3	2.16	0.46
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.97	0.46
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.97	0.46
3:D:45:ASN:HB3	3:D:48:THR:O	2.15	0.46
3:D:277:ASN:HA	3:D:280:LYS:HG3	1.96	0.46
3:D:400:MET:HE2	3:D:400:MET:HB3	1.81	0.46
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.96	0.46
3:D:1170:LYS:C	3:D:1172:LYS:H	2.22	0.46
5:F:580:PHE:C	5:F:582:VAL:H	2.23	0.46
2:I:384:LEU:O	2:I:388:LEU:HG	2.15	0.46
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.98	0.46
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.98	0.46
2:I:1151:LEU:HD23	2:I:1151:LEU:HA	1.82	0.46
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.50	0.46
3:J:522:GLY:O	3:J:525:MET:HG2	2.14	0.46
3:J:665:GLN:HG3	3:J:678:ARG:HH21	1.80	0.46
3:J:1170:LYS:C	3:J:1172:LYS:H	2.22	0.46
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.47	0.46
5:L:320:ILE:HG23	5:L:327:SER:O	2.15	0.46
6:N:140:THR:O	6:N:144:ILE:HG12	2.15	0.46
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.30	0.46
3:D:510:LEU:O	3:D:514:THR:HG22	2.15	0.46
5:F:130:VAL:HA	5:F:133:SER:HB2	1.96	0.46
2:I:998:LEU:H	2:I:998:LEU:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:504:GLN:OE1	3:J:731:ARG:NH1	2.48	0.46
3:J:559:ALA:HB3	3:J:562:GLU:HB3	1.97	0.46
3:J:664:ILE:HD11	3:J:685:ILE:HD12	1.96	0.46
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.44	0.46
1:A:118:ASP:H	1:A:121:VAL:HB	1.80	0.46
1:A:195:ARG:HD2	1:A:196:THR:N	2.31	0.46
2:C:9:LYS:O	2:C:1172:LEU:HD23	2.15	0.46
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.30	0.46
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.97	0.46
3:D:733:SER:O	3:D:736:GLN:N	2.48	0.46
3:D:850:LYS:HB2	3:D:852:GLY:O	2.15	0.46
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.51	0.46
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.80	0.46
1:A:163:GLU:O	1:A:164:ASP:HB2	2.14	0.46
2:C:14:ASP:OD2	2:C:1156:ARG:NE	2.49	0.46
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.73	0.46
2:C:338:THR:HG22	2:C:345:PRO:HB3	1.98	0.46
2:C:998:LEU:H	2:C:998:LEU:HD12	1.80	0.46
3:D:365:GLN:O	3:D:437:PHE:HD1	1.98	0.46
3:D:395:LYS:NZ	5:F:612:ASP:HB3	2.31	0.46
3:D:518:VAL:HG22	3:D:709:ARG:HB2	1.96	0.46
2:I:678:ARG:HA	2:I:678:ARG:HD3	1.79	0.46
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.16	0.46
2:I:957:LYS:HG3	2:I:1029:LEU:HD11	1.97	0.46
3:J:827:GLU:O	3:J:829:GLY:N	2.44	0.46
6:M:12:LEU:C	6:M:14:ILE:H	2.23	0.46
2:C:42:ASP:C	2:C:44:GLU:H	2.24	0.46
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.46
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.31	0.46
2:C:846:GLY:C	2:C:889:PRO:HG3	2.40	0.46
2:C:1124:ILE:O	2:C:1128:ILE:HG13	2.15	0.46
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.35	0.46
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.49	0.46
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.16	0.46
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.81	0.46
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.97	0.46
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.46	0.46
2:I:246:LEU:HB2	2:I:269:ILE:HG21	1.97	0.46
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.97	0.46
3:J:53:ARG:HA	3:J:54:ASP:HA	1.56	0.46
3:J:599:LYS:CE	6:N:69:PHE:HE1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.97	0.46
2:C:936:ARG:HD2	2:C:939:VAL:CG2	2.44	0.46
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.51	0.46
2:C:151:ARG:HH12	2:C:175:ARG:HH11	1.64	0.46
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.45	0.46
2:C:517:GLN:HG3	2:C:523:GLU:OE2	2.16	0.46
2:C:972:PHE:CB	2:C:994:ARG:HH21	2.28	0.46
3:D:120:LEU:HG	3:D:1330:ARG:HH21	1.81	0.46
3:D:500:ILE:HG22	3:D:500:ILE:O	2.16	0.46
3:D:659:ALA:O	3:D:663:GLU:N	2.49	0.46
3:D:1361:THR:HG22	4:E:21:LEU:HD22	1.97	0.46
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.27	0.46
3:J:81:ARG:C	3:J:83:VAL:H	2.23	0.46
3:J:227:PHE:O	3:J:230:SER:HB3	2.16	0.46
5:L:166:VAL:O	5:L:167:ASP:HB2	2.15	0.46
6:N:25:GLU:H	6:N:25:GLU:HG2	1.44	0.46
1:A:11:PRO:HA	1:A:30:PRO:CG	2.46	0.46
1:A:211:ILE:HA	1:A:211:ILE:HD13	1.63	0.46
2:C:667:LEU:HD23	2:C:667:LEU:HA	1.69	0.46
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.80	0.46
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.98	0.46
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.51	0.46
3:J:197:GLU:O	3:J:201:LEU:HG	2.16	0.46
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.98	0.46
6:N:12:LEU:C	6:N:14:ILE:N	2.74	0.46
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.97	0.45
1:A:315:GLY:C	1:A:316:MET:HG3	2.40	0.45
2:C:27:LEU:HD23	2:C:27:LEU:HA	1.68	0.45
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.81	0.45
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.80	0.45
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.62	0.45
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.98	0.45
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.45
3:D:1301:THR:HG21	3:J:1299:GLY:O	2.16	0.45
5:F:354:THR:O	5:F:358:VAL:HG23	2.16	0.45
5:F:377:LYS:O	5:F:381:GLU:HG3	2.16	0.45
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.22	0.45
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.80	0.45
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.98	0.45
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.31	0.45
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.98	0.45
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.46	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.17	0.45
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.30	0.45
3:D:418:GLU:OE1	4:E:3:ARG:NH2	2.49	0.45
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.35	0.45
3:D:929:GLN:HG2	6:M:75:ARG:HD2	1.98	0.45
3:D:935:PHE:C	6:M:86:LEU:HD21	2.42	0.45
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.98	0.45
5:F:310:GLU:O	5:F:344:LEU:HD21	2.16	0.45
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.46	0.45
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.98	0.45
2:I:1286:THR:N	3:J:479:GLU:OE2	2.44	0.45
3:J:358:GLY:N	3:J:359:PRO:HD3	2.31	0.45
3:J:418:GLU:HB2	4:K:45:LYS:HB2	1.98	0.45
3:J:826:ILE:HD12	3:J:826:ILE:O	2.16	0.45
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.17	0.45
2:C:438:GLY:O	6:M:148:GLN:NE2	2.49	0.45
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.45	0.45
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.97	0.45
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.45	0.45
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.98	0.45
3:D:555:TYR:HB2	3:D:586:GLY:HA2	1.98	0.45
3:D:638:SER:OG	3:D:639:VAL:N	2.50	0.45
5:F:363:ARG:O	5:F:367:ILE:HG13	2.16	0.45
5:F:513:ASP:C	5:F:515:GLU:H	2.23	0.45
1:H:57:THR:HG22	1:H:58:GLU:OE1	2.16	0.45
1:H:84:ASN:CG	3:J:551:ARG:HH22	2.24	0.45
2:I:250:THR:HA	2:I:268:ARG:HA	1.98	0.45
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.97	0.45
5:L:311:THR:HG21	5:L:348:GLU:CD	2.41	0.45
5:L:513:ASP:C	5:L:515:GLU:H	2.25	0.45
2:C:297:VAL:HG12	2:C:315:MET:O	2.15	0.45
3:D:1344:LEU:O	3:D:1346:GLY:N	2.46	0.45
1:H:7:GLU:HG2	1:H:8:PHE:H	1.82	0.45
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.50	0.45
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.98	0.45
3:J:1290:ARG:HD2	3:J:1298:VAL:HG12	1.96	0.45
5:L:310:GLU:OE2	5:L:355:ILE:HG21	2.16	0.45
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.46	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:670:PHE:CZ	2:C:1195:ILE:HD11	2.51	0.45
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.78	0.45
3:D:81:ARG:O	3:D:83:VAL:N	2.50	0.45
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.81	0.45
5:F:525:ASP:CG	5:F:528:LEU:HG	2.42	0.45
5:F:532:LEU:O	5:F:536:THR:HG23	2.16	0.45
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.46	0.45
2:I:678:ARG:NH1	2:I:1071:GLY:O	2.35	0.45
3:J:466:MET:HE2	3:J:466:MET:HB3	1.87	0.45
3:J:599:LYS:HE2	6:N:69:PHE:HE1	1.81	0.45
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.97	0.45
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.98	0.45
1:G:65:LEU:HA	1:G:65:LEU:HD13	1.82	0.45
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.97	0.45
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.88	0.45
3:J:316:ILE:HA	3:J:323:PRO:HA	1.99	0.45
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.98	0.45
3:J:843:VAL:HG13	3:J:883:ARG:HD3	1.99	0.45
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.49	0.45
1:A:89:ALA:O	1:A:124:VAL:HG12	2.17	0.45
2:C:151:ARG:HH12	2:C:175:ARG:NH1	2.15	0.45
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.53	0.45
3:D:664:ILE:CD1	3:D:681:LYS:HG2	2.44	0.45
3:D:1332:LEU:O	3:D:1336:ALA:N	2.44	0.45
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.51	0.45
3:J:749:LYS:HB3	3:J:755:ILE:HD11	1.99	0.45
3:J:923:ILE:O	3:J:926:PRO:HD2	2.17	0.45
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.99	0.45
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.32	0.45
6:M:145:ARG:O	6:M:149:MET:N	2.32	0.45
2:C:518:ASN:OD1	2:C:518:ASN:N	2.50	0.45
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.75	0.45
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.47	0.45
3:D:161:THR:HG23	3:D:164:GLN:H	1.82	0.45
5:F:166:VAL:O	5:F:167:ASP:HB2	2.17	0.45
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.98	0.45
2:I:1106:ARG:O	2:I:1108:ASN:N	2.46	0.45
3:J:156:ARG:NH1	3:J:157:GLN:HE21	2.14	0.45
3:J:342:LEU:HA	3:J:343:LEU:HA	1.69	0.45
3:J:1365:TYR:OH	3:J:1369:ARG:NH1	2.49	0.45
1:A:135:ASP:HB2	2:C:726:TYR:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:SER:OG	1:A:180:VAL:HG23	2.17	0.45
1:A:224:LEU:HG	1:A:228:LEU:HD12	1.98	0.45
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.47	0.45
2:C:88:ARG:HB2	2:C:88:ARG:HH11	1.81	0.45
2:C:744:GLY:C	2:C:746:ALA:H	2.25	0.45
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.47	0.45
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.51	0.45
3:D:739:GLN:OE1	3:D:744:ARG:HB2	2.17	0.45
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.32	0.45
5:F:94:THR:HG21	5:F:99:ARG:HG2	1.99	0.45
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.99	0.45
2:I:655:VAL:N	2:I:659:GLN:OE1	2.50	0.45
3:J:205:LEU:HD23	3:J:217:LEU:HG	1.99	0.45
3:J:657:ALA:O	3:J:661:VAL:HG23	2.16	0.45
3:J:789:LYS:HZ3	3:J:932:MET:CB	2.29	0.45
5:L:233:ASP:O	5:L:236:LYS:HE2	2.16	0.45
1:B:69:SER:H	1:B:78:ILE:HD12	1.82	0.45
2:C:290:GLU:HG2	2:C:319:LEU:CD1	2.47	0.45
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.99	0.45
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.82	0.45
3:D:650:LYS:HZ3	3:D:762:ASN:HD22	1.64	0.45
1:H:49:SER:O	1:H:151:GLY:HA2	2.17	0.45
1:H:59:VAL:HG23	1:H:173:VAL:HG21	1.98	0.45
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.99	0.45
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.52	0.45
3:J:494:ALA:CB	3:J:922:SER:HB3	2.46	0.45
3:J:1292:LEU:O	3:J:1293:GLU:HB2	2.17	0.45
5:L:225:ARG:O	5:L:229:VAL:HG13	2.17	0.45
5:L:493:LYS:HG2	5:L:496:LYS:HE2	1.99	0.45
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.66	0.44
2:C:42:ASP:OD1	2:C:44:GLU:HG2	2.17	0.44
2:C:565:GLU:HG2	2:C:565:GLU:O	2.17	0.44
3:D:73:GLY:O	3:D:76:LYS:HG3	2.17	0.44
3:D:372:MET:O	3:D:376:LEU:HD12	2.17	0.44
1:G:69:SER:O	1:G:78:ILE:HG12	2.18	0.44
2:I:153:PRO:HA	2:I:177:ILE:O	2.18	0.44
2:I:637:ARG:HA	2:I:642:SER:HA	1.98	0.44
2:I:891:GLY:O	2:I:892:GLU:HG3	2.17	0.44
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.49	0.44
5:L:276:MET:O	5:L:280:VAL:HG23	2.17	0.44
1:A:169:GLY:O	1:A:171:LEU:HD22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PHE:HE2	1:A:254:LEU:HG	1.81	0.44
2:C:395:TYR:HB3	2:C:419:ILE:HG22	1.97	0.44
2:C:800:MET:SD	2:C:1096:ILE:HD11	2.57	0.44
3:D:513:MET:HE2	3:D:513:MET:HB3	1.78	0.44
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.56	0.44
3:D:678:ARG:O	3:D:682:VAL:HG23	2.17	0.44
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.99	0.44
2:I:705:GLU:HB2	2:I:794:LEU:H	1.81	0.44
2:I:810:TYR:HE2	3:J:359:PRO:HD2	1.81	0.44
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.98	0.44
3:J:268:LEU:HA	3:J:268:LEU:HD23	1.71	0.44
2:C:92:TYR:CD2	2:C:129:LEU:HB2	2.52	0.44
2:C:221:LEU:HD12	2:C:298:ALA:O	2.18	0.44
2:C:620:ASN:ND2	2:C:620:ASN:O	2.50	0.44
2:C:741:MET:HE3	2:C:974:ARG:NH2	2.32	0.44
2:C:1164:PHE:HD1	2:C:1164:PHE:HA	1.67	0.44
2:C:1240:ASP:OD1	2:C:1240:ASP:N	2.45	0.44
5:F:310:GLU:OE2	5:F:355:ILE:HG21	2.17	0.44
5:F:456:MET:HE1	5:F:497:VAL:HG13	1.99	0.44
2:I:227:LYS:NZ	2:I:298:ALA:HB1	2.31	0.44
2:I:479:LEU:HD21	2:I:492:MET:HE1	1.99	0.44
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.18	0.44
3:J:1266:ILE:HD12	3:J:1273:ASP:C	2.42	0.44
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.61	0.44
6:N:98:LYS:NZ	6:N:101:LYS:HD3	2.32	0.44
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.53	0.44
1:A:239:GLN:HG3	1:A:240:PRO:HD2	2.00	0.44
1:A:253:LEU:HA	1:A:278:ILE:HD11	1.99	0.44
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.99	0.44
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.33	0.44
2:C:1273:MET:HE3	2:C:1273:MET:HB2	1.90	0.44
3:D:744:ARG:HG3	3:D:744:ARG:O	2.18	0.44
3:J:1167:LYS:HZ1	3:J:1170:LYS:HB2	1.82	0.44
2:C:367:TYR:HA	2:C:384:LEU:HD22	2.00	0.44
3:D:37:GLU:HA	3:D:104:HIS:O	2.18	0.44
3:D:707:ILE:HD12	3:D:707:ILE:H	1.82	0.44
1:G:181:GLU:HB3	1:G:206:GLU:HG2	1.99	0.44
2:I:202:ARG:NH2	2:I:368:ARG:HH12	2.16	0.44
2:I:356:THR:HG21	2:I:362:ALA:HA	2.00	0.44
2:I:724:VAL:HG23	2:I:775:GLU:N	2.28	0.44
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.82	0.44
5:L:357:GLN:HA	5:L:360:ASP:HB2	2.00	0.44
1:A:67:GLU:HG2	1:A:171:LEU:HD12	1.98	0.44
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.51	0.44
2:C:320:ASP:OD1	2:C:324:LYS:HE3	2.17	0.44
3:D:259:ARG:NH1	5:F:502:LYS:HB3	2.31	0.44
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.98	0.44
1:G:9:LEU:O	1:H:227:GLN:NE2	2.51	0.44
2:I:107:ARG:HA	2:I:108:GLU:HA	1.61	0.44
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.48	0.44
2:I:744:GLY:C	2:I:746:ALA:H	2.26	0.44
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.29	0.44
3:J:331:ILE:O	3:J:337:ARG:HA	2.18	0.44
3:J:435:GLN:HE21	3:J:486:SER:HA	1.83	0.44
3:J:594:GLN:HB2	3:J:595:ALA:H	1.59	0.44
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.47	0.44
1:A:162:GLU:HB3	1:A:163:GLU:H	1.62	0.44
1:B:64:VAL:HG11	1:B:69:SER:CB	2.48	0.44
2:C:739:ASP:N	2:C:739:ASP:OD1	2.49	0.44
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.82	0.44
2:C:1287:LEU:HD22	3:D:1357:ILE:CG1	2.48	0.44
5:F:316:PHE:CZ	5:F:334:SER:HA	2.52	0.44
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.99	0.44
3:J:528:THR:O	3:J:551:ARG:HB3	2.17	0.44
3:J:748:ALA:O	3:J:777:HIS:HD2	2.00	0.44
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.99	0.44
1:B:22:THR:O	1:B:213:PRO:HG3	2.18	0.44
1:B:41:ASN:O	1:B:45:ARG:HG3	2.18	0.44
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	2.01	0.44
3:D:239:LEU:HA	3:D:239:LEU:HD23	1.49	0.44
2:I:800:MET:HG3	2:I:1096:ILE:HD11	2.00	0.44
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.18	0.44
3:J:604:MET:HE3	3:J:604:MET:HB2	1.74	0.44
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.75	0.44
6:N:12:LEU:C	6:N:14:ILE:H	2.25	0.44
6:N:69:PHE:HA	6:N:70:PRO:HD3	1.85	0.44
1:B:31:LEU:HD13	1:B:31:LEU:HA	1.85	0.44
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.53	0.44
3:D:358:GLY:N	3:D:359:PRO:HD3	2.33	0.44
3:D:1166:GLY:O	3:D:1174:ARG:HB2	2.18	0.44
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:50:ALA:O	4:E:54:ILE:HG12	2.17	0.44
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.66	0.44
1:H:67:GLU:HA	1:H:78:ILE:HG21	2.00	0.44
1:H:88:LEU:HD12	1:H:89:ALA:H	1.83	0.44
2:I:550:VAL:HB	3:J:780:ARG:CZ	2.48	0.44
3:J:617:THR:O	3:J:620:PHE:HB3	2.18	0.44
5:L:115:GLY:HA2	5:L:118:ASP:HB2	2.00	0.44
1:B:44:ARG:CG	1:B:183:ILE:HD13	2.48	0.43
2:C:750:ILE:HD13	2:C:963:GLU:OE2	2.18	0.43
3:D:528:THR:O	3:D:551:ARG:HB3	2.17	0.43
3:D:1284:ARG:HE	3:D:1304:ARG:NH2	2.16	0.43
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.53	0.43
5:F:608:ARG:HH11	5:F:608:ARG:CG	2.30	0.43
2:I:13:LYS:HD3	2:I:1149:TYR:HA	1.99	0.43
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.18	0.43
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.52	0.43
3:D:309:ASN:HD21	3:D:315:ALA:N	2.15	0.43
3:D:317:THR:HA	3:D:324:LEU:HD23	2.00	0.43
1:G:166:ARG:O	1:G:167:PRO:C	2.60	0.43
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.83	0.43
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.45	0.43
5:L:147:GLN:HE22	5:L:150:ARG:HH11	1.66	0.43
2:C:149:LEU:HD12	2:C:452:ARG:O	2.17	0.43
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.32	0.43
2:C:1290:MET:SD	2:C:1294:LYS:HE3	2.58	0.43
3:D:159:ILE:O	3:D:159:ILE:HG13	2.18	0.43
3:D:705:THR:OG1	3:D:718:SER:HA	2.18	0.43
5:F:111:LEU:HD13	5:F:116:GLU:HA	2.00	0.43
1:G:16:ILE:HG23	1:G:26:VAL:HG12	2.00	0.43
2:I:65:ASN:HB3	2:I:105:TYR:HB2	2.00	0.43
2:I:119:GLU:CG	2:I:488:MET:HB3	2.49	0.43
2:I:225:PHE:HZ	2:I:348:SER:H	1.65	0.43
3:J:288:PRO:O	3:J:292:VAL:HG13	2.18	0.43
3:J:475:GLU:CD	4:K:28:ARG:HH22	2.26	0.43
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.42	0.43
2:C:15:PHE:HE2	2:C:1182:ILE:HG21	1.84	0.43
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.81	0.43
2:C:533:LEU:HD11	2:C:540:ARG:HD2	2.00	0.43
2:C:1101:LEU:CB	3:D:731:ARG:HD3	2.39	0.43
2:C:1269:ARG:HD3	3:D:343:LEU:HB2	2.00	0.43
3:D:1257:VAL:HG22	3:D:1260:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:814:ASP:HB3	2:I:1073:LYS:O	2.19	0.43
2:I:841:ARG:HA	2:I:1046:VAL:HA	2.00	0.43
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	2.00	0.43
2:I:1151:LEU:HD11	2:I:1198:LEU:HB2	1.99	0.43
3:J:275:ARG:HD3	3:J:298:MET:HB3	2.00	0.43
1:A:125:LYS:HE3	1:A:128:HIS:HB2	2.01	0.43
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.18	0.43
3:D:518:VAL:HG11	3:D:707:ILE:HD13	2.01	0.43
3:D:1219:ASP:O	3:D:1222:ARG:N	2.50	0.43
4:E:38:LEU:HB2	4:E:53:GLU:OE1	2.18	0.43
5:F:100:MET:HE2	5:F:100:MET:HB3	1.88	0.43
2:I:75:LEU:HD13	2:I:75:LEU:HA	1.85	0.43
2:I:234:ASP:OD1	2:I:235:ASN:N	2.51	0.43
2:I:748:ILE:HD13	2:I:970:GLY:HA3	2.01	0.43
2:I:933:VAL:HG11	2:I:945:ALA:HB2	2.00	0.43
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.48	0.43
6:M:12:LEU:C	6:M:14:ILE:N	2.75	0.43
6:N:32:MET:SD	6:N:37:LEU:HD11	2.58	0.43
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.48	0.43
1:A:321:TRP:HA	1:A:322:PRO:HA	1.86	0.43
1:B:190:ALA:O	1:B:198:LEU:HB2	2.19	0.43
3:D:119:SER:O	3:D:120:LEU:C	2.61	0.43
4:E:56:GLU:HB2	4:E:58:LEU:HD11	2.01	0.43
1:G:207:THR:HG21	1:G:211:ILE:HG22	2.00	0.43
2:I:778:GLU:HB3	2:I:781:ASP:OD1	2.18	0.43
2:I:1075:VAL:HG21	3:J:463:GLY:HA2	2.00	0.43
3:J:382:TYR:HE1	3:J:401:VAL:HG21	1.84	0.43
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.01	0.43
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.19	0.43
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.53	0.43
2:C:1161:LEU:HD21	2:C:1165:SER:HB3	2.01	0.43
3:D:809:VAL:HA	3:D:894:VAL:O	2.18	0.43
3:D:835:LEU:O	3:D:839:VAL:HG23	2.19	0.43
3:D:902:ASP:OD1	3:D:903:LEU:N	2.52	0.43
3:D:929:GLN:HG2	6:M:75:ARG:CD	2.49	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:CG2	2.49	0.43
5:F:141:ILE:HG21	5:F:228:TYR:CD1	2.54	0.43
5:F:584:ARG:O	5:F:588:ARG:HG3	2.19	0.43
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.87	0.43
2:I:936:ARG:NH1	5:L:495:ARG:HE	2.15	0.43
3:J:363:LEU:HD11	3:J:500:ILE:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:421:VAL:HG22	3:J:439:PRO:HG3	2.00	0.43
3:J:825:VAL:HG22	3:J:833:GLU:H	1.83	0.43
3:J:872:LEU:HD23	3:J:872:LEU:HA	1.77	0.43
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.34	0.43
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.82	0.43
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.49	0.43
2:C:246:LEU:HB2	2:C:269:ILE:HG21	2.01	0.43
2:C:349:GLU:O	2:C:353:VAL:HG23	2.17	0.43
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.54	0.43
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.72	0.43
3:D:525:MET:O	3:D:548:VAL:HG13	2.19	0.43
3:D:872:LEU:HD23	3:D:872:LEU:HA	1.77	0.43
3:D:1183:SER:CB	3:J:206:ASN:HD21	2.31	0.43
3:D:1292:LEU:O	3:J:1227:HIS:HD2	2.01	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.01	0.43
2:I:678:ARG:NH2	6:N:73:VAL:HG11	2.33	0.43
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.34	0.43
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.50	0.43
3:J:716:GLN:HG3	3:J:717:VAL:O	2.19	0.43
3:J:1143:ASP:HA	3:J:1148:ARG:NH1	2.33	0.43
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.65	0.43
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.18	0.43
2:C:131:THR:OG1	2:C:135:THR:O	2.37	0.43
2:C:153:PRO:HB2	2:C:401:GLY:HA2	2.00	0.43
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.84	0.43
2:C:1112:ILE:HD11	3:D:639:VAL:HG22	2.01	0.43
3:D:316:ILE:HA	3:D:323:PRO:HA	2.00	0.43
3:D:929:GLN:O	6:M:79:GLU:OE2	2.36	0.43
1:H:47:LEU:HD13	1:H:183:ILE:HG21	2.01	0.43
2:I:47:TYR:OH	2:I:398:SER:HB2	2.18	0.43
2:I:921:PRO:O	2:I:924:VAL:HG22	2.18	0.43
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.52	0.43
3:J:338:PHE:O	3:J:340:GLN:N	2.52	0.43
5:L:474:MET:C	5:L:476:ARG:H	2.25	0.43
1:A:104:LYS:HD3	1:A:114:ASP:OD2	2.19	0.43
2:C:143:ARG:NH2	2:C:512:SER:O	2.52	0.43
2:C:403:MET:HE3	2:C:403:MET:HB3	1.95	0.43
3:D:218:THR:HA	3:D:221:ILE:HG22	2.01	0.43
3:D:731:ARG:NH2	6:M:73:VAL:HG11	2.31	0.43
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.49	0.43
5:F:316:PHE:HZ	5:F:334:SER:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:561:MET:HE3	5:F:561:MET:HB2	1.83	0.43
1:H:155:ALA:HB2	1:H:174:ASP:N	2.34	0.43
2:I:149:LEU:HD13	2:I:453:ILE:HG13	2.00	0.43
2:I:227:LYS:HA	2:I:335:THR:O	2.18	0.43
2:I:228:VAL:HB	2:I:335:THR:OG1	2.18	0.43
2:I:678:ARG:CG	2:I:1108:ASN:HD22	2.29	0.43
3:J:1147:ALA:O	3:J:1218:HIS:NE2	2.52	0.43
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	2.00	0.43
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.54	0.43
1:A:76:GLU:N	1:A:76:GLU:OE2	2.52	0.42
2:C:185:ASP:HB2	2:C:197:ARG:HG3	2.00	0.42
2:C:800:MET:HE3	2:C:800:MET:HB3	1.63	0.42
3:D:357:VAL:HB	3:D:358:GLY:H	1.69	0.42
3:D:604:MET:HE3	3:D:604:MET:HB2	1.88	0.42
5:F:341:LEU:CD2	5:F:344:LEU:HD23	2.49	0.42
1:G:154:PRO:HB2	2:I:1059:ARG:HH21	1.84	0.42
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.54	0.42
2:I:802:VAL:HA	2:I:1096:ILE:O	2.19	0.42
3:J:161:THR:HG22	3:J:164:GLN:CD	2.44	0.42
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.76	0.42
6:M:144:ILE:HG23	6:M:147:LYS:HE2	2.01	0.42
6:N:24:GLN:HG3	6:N:24:GLN:O	2.19	0.42
6:N:144:ILE:HG23	6:N:147:LYS:HE2	2.01	0.42
1:A:220:ALA:O	1:A:223:ILE:HG13	2.18	0.42
2:C:39:ILE:HD11	2:C:75:LEU:HG	2.00	0.42
2:C:517:GLN:O	2:C:517:GLN:HG2	2.19	0.42
3:D:337:ARG:NH2	3:D:1323:ALA:HB3	2.34	0.42
3:D:356:THR:OG1	3:D:357:VAL:N	2.52	0.42
3:D:395:LYS:HZ1	5:F:612:ASP:HB3	1.84	0.42
3:D:1136:GLY:HA2	3:D:1140:ARG:HG2	2.00	0.42
5:F:458:GLU:O	5:F:462:LYS:HG3	2.19	0.42
3:J:24:LEU:HB2	3:J:232:ASN:OD1	2.20	0.42
3:J:195:GLU:H	3:J:195:GLU:HG3	1.65	0.42
3:J:338:PHE:C	3:J:340:GLN:H	2.27	0.42
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.44	0.42
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.84	0.42
6:M:33:ASN:OD1	6:M:36:GLN:HB2	2.18	0.42
2:C:107:ARG:HA	2:C:108:GLU:HA	1.28	0.42
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.75	0.42
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.00	0.42
2:C:1222:GLU:HG3	3:D:634:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.54	0.42
3:D:16:GLU:O	3:D:1369:ARG:NH2	2.46	0.42
3:D:194:LEU:HD13	3:D:228:VAL:HG22	2.01	0.42
3:D:903:LEU:HD23	3:D:905:ARG:HD3	2.01	0.42
2:I:678:ARG:HH21	6:N:73:VAL:HG11	1.84	0.42
3:J:268:LEU:CB	3:J:306:LEU:HD23	2.49	0.42
3:J:395:LYS:NZ	5:L:612:ASP:OD2	2.39	0.42
3:J:650:LYS:O	3:J:654:ILE:HG13	2.19	0.42
3:J:743:MET:HE2	3:J:743:MET:HB3	1.91	0.42
3:J:809:VAL:HA	3:J:894:VAL:O	2.20	0.42
3:J:1372:ARG:HE	3:J:1372:ARG:HB2	1.64	0.42
6:N:55:VAL:O	6:N:59:VAL:HG23	2.18	0.42
1:A:142:MET:HG3	1:A:144:ILE:HG13	2.01	0.42
2:C:117:ILE:H	2:C:117:ILE:HG12	1.66	0.42
2:C:153:PRO:HB2	2:C:401:GLY:CA	2.49	0.42
2:C:230:PHE:CE1	2:C:239:MET:HB2	2.53	0.42
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.01	0.42
2:C:466:VAL:HA	2:C:469:VAL:HG22	2.01	0.42
2:C:606:LEU:HD21	2:C:614:TYR:HD1	1.84	0.42
2:C:882:ILE:HD12	2:C:882:ILE:H	1.83	0.42
3:D:342:LEU:HA	3:D:343:LEU:HA	1.66	0.42
3:D:478:LEU:HG	4:E:47:THR:HG23	2.00	0.42
3:D:529:GLY:HA2	3:D:551:ARG:O	2.19	0.42
3:D:743:MET:HE2	3:D:743:MET:HB3	1.93	0.42
3:D:826:ILE:HD12	3:D:826:ILE:O	2.18	0.42
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.27	0.42
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.78	0.42
2:I:490:GLN:CG	5:L:472:GLN:HG3	2.50	0.42
2:I:490:GLN:HG2	5:L:472:GLN:HG3	2.00	0.42
2:I:992:LEU:HD12	2:I:996:ARG:HB3	2.00	0.42
3:J:591:ILE:HG23	3:J:604:MET:HE2	2.01	0.42
5:L:476:ARG:HB3	5:L:476:ARG:HH11	1.84	0.42
6:N:30:GLU:HG3	6:N:32:MET:H	1.85	0.42
1:A:153:VAL:O	1:A:175:ALA:HB3	2.20	0.42
1:A:251:PRO:HD2	5:F:605:GLU:HG3	2.00	0.42
1:A:285:THR:O	1:A:289:LEU:HG	2.20	0.42
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.62	0.42
2:C:1252:SER:HB3	2:C:1255:THR:O	2.20	0.42
3:D:81:ARG:C	3:D:83:VAL:N	2.77	0.42
3:D:153:ASN:C	3:D:154:LEU:HG	2.44	0.42
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.55	0.42
1:H:60:GLU:O	1:H:142:MET:HB2	2.20	0.42
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.20	0.42
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.34	0.42
3:J:322:ARG:HG3	3:J:323:PRO:HD2	2.01	0.42
3:J:773:PHE:O	3:J:776:THR:HB	2.19	0.42
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.33	0.42
6:N:125:ARG:NH2	6:N:134:LEU:O	2.39	0.42
2:C:103:VAL:C	2:C:104:ILE:HD12	2.44	0.42
2:C:580:GLN:HB2	2:C:605:TYR:HE1	1.83	0.42
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.53	0.42
3:D:266:ASN:O	3:D:270:ARG:HB2	2.19	0.42
3:D:511:TYR:CD2	3:D:728:SER:HB3	2.54	0.42
3:D:511:TYR:HE1	3:D:724:MET:HG2	1.85	0.42
2:I:42:ASP:C	2:I:44:GLU:H	2.26	0.42
2:I:559:CYS:HA	2:I:560:PRO:HD3	1.90	0.42
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.55	0.42
2:I:810:TYR:O	2:I:1077:SER:OG	2.31	0.42
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.96	0.42
3:J:491:LEU:HD23	3:J:491:LEU:HA	1.87	0.42
3:J:491:LEU:HD22	3:J:496:GLY:O	2.20	0.42
3:J:514:THR:O	3:J:514:THR:OG1	2.32	0.42
3:J:1156:LEU:HD22	3:J:1156:LEU:N	2.35	0.42
2:C:5:TYR:O	2:C:8:LYS:HG2	2.20	0.42
2:C:87:ILE:H	2:C:87:ILE:HG13	1.65	0.42
2:C:672:GLU:HG2	2:C:1187:PHE:HA	2.01	0.42
2:C:681:MET:O	2:C:685:MET:HE2	2.19	0.42
2:C:706:ARG:HG3	2:C:793:GLU:HG2	2.00	0.42
2:C:886:LYS:H	2:C:917:SER:HB3	1.84	0.42
3:D:436:ALA:HB3	3:D:485:MET:HA	2.01	0.42
3:D:442:ILE:HD13	3:D:442:ILE:HA	1.89	0.42
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.19	0.42
2:I:465:ARG:O	2:I:469:VAL:HG13	2.19	0.42
2:I:1293:VAL:HG13	2:I:1301:ARG:HA	2.00	0.42
2:I:1304:MET:HE2	3:J:472:LEU:HB3	2.01	0.42
3:J:239:LEU:HD23	3:J:239:LEU:HA	1.78	0.42
5:L:394:TYR:CD2	5:L:439:ILE:HG21	2.55	0.42
2:C:145:ILE:HG22	2:C:456:VAL:HG22	2.00	0.42
2:C:208:ILE:HG13	2:C:354:ASP:OD1	2.19	0.42
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.01	0.42
2:C:805:MET:HE1	2:C:1221:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:614:LEU:HD23	4:E:5:THR:HB	2.01	0.42
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	2.01	0.42
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.20	0.42
1:H:52:PRO:CG	1:H:150:ARG:HG2	2.49	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.85	0.42
3:J:30:ILE:HD13	3:J:243:PRO:HG3	2.00	0.42
3:J:118:LYS:HB3	3:J:118:LYS:HE2	1.93	0.42
3:J:824:PRO:HD3	3:J:835:LEU:HB2	2.02	0.42
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.34	0.42
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	2.00	0.42
1:A:12:ARG:H	1:A:30:PRO:CD	2.33	0.42
1:A:224:LEU:HD23	1:B:228:LEU:HD11	2.02	0.42
2:C:91:THR:HB	2:C:138:ILE:O	2.20	0.42
3:D:114:ILE:HD11	3:D:311:ARG:HB2	2.01	0.42
3:D:493:PRO:O	3:D:1252:HIS:NE2	2.36	0.42
5:F:306:PHE:CE1	5:F:310:GLU:HG3	2.54	0.42
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.54	0.42
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.42
3:J:646:ILE:HG22	3:J:650:LYS:HD2	2.02	0.42
3:J:903:LEU:HD21	3:J:913:GLU:OE1	2.20	0.42
5:L:577:GLY:O	5:L:581:ASP:N	2.49	0.42
6:N:18:ALA:C	6:N:20:VAL:H	2.27	0.42
6:N:31:TYR:O	6:N:31:TYR:CG	2.73	0.42
1:A:187:VAL:O	1:A:187:VAL:HG23	2.20	0.42
2:C:42:ASP:O	2:C:44:GLU:N	2.52	0.42
2:C:211:ARG:NH1	2:C:357:ASN:O	2.53	0.42
2:C:363:LEU:HB3	2:C:381:ALA:HB1	2.02	0.42
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.35	0.42
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.55	0.42
3:D:279:LEU:HD12	3:D:295:GLU:HG3	2.01	0.42
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.01	0.42
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.19	0.42
5:F:276:MET:O	5:F:280:VAL:HG23	2.20	0.42
5:F:471:LEU:HD23	5:F:476:ARG:O	2.20	0.42
1:G:151:GLY:O	1:G:177:TYR:HB2	2.19	0.42
1:H:56:VAL:HG11	1:H:144:ILE:HD11	2.02	0.42
2:I:896:THR:O	2:I:897:PRO:C	2.62	0.42
2:I:1276:TRP:CH2	3:J:798:ARG:HG3	2.53	0.42
3:J:591:ILE:HD11	3:J:603:LYS:HE3	2.00	0.42
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.85	0.42
5:L:401:PHE:O	5:L:405:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:HE1	1:A:69:SER:HB3	1.83	0.41
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.85	0.41
2:C:685:MET:HE3	2:C:685:MET:HB2	1.81	0.41
3:D:215:LYS:HE2	3:D:215:LYS:HB3	1.93	0.41
3:D:748:ALA:HA	3:D:754:ILE:HA	2.02	0.41
5:F:561:MET:HA	5:F:567:MET:CE	2.48	0.41
1:G:57:THR:HG22	1:G:58:GLU:HG3	2.02	0.41
1:H:59:VAL:HG21	1:H:85:LEU:HD13	2.02	0.41
1:H:64:VAL:HG12	1:H:66:HIS:H	1.85	0.41
2:I:731:ARG:NH1	2:I:962:GLU:OE1	2.53	0.41
3:J:442:ILE:HD13	3:J:442:ILE:HA	1.92	0.41
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.50	0.41
5:L:161:LEU:C	5:L:262:VAL:HG23	2.45	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.79	0.41
6:M:108:ASP:CG	6:M:109:GLU:N	2.77	0.41
1:A:226:GLU:HB3	1:B:10:LYS:HE2	2.03	0.41
1:A:290:LEU:HB3	1:A:291:LYS:HE2	2.02	0.41
2:C:80:PHE:HB3	2:C:84:GLU:CB	2.50	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.20	0.41
2:C:458:GLU:O	2:C:461:GLU:HB3	2.21	0.41
2:C:643:SER:HG	2:C:645:PHE:HE1	1.66	0.41
2:C:714:VAL:HB	2:C:787:PRO:HD2	2.01	0.41
2:C:937:ASP:CB	2:C:1039:GLY:HA3	2.50	0.41
2:C:1069:ARG:HH21	2:C:1114:GLU:CD	2.29	0.41
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.53	0.41
1:H:48:LEU:CD2	3:J:535:ARG:HG3	2.50	0.41
2:I:79:VAL:HG23	2:I:80:PHE:H	1.85	0.41
2:I:870:ILE:CG2	2:I:944:ARG:HD3	2.50	0.41
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.85	0.41
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.48	0.41
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.35	0.41
3:J:594:GLN:HG3	3:J:596:LEU:HD22	2.02	0.41
5:L:354:THR:O	5:L:358:VAL:HG23	2.19	0.41
5:L:511:ILE:HD12	5:L:511:ILE:HA	1.86	0.41
6:N:108:ASP:CG	6:N:109:GLU:N	2.78	0.41
1:A:323:PRO:HB2	1:A:324:ALA:HB2	2.02	0.41
1:B:51:MET:HB3	1:B:178:SER:HB2	2.01	0.41
2:C:247:ARG:NH2	2:C:274:ILE:HD12	2.36	0.41
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.20	0.41
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.90	0.41
3:D:544:LEU:HD12	3:D:544:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.02	0.41
1:G:51:MET:HA	1:G:52:PRO:HD3	1.91	0.41
3:J:647:PRO:CG	3:J:697:MET:HB3	2.50	0.41
5:L:151:VAL:HG22	5:L:156:ALA:HB3	2.02	0.41
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.86	0.41
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.54	0.41
2:C:79:VAL:HG23	2:C:80:PHE:H	1.84	0.41
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.35	0.41
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.79	0.41
3:D:305:ALA:O	3:D:309:ASN:HB2	2.19	0.41
3:D:495:ASN:C	3:D:497:GLU:H	2.26	0.41
2:I:646:SER:HB3	2:I:649:GLN:HG3	2.02	0.41
2:I:814:ASP:OD1	2:I:814:ASP:N	2.53	0.41
2:I:946:LEU:HD23	2:I:946:LEU:HA	1.90	0.41
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.85	0.41
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.84	0.41
3:J:324:LEU:O	3:J:324:LEU:HD12	2.20	0.41
3:J:343:LEU:H	3:J:343:LEU:HG	1.72	0.41
3:J:1167:LYS:HZ1	3:J:1170:LYS:CB	2.32	0.41
5:L:474:MET:O	5:L:476:ARG:N	2.49	0.41
6:M:70:PRO:HG2	6:M:78:GLN:HG3	2.01	0.41
1:B:181:GLU:HA	3:D:535:ARG:HH21	1.85	0.41
2:C:903:ARG:HD2	2:C:908:GLU:HB3	2.02	0.41
2:C:1101:LEU:O	2:C:1104:PRO:HD2	2.21	0.41
3:D:403:ARG:HB3	3:D:405:GLU:HG3	2.02	0.41
3:D:710:ASP:OD1	3:D:711:GLY:N	2.53	0.41
4:E:2:ALA:HB2	4:E:55:GLU:OE2	2.19	0.41
1:G:77:ASP:OD2	2:I:755:LYS:NZ	2.47	0.41
1:H:35:PHE:HA	1:H:38:THR:HG22	2.01	0.41
2:I:325:LEU:HA	2:I:328:SER:OG	2.20	0.41
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.20	0.41
3:J:902:ASP:OD1	3:J:903:LEU:N	2.53	0.41
3:J:1192:LYS:HB2	3:J:1192:LYS:HE3	1.83	0.41
3:J:1250:ASP:O	3:J:1251:LYS:C	2.63	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41
1:A:105:SER:HB3	1:A:139:SER:OG	2.20	0.41
1:A:106:GLY:HA2	1:A:136:GLU:O	2.20	0.41
1:A:112:ALA:O	1:A:115:ILE:HG13	2.20	0.41
1:B:133:LEU:HD11	1:B:140:ILE:HG21	2.02	0.41
2:C:81:ASP:HA	2:C:92:TYR:HE1	1.86	0.41
2:C:159:SER:HB2	6:M:151:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.78	0.41
2:C:960:LEU:O	2:C:963:GLU:HB2	2.21	0.41
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.02	0.41
3:D:27:PRO:HB3	3:D:241:VAL:HG23	2.03	0.41
3:D:259:ARG:NH1	5:F:503:GLU:O	2.53	0.41
1:G:179:PRO:O	1:G:207:THR:HA	2.21	0.41
1:H:7:GLU:HG2	1:H:8:PHE:N	2.36	0.41
2:I:404:LYS:HD2	2:I:404:LYS:HA	1.80	0.41
2:I:850:ILE:HG22	2:I:850:ILE:O	2.20	0.41
3:J:500:ILE:HG22	3:J:500:ILE:O	2.21	0.41
3:J:865:HIS:HE1	3:J:867:GLN:HB2	1.85	0.41
3:J:901:ARG:HD2	3:J:906:GLY:O	2.20	0.41
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.35	0.41
1:A:262:LEU:H	1:A:262:LEU:HD12	1.86	0.41
1:B:99:ILE:HD12	1:B:145:LYS:HB2	2.02	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.85	0.41
2:C:75:LEU:HD11	2:C:127:ILE:HD11	2.03	0.41
2:C:1253:LEU:HA	5:F:525:ASP:HB2	2.01	0.41
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.49	0.41
5:F:292:VAL:HG21	5:F:299:LYS:HG2	2.02	0.41
5:F:309:ASN:HB3	5:F:310:GLU:H	1.69	0.41
5:F:489:MET:HB2	5:F:490:PRO:HD2	2.02	0.41
2:I:55:SER:OG	2:I:56:VAL:N	2.54	0.41
2:I:146:VAL:HG13	2:I:529:ARG:HB3	2.02	0.41
2:I:344:GLY:O	2:I:346:TYR:N	2.53	0.41
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.44	0.41
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	2.01	0.41
3:J:511:TYR:HE1	3:J:724:MET:HG2	1.85	0.41
3:J:525:MET:O	3:J:548:VAL:HG13	2.20	0.41
5:L:110:LEU:HD23	5:L:382:ALA:O	2.21	0.41
5:L:511:ILE:HG21	5:L:522:PHE:CE2	2.55	0.41
6:M:139:LYS:NZ	6:M:143:GLU:CD	2.78	0.41
1:A:284:ARG:HG3	1:A:288:GLU:HG3	2.03	0.41
2:C:528:ARG:NH2	2:C:576:SER:O	2.54	0.41
2:C:578:TYR:HB3	2:C:590:PRO:HG2	2.03	0.41
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.54	0.41
3:D:412:LEU:O	3:D:415:VAL:HG22	2.20	0.41
3:D:580:TRP:HH2	3:D:587:LEU:O	2.04	0.41
5:F:130:VAL:O	5:F:134:VAL:N	2.49	0.41
5:F:507:MET:HE2	5:F:507:MET:HB3	1.70	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.86	0.41
2:I:1222:GLU:O	3:J:636:GLY:HA3	2.21	0.41
3:J:381:ILE:O	3:J:385:LEU:HB2	2.20	0.41
3:J:400:MET:HE2	3:J:400:MET:HB3	1.78	0.41
3:J:418:GLU:H	4:K:45:LYS:NZ	2.19	0.41
5:L:299:LYS:HA	5:L:302:PHE:HB3	2.03	0.41
1:A:70:THR:CG2	2:C:755:LYS:HE2	2.51	0.41
1:A:185:TYR:HA	1:A:202:VAL:O	2.20	0.41
1:A:289:LEU:CD1	1:A:314:LEU:HD21	2.51	0.41
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.20	0.41
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.36	0.41
2:C:921:PRO:O	2:C:924:VAL:HG22	2.20	0.41
3:D:110:PRO:HD2	3:D:183:GLU:HG2	2.02	0.41
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.85	0.41
3:D:275:ARG:HD3	3:D:298:MET:HB3	2.02	0.41
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.54	0.41
3:D:1168:GLU:O	3:D:1170:LYS:N	2.54	0.41
4:E:26:ARG:NH2	4:E:38:LEU:HD13	2.35	0.41
5:F:274:ARG:HA	5:F:277:MET:HB2	2.03	0.41
5:F:404:LEU:HD22	5:F:443:ILE:HD11	2.02	0.41
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.02	0.41
1:G:75:GLN:HA	2:I:729:ALA:N	2.36	0.41
2:I:103:VAL:C	2:I:104:ILE:HD12	2.46	0.41
2:I:135:THR:HG22	2:I:527:LYS:HE2	2.03	0.41
2:I:389:PHE:HD1	2:I:395:TYR:CE1	2.39	0.41
2:I:591:TYR:HA	2:I:655:VAL:HG23	2.03	0.41
2:I:745:GLU:HA	2:I:971:LEU:HD12	2.03	0.41
2:I:796:LEU:H	2:I:796:LEU:HD12	1.86	0.41
2:I:848:GLU:HG2	2:I:888:THR:HG22	2.02	0.41
2:I:886:LYS:H	2:I:917:SER:HB3	1.85	0.41
2:I:985:GLU:HG2	2:I:988:LYS:HD2	2.02	0.41
2:I:1066:MET:HE1	2:I:1076:ILE:HD12	2.03	0.41
2:I:1103:VAL:HB	2:I:1104:PRO:HD3	2.03	0.41
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.86	0.41
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.89	0.41
5:L:503:GLU:OE1	5:L:504:PRO:HD2	2.20	0.41
6:M:49:ASN:HA	6:M:52:ARG:NH1	2.35	0.41
2:C:226:GLU:HB2	2:C:245:ARG:HH22	1.86	0.41
2:C:548:ARG:HG2	2:C:571:LEU:HD21	2.02	0.41
3:D:126:LEU:H	3:D:126:LEU:HG	1.70	0.41
3:D:205:LEU:CD2	3:D:214:ARG:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.78	0.41
1:H:50:SER:HA	1:H:150:ARG:O	2.21	0.41
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.95	0.41
2:I:88:ARG:HB2	2:I:88:ARG:NH1	2.36	0.41
2:I:896:THR:HB	2:I:897:PRO:HD2	2.03	0.41
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.02	0.41
3:J:674:THR:HG22	6:N:136:ILE:CD1	2.50	0.41
3:J:796:LEU:HA	3:J:796:LEU:HD12	1.79	0.41
3:J:850:LYS:HB2	3:J:852:GLY:O	2.20	0.41
2:C:169:LYS:HE2	2:C:190:PRO:O	2.21	0.40
2:C:503:LYS:HD2	2:C:503:LYS:HA	1.91	0.40
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.85	0.40
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.56	0.40
3:D:581:MET:HE2	3:D:581:MET:HB3	1.98	0.40
3:D:762:ASN:OD1	3:D:764:ARG:N	2.54	0.40
3:D:860:ARG:HA	3:D:860:ARG:HD2	1.81	0.40
5:F:100:MET:H	5:F:100:MET:HG2	1.65	0.40
2:I:221:LEU:HB3	2:I:336:LEU:HD21	2.03	0.40
2:I:379:GLU:CD	2:I:379:GLU:H	2.28	0.40
2:I:818:VAL:HB	2:I:1076:ILE:HD11	2.04	0.40
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.93	0.40
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.86	0.40
3:J:638:SER:OG	3:J:639:VAL:N	2.52	0.40
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.85	0.40
1:B:62:ASP:OD2	1:B:140:ILE:HD12	2.20	0.40
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.21	0.40
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.54	0.40
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	2.03	0.40
3:D:19:ALA:HB2	3:D:1373:ARG:NH2	2.36	0.40
3:D:84:ILE:H	3:D:84:ILE:HG13	1.70	0.40
3:D:347:VAL:HG12	3:D:348:ASP:O	2.21	0.40
3:D:1319:PHE:CD1	3:D:1319:PHE:C	2.99	0.40
5:F:383:ASN:HB2	5:F:412:LEU:HD21	2.03	0.40
5:F:463:LEU:HD23	5:F:463:LEU:HA	1.93	0.40
1:G:43:LEU:HA	1:G:43:LEU:HD23	1.78	0.40
1:G:133:LEU:HD12	1:G:138:ALA:HB3	2.03	0.40
2:I:607:SER:OG	2:I:609:ILE:HG13	2.21	0.40
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.67	0.40
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	2.03	0.40
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.03	0.40
5:L:348:GLU:HA	5:L:353:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:15:LEU:HD23	6:N:15:LEU:HA	1.97	0.40
1:A:59:VAL:HG22	1:A:144:ILE:HA	2.03	0.40
1:B:73:GLY:C	1:B:134:THR:HG22	2.46	0.40
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.54	0.40
3:D:224:LEU:O	3:D:227:PHE:N	2.54	0.40
3:D:860:ARG:HB3	3:D:861:ASN:H	1.72	0.40
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.86	0.40
3:D:1186:TYR:HE2	3:D:1188:GLU:HB2	1.85	0.40
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.36	0.40
5:F:320:ILE:HG23	5:F:327:SER:O	2.22	0.40
2:I:193:ASN:ND2	2:I:353:VAL:HG21	2.36	0.40
2:I:503:LYS:HA	2:I:503:LYS:HD2	1.80	0.40
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.83	0.40
2:I:883:LEU:HG	2:I:920:VAL:HG23	2.03	0.40
2:I:897:PRO:HG3	5:L:564:GLY:C	2.47	0.40
3:J:517:CYS:HA	3:J:716:GLN:OE1	2.21	0.40
3:J:1259:GLN:NE2	3:J:1262:ARG:NH1	2.70	0.40
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.21	0.40
5:L:119:ILE:HG23	5:L:375:ALA:HB1	2.04	0.40
1:A:166:ARG:N	1:A:167:PRO:HD2	2.36	0.40
1:B:88:LEU:HD12	1:B:89:ALA:H	1.86	0.40
2:C:462:ASN:O	2:C:466:VAL:HG23	2.21	0.40
2:C:1211:ARG:HE	2:C:1220:GLN:HE21	1.70	0.40
3:D:117:LEU:O	3:D:117:LEU:HG	2.20	0.40
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.48	0.40
3:D:363:LEU:O	3:D:363:LEU:HG	2.21	0.40
3:D:429:LEU:HD13	3:D:429:LEU:HA	1.73	0.40
3:D:786:THR:HA	3:D:789:LYS:HG3	2.03	0.40
2:I:80:PHE:HB3	2:I:84:GLU:HB2	2.04	0.40
2:I:646:SER:HB3	2:I:649:GLN:CD	2.45	0.40
2:I:705:GLU:CD	2:I:705:GLU:H	2.30	0.40
2:I:800:MET:HE1	2:I:822:VAL:HG13	2.03	0.40
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	2.03	0.40
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	2.01	0.40
3:J:201:LEU:HD11	3:J:220:ARG:NH1	2.36	0.40
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.35	0.40
5:L:585:GLU:O	5:L:589:GLN:HG3	2.22	0.40
6:M:144:ILE:HD12	6:M:147:LYS:HE2	2.03	0.40
6:N:139:LYS:NZ	6:N:143:GLU:CD	2.78	0.40
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.56	0.40
2:C:139:ASN:HD22	2:C:139:ASN:HA	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1075:VAL:HG23	3:D:461:PHE:O	2.22	0.40
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.40
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.84	0.40
5:F:111:LEU:HD23	5:F:111:LEU:HA	1.93	0.40
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.52	0.40
2:I:256:GLU:HB3	2:I:261:VAL:HG22	2.04	0.40
2:I:745:GLU:H	2:I:1017:GLN:HG3	1.85	0.40
3:J:45:ASN:O	3:J:46:TYR:HB3	2.21	0.40
3:J:679:TYR:O	3:J:683:ILE:HG13	2.22	0.40
5:L:469:GLN:O	5:L:473:GLU:HB2	2.21	0.40
5:L:511:ILE:HG13	5:L:512:GLY:H	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:O	1:G:101:THR:OG1[4_545]	1.98	0.22
2:C:44:GLU:OE2	5:F:596:ARG:NH1[4_555]	2.17	0.03
2:C:1006:GLU:OE1	3:D:68:TYR:OH[4_555]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/329 (96%)	248 (78%)	52 (16%)	17 (5%)	1	15
1	B	213/329 (65%)	195 (92%)	14 (7%)	4 (2%)	6	32
1	G	225/329 (68%)	202 (90%)	18 (8%)	5 (2%)	5	29
1	H	212/329 (64%)	197 (93%)	11 (5%)	4 (2%)	6	32
2	C	1338/1342 (100%)	1202 (90%)	118 (9%)	18 (1%)	9	41
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1167/1407 (83%)	1037 (89%)	103 (9%)	27 (2%)	5	28
3	J	1155/1407 (82%)	1029 (89%)	100 (9%)	26 (2%)	5	28
4	E	87/91 (96%)	80 (92%)	5 (6%)	2 (2%)	5	28
4	K	77/91 (85%)	69 (90%)	4 (5%)	4 (5%)	1	15
5	F	462/613 (75%)	426 (92%)	28 (6%)	8 (2%)	7	35
5	L	463/613 (76%)	425 (92%)	31 (7%)	7 (2%)	8	38
6	M	138/151 (91%)	128 (93%)	8 (6%)	2 (1%)	9	39
6	N	138/151 (91%)	129 (94%)	6 (4%)	3 (2%)	5	29
All	All	7330/8524 (86%)	6564 (90%)	618 (8%)	148 (2%)	6	31

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO
1	A	242	VAL
1	B	193	GLU
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1153	ALA
2	C	1154	ASP
2	C	1159	VAL
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	669	GLN
3	D	673	VAL
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR

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Mol	Chain	Res	Type
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	569	THR
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	496	GLY
3	J	710	ASP
3	J	712	GLN
3	J	805	GLN
3	J	850	LYS
3	J	1294	ALA
4	K	4	VAL
4	K	15	ASN
4	K	33	GLY
5	L	584	ARG
6	M	30	GLU
6	N	30	GLU
6	N	31	TYR
1	A	50	SER
1	A	119	GLY
1	A	164	ASP
1	A	232	VAL
1	A	315	GLY
1	A	320	ASN
1	B	13	LEU
2	C	121	GLU
3	D	89	GLY
3	D	805	GLN
3	D	1274	PHE

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Mol	Chain	Res	Type
5	F	566	ASP
5	F	584	ARG
1	G	162	GLU
1	G	167	PRO
1	H	138	ALA
1	H	193	GLU
2	I	1059	ARG
2	I	1165	SER
3	J	314	ARG
3	J	339	ARG
3	J	745	GLY
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
1	A	62	ASP
1	B	136	GLU
2	C	163	LYS
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY
3	D	314	ARG
3	D	417	ARG
3	D	1344	LEU
1	G	229	GLU
2	I	892	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	89	GLY
3	J	417	ARG
4	K	14	GLY
1	A	324	ALA
1	B	138	ALA
2	C	813	GLU
2	C	1059	ARG
3	D	1297	LYS
1	H	20	SER
2	I	696	ASP

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Mol	Chain	Res	Type
2	I	813	GLU
3	J	332	LYS
3	J	344	GLY
3	J	1344	LEU
1	A	318	LEU
1	A	319	GLU
2	C	983	GLY
2	C	1158	LYS
3	D	46	TYR
5	F	602	SER
2	I	160	ASP
3	J	338	PHE
3	J	357	VAL
6	N	27	PRO
1	A	19	VAL
3	D	345	LYS
3	D	357	VAL
2	I	201	ARG
2	I	756	TYR
3	J	333	GLY
5	L	585	GLU
6	M	27	PRO
3	D	826	ILE
3	D	828	GLY
5	F	96	ASP
3	J	173	GLY
3	J	336	GLY
3	D	82	GLY
3	D	120	LEU
3	D	831	VAL
5	F	361	ILE
3	J	639	VAL
5	L	475	GLY
1	G	14	VAL
2	I	1202	GLY
4	E	86	ILE
5	F	475	GLY
1	H	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	222 (80%)	56 (20%)	1	8
1	B	186/286 (65%)	163 (88%)	23 (12%)	4	18
1	G	193/286 (68%)	162 (84%)	31 (16%)	2	12
1	H	183/286 (64%)	168 (92%)	15 (8%)	10	31
2	C	1155/1157 (100%)	1024 (89%)	131 (11%)	5	20
2	I	1154/1157 (100%)	1031 (89%)	123 (11%)	6	22
3	D	962/1168 (82%)	860 (89%)	102 (11%)	6	22
3	J	960/1168 (82%)	859 (90%)	101 (10%)	6	22
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	17
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	22
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	23
5	L	418/540 (77%)	373 (89%)	45 (11%)	6	22
6	M	121/131 (92%)	110 (91%)	11 (9%)	9	28
6	N	121/131 (92%)	109 (90%)	12 (10%)	7	24
All	All	6287/7286 (86%)	5579 (89%)	708 (11%)	5	20

All (708) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	9	LEU
1	A	18	GLN
1	A	26	VAL
1	A	29	GLU
1	A	32	GLU
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	70	THR

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Mol	Chain	Res	Type
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	75	GLN
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL
1	A	99	ILE
1	A	105	SER
1	A	110	VAL
1	A	116	THR
1	A	133	LEU
1	A	137	ASN
1	A	159	ILE
1	A	165	GLU
1	A	168	ILE
1	A	171	LEU
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL
1	A	195	ARG
1	A	207	THR
1	A	211	ILE
1	A	223	ILE
1	A	227	GLN
1	A	231	PHE
1	A	239	GLN
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	252	ILE
1	A	262	LEU
1	A	264	VAL
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU
1	A	302	GLU
1	A	306	VAL

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Mol	Chain	Res	Type
1	A	316	MET
1	A	318	LEU
1	A	320	ASN
1	B	9	LEU
1	B	14	VAL
1	B	16	ILE
1	B	26	VAL
1	B	27	THR
1	B	50	SER
1	B	60	GLU
1	B	62	ASP
1	B	64	VAL
1	B	72	GLU
1	B	79	LEU
1	B	92	VAL
1	B	95	LYS
1	B	102	LEU
1	B	121	VAL
1	B	124	VAL
1	B	133	LEU
1	B	139	SER
1	B	146	VAL
1	B	183	ILE
1	B	191	ARG
1	B	196	THR
1	B	233	ASP
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	22	LEU
2	C	23	ASP
2	C	39	ILE
2	C	46	GLN
2	C	56	VAL
2	C	81	ASP
2	C	90	VAL
2	C	103	VAL
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR

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Mol	Chain	Res	Type
2	C	135	THR
2	C	138	ILE
2	C	145	ILE
2	C	164	THR
2	C	170	VAL
2	C	201	ARG
2	C	208	ILE
2	C	285	ILE
2	C	292	ILE
2	C	302	ILE
2	C	306	THR
2	C	316	GLU
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	377	THR
2	C	384	LEU
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	453	ILE
2	C	455	SER
2	C	456	VAL
2	C	471	VAL
2	C	481	LEU
2	C	484	LEU
2	C	490	GLN
2	C	492	MET
2	C	493	ILE
2	C	518	ASN
2	C	521	LEU
2	C	525	THR
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	550	VAL
2	C	553	THR
2	C	558	VAL
2	C	561	ILE
2	C	575	LEU
2	C	600	THR
2	C	609	ILE

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Mol	Chain	Res	Type
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	633	LEU
2	C	634	VAL
2	C	657	THR
2	C	660	VAL
2	C	663	VAL
2	C	672	GLU
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	781	ASP
2	C	783	LEU
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	817	LEU
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	922	ASN
2	C	948	ILE
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1050	VAL
2	C	1054	LEU
2	C	1072	ASN
2	C	1076	ILE
2	C	1078	LYS
2	C	1082	ILE
2	C	1098	LEU

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Mol	Chain	Res	Type
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1141	LEU
2	C	1145	ILE
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1172	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1225	VAL
2	C	1227	VAL
2	C	1233	LEU
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1291	LEU
2	C	1296	ASP
2	C	1313	HIS
2	C	1327	LEU
3	D	8	LEU
3	D	11	GLN
3	D	12	THR
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
3	D	93	THR
3	D	95	THR

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Mol	Chain	Res	Type
3	D	96	LYS
3	D	97	VAL
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	259	ARG
3	D	292	VAL
3	D	306	LEU
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	363	LEU
3	D	374	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	407	VAL
3	D	413	ASP
3	D	416	ILE
3	D	423	LEU
3	D	425	ARG
3	D	429	LEU
3	D	442	ILE
3	D	490	ILE
3	D	505	ASP
3	D	507	VAL
3	D	510	LEU
3	D	514	THR
3	D	532	GLU
3	D	536	LEU
3	D	545	HIS
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	594	GLN
3	D	615	LYS
3	D	639	VAL

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Mol	Chain	Res	Type
3	D	641	ILE
3	D	678	ARG
3	D	685	ILE
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	721	SER
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	790	THR
3	D	797	THR
3	D	801	VAL
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG
3	D	890	THR
3	D	903	LEU
3	D	908	ILE
3	D	918	ILE
3	D	1135	THR
3	D	1146	GLU
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1194	ARG
3	D	1221	LEU
3	D	1251	LYS
3	D	1255	VAL
3	D	1257	VAL
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN

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Mol	Chain	Res	Type
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1361	THR
3	D	1366	HIS
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU
5	F	98	VAL
5	F	114	GLU
5	F	127	ILE
5	F	152	GLU
5	F	154	GLU
5	F	163	THR
5	F	230	VAL
5	F	261	LEU
5	F	277	MET
5	F	305	LEU
5	F	306	PHE
5	F	335	GLU
5	F	341	LEU
5	F	399	LEU
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	494	ILE
5	F	507	MET
5	F	516	ASP
5	F	526	THR

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Mol	Chain	Res	Type
5	F	527	THR
5	F	530	LEU
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	559	LEU
5	F	561	MET
5	F	568	ASN
5	F	569	THR
5	F	572	THR
5	F	578	LYS
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	27	THR
1	G	33	ARG
1	G	50	SER
1	G	64	VAL
1	G	65	LEU
1	G	70	THR
1	G	79	LEU
1	G	90	VAL
1	G	101	THR
1	G	121	VAL
1	G	124	VAL
1	G	129	VAL
1	G	133	LEU
1	G	137	ASN
1	G	145	LYS
1	G	156	SER
1	G	168	ILE
1	G	178	SER
1	G	183	ILE
1	G	187	VAL
1	G	192	VAL

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Mol	Chain	Res	Type
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	217	ILE
1	G	219	ARG
1	H	16	ILE
1	H	27	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	66	HIS
1	H	75	GLN
1	H	95	LYS
1	H	102	LEU
1	H	121	VAL
1	H	124	VAL
1	H	133	LEU
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	21	VAL
2	I	22	LEU
2	I	39	ILE
2	I	46	GLN
2	I	56	VAL
2	I	86	GLN
2	I	90	VAL
2	I	103	VAL
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	119	GLU
2	I	131	THR
2	I	132	ASP
2	I	135	THR
2	I	138	ILE
2	I	156	PHE
2	I	164	THR
2	I	170	VAL

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Mol	Chain	Res	Type
2	I	208	ILE
2	I	285	ILE
2	I	292	ILE
2	I	302	ILE
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	343	HIS
2	I	360	LEU
2	I	384	LEU
2	I	423	ASP
2	I	445	ILE
2	I	453	ILE
2	I	455	SER
2	I	456	VAL
2	I	471	VAL
2	I	481	LEU
2	I	484	LEU
2	I	492	MET
2	I	493	ILE
2	I	518	ASN
2	I	521	LEU
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	542	ARG
2	I	550	VAL
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	575	LEU
2	I	596	ASP
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	633	LEU
2	I	635	THR

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Mol	Chain	Res	Type
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	705	GLU
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	799	ASN
2	I	800	MET
2	I	817	LEU
2	I	828	PHE
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	922	ASN
2	I	951	MET
2	I	984	VAL
2	I	1002	LEU
2	I	1037	THR
2	I	1050	VAL
2	I	1054	LEU
2	I	1078	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1172	LEU
2	I	1180	MET
2	I	1198	LEU

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Mol	Chain	Res	Type
2	I	1206	THR
2	I	1210	ILE
2	I	1225	VAL
2	I	1227	VAL
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER
2	I	1254	VAL
2	I	1287	LEU
2	I	1296	ASP
2	I	1299	ASN
2	I	1313	HIS
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	93	THR
3	J	95	THR
3	J	96	LYS
3	J	97	VAL
3	J	162	GLU
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	283	LEU
3	J	292	VAL
3	J	306	LEU
3	J	324	LEU
3	J	343	LEU

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Mol	Chain	Res	Type
3	J	357	VAL
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE
3	J	415	VAL
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	505	ASP
3	J	506	VAL
3	J	507	VAL
3	J	510	LEU
3	J	514	THR
3	J	532	GLU
3	J	536	LEU
3	J	545	HIS
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	591	ILE
3	J	594	GLN
3	J	605	LEU
3	J	615	LYS
3	J	639	VAL
3	J	641	ILE
3	J	678	ARG
3	J	685	ILE
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	797	THR
3	J	801	VAL
3	J	810	THR

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Mol	Chain	Res	Type
3	J	827	GLU
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	897	HIS
3	J	898	CYS
3	J	903	LEU
3	J	908	ILE
3	J	910	ASN
3	J	913	GLU
3	J	918	ILE
3	J	1146	GLU
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1194	ARG
3	J	1204	VAL
3	J	1221	LEU
3	J	1243	LEU
3	J	1251	LYS
3	J	1255	VAL
3	J	1257	VAL
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL

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Mol	Chain	Res	Type
5	L	102	MET
5	L	114	GLU
5	L	127	ILE
5	L	152	GLU
5	L	154	GLU
5	L	163	THR
5	L	261	LEU
5	L	277	MET
5	L	305	LEU
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	405	ILE
5	L	429	THR
5	L	445	ASP
5	L	450	ILE
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP
5	L	494	ILE
5	L	507	MET
5	L	526	THR
5	L	527	THR
5	L	547	VAL
5	L	552	THR
5	L	558	VAL
5	L	559	LEU
5	L	561	MET
5	L	568	ASN
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG

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Mol	Chain	Res	Type
5	L	606	VAL
5	L	607	LEU
6	M	25	GLU
6	M	42	ARG
6	M	50	GLN
6	M	52	ARG
6	M	69	PHE
6	M	72	PRO
6	M	78	GLN
6	M	88	ASN
6	M	123	ILE
6	M	136	ILE
6	M	146	GLU
6	N	25	GLU
6	N	42	ARG
6	N	50	GLN
6	N	52	ARG
6	N	69	PHE
6	N	72	PRO
6	N	73	VAL
6	N	78	GLN
6	N	88	ASN
6	N	123	ILE
6	N	136	ILE
6	N	146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	37	HIS
1	A	66	HIS
1	A	75	GLN
1	A	268	ASN
1	B	23	HIS
1	B	147	GLN
2	C	46	GLN
2	C	133	ASN
2	C	139	ASN
2	C	314	ASN
2	C	343	HIS
2	C	513	GLN

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Mol	Chain	Res	Type
2	C	620	ASN
2	C	677	ASN
2	C	766	ASN
2	C	1116	HIS
2	C	1209	GLN
2	C	1220	GLN
2	C	1237	HIS
2	C	1288	GLN
2	C	1314	GLN
2	C	1336	ASN
3	D	200	GLN
3	D	320	ASN
3	D	365	GLN
3	D	419	HIS
3	D	424	ASN
3	D	450	HIS
3	D	489	ASN
3	D	606	ASN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	861	ASN
3	D	865	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1235	ASN
4	E	15	ASN
5	F	131	GLN
5	F	294	GLN
5	F	383	ASN
5	F	406	GLN
5	F	446	GLN
5	F	455	HIS
5	F	464	ASN
5	F	579	GLN
5	F	600	HIS
1	G	66	HIS
1	G	132	HIS
1	G	186	ASN
2	I	46	GLN
2	I	139	ASN
2	I	150	HIS

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Mol	Chain	Res	Type
2	I	490	GLN
2	I	510	GLN
2	I	618	GLN
2	I	620	ASN
2	I	673	HIS
2	I	760	ASN
2	I	766	ASN
2	I	799	ASN
2	I	1013	GLN
2	I	1038	GLN
2	I	1116	HIS
2	I	1146	GLN
2	I	1209	GLN
2	I	1220	GLN
2	I	1288	GLN
2	I	1314	GLN
2	I	1336	ASN
3	J	157	GLN
3	J	158	GLN
3	J	200	GLN
3	J	206	ASN
3	J	294	ASN
3	J	365	GLN
3	J	430	HIS
3	J	448	GLN
3	J	450	HIS
3	J	594	GLN
3	J	606	ASN
3	J	739	GLN
3	J	771	GLN
3	J	1235	ASN
3	J	1366	HIS
5	L	283	GLN
5	L	294	GLN
5	L	301	ASN
5	L	362	ASN
5	L	446	GLN
5	L	579	GLN
6	M	78	GLN
6	N	50	GLN
6	N	78	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	-0.38	1 (0%) 90 80	230, 295, 400, 420	0
1	B	217/329 (65%)	-0.35	0 100 100	243, 301, 356, 388	0
1	G	227/329 (68%)	-0.23	3 (1%) 75 60	270, 312, 357, 389	0
1	H	216/329 (65%)	-0.26	0 100 100	287, 356, 409, 427	0
2	C	1340/1342 (99%)	-0.37	5 (0%) 88 77	166, 255, 352, 403	0
2	I	1340/1342 (99%)	-0.45	3 (0%) 91 83	203, 302, 382, 423	0
3	D	1171/1407 (83%)	-0.30	11 (0%) 81 67	169, 238, 355, 404	0
3	J	1159/1407 (82%)	-0.41	3 (0%) 90 80	183, 262, 356, 405	0
4	E	89/91 (97%)	-0.43	0 100 100	225, 281, 318, 330	0
4	K	79/91 (86%)	-0.34	0 100 100	320, 426, 502, 516	0
5	F	468/613 (76%)	-0.41	1 (0%) 91 83	199, 288, 436, 472	0
5	L	469/613 (76%)	-0.42	3 (0%) 85 73	212, 309, 420, 437	0
6	M	140/151 (92%)	-0.20	1 (0%) 84 71	374, 435, 492, 503	0
6	N	140/151 (92%)	-0.13	0 100 100	417, 439, 458, 465	0
All	All	7374/8524 (86%)	-0.37	31 (0%) 88 77	166, 283, 416, 516	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	GLU	3.8
3	D	502	PRO	3.7
3	D	508	LEU	3.5
3	D	877	VAL	3.3
2	I	796	LEU	3.2
1	G	205	MET	3.0
2	I	1233	LEU	2.9
3	D	879	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	112	ALA	2.6
1	G	43	LEU	2.6
3	J	160	LEU	2.6
2	C	317	LEU	2.5
5	L	604	SER	2.5
3	J	154	LEU	2.5
6	M	72	PRO	2.4
3	D	113	HIS	2.4
1	G	26	VAL	2.4
3	D	482	ALA	2.4
2	C	1233	LEU	2.4
3	D	242	LEU	2.2
2	C	499	SER	2.2
5	L	598	LEU	2.2
2	C	1049	ILE	2.2
5	F	269	LEU	2.2
5	L	224	LEU	2.2
2	I	1232	MET	2.1
3	D	423	LEU	2.0
3	D	872	LEU	2.0
2	C	429	MET	2.0
3	J	415	VAL	2.0
3	D	99	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	J	2001	1/1	0.71	0.14	335,335,335,335	0
7	MG	D	2001	1/1	0.76	0.14	268,268,268,268	0
8	ZN	M	200	1/1	0.91	0.08	512,512,512,512	0
8	ZN	N	200	1/1	0.93	0.05	506,506,506,506	0
8	ZN	D	2003	1/1	0.99	0.08	245,245,245,245	0
8	ZN	J	2003	1/1	0.99	0.05	211,211,211,211	0
8	ZN	J	2002	1/1	1.00	0.02	269,269,269,269	0
8	ZN	D	2002	1/1	1.00	0.06	271,271,271,271	0

6.5 Other polymers [i](#)

There are no such residues in this entry.