



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 11:15 PM EST

PDB ID : 5UAC
Title : Escherichia coli RNA polymerase and Rifampin complex, wild-type
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

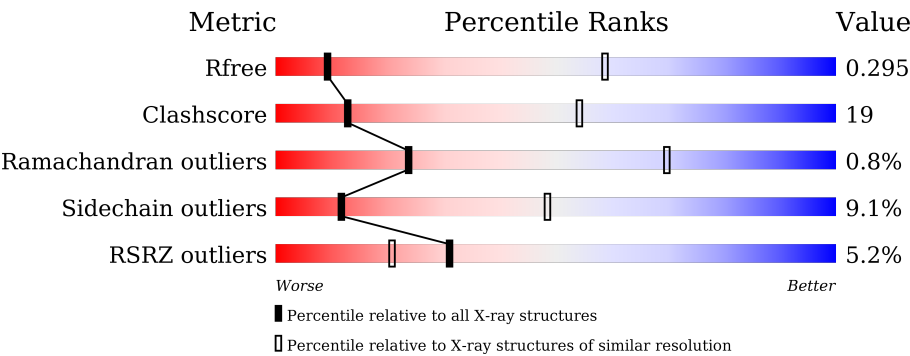
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	329	<div><div>0.1%</div><div><div></div><div>40%</div><div>26%</div><div>•</div><div>31%</div></div></div>
1	B	329	<div><div>2%</div><div><div></div><div>36%</div><div>27%</div><div>•</div><div>35%</div></div></div>
1	G	329	<div><div></div><div><div></div><div>39%</div><div>25%</div><div>•</div><div>32%</div></div></div>
1	H	329	<div><div>3%</div><div><div></div><div>31%</div><div>32%</div><div>•</div><div>35%</div></div></div>
2	C	1342	<div><div>4%</div><div><div></div><div>58%</div><div>36%</div><div>6%</div></div></div>
2	I	1342	<div><div>7%</div><div><div></div><div>60%</div><div>36%</div><div>•</div></div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	D	1503	-	-	X	-
8	ZN	J	1503	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1342	Total	C	N	O	S	0	0	0
			10585	6641	1843	2057	44			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

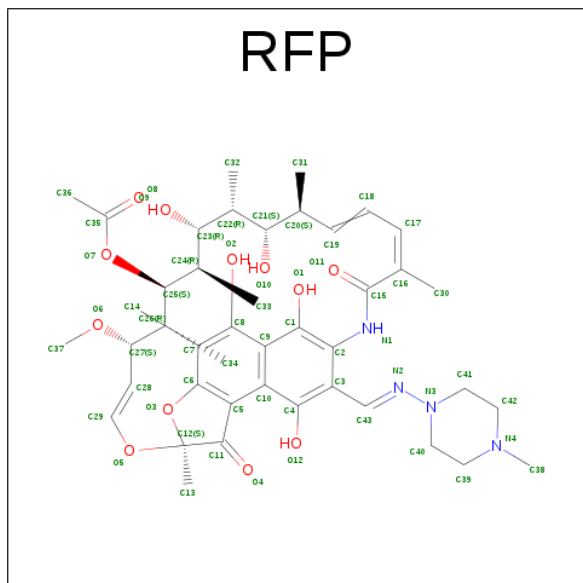
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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

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

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

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



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

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

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

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

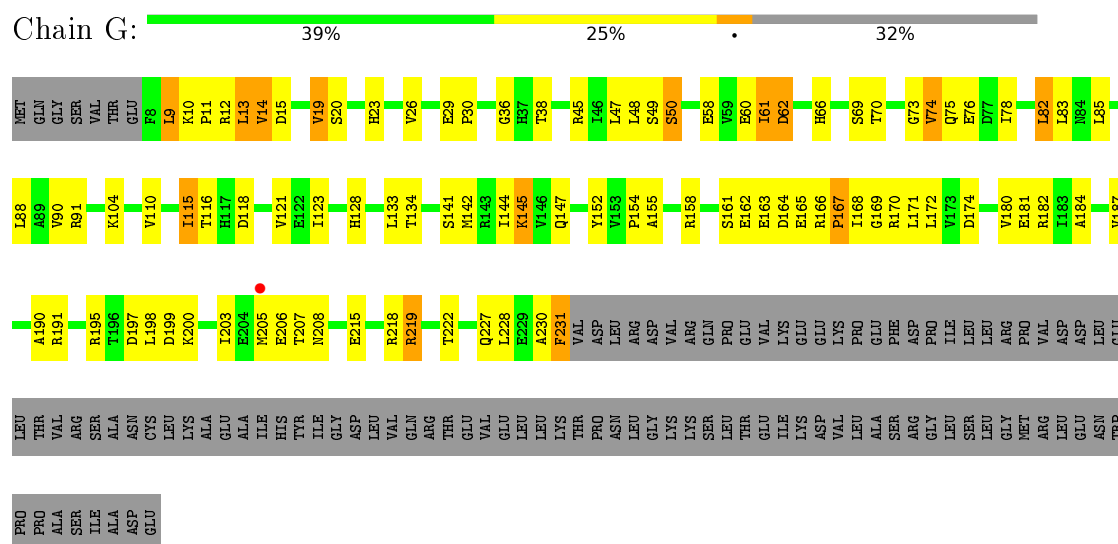
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		

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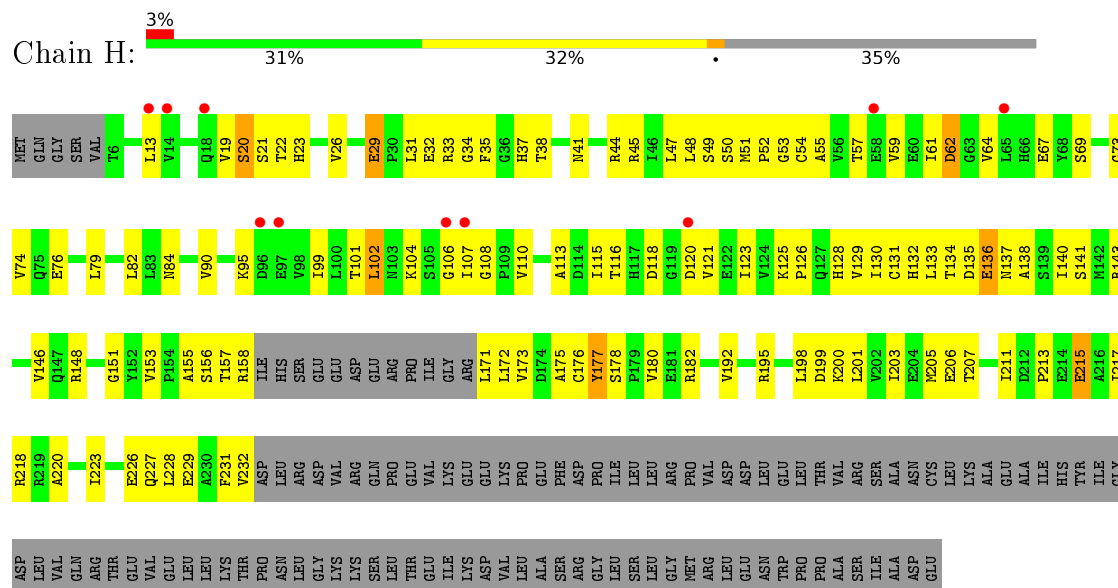
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		

Chain G:



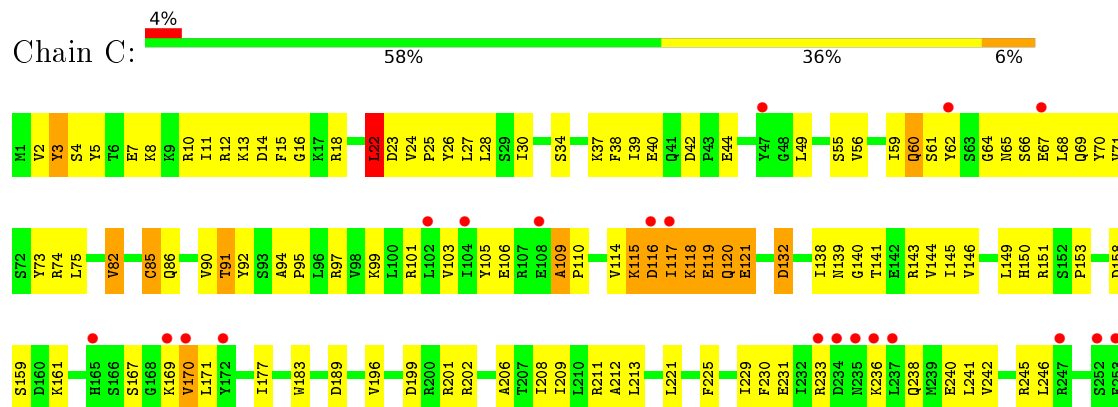
- Molecule 1: DNA-directed RNA polymerase subunit alpha

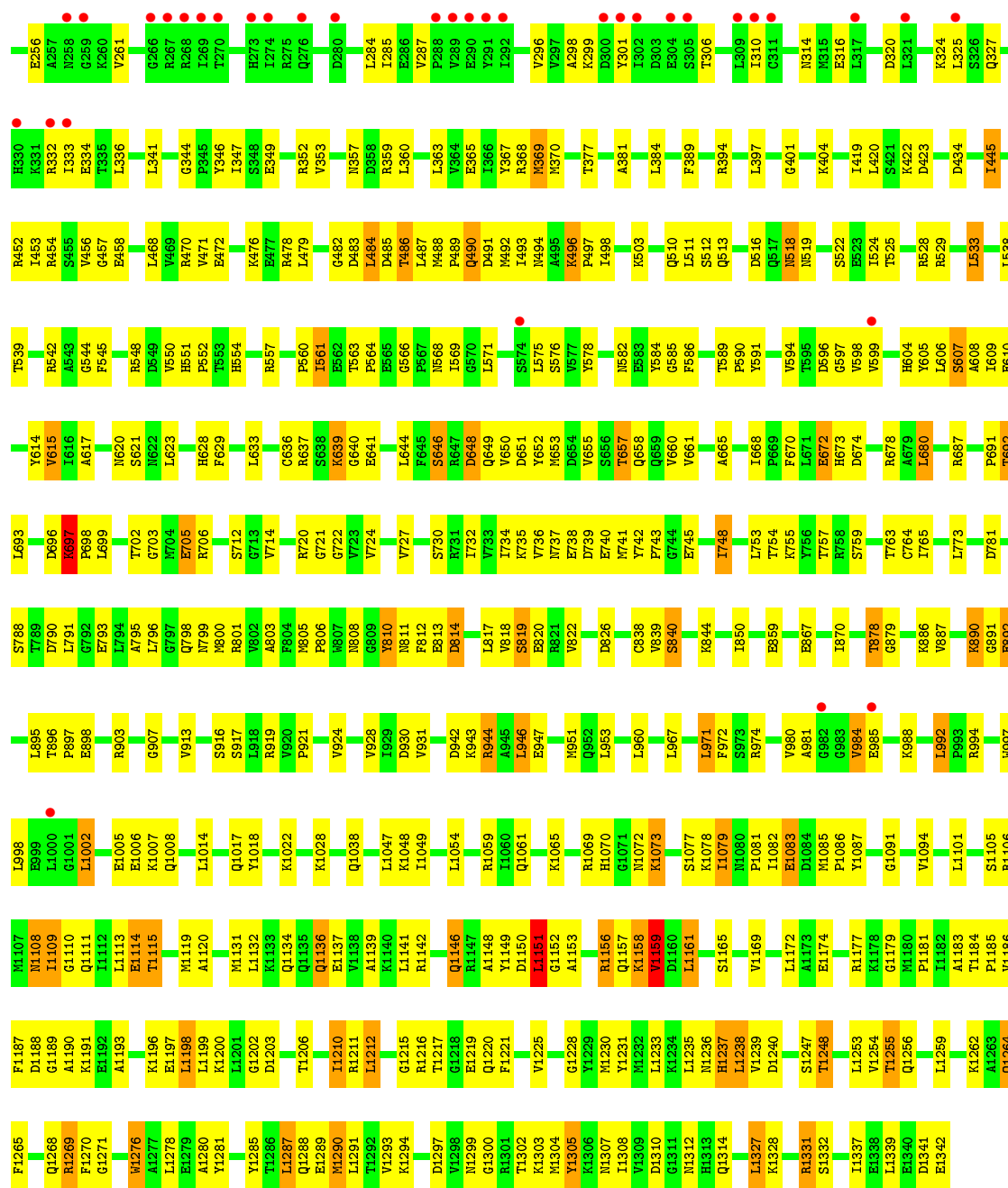
Chain H:



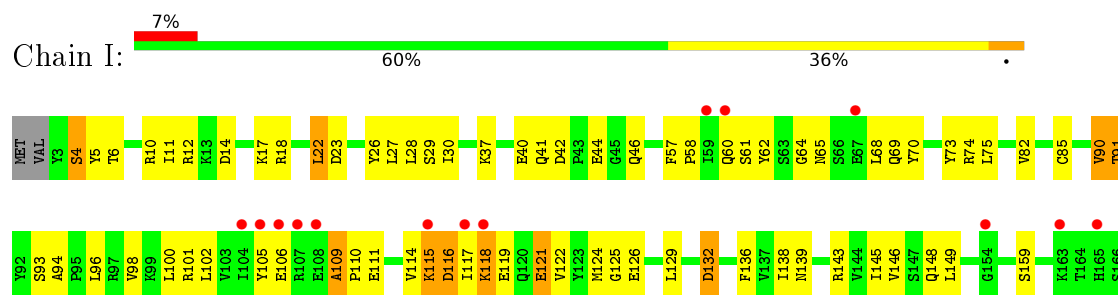
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



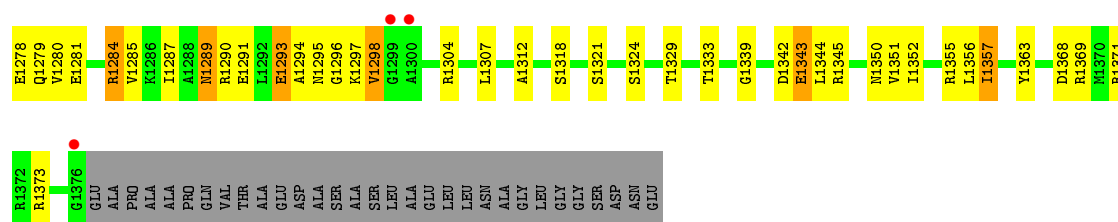


- Molecule 2: DNA-directed RNA polymerase subunit beta

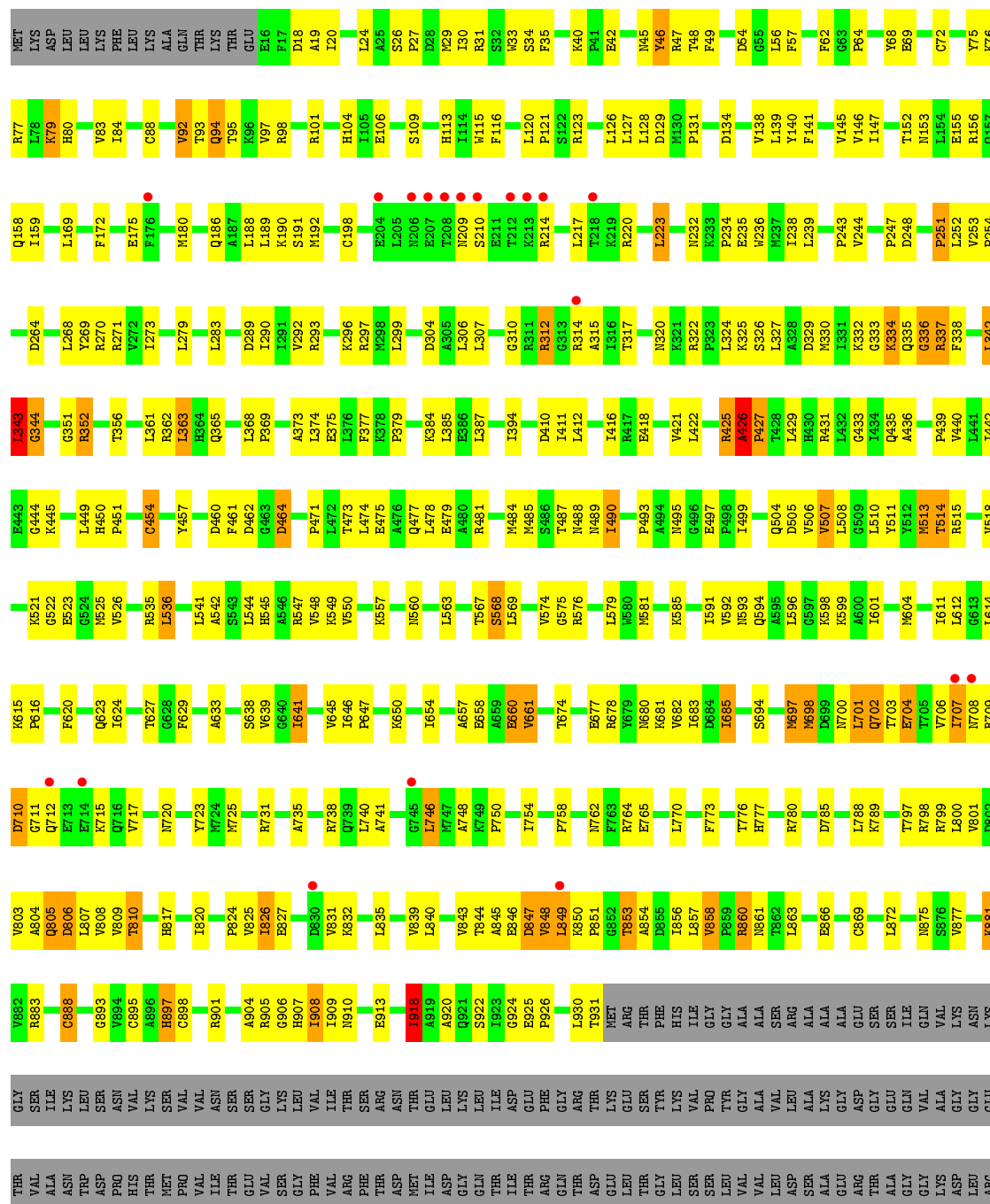


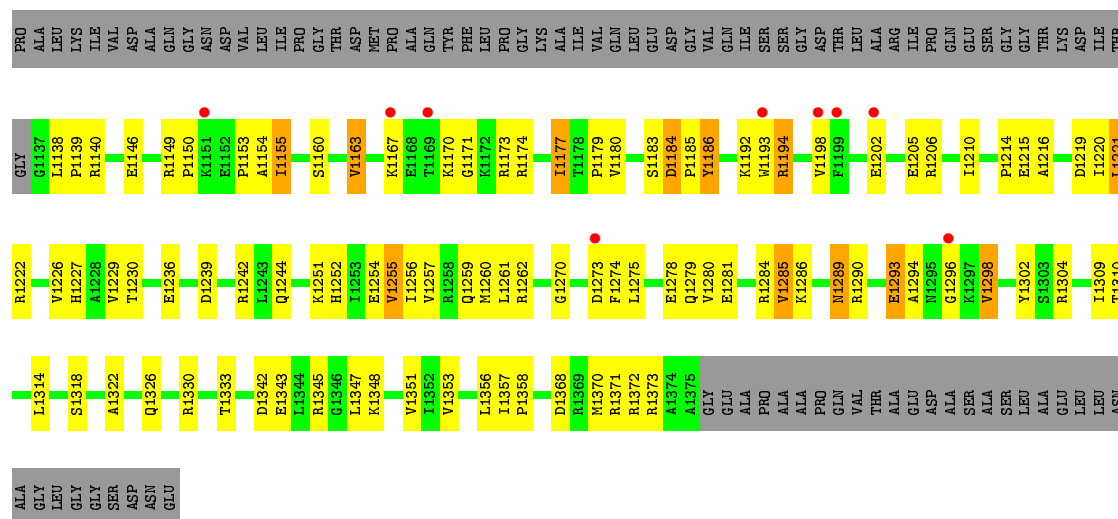






- Molecule 3: DNA-directed RNA polymerase subunit beta'





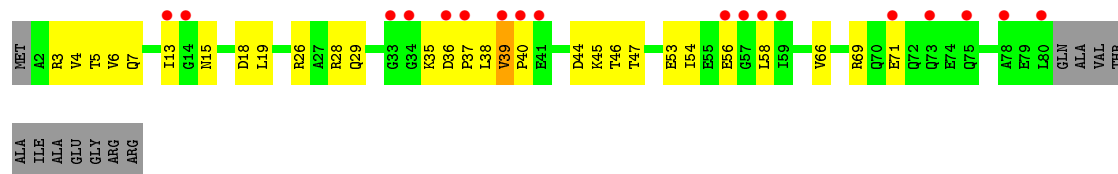
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 69% 23%



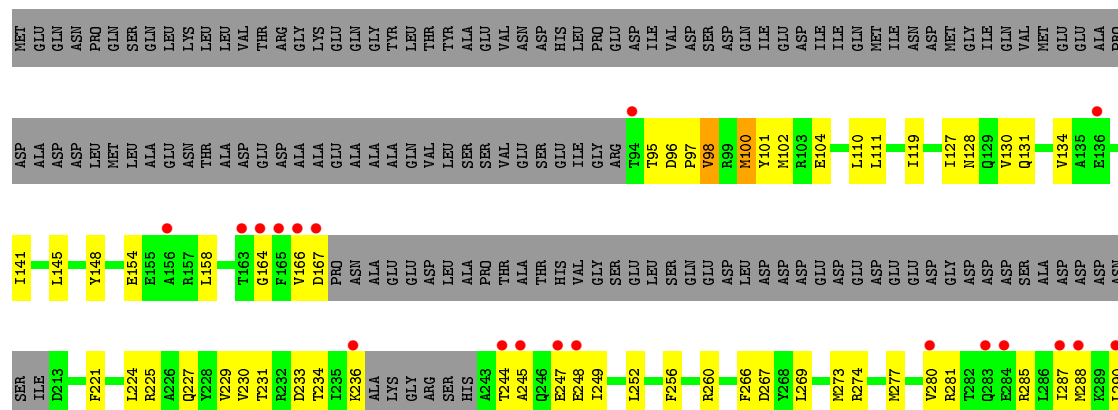
- Molecule 4: DNA-directed RNA polymerase subunit omega

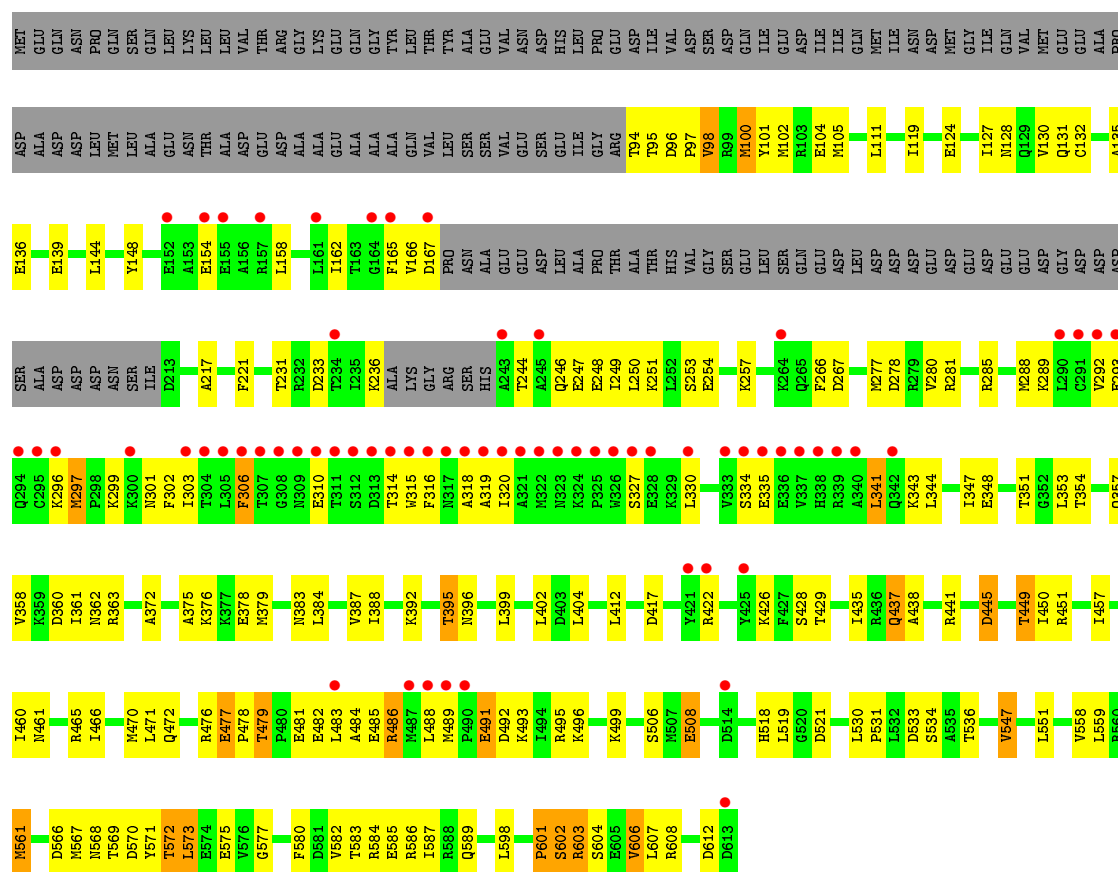
Chain K: 20% 55% 31% 13%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 10% 48% 24% 24%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	188.96Å 204.43Å 313.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.80 29.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.98-3.80) 99.8 (29.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.75Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.248 , 0.295 0.245 , 0.295	Depositor DCC
R_{free} test set	1994 reflections (1.67%)	DCC
Wilson B-factor (Å ²)	159.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 102.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55049	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.73	2/1774 (0.1%)	0.86	2/2405 (0.1%)
1	B	0.66	0/1668	0.91	1/2260 (0.0%)
1	G	0.54	0/1751	0.77	1/2373 (0.0%)
1	H	0.53	0/1678	0.85	2/2274 (0.1%)
2	C	0.89	12/10754 (0.1%)	0.92	25/14509 (0.2%)
2	I	0.58	4/10735 (0.0%)	0.71	2/14484 (0.0%)
3	D	0.96	20/9229 (0.2%)	0.98	27/12459 (0.2%)
3	J	0.74	4/9140 (0.0%)	0.86	14/12341 (0.1%)
4	E	0.69	0/693	0.81	1/935 (0.1%)
4	K	0.31	0/629	0.55	0/847
5	F	0.50	0/3864	0.69	3/5194 (0.1%)
5	L	0.46	0/3872	0.63	1/5205 (0.0%)
All	All	0.74	42/55787 (0.1%)	0.84	79/75286 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	6
2	I	0	2
3	D	0	6
3	J	0	2
4	E	0	1
5	F	0	1
5	L	0	1
All	All	0	20

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	764	CYS	CB-SG	-11.76	1.62	1.82
3	D	454	CYS	CB-SG	-8.90	1.67	1.82
2	C	636	CYS	CB-SG	-8.85	1.67	1.82
3	J	888	CYS	CB-SG	-8.72	1.67	1.82
2	C	838	CYS	CB-SG	-8.60	1.67	1.82
2	C	1276	TRP	CB-CG	-7.97	1.35	1.50
3	J	343	LEU	CG-CD2	7.45	1.79	1.51
2	I	373	GLY	C-N	7.00	1.50	1.34
3	D	1363	TYR	CD1-CE1	-6.99	1.28	1.39
1	A	9	LEU	C-N	6.93	1.50	1.34
2	C	85	CYS	CB-SG	-6.45	1.71	1.82
3	D	898	CYS	CB-SG	-6.19	1.71	1.82
3	D	517	CYS	CB-SG	-6.01	1.72	1.82
3	D	1363	TYR	CE1-CZ	-5.85	1.30	1.38
3	D	198	CYS	CB-SG	-5.85	1.72	1.81
2	I	813	GLU	CB-CG	-5.83	1.41	1.52
1	A	29	GLU	C-N	5.82	1.45	1.34
3	D	1241	TYR	CD2-CE2	-5.75	1.30	1.39
2	I	1270	PHE	CD2-CE2	-5.68	1.27	1.39
3	D	888	CYS	CB-SG	-5.68	1.72	1.81
2	C	822	VAL	CB-CG2	-5.52	1.41	1.52
2	C	1079	ILE	C-N	-5.52	1.21	1.34
3	D	468	VAL	CB-CG2	-5.45	1.41	1.52
3	D	115	TRP	CB-CG	-5.44	1.40	1.50
3	D	586	GLY	C-N	-5.42	1.21	1.34
3	J	454	CYS	CB-SG	-5.42	1.73	1.81
3	D	366	CYS	CB-SG	-5.38	1.73	1.81
2	C	810	TYR	CE2-CZ	-5.36	1.31	1.38
3	D	457	TYR	CD2-CE2	-5.35	1.31	1.39
2	C	1305	TYR	CD1-CE1	-5.29	1.31	1.39
3	D	639	VAL	CB-CG1	-5.28	1.41	1.52
3	J	198	CYS	CB-SG	-5.28	1.73	1.81
3	D	437	PHE	C-N	-5.28	1.22	1.34
3	D	801	VAL	CB-CG2	-5.24	1.41	1.52
2	C	144	VAL	CB-CG1	-5.23	1.41	1.52
2	C	811	ASN	CB-CG	-5.20	1.39	1.51
3	D	809	VAL	CB-CG1	-5.18	1.42	1.52
3	D	869	CYS	CB-SG	-5.15	1.73	1.81
3	D	773	PHE	CB-CG	-5.13	1.42	1.51
3	D	421	VAL	CB-CG1	-5.08	1.42	1.52
2	I	344	GLY	C-N	-5.05	1.24	1.34
2	C	1305	TYR	CE1-CZ	-5.04	1.32	1.38

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	343	LEU	CA-CB-CG	-8.74	95.19	115.30
3	D	807	LEU	CB-CG-CD2	-8.46	96.62	111.00
3	J	327	LEU	CB-CG-CD2	-8.45	96.64	111.00
3	D	888	CYS	CA-CB-SG	-8.38	98.92	114.00
3	J	426	ALA	C-N-CD	-8.01	102.98	120.60
3	D	368	LEU	CB-CG-CD2	-7.55	98.16	111.00
3	D	1261	LEU	CB-CG-CD2	-7.54	98.17	111.00
3	D	242	LEU	CB-CG-CD1	-7.39	98.43	111.00
3	D	239	LEU	CB-CG-CD2	-7.26	98.66	111.00
2	C	1259	LEU	CA-CB-CG	-7.26	98.61	115.30
3	D	426	ALA	C-N-CD	-7.24	104.68	120.60
2	C	1151	LEU	CA-CB-CG	-7.17	98.80	115.30
2	C	511	LEU	CB-CG-CD2	-7.01	99.08	111.00
2	C	1269	ARG	NE-CZ-NH2	-6.84	116.88	120.30
3	J	464	ASP	CB-CG-OD2	6.84	124.45	118.30
3	D	449	LEU	CB-CG-CD2	-6.79	99.45	111.00
3	D	432	LEU	CB-CG-CD2	-6.72	99.57	111.00
3	D	1357	ILE	CG1-CB-CG2	-6.69	96.67	111.40
3	J	888	CYS	CA-CB-SG	-6.60	102.11	114.00
3	D	608	CYS	CA-CB-SG	-6.55	102.21	114.00
2	C	1287	LEU	CB-CG-CD2	-6.30	100.30	111.00
2	C	27	LEU	CB-CG-CD2	-6.26	100.36	111.00
3	D	330	MET	CA-CB-CG	-6.13	102.87	113.30
5	L	602	SER	N-CA-C	-6.11	94.52	111.00
4	E	16	ARG	NE-CZ-NH1	6.09	123.34	120.30
2	I	1270	PHE	CB-CG-CD2	-6.09	116.54	120.80
2	C	1069	ARG	NE-CZ-NH1	-6.07	117.26	120.30
3	D	605	LEU	CA-CB-CG	-6.06	101.36	115.30
3	J	918	ILE	CG1-CB-CG2	-5.95	98.31	111.40
1	H	29	GLU	C-N-CD	-5.91	107.60	120.60
2	C	680	LEU	CB-CG-CD1	-5.89	100.99	111.00
1	G	82	LEU	CB-CG-CD2	-5.88	101.01	111.00
5	F	602	SER	N-CA-C	-5.82	95.28	111.00
2	C	706	ARG	NE-CZ-NH1	-5.80	117.40	120.30
2	C	648	ASP	CB-CG-OD1	-5.74	113.14	118.30
2	C	1259	LEU	CB-CG-CD2	-5.74	101.25	111.00
3	D	307	LEU	CB-CG-CD1	-5.66	101.38	111.00
2	C	533	LEU	CB-CG-CD2	-5.65	101.39	111.00
2	C	946	LEU	CB-CG-CD1	-5.62	101.44	111.00
3	J	508	LEU	CB-CG-CD1	-5.59	101.50	111.00
3	D	361	LEU	CB-CG-CD1	-5.57	101.53	111.00
2	C	1047	LEU	CA-CB-CG	-5.52	102.60	115.30
3	J	449	LEU	CB-CG-CD2	-5.52	101.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	740	LEU	CB-CG-CD1	-5.50	101.64	111.00
3	D	807	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	H	102	LEU	CA-CB-CG	5.46	127.85	115.30
3	D	423	LEU	CB-CG-CD1	-5.41	101.80	111.00
3	J	1261	LEU	CB-CG-CD2	-5.39	101.83	111.00
2	C	706	ARG	CB-CG-CD	-5.39	97.60	111.60
3	J	223	LEU	CB-CG-CD2	-5.38	101.86	111.00
2	C	1161	LEU	CA-CB-CG	-5.36	102.98	115.30
2	C	1287	LEU	CB-CG-CD1	-5.34	101.93	111.00
3	D	487	THR	CA-CB-CG2	-5.32	104.95	112.40
5	F	519	LEU	CB-CG-CD1	-5.30	101.99	111.00
3	D	605	LEU	CB-CG-CD2	-5.27	102.04	111.00
5	F	532	LEU	CA-CB-CG	5.26	127.41	115.30
2	C	971	LEU	CB-CG-CD2	-5.26	102.06	111.00
2	C	1248	THR	CA-CB-CG2	-5.25	105.05	112.40
3	D	385	LEU	CB-CG-CD1	-5.25	102.08	111.00
3	D	508	LEU	CB-CG-CD1	-5.25	102.08	111.00
3	D	412	LEU	CB-CG-CD2	-5.24	102.09	111.00
2	C	1115	THR	CA-CB-CG2	-5.24	105.06	112.40
2	C	1278	LEU	CB-CG-CD2	5.24	119.90	111.00
2	C	1269	ARG	NE-CZ-NH1	5.23	122.91	120.30
3	J	909	ILE	CG1-CB-CG2	-5.20	99.97	111.40
3	J	800	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	I	1287	LEU	CB-CG-CD2	-5.15	102.24	111.00
3	D	1258	ARG	NE-CZ-NH1	-5.14	117.73	120.30
3	J	299	LEU	CB-CG-CD2	-5.13	102.27	111.00
3	J	343	LEU	CB-CG-CD1	5.12	119.70	111.00
2	C	561	ILE	CB-CA-C	-5.12	101.37	111.60
3	D	1233	ILE	CG1-CB-CG2	-5.10	100.17	111.40
1	B	13	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	47	LEU	CB-CG-CD1	-5.09	102.34	111.00
2	C	1212	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	A	131	CYS	CA-CB-SG	-5.07	104.88	114.00
3	D	746	LEU	CB-CG-CD2	-5.07	102.38	111.00
3	J	412	LEU	CB-CG-CD2	-5.05	102.42	111.00
2	C	22	LEU	CB-CG-CD2	-5.04	102.43	111.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	1239	VAL	Mainchain
2	C	1255	THR	Mainchain
2	C	1290	MET	Mainchain
2	C	236	LYS	Peptide
2	C	646	SER	Mainchain
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
3	D	1321	SER	Mainchain
3	D	471	PRO	Mainchain
3	D	593	ASN	Mainchain
3	D	808	VAL	Mainchain
4	E	32	VAL	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	601	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1780	90	0
1	B	1649	0	1674	101	0
1	G	1730	0	1756	82	0
1	H	1659	0	1692	91	0
2	C	10585	0	10603	425	0
2	I	10566	0	10576	385	0
3	D	9089	0	9264	449	0
3	J	9001	0	9170	378	0
4	E	691	0	695	16	0
4	K	627	0	634	24	0
5	F	3813	0	3880	132	0
5	L	3821	0	3884	134	0
6	C	59	0	54	14	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	1	0	0	0	0
8	D	2	0	0	2	0
8	J	2	0	0	1	0
All	All	55049	0	55662	2119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (2119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:343:LEU:CG	3:J:343:LEU:CD2	1.79	1.59
3:D:426:ALA:CB	3:D:427:PRO:CD	2.12	1.26
3:J:426:ALA:CB	3:J:427:PRO:HD3	1.69	1.19
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.16	1.16
3:D:426:ALA:HB3	3:D:427:PRO:CD	1.70	1.13
2:C:1271:GLY:HA2	3:D:343:LEU:CD2	1.78	1.13
3:J:426:ALA:HB3	3:J:427:PRO:CD	1.78	1.13
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.10	1.09
3:D:426:ALA:CB	3:D:427:PRO:HD3	1.82	1.07
3:D:426:ALA:HB1	3:D:427:PRO:HD3	1.32	1.07
2:C:1269:ARG:HG3	3:D:343:LEU:HD12	1.31	1.06
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.38	1.02
1:A:223:ILE:HG21	1:B:8:PHE:CE1	1.95	1.02
3:D:343:LEU:CD2	3:D:344:GLY:HA3	1.92	1.00
3:D:888:CYS:HG	8:D:1503:ZN:ZN	0.70	0.99
3:D:426:ALA:HB3	3:D:427:PRO:HD2	1.01	0.97
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.44	0.97
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.45	0.97
3:D:576:ARG:NH1	3:D:593:ASN:O	1.97	0.97
1:A:223:ILE:HG21	1:B:8:PHE:HE1	1.28	0.97
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.43	0.96
1:A:150:ARG:CD	1:B:8:PHE:HE2	1.78	0.96
3:J:343:LEU:CD2	3:J:343:LEU:CD1	2.43	0.96
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.32	0.95
3:D:426:ALA:CB	3:D:427:PRO:HD2	1.80	0.94
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.34	0.92
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.52	0.92
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.53	0.91
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.36	0.90
1:G:45:ARG:HG2	1:H:38:THR:HB	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.53	0.90
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.53	0.89
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.55	0.88
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.57	0.87
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.07	0.86
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.58	0.86
3:J:576:ARG:NH1	3:J:593:ASN:O	2.10	0.85
3:D:343:LEU:HD22	3:D:344:GLY:CA	2.06	0.84
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.10	0.84
2:I:324:LYS:O	2:I:327:GLN:NE2	2.11	0.84
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.11	0.83
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.61	0.82
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.61	0.82
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.61	0.82
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.43	0.82
1:A:150:ARG:NE	1:B:8:PHE:CE2	2.47	0.82
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.62	0.81
3:J:817:HIS:CE1	3:J:860:ARG:HE	1.97	0.81
1:A:150:ARG:NE	1:B:8:PHE:HE2	1.77	0.81
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.43	0.81
3:J:425:ARG:O	3:J:426:ALA:O	1.98	0.81
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.60	0.81
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.63	0.81
3:J:436:ALA:HB3	3:J:485:MET:HA	1.61	0.81
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.13	0.80
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	1.63	0.80
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.61	0.80
6:C:3001:RFP:O1	6:C:3001:RFP:O11	1.99	0.80
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.61	0.80
1:A:150:ARG:CD	1:B:8:PHE:CE2	2.65	0.80
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.46	0.80
3:J:700:ASN:O	3:J:704:GLU:HB2	1.81	0.80
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.47	0.79
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.64	0.79
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.62	0.79
3:D:418:GLU:HG3	4:E:45:LYS:H	1.46	0.79
5:F:97:PRO:HA	5:F:100:MET:HG3	1.64	0.79
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.62	0.79
5:F:316:PHE:HZ	5:F:334:SER:HA	1.47	0.78
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.48	0.78
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.66	0.78
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.66	0.77
3:J:418:GLU:HG3	4:K:45:LYS:H	1.49	0.77
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.66	0.77
2:I:560:PRO:O	3:J:780:ARG:NH2	2.15	0.77
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.67	0.77
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.67	0.76
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.66	0.76
1:G:166:ARG:O	1:G:168:ILE:N	2.18	0.76
3:J:905:ARG:HH21	3:J:907:HIS:CB	1.96	0.76
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.66	0.76
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.65	0.76
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.66	0.76
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.50	0.76
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.67	0.76
3:J:156:ARG:NH2	3:J:191:SER:OG	2.18	0.76
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.51	0.75
1:H:57:THR:HG21	1:H:158:ARG:HE	1.51	0.75
1:A:166:ARG:O	1:A:168:ILE:N	2.18	0.75
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.67	0.75
2:C:721:GLY:N	2:C:740:GLU:OE1	2.17	0.75
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.01	0.75
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.68	0.75
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.69	0.74
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.19	0.74
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.20	0.74
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.69	0.74
3:D:156:ARG:NH2	3:D:191:SER:OG	2.19	0.74
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.05	0.74
3:D:129:ASP:HB2	3:D:220:ARG:CZ	2.18	0.74
1:A:223:ILE:CG2	1:B:8:PHE:CE1	2.70	0.73
2:I:18:ARG:NH1	2:I:621:SER:O	2.21	0.73
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.23	0.73
3:D:56:LEU:HD12	3:D:56:LEU:H	1.52	0.73
2:I:1211:ARG:HE	2:I:1220:GLN:HE21	1.36	0.73
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.68	0.73
1:A:45:ARG:HG2	1:B:38:THR:HB	1.71	0.73
2:C:930:ASP:OD2	2:C:931:VAL:N	2.21	0.73
3:D:700:ASN:O	3:D:704:GLU:HB2	1.89	0.73
3:D:264:ASP:OD2	5:F:506:SER:OG	2.05	0.73
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:30:ILE:HD12	2:I:30:ILE:H	1.53	0.73
1:A:233:ASP:N	1:A:233:ASP:OD2	2.19	0.73
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.52	0.73
2:C:886:LYS:H	2:C:917:SER:HB3	1.52	0.72
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.89	0.72
2:C:510:GLN:HE21	6:C:3001:RFP:H131	1.54	0.72
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.72	0.72
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.70	0.72
1:A:23:HIS:HB2	1:A:205:MET:O	1.89	0.72
1:B:64:VAL:HG11	1:B:69:SER:HB2	1.70	0.72
2:C:12:ARG:NE	2:C:793:GLU:OE1	2.16	0.72
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.71	0.72
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.55	0.71
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.55	0.71
1:B:23:HIS:HB2	1:B:205:MET:O	1.89	0.71
3:D:336:GLY:HA3	3:D:1324:SER:O	1.91	0.71
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.22	0.71
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.56	0.71
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.06	0.71
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.70	0.71
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.72	0.71
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.71	0.71
3:D:342:LEU:HA	3:D:343:LEU:HD23	1.71	0.71
3:J:343:LEU:CD2	3:J:343:LEU:CB	2.69	0.71
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.06	0.71
2:C:324:LYS:O	2:C:327:GLN:NE2	2.22	0.71
2:I:40:GLU:O	2:I:73:TYR:OH	2.09	0.71
3:J:35:PHE:HD1	3:J:101:ARG:HB3	1.55	0.70
3:D:36:GLY:HA3	3:D:61:ILE:HG23	1.73	0.70
3:J:244:VAL:HA	3:J:269:TYR:OH	1.91	0.70
3:J:888:CYS:SG	8:J:1503:ZN:ZN	1.79	0.70
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.72	0.70
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.24	0.70
1:B:13:LEU:HG	1:B:29:GLU:HB3	1.73	0.70
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.71	0.70
3:D:210:SER:O	3:D:214:ARG:HG2	1.91	0.70
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.74	0.70
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.74	0.70
3:D:77:ARG:HG3	3:D:79:LYS:H	1.54	0.70
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.22	0.69
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.74	0.69
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.74	0.69
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.58	0.69
3:D:11:GLN:HG3	3:D:12:THR:H	1.55	0.69
3:J:384:LYS:HD2	3:J:387:LEU:HD23	1.74	0.69
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	1.92	0.69
5:L:533:ASP:O	5:L:536:THR:N	2.25	0.69
2:I:452:ARG:NH1	2:I:584:TYR:O	2.24	0.69
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.74	0.69
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.75	0.69
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.08	0.69
3:J:843:VAL:HG11	3:J:897:HIS:O	1.93	0.69
1:A:150:ARG:CZ	1:B:8:PHE:CE2	2.76	0.69
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.07	0.69
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.75	0.69
2:I:808:ASN:H	3:J:633:ALA:HB2	1.57	0.69
3:J:426:ALA:HB1	3:J:427:PRO:HD3	1.72	0.69
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.27	0.68
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.75	0.68
2:C:1247:SER:HB3	3:D:375:GLU:O	1.94	0.68
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.27	0.68
2:C:30:ILE:H	2:C:30:ILE:HD12	1.59	0.68
1:G:62:ASP:OD1	1:G:141:SER:OG	2.11	0.68
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.76	0.68
5:L:97:PRO:HA	5:L:100:MET:HG3	1.74	0.68
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.74	0.68
2:I:1289:GLU:OE2	3:J:473:THR:HG22	1.94	0.68
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.09	0.68
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.77	0.67
5:F:601:PRO:HA	5:F:604:SER:HB2	1.77	0.67
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.74	0.67
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.77	0.67
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.77	0.67
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.76	0.67
2:I:1157:GLN:O	2:I:1158:LYS:HG2	1.94	0.67
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.76	0.67
3:J:210:SER:O	3:J:214:ARG:HG2	1.94	0.67
5:L:94:THR:OG1	5:L:95:THR:N	2.28	0.67
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.75	0.67
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	1.94	0.67
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.59	0.67
1:B:57:THR:HG21	1:B:158:ARG:HE	1.59	0.67
3:D:901:ARG:HA	3:D:908:ILE:HA	1.76	0.67
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.75	0.67
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.22	0.67
2:C:1202:GLY:O	2:C:1203:ASP:HB2	1.95	0.67
5:F:533:ASP:O	5:F:536:THR:N	2.28	0.67
3:J:45:ASN:HB3	3:J:48:THR:O	1.95	0.67
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.10	0.67
3:D:843:VAL:HG11	3:D:897:HIS:O	1.95	0.67
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.59	0.67
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.95	0.67
3:J:98:ARG:HB3	3:J:248:ASP:OD2	1.95	0.67
3:J:94:GLN:O	3:J:97:VAL:HG23	1.95	0.67
2:I:250:THR:HA	2:I:268:ARG:HA	1.77	0.66
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.76	0.66
5:L:316:PHE:HZ	5:L:334:SER:HA	1.59	0.66
2:C:1307:ASN:HB3	2:C:1312:ASN:O	1.95	0.66
2:C:563:THR:OG1	2:C:564:PRO:HD2	1.96	0.66
1:B:11:PRO:CB	1:B:28:LEU:HD21	2.25	0.66
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.31	0.66
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.78	0.66
2:C:557:ARG:HH21	2:C:607:SER:C	1.98	0.66
1:H:32:GLU:OE2	1:H:195:ARG:NH2	2.28	0.66
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.29	0.66
2:I:183:TRP:N	2:I:199:ASP:OD1	2.28	0.66
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.76	0.66
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.28	0.66
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.78	0.66
2:I:1247:SER:HB3	3:J:375:GLU:O	1.94	0.66
1:H:106:GLY:N	1:H:137:ASN:O	2.26	0.66
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.11	0.66
2:C:528:ARG:NH2	2:C:576:SER:O	2.29	0.66
2:C:490:GLN:HE21	5:F:472:GLN:HE21	1.43	0.66
3:J:186:GLN:HB2	3:J:238:ILE:HG21	1.77	0.66
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.61	0.65
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.25	0.65
3:D:895:CYS:SG	8:D:1503:ZN:ZN	1.84	0.65
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.79	0.65
2:C:806:PRO:HB3	3:D:505:ASP:OD1	1.95	0.65
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.77	0.65
2:C:703:GLY:N	2:C:705:GLU:OE2	2.28	0.65
2:C:91:THR:HG21	2:C:503:LYS:HZ3	1.61	0.65
2:I:109:ALA:HB1	2:I:110:PRO:C	2.17	0.65
2:I:314:ASN:O	2:I:352:ARG:NH1	2.21	0.65
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.31	0.65
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.60	0.65
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.78	0.65
1:A:161:SER:O	1:A:163:GLU:N	2.29	0.65
2:C:928:VAL:HG22	2:C:1054:LEU:HD11	1.79	0.65
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.32	0.65
3:D:789:LYS:NZ	3:D:931:THR:O	2.28	0.65
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.62	0.64
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.78	0.64
5:F:274:ARG:NH2	5:F:369:GLU:OE2	2.30	0.64
5:F:479:THR:HG23	5:F:481:GLU:H	1.62	0.64
1:G:227:GLN:HE21	1:H:35:PHE:HD2	1.42	0.64
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.30	0.64
3:D:98:ARG:HB3	3:D:248:ASP:OD2	1.97	0.64
5:F:573:LEU:H	5:F:573:LEU:HD23	1.60	0.64
3:J:817:HIS:CD2	3:J:860:ARG:HH21	2.15	0.64
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.79	0.64
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.78	0.64
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.11	0.64
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.79	0.64
1:A:10:LYS:HA	1:B:227:GLN:NE2	2.12	0.64
2:I:1072:ASN:N	2:I:1072:ASN:OD1	2.24	0.64
1:A:13:LEU:H	1:A:13:LEU:HD23	1.63	0.64
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.79	0.64
1:A:27:THR:C	1:A:28:LEU:HD12	2.18	0.64
3:D:658:GLU:O	3:D:661:VAL:HG13	1.98	0.64
3:J:1252:HIS:O	3:J:1255:VAL:HG13	1.98	0.64
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.63	0.63
5:F:598:LEU:O	5:F:604:SER:OG	2.12	0.63
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.79	0.63
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.63	0.63
1:H:59:VAL:O	1:H:171:LEU:N	2.29	0.63
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.79	0.63
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.63	0.63
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.80	0.63
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.63	0.63
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.79	0.63
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.31	0.63
2:C:566:GLY:O	2:C:569:ILE:HG13	1.99	0.63
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.32	0.63
3:J:425:ARG:HG2	3:J:426:ALA:H	1.64	0.63
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.64	0.63
2:C:692:THR:OG1	2:C:693:LEU:N	2.29	0.63
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.78	0.63
3:D:30:ILE:CG2	3:D:243:PRO:HG3	2.29	0.63
3:D:270:ARG:HH21	5:F:449:THR:HG23	1.63	0.63
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.61	0.63
3:J:901:ARG:HA	3:J:908:ILE:HA	1.79	0.63
1:H:176:CYS:O	1:H:178:SER:N	2.32	0.63
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.64	0.63
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.79	0.63
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.13	0.63
1:G:218:ARG:HH11	1:H:232:VAL:HG21	1.62	0.63
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.31	0.63
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.63	0.63
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.22	0.62
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.79	0.62
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.79	0.62
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.81	0.62
2:C:1269:ARG:CG	3:D:343:LEU:HD12	2.19	0.62
1:G:19:VAL:HG11	1:G:23:HIS:CE1	2.33	0.62
1:H:205:MET:HG2	1:H:206:GLU:H	1.64	0.62
1:G:49:SER:OG	1:G:50:SER:N	2.31	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.81	0.62
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.10	0.62
3:D:9:LYS:HZ2	3:D:11:GLN:HA	1.64	0.62
1:B:11:PRO:HB2	1:B:28:LEU:HD11	1.82	0.62
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.34	0.62
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.82	0.62
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.80	0.62
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.33	0.62
2:C:1291:LEU:HD21	3:D:1351:VAL:HG13	1.82	0.62
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.82	0.62
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.82	0.62
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.35	0.62
2:C:60:GLN:HA	2:C:67:GLU:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:HIS:HB2	1:G:205:MET:O	1.98	0.62
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.35	0.62
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.82	0.62
3:J:697:MET:SD	3:J:741:ALA:HB3	2.39	0.62
3:D:368:LEU:C	3:D:368:LEU:HD23	2.21	0.61
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.80	0.61
1:G:13:LEU:H	1:G:13:LEU:HD23	1.65	0.61
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.65	0.61
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.00	0.61
3:J:264:ASP:OD2	5:L:506:SER:OG	2.17	0.61
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.81	0.61
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.82	0.61
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.31	0.61
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.35	0.61
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.82	0.61
3:D:888:CYS:SG	3:D:889:ASP:N	2.74	0.61
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.83	0.61
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.33	0.61
3:D:709:ARG:O	3:D:711:GLY:N	2.34	0.61
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.83	0.61
2:I:930:ASP:OD2	2:I:931:VAL:N	2.34	0.61
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.82	0.61
1:H:192:VAL:HG21	1:H:198:LEU:HD12	1.82	0.61
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.82	0.61
5:F:343:LYS:H	5:F:343:LYS:HD2	1.65	0.61
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.15	0.61
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.83	0.61
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.66	0.61
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.40	0.61
5:L:573:LEU:H	5:L:573:LEU:HD23	1.66	0.61
2:C:55:SER:OG	2:C:56:VAL:N	2.34	0.60
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.01	0.60
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.82	0.60
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.36	0.60
2:I:886:LYS:H	2:I:917:SER:HB3	1.66	0.60
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.01	0.60
3:D:45:ASN:HB3	3:D:48:THR:O	2.01	0.60
5:L:105:MET:HE3	5:L:384:LEU:HB2	1.83	0.60
3:D:709:ARG:C	3:D:711:GLY:H	2.04	0.60
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.83	0.60
3:J:126:LEU:HD13	3:J:223:LEU:CD2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:395:THR:OG1	5:L:396:ASN:N	2.34	0.60
2:C:1271:GLY:HA2	3:D:343:LEU:CG	2.31	0.60
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.83	0.60
1:G:230:ALA:HB3	1:G:231:PHE:CE2	2.37	0.60
2:I:215:TYR:HE2	2:I:422:LYS:HD2	1.65	0.60
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.66	0.60
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.34	0.60
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.01	0.60
3:J:426:ALA:CB	3:J:427:PRO:CD	2.32	0.60
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.82	0.60
2:I:615:VAL:HA	2:I:638:SER:HA	1.84	0.60
3:J:1155:ILE:HD12	3:J:1210:ILE:HB	1.84	0.60
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.17	0.60
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.84	0.60
2:C:91:THR:HG21	2:C:503:LYS:NZ	2.17	0.60
2:C:980:VAL:O	2:C:984:VAL:HB	2.02	0.60
3:D:436:ALA:HB3	3:D:485:MET:HA	1.84	0.60
2:I:296:VAL:HB	2:I:336:LEU:HD12	1.84	0.60
2:C:109:ALA:HB1	2:C:110:PRO:C	2.22	0.60
1:B:102:LEU:O	1:B:141:SER:HA	2.01	0.60
1:B:53:GLY:HA3	1:B:177:TYR:O	2.02	0.60
1:H:53:GLY:HA3	1:H:177:TYR:O	2.02	0.60
3:J:514:THR:HB	3:J:576:ARG:HG2	1.83	0.60
1:A:14:VAL:HG22	1:A:15:ASP:H	1.67	0.59
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.84	0.59
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.66	0.59
3:D:931:THR:OG1	3:D:931:THR:O	2.18	0.59
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.82	0.59
5:F:316:PHE:CZ	5:F:334:SER:HA	2.34	0.59
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.84	0.59
3:J:846:GLU:HA	3:J:860:ARG:HD3	1.84	0.59
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.17	0.59
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.51	0.59
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.67	0.59
1:G:73:GLY:O	1:G:134:THR:HG22	2.00	0.59
2:I:93:SER:OG	2:I:126:GLU:OE1	2.13	0.59
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.67	0.59
2:C:452:ARG:NH1	2:C:584:TYR:O	2.36	0.59
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.66	0.59
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.84	0.59
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.84	0.59
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.83	0.59
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.85	0.59
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.84	0.59
5:L:492:ASP:O	5:L:495:ARG:NH1	2.35	0.59
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.84	0.59
1:H:49:SER:O	1:H:151:GLY:HA2	2.03	0.59
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.17	0.59
4:K:39:VAL:HG21	4:K:56:GLU:HG3	1.84	0.59
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.85	0.59
1:G:12:ARG:H	1:G:30:PRO:HD2	1.68	0.59
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.85	0.59
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.17	0.59
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.84	0.59
3:J:336:GLY:O	3:J:337:ARG:HB2	2.03	0.59
5:L:244:THR:O	5:L:247:GLU:HG2	2.03	0.59
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.32	0.59
3:D:363:LEU:HG	3:D:363:LEU:O	2.02	0.59
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.85	0.59
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.38	0.59
2:C:18:ARG:NH1	2:C:621:SER:O	2.36	0.59
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.85	0.59
1:B:62:ASP:HB2	1:B:141:SER:O	2.03	0.58
5:F:561:MET:HA	5:F:567:MET:HE1	1.84	0.58
1:B:20:SER:OG	1:B:21:SER:N	2.36	0.58
2:C:566:GLY:H	2:C:569:ILE:CG1	2.16	0.58
3:D:460:ASP:HB2	3:D:464:ASP:OD2	2.03	0.58
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.84	0.58
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.51	0.58
3:J:42:GLU:CG	5:L:451:ARG:HE	2.16	0.58
3:D:428:THR:HG22	3:D:428:THR:O	2.02	0.58
1:G:231:PHE:N	1:G:231:PHE:CD2	2.70	0.58
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.84	0.58
3:J:279:LEU:HD23	3:J:279:LEU:O	2.02	0.58
1:A:227:GLN:NE2	1:B:9:LEU:O	2.35	0.58
1:A:150:ARG:HD3	1:B:8:PHE:HE2	1.65	0.58
2:C:256:GLU:HB3	2:C:261:VAL:HG22	1.85	0.58
3:D:510:LEU:HD22	3:D:601:ILE:CD1	2.32	0.58
2:I:878:THR:OG1	2:I:879:GLY:N	2.34	0.58
1:B:90:VAL:HG12	1:B:91:ARG:H	1.68	0.58
2:C:594:VAL:HG22	2:C:599:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.85	0.58
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.68	0.58
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.85	0.58
3:J:129:ASP:HB2	3:J:220:ARG:NH2	2.19	0.58
3:J:460:ASP:HB2	3:J:464:ASP:OD2	2.03	0.58
2:I:963:GLU:O	2:I:967:LEU:HB2	2.03	0.58
3:J:598:LYS:O	3:J:601:ILE:HG22	2.03	0.58
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.83	0.58
2:C:878:THR:OG1	2:C:879:GLY:N	2.34	0.58
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.18	0.58
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.36	0.58
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.36	0.58
3:J:304:ASP:OD2	3:J:312:ARG:NE	2.37	0.58
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.36	0.58
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.34	0.58
1:A:49:SER:OG	1:A:50:SER:N	2.36	0.58
2:C:1236:ASN:O	2:C:1237:HIS:ND1	2.34	0.58
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.85	0.58
3:D:744:ARG:NH1	3:D:763:PHE:HZ	2.00	0.58
1:G:14:VAL:HG22	1:G:15:ASP:H	1.68	0.58
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.04	0.58
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.33	0.58
2:C:524:ILE:HD12	2:C:712:SER:HB2	1.85	0.58
2:C:808:ASN:H	3:D:633:ALA:HB2	1.68	0.58
1:G:45:ARG:NH1	1:H:34:GLY:O	2.37	0.58
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.36	0.58
2:C:529:ARG:HH12	6:C:3001:RFP:C18	2.16	0.57
3:D:614:LEU:O	3:D:617:THR:N	2.37	0.57
3:D:789:LYS:NZ	3:D:931:THR:OG1	2.35	0.57
1:H:101:THR:H	1:H:116:THR:HG22	1.69	0.57
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.69	0.57
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.87	0.57
2:C:516:ASP:HB2	6:C:3001:RFP:H20C	1.85	0.57
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.37	0.57
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.33	0.57
2:I:566:GLY:O	2:I:569:ILE:HG13	2.04	0.57
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.86	0.57
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.87	0.57
1:G:218:ARG:HH11	1:H:232:VAL:CG2	2.18	0.57
1:H:73:GLY:O	1:H:134:THR:HG22	2.05	0.57
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.14	0.57
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.86	0.57
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.40	0.57
2:I:148:GLN:NE2	2:I:535:PRO:O	2.28	0.57
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.86	0.57
3:J:901:ARG:HD2	3:J:906:GLY:O	2.05	0.57
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.44	0.57
3:D:362:ARG:H	3:D:365:GLN:HE21	1.53	0.57
1:H:102:LEU:O	1:H:141:SER:HA	2.04	0.57
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.86	0.57
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.87	0.57
1:H:48:LEU:HD22	3:J:535:ARG:HD3	1.87	0.57
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.86	0.57
5:L:281:ARG:O	5:L:285:ARG:HG3	2.05	0.57
3:J:34:SER:HG	3:J:104:HIS:CG	2.22	0.57
2:I:844:LYS:HD3	3:J:49:PHE:HE2	1.69	0.57
2:C:2:VAL:O	2:C:3:TYR:HB2	2.04	0.57
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.40	0.57
5:L:314:THR:O	5:L:318:ALA:HB3	2.05	0.57
3:D:360:TYR:OH	3:D:448:GLN:OE1	2.03	0.57
1:H:55:ALA:O	1:H:146:VAL:HG13	2.04	0.57
1:H:20:SER:OG	1:H:21:SER:N	2.36	0.57
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.40	0.56
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.86	0.56
5:F:547:VAL:HG23	5:F:603:ARG:NH1	2.18	0.56
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.05	0.56
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.86	0.56
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.34	0.56
1:A:38:THR:OG1	1:B:45:ARG:HG2	2.04	0.56
2:I:149:LEU:HD12	2:I:452:ARG:O	2.05	0.56
2:I:617:ALA:HA	2:I:636:CYS:SG	2.44	0.56
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.87	0.56
2:C:201:ARG:NH2	2:C:370:MET:O	2.29	0.56
1:H:153:VAL:O	1:H:175:ALA:N	2.32	0.56
1:H:74:VAL:HG12	1:H:76:GLU:H	1.70	0.56
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.20	0.56
1:B:102:LEU:HD11	1:B:110:VAL:HG11	1.86	0.56
3:D:11:GLN:HG3	3:D:12:THR:N	2.19	0.56
3:D:697:MET:SD	3:D:741:ALA:HB3	2.45	0.56
3:D:748:ALA:O	3:D:777:HIS:HD2	1.88	0.56
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:GLU:OE2	1:H:200:LYS:HE3	2.04	0.56
2:I:1065:LYS:HD3	2:I:1235:LEU:HD12	1.87	0.56
2:I:1131:MET:HE1	2:I:1141:LEU:HD12	1.87	0.56
1:H:23:HIS:HB2	1:H:205:MET:O	2.06	0.56
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.87	0.56
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.71	0.56
5:L:254:GLU:HA	5:L:257:LYS:HD3	1.87	0.56
3:D:744:ARG:NH1	3:D:763:PHE:CZ	2.73	0.56
2:I:101:ARG:HG3	2:I:118:LYS:HD2	1.88	0.56
3:J:514:THR:OG1	3:J:594:GLN:O	2.24	0.56
1:A:181:GLU:HB3	1:A:206:GLU:HG3	1.88	0.56
6:C:3001:RFP:O9	6:C:3001:RFP:O10	2.21	0.56
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.69	0.56
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.88	0.56
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.87	0.56
1:B:182:ARG:O	1:B:183:ILE:HD12	2.04	0.56
1:B:190:ALA:N	1:B:198:LEU:O	2.34	0.56
3:D:1280:VAL:CG1	3:D:1304:ARG:HH21	2.16	0.56
3:D:772:TYR:O	3:D:775:SER:HB3	2.04	0.56
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.88	0.56
5:F:562:ARG:HH21	5:F:573:LEU:HD22	1.71	0.56
1:G:165:GLU:OE2	1:G:172:LEU:HD11	2.04	0.56
2:I:411:ARG:NH2	2:I:427:ASP:OD2	2.34	0.56
3:J:209:ASN:HA	3:J:214:ARG:HE	1.71	0.56
1:A:50:SER:HB2	1:B:8:PHE:HZ	1.70	0.56
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.88	0.56
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.86	0.56
2:I:516:ASP:H	2:I:526:HIS:HD1	1.54	0.56
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.46	0.56
3:J:905:ARG:NH1	3:J:910:ASN:HD21	2.03	0.56
3:D:18:ASP:HB2	3:D:1373:ARG:NH2	2.21	0.56
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.88	0.56
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.88	0.56
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.88	0.55
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.87	0.55
1:B:182:ARG:C	1:B:183:ILE:HD12	2.26	0.55
2:C:146:VAL:HG21	2:C:513:GLN:NE2	2.21	0.55
2:C:516:ASP:OD2	2:C:522:SER:OG	2.23	0.55
2:C:596:ASP:OD2	2:C:597:GLY:N	2.38	0.55
2:C:844:LYS:HD3	3:D:49:PHE:HE2	1.71	0.55
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:703:GLY:N	2:I:705:GLU:OE2	2.39	0.55
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.41	0.55
2:C:560:PRO:O	3:D:780:ARG:NH2	2.37	0.55
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.89	0.55
1:H:57:THR:O	1:H:173:VAL:HG22	2.06	0.55
5:L:569:THR:OG1	5:L:570:ASP:N	2.38	0.55
1:A:12:ARG:H	1:A:30:PRO:HD2	1.71	0.55
2:C:169:LYS:O	2:C:170:VAL:HG22	2.07	0.55
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.72	0.55
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.71	0.55
3:J:510:LEU:HG	3:J:513:MET:CE	2.35	0.55
3:D:1158:GLU:HB3	3:D:1186:TYR:CE1	2.42	0.55
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.88	0.55
2:I:490:GLN:HG2	2:I:491:ASP:N	2.22	0.55
2:I:594:VAL:HG22	2:I:599:VAL:HA	1.89	0.55
5:L:135:ALA:HB1	5:L:253:SER:HA	1.88	0.55
2:C:23:ASP:N	2:C:23:ASP:OD1	2.39	0.55
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.29	0.55
3:D:19:ALA:O	3:D:20:ILE:HG13	2.07	0.55
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.88	0.55
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.41	0.55
5:L:479:THR:HG23	5:L:481:GLU:H	1.72	0.55
3:D:847:ASP:HA	3:D:860:ARG:H	1.72	0.55
5:F:572:THR:O	5:F:576:VAL:HG23	2.07	0.55
2:C:615:VAL:HG13	2:C:651:ASP:H	1.71	0.55
2:I:23:ASP:N	2:I:23:ASP:OD1	2.40	0.55
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.41	0.55
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.40	0.55
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.71	0.55
5:L:602:SER:OG	5:L:603:ARG:N	2.39	0.55
5:L:601:PRO:HA	5:L:604:SER:HB2	1.88	0.55
1:B:29:GLU:HG3	1:B:30:PRO:HG3	1.89	0.55
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.22	0.55
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.88	0.55
5:F:320:ILE:HG12	5:F:330:LEU:HD12	1.88	0.55
1:G:155:ALA:N	1:G:174:ASP:OD1	2.30	0.55
1:H:64:VAL:HG11	1:H:69:SER:OG	2.07	0.55
2:I:972:PHE:CZ	2:I:998:LEU:HD11	2.41	0.55
3:J:77:ARG:HE	5:L:569:THR:HA	1.71	0.55
5:L:584:ARG:HA	5:L:584:ARG:HH11	1.72	0.54
1:A:223:ILE:HG23	1:B:8:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.21	0.54
3:D:56:LEU:HD12	3:D:56:LEU:N	2.21	0.54
2:I:367:TYR:CE2	2:I:376:PRO:HA	2.43	0.54
3:J:152:THR:OG1	3:J:153:ASN:N	2.40	0.54
5:L:127:ILE:O	5:L:130:VAL:HG22	2.06	0.54
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.73	0.54
3:D:767:LEU:HD12	3:D:767:LEU:N	2.22	0.54
1:H:104:LYS:HB3	1:H:140:ILE:HD11	1.90	0.54
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.89	0.54
1:B:101:THR:O	1:B:116:THR:HG22	2.07	0.54
2:C:483:ASP:HB2	2:C:486:THR:HG21	1.89	0.54
2:C:582:ASN:HB3	2:C:586:PHE:H	1.72	0.54
5:F:166:VAL:O	5:F:167:ASP:HB2	2.07	0.54
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.23	0.54
3:J:504:GLN:OE1	3:J:731:ARG:NH1	2.40	0.54
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.89	0.54
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.89	0.54
2:C:213:LEU:HB3	2:C:422:LYS:HD2	1.89	0.54
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.90	0.54
3:D:34:SER:HG	3:D:104:HIS:CG	2.26	0.54
3:D:36:GLY:CA	3:D:61:ILE:HG23	2.37	0.54
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.89	0.54
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.90	0.54
5:L:166:VAL:O	5:L:167:ASP:HB2	2.07	0.54
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.90	0.54
3:D:317:THR:HB	3:D:324:LEU:HB3	1.89	0.54
3:D:888:CYS:SG	3:D:895:CYS:SG	3.06	0.54
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.72	0.54
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.22	0.54
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	1.90	0.54
2:C:840:SER:OG	2:C:840:SER:O	2.19	0.54
3:D:474:LEU:HA	3:D:477:GLN:HG3	1.89	0.54
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.89	0.54
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.89	0.54
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.88	0.54
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.89	0.54
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.89	0.54
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.08	0.54
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.90	0.54
2:I:528:ARG:NH2	2:I:576:SER:O	2.40	0.54
3:J:271:ARG:HH12	3:J:315:ALA:HB1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:437:GLN:HG3	5:L:438:ALA:N	2.22	0.54
5:L:441:ARG:NH1	5:L:445:ASP:OD1	2.30	0.54
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.89	0.54
2:C:143:ARG:NH2	2:C:512:SER:O	2.41	0.54
3:D:515:ARG:O	3:D:545:HIS:HB3	2.07	0.54
3:D:801:VAL:HG12	3:D:920:ALA:HB3	1.89	0.54
5:F:461:ASN:O	5:F:465:ARG:HG2	2.07	0.54
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.43	0.54
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.08	0.54
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.88	0.54
1:G:161:SER:O	1:G:163:GLU:N	2.41	0.54
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.41	0.53
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.44	0.53
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.72	0.53
2:I:98:VAL:O	2:I:121:GLU:HA	2.07	0.53
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.90	0.53
3:J:129:ASP:HB2	3:J:220:ARG:CZ	2.38	0.53
3:J:56:LEU:H	3:J:56:LEU:HD12	1.72	0.53
1:A:223:ILE:CG2	1:B:8:PHE:CD1	2.92	0.53
5:F:127:ILE:O	5:F:130:VAL:HG22	2.08	0.53
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.73	0.53
3:J:918:ILE:O	3:J:922:SER:OG	2.18	0.53
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.89	0.53
5:L:483:LEU:H	5:L:483:LEU:HD12	1.72	0.53
2:C:561:ILE:HD11	2:C:665:ALA:HB1	1.89	0.53
2:C:696:ASP:HB2	2:C:798:GLN:CG	2.34	0.53
3:D:137:ARG:HD3	3:D:143:SER:OG	2.09	0.53
3:D:665:GLN:HG3	3:D:669:GLN:NE2	2.24	0.53
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.90	0.53
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.74	0.53
3:J:525:MET:O	3:J:548:VAL:HG13	2.08	0.53
2:C:5:TYR:HD1	2:C:8:LYS:HD3	1.74	0.53
3:D:316:ILE:HA	3:D:323:PRO:HA	1.89	0.53
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.42	0.53
5:F:540:LEU:HD12	5:F:610:PHE:CD1	2.44	0.53
2:I:4:SER:OG	2:I:5:TYR:N	2.40	0.53
3:J:270:ARG:HH21	5:L:449:THR:HG23	1.74	0.53
1:B:35:PHE:HA	1:B:38:THR:HG22	1.90	0.53
2:C:564:PRO:HG2	2:C:568:ASN:O	2.08	0.53
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.72	0.53
2:I:225:PHE:CE2	2:I:347:ILE:HB	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:64:PRO:HG2	3:J:93:THR:H	1.74	0.53
5:L:101:TYR:O	5:L:104:GLU:N	2.40	0.53
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.36	0.53
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.91	0.53
1:A:19:VAL:HG11	1:A:23:HIS:CE1	2.43	0.53
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.90	0.53
4:E:8:ASP:HB2	4:E:55:GLU:HG2	1.90	0.53
2:I:598:VAL:HG22	2:I:628:HIS:HE1	1.73	0.53
1:B:6:THR:O	1:B:6:THR:OG1	2.25	0.53
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.09	0.53
2:C:759:SER:OG	2:C:763:THR:N	2.38	0.53
3:D:343:LEU:HD13	3:D:343:LEU:C	2.29	0.53
3:D:9:LYS:HD3	3:D:10:ALA:O	2.08	0.53
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.48	0.53
2:I:519:ASN:HB3	2:I:522:SER:HB2	1.91	0.53
2:I:607:SER:HB3	2:I:610:GLU:OE1	2.09	0.53
2:I:705:GLU:HB2	2:I:794:LEU:H	1.74	0.53
2:I:891:GLY:O	2:I:892:GLU:HG3	2.09	0.53
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.56	0.53
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.43	0.53
3:J:840:LEU:HD12	3:J:869:CYS:SG	2.48	0.53
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.09	0.53
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.73	0.53
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.91	0.53
1:G:90:VAL:HG22	1:G:91:ARG:H	1.73	0.53
1:A:86:LYS:NZ	1:A:174:ASP:OD2	2.40	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.44	0.53
2:C:796:LEU:H	2:C:796:LEU:HD12	1.74	0.53
3:D:473:THR:HG23	3:D:476:ALA:H	1.73	0.53
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.34	0.52
2:C:1247:SER:OG	2:C:1248:THR:N	2.42	0.52
2:C:548:ARG:HB3	2:C:569:ILE:O	2.09	0.52
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.91	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.91	0.52
2:I:1337:ILE:O	2:I:1337:ILE:HG23	2.09	0.52
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.29	0.52
3:J:709:ARG:C	3:J:711:GLY:H	2.11	0.52
2:C:1293:VAL:HG11	2:C:1304:MET:HG2	1.91	0.52
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.91	0.52
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.24	0.52
4:E:16:ARG:HG2	4:E:16:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:168:GLY:C	2:I:170:VAL:H	2.10	0.52
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.43	0.52
1:A:167:PRO:HB2	1:A:170:ARG:HB2	1.91	0.52
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.44	0.52
2:C:498:ILE:HD12	2:C:498:ILE:H	1.74	0.52
2:C:687:ARG:HH22	6:C:3001:RFP:H301	1.74	0.52
3:D:1291:GLU:HG2	3:J:1302:TYR:OH	2.09	0.52
3:D:306:LEU:O	3:D:326:SER:HB2	2.10	0.52
3:D:800:LEU:HB3	3:D:920:ALA:CB	2.40	0.52
3:D:857:LEU:HD12	3:D:858:VAL:H	1.73	0.52
2:I:1086:PRO:O	2:I:1094:VAL:HG12	2.09	0.52
2:I:498:ILE:H	2:I:498:ILE:HD12	1.74	0.52
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.91	0.52
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.91	0.52
3:J:748:ALA:O	3:J:777:HIS:HD2	1.93	0.52
1:A:177:TYR:O	1:A:178:SER:HB2	2.09	0.52
1:A:45:ARG:HG2	1:B:38:THR:CB	2.38	0.52
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.90	0.52
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	1.90	0.52
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.92	0.52
3:D:1262:ARG:HD2	3:D:1279:GLN:HE22	1.75	0.52
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.90	0.52
1:H:107:ILE:HD11	1:H:136:GLU:H	1.73	0.52
1:H:57:THR:HG21	1:H:158:ARG:NE	2.21	0.52
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.90	0.52
2:I:819:SER:HB2	2:I:1085:MET:SD	2.50	0.52
3:J:290:ILE:H	3:J:290:ILE:HD12	1.74	0.52
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.74	0.52
1:A:207:THR:HG22	1:A:209:GLY:H	1.74	0.52
2:C:529:ARG:HH12	6:C:3001:RFP:C17	2.22	0.52
2:C:12:ARG:HH21	2:C:793:GLU:CD	2.13	0.52
5:F:571:TYR:CD1	5:F:575:GLU:HG2	2.43	0.52
1:B:29:GLU:OE1	1:B:200:LYS:HG3	2.10	0.52
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.91	0.52
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.39	0.52
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.38	0.52
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.40	0.52
1:G:115:ILE:HG22	1:G:116:THR:H	1.74	0.52
2:I:1002:LEU:N	2:I:1008:GLN:OE1	2.43	0.52
2:I:90:VAL:HG12	2:I:91:THR:H	1.75	0.52
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:687:ARG:NH2	6:C:3001:RFP:H301	2.25	0.52
2:C:1270:PHE:O	3:D:343:LEU:HD11	2.08	0.52
2:I:132:ASP:N	2:I:132:ASP:OD1	2.36	0.52
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.92	0.52
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.09	0.52
2:C:1149:TYR:CB	2:C:1159:VAL:HG11	2.39	0.52
2:C:730:SER:O	2:C:753:LEU:HB2	2.10	0.52
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.42	0.52
2:I:818:VAL:O	2:I:1079:ILE:HD12	2.09	0.52
2:I:159:SER:HB2	2:I:442:VAL:HG21	1.92	0.52
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.91	0.52
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.43	0.52
3:J:93:THR:HG22	3:J:94:GLN:H	1.75	0.52
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.92	0.52
2:C:1285:TYR:CE2	3:D:1356:LEU:HD11	2.45	0.52
3:D:490:ILE:HB	3:D:500:ILE:HG13	1.92	0.52
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.28	0.52
2:I:1114:GLU:OE1	2:I:1230:MET:HA	2.10	0.52
2:I:27:LEU:HB2	2:I:524:ILE:HD11	1.91	0.52
2:I:724:VAL:HG23	2:I:775:GLU:O	2.10	0.52
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.92	0.52
3:J:1177:ILE:HG13	3:J:1186:TYR:O	2.10	0.52
3:J:510:LEU:HG	3:J:513:MET:HE2	1.90	0.52
1:A:19:VAL:HG13	1:A:20:SER:H	1.75	0.51
2:C:2:VAL:HG13	2:C:1158:LYS:NZ	2.25	0.51
2:C:60:GLN:O	2:C:476:LYS:HG2	2.10	0.51
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.92	0.51
5:F:96:ASP:O	5:F:98:VAL:N	2.44	0.51
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.92	0.51
2:I:146:VAL:HG21	2:I:513:GLN:NE2	2.25	0.51
2:I:169:LYS:O	2:I:170:VAL:HG22	2.10	0.51
2:I:370:MET:HG3	2:I:384:LEU:HD21	1.92	0.51
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.75	0.51
2:C:1038:GLN:O	2:C:1038:GLN:HG3	2.08	0.51
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.93	0.51
5:F:584:ARG:HA	5:F:584:ARG:NH1	2.25	0.51
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.46	0.51
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.92	0.51
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.93	0.51
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.46	0.51
2:C:698:PRO:HG3	2:C:1231:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.91	0.51
3:D:1344:LEU:HD12	3:D:1344:LEU:N	2.25	0.51
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.93	0.51
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.11	0.51
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.08	0.51
1:G:172:LEU:HD12	1:G:172:LEU:H	1.75	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.10	0.51
2:I:593:LYS:HB3	2:I:602:GLU:HG3	1.92	0.51
3:J:638:SER:OG	3:J:639:VAL:N	2.43	0.51
5:L:250:LEU:O	5:L:254:GLU:HG2	2.10	0.51
5:L:379:MET:HG3	5:L:383:ASN:ND2	2.25	0.51
2:C:1197:GLU:O	2:C:1200:LYS:HB2	2.10	0.51
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.40	0.51
3:D:94:GLN:O	3:D:97:VAL:HG23	2.11	0.51
3:J:342:LEU:N	3:J:344:GLY:HA2	2.26	0.51
2:C:1299:ASN:HD22	2:C:1303:LYS:HE2	1.75	0.51
3:D:748:ALA:O	3:D:777:HIS:CD2	2.63	0.51
3:D:93:THR:HG22	3:D:94:GLN:H	1.74	0.51
5:F:314:THR:O	5:F:318:ALA:HB3	2.11	0.51
2:C:490:GLN:HE21	5:F:472:GLN:NE2	2.09	0.51
5:F:483:LEU:H	5:F:483:LEU:HD12	1.76	0.51
2:I:396:ASP:HA	2:I:418:GLY:O	2.10	0.51
2:I:462:ASN:O	2:I:466:VAL:HG23	2.09	0.51
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.45	0.51
5:L:292:VAL:HA	5:L:297:MET:O	2.11	0.51
3:D:209:ASN:HA	3:D:214:ARG:HE	1.74	0.51
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.75	0.51
3:D:97:VAL:HG11	3:D:101:ARG:NH2	2.26	0.51
2:I:402:ARG:NE	2:I:417:SER:O	2.41	0.51
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.41	0.51
2:I:812:PHE:CE2	3:J:451:PRO:HB3	2.45	0.51
1:A:54:CYS:HB3	1:A:148:ARG:HG3	1.93	0.51
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.35	0.51
3:D:1167:LYS:HZ3	3:D:1170:LYS:HB2	1.75	0.51
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.73	0.51
2:I:499:SER:O	2:I:503:LYS:HB2	2.10	0.51
2:I:62:TYR:C	2:I:64:GLY:H	2.14	0.51
2:I:944:ARG:HE	2:I:948:ILE:HD11	1.76	0.51
3:J:79:LYS:CB	5:L:569:THR:HB	2.41	0.51
2:C:998:LEU:HD12	2:C:998:LEU:H	1.76	0.51
3:D:622:ASP:HB3	3:D:626:TYR:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.75	0.51
5:F:101:TYR:O	5:F:104:GLU:N	2.44	0.51
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.76	0.51
2:C:696:ASP:O	2:C:697:LYS:HB3	2.10	0.51
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.40	0.51
3:J:1173:ARG:HB2	3:J:1192:LYS:HD2	1.93	0.51
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.76	0.51
3:J:827:GLU:HG2	3:J:832:LYS:HD2	1.93	0.51
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.92	0.51
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.10	0.51
2:I:125:GLY:CA	2:I:499:SER:HB2	2.38	0.51
2:I:402:ARG:NH2	2:I:419:ILE:O	2.43	0.51
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.93	0.51
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.26	0.50
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.93	0.50
5:F:572:THR:HG23	5:F:575:GLU:HB2	1.91	0.50
2:I:684:ASN:OD1	2:I:687:ARG:NH1	2.43	0.50
3:J:77:ARG:HG3	3:J:79:LYS:H	1.76	0.50
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.93	0.50
5:F:245:ALA:O	5:F:249:ILE:HG13	2.11	0.50
5:F:292:VAL:HA	5:F:297:MET:O	2.11	0.50
2:I:618:GLN:HG3	2:I:620:ASN:H	1.77	0.50
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.50
3:J:810:THR:HG21	3:J:893:GLY:HA3	1.92	0.50
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	1.92	0.50
1:B:182:ARG:HD3	1:B:206:GLU:OE2	2.11	0.50
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.93	0.50
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.94	0.50
2:C:739:ASP:OD1	2:C:739:ASP:N	2.33	0.50
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.11	0.50
5:F:316:PHE:O	5:F:320:ILE:HG13	2.11	0.50
3:J:846:GLU:HA	3:J:860:ARG:CD	2.41	0.50
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.11	0.50
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.93	0.50
3:D:215:LYS:O	3:D:218:THR:HG22	2.12	0.50
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.92	0.50
2:C:898:GLU:OE2	5:F:541:ARG:NH1	2.44	0.50
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.76	0.50
5:L:316:PHE:CZ	5:L:334:SER:HA	2.44	0.50
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.26	0.50
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.47	0.50
5:F:141:ILE:HG23	5:F:224:LEU:HD11	1.94	0.50
2:I:810:TYR:CD1	2:I:1078:LYS:HB2	2.47	0.50
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.58	0.50
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.92	0.50
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.23	0.50
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.76	0.50
3:D:814:CYS:SG	3:D:895:CYS:SG	3.10	0.50
3:D:903:LEU:HD23	3:D:905:ARG:HD3	1.93	0.50
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.42	0.50
1:H:73:GLY:C	1:H:134:THR:HG22	2.32	0.50
1:H:223:ILE:HA	1:H:226:GLU:HB2	1.94	0.50
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.94	0.50
3:J:270:ARG:NH2	5:L:449:THR:HG23	2.27	0.50
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.27	0.50
2:C:1131:MET:CE	2:C:1141:LEU:HD12	2.42	0.50
1:H:76:GLU:N	1:H:76:GLU:OE1	2.45	0.50
3:J:1221:LEU:HD22	3:J:1221:LEU:O	2.11	0.50
3:J:694:SER:OG	3:J:738:ARG:NE	2.44	0.50
1:A:108:GLY:O	1:A:133:LEU:HB2	2.11	0.50
2:C:658:GLN:O	2:C:660:VAL:N	2.45	0.50
3:D:254:PRO:O	3:D:255:LEU:HD22	2.12	0.50
3:D:518:VAL:HG23	3:D:547:ARG:NH2	2.27	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.94	0.50
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.94	0.50
2:I:468:LEU:O	2:I:471:VAL:HG12	2.12	0.50
2:I:778:GLU:O	2:I:781:ASP:HB2	2.11	0.50
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.76	0.50
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.92	0.50
3:D:623:GLN:O	3:D:627:THR:HG22	2.12	0.50
1:H:35:PHE:HA	1:H:38:THR:HG22	1.94	0.50
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.75	0.50
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.42	0.50
1:B:55:ALA:O	1:B:146:VAL:HG13	2.12	0.49
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.93	0.49
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.30	0.49
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.94	0.49
1:G:45:ARG:HG2	1:H:38:THR:CB	2.35	0.49
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.77	0.49
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	1.94	0.49
2:I:566:GLY:H	2:I:569:ILE:CG1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:281:ARG:O	5:F:285:ARG:HG3	2.12	0.49
1:G:219:ARG:HA	1:G:222:THR:HB	1.94	0.49
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.47	0.49
3:J:362:ARG:H	3:J:365:GLN:NE2	2.09	0.49
5:L:320:ILE:O	5:L:327:SER:HB3	2.12	0.49
5:L:601:PRO:HB3	5:L:608:ARG:HH22	1.77	0.49
1:A:150:ARG:CZ	1:B:8:PHE:HE2	2.20	0.49
2:C:138:ILE:HG22	2:C:139:ASN:N	2.27	0.49
5:F:395:THR:OG1	5:F:396:ASN:N	2.45	0.49
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.95	0.49
2:I:41:GLN:NE2	2:I:73:TYR:O	2.45	0.49
3:D:1297:LYS:HD3	3:J:1302:TYR:CE1	2.47	0.49
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.10	0.49
1:A:73:GLY:O	1:A:134:THR:HG22	2.13	0.49
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.11	0.49
2:C:470:ARG:NE	2:C:497:PRO:HB3	2.27	0.49
2:C:614:TYR:CD1	2:C:652:TYR:CE1	3.01	0.49
2:C:720:ARG:NE	2:C:736:VAL:HG11	2.26	0.49
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.95	0.49
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.94	0.49
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.95	0.49
5:L:343:LYS:HD2	5:L:343:LYS:H	1.77	0.49
5:L:470:MET:HE2	5:L:478:PRO:HB3	1.93	0.49
2:C:115:LYS:HE3	2:C:116:ASP:H	1.78	0.49
2:C:1255:THR:O	2:C:1255:THR:OG1	2.29	0.49
2:C:533:LEU:HB2	6:C:3001:RFP:H143	1.94	0.49
3:D:79:LYS:HD3	5:F:568:ASN:HB3	1.94	0.49
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.12	0.49
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.43	0.49
1:H:110:VAL:HG21	1:H:140:ILE:CD1	2.42	0.49
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.43	0.49
3:J:875:ASN:OD1	3:J:875:ASN:N	2.45	0.49
1:A:197:ASP:O	1:A:198:LEU:HD23	2.12	0.49
1:A:45:ARG:HG3	1:A:46:ILE:HD13	1.94	0.49
2:C:1253:LEU:HD22	2:C:1253:LEU:O	2.13	0.49
2:C:510:GLN:NE2	6:C:3001:RFP:H131	2.23	0.49
2:C:490:GLN:HG2	2:C:491:ASP:N	2.26	0.49
3:D:198:CYS:O	3:D:202:ARG:HG3	2.12	0.49
4:E:79:GLU:O	4:E:83:VAL:HG12	2.12	0.49
2:I:666:SER:OG	2:I:704:MET:HG3	2.12	0.49
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.46	0.49
3:D:152:THR:OG1	3:D:153:ASN:N	2.44	0.49
2:C:844:LYS:HD3	3:D:49:PHE:CE2	2.46	0.49
4:E:32:VAL:O	4:E:34:GLY:N	2.43	0.49
5:F:562:ARG:NH2	5:F:573:LEU:HD22	2.27	0.49
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.95	0.49
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.93	0.49
5:L:139:GLU:HG2	5:L:351:THR:HA	1.93	0.49
1:A:51:MET:HE3	1:A:52:PRO:HD2	1.95	0.49
2:C:607:SER:HB3	2:C:610:GLU:OE1	2.12	0.49
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.28	0.49
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.26	0.49
3:D:849:LEU:HD13	3:D:849:LEU:H	1.77	0.49
5:F:412:LEU:HB2	5:F:435:ILE:HD11	1.95	0.49
2:I:188:PHE:CZ	2:I:194:LEU:HD13	2.48	0.49
2:I:239:MET:O	2:I:284:LEU:HD12	2.13	0.49
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.33	0.49
3:J:1257:VAL:O	3:J:1260:MET:N	2.45	0.49
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.95	0.49
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.93	0.49
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.49
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.43	0.49
2:C:1271:GLY:CA	3:D:343:LEU:HD21	2.26	0.49
3:D:8:LEU:HD22	3:D:9:LYS:O	2.12	0.49
1:H:205:MET:HG2	1:H:206:GLU:N	2.28	0.49
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.95	0.49
3:D:218:THR:HA	3:D:221:ILE:HG22	1.95	0.49
1:H:107:ILE:HG13	1:H:136:GLU:O	2.13	0.49
1:H:192:VAL:HB	1:H:195:ARG:HB2	1.95	0.49
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.46	0.49
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.48	0.49
3:J:362:ARG:H	3:J:365:GLN:HE21	1.61	0.49
3:J:426:ALA:HB3	3:J:427:PRO:HD2	1.84	0.49
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.78	0.49
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.94	0.48
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.95	0.48
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.78	0.48
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.94	0.48
3:J:735:ALA:O	3:J:738:ARG:HB3	2.12	0.48
3:J:888:CYS:HB2	3:J:898:CYS:SG	2.53	0.48
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.43	0.48
1:B:68:TYR:O	1:B:69:SER:OG	2.23	0.48
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.47	0.48
2:C:42:ASP:OD2	2:C:44:GLU:HG2	2.13	0.48
2:C:561:ILE:HD11	2:C:665:ALA:CB	2.43	0.48
2:C:791:LEU:HD23	2:C:791:LEU:HA	1.59	0.48
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.43	0.48
3:D:129:ASP:HB2	3:D:220:ARG:NH2	2.28	0.48
5:F:234:THR:O	5:F:245:ALA:HB2	2.13	0.48
1:H:67:GLU:OE2	1:H:171:LEU:HB2	2.14	0.48
2:I:701:GLY:O	2:I:1184:THR:N	2.30	0.48
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.94	0.48
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.96	0.48
1:B:90:VAL:HG12	1:B:91:ARG:N	2.27	0.48
2:C:316:GLU:H	2:C:316:GLU:CD	2.17	0.48
5:F:601:PRO:CA	5:F:604:SER:HB2	2.41	0.48
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.94	0.48
2:I:1174:GLU:OE2	2:I:1177:ARG:NH1	2.44	0.48
2:I:1238:LEU:H	2:I:1238:LEU:CD1	2.20	0.48
2:I:211:ARG:HD3	2:I:357:ASN:O	2.14	0.48
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.95	0.48
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.27	0.48
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.29	0.48
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.46	0.48
3:J:741:ALA:O	3:J:762:ASN:ND2	2.46	0.48
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.14	0.48
2:C:486:THR:HG23	2:C:487:LEU:H	1.78	0.48
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.94	0.48
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.96	0.48
1:G:49:SER:HG	1:G:50:SER:N	2.10	0.48
2:I:848:GLU:CD	2:I:886:LYS:HZ3	2.12	0.48
2:C:149:LEU:HD13	2:C:453:ILE:CG1	2.44	0.48
2:C:314:ASN:O	2:C:352:ARG:NH1	2.41	0.48
3:D:411:ILE:HG23	3:D:411:ILE:HD12	1.54	0.48
5:F:354:THR:O	5:F:358:VAL:HG23	2.13	0.48
2:I:842:ASP:N	2:I:1045:GLY:O	2.46	0.48
3:J:773:PHE:O	3:J:776:THR:HB	2.13	0.48
5:L:466:ILE:HG22	5:L:470:MET:HG3	1.95	0.48
1:B:214:GLU:O	1:B:218:ARG:HG3	2.14	0.48
2:C:365:GLU:CD	2:C:368:ARG:HH21	2.16	0.48
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:614:TYR:CD1	2:C:652:TYR:HE1	2.31	0.48
3:D:902:ASP:OD1	3:D:903:LEU:N	2.46	0.48
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.96	0.48
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.95	0.48
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.96	0.48
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.94	0.48
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.51	0.48
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.87	0.48
5:F:164:GLY:O	5:F:260:ARG:HB2	2.12	0.48
5:F:244:THR:O	5:F:247:GLU:HG2	2.13	0.48
2:I:1337:ILE:HG21	2:I:1337:ILE:HD13	1.60	0.48
3:J:488:ASN:HD21	4:K:6:VAL:HG22	1.79	0.48
1:B:74:VAL:HG12	1:B:76:GLU:H	1.79	0.48
1:A:150:ARG:CZ	1:B:8:PHE:CD2	2.96	0.48
3:D:314:ARG:NH2	3:D:323:PRO:HG3	2.28	0.48
3:D:515:ARG:CZ	3:D:719:PHE:CE2	2.97	0.48
3:D:888:CYS:HB2	3:D:898:CYS:SG	2.53	0.48
4:E:54:ILE:HD13	4:E:59:ILE:O	2.12	0.48
5:F:292:VAL:HG21	5:F:299:LYS:HG2	1.96	0.48
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.48	0.48
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.95	0.48
5:L:96:ASP:O	5:L:98:VAL:N	2.47	0.48
1:B:90:VAL:HG13	1:B:122:GLU:O	2.13	0.48
2:C:488:MET:O	2:C:490:GLN:N	2.44	0.48
3:D:528:THR:HG22	3:D:532:GLU:CD	2.34	0.48
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.96	0.48
5:F:320:ILE:HG23	5:F:327:SER:O	2.13	0.48
2:I:1077:SER:OG	2:I:1078:LYS:N	2.47	0.48
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.48	0.48
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.95	0.48
2:I:62:TYR:O	2:I:64:GLY:N	2.47	0.48
2:I:721:GLY:N	2:I:740:GLU:OE1	2.37	0.48
3:J:847:ASP:OD1	3:J:847:ASP:N	2.41	0.48
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.94	0.48
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.95	0.48
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.95	0.48
1:A:150:ARG:HD2	1:B:8:PHE:CE2	2.48	0.48
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.44	0.48
3:J:801:VAL:HG12	3:J:920:ALA:HB3	1.96	0.48
5:L:348:GLU:HG2	5:L:354:THR:HA	1.96	0.48
2:C:1238:LEU:HD12	2:C:1238:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.95	0.47
1:H:41:ASN:ND2	2:I:1217:THR:HA	2.29	0.47
2:I:170:VAL:HG23	2:I:171:LEU:N	2.29	0.47
3:J:1347:LEU:HG	3:J:1357:ILE:HG23	1.95	0.47
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.14	0.47
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.49	0.47
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.96	0.47
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.50	0.47
1:H:34:GLY:HA3	2:I:1083:GLU:OE1	2.14	0.47
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.48	0.47
2:I:593:LYS:HA	2:I:652:TYR:CD2	2.49	0.47
3:J:1219:ASP:O	3:J:1222:ARG:N	2.47	0.47
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.96	0.47
1:B:29:GLU:HG3	1:B:30:PRO:CG	2.44	0.47
1:B:73:GLY:O	1:B:134:THR:HG22	2.15	0.47
2:C:1185:PRO:CB	2:C:1188:ASP:HB3	2.43	0.47
2:C:896:THR:HB	2:C:897:PRO:HD2	1.96	0.47
3:D:101:ARG:O	3:D:246:PRO:HG3	2.12	0.47
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.50	0.47
3:D:854:ALA:HB2	3:J:1372:ARG:HE	1.79	0.47
1:H:62:ASP:HB2	1:H:141:SER:O	2.13	0.47
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.46	0.47
2:I:260:LYS:HE3	2:I:262:TYR:CE1	2.49	0.47
2:I:1281:TYR:OH	3:J:431:ARG:O	2.11	0.47
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.76	0.47
3:J:658:GLU:O	3:J:661:VAL:HG13	2.14	0.47
3:J:702:GLN:HG2	3:J:703:THR:N	2.27	0.47
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.96	0.47
1:A:28:LEU:N	1:A:28:LEU:HD12	2.29	0.47
1:B:54:CYS:SG	1:B:92:VAL:HG22	2.54	0.47
2:C:1110:GLY:O	2:C:1113:LEU:N	2.48	0.47
2:C:59:ILE:HD13	2:C:472:GLU:HA	1.96	0.47
3:D:1295:ASN:OD1	3:J:1206:ARG:NH2	2.47	0.47
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.96	0.47
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.27	0.47
2:I:1276:TRP:O	2:I:1279:GLU:N	2.45	0.47
3:J:19:ALA:HB2	3:J:1373:ARG:HH22	1.79	0.47
3:J:568:SER:OG	3:J:569:LEU:N	2.45	0.47
2:C:1337:ILE:O	2:C:1337:ILE:HG23	2.14	0.47
2:C:801:ARG:HD3	2:C:1094:VAL:HA	1.96	0.47
2:C:953:LEU:HD12	2:C:953:LEU:HA	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:992:LEU:HD23	2:C:992:LEU:H	1.79	0.47
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.47	0.47
1:H:101:THR:H	1:H:116:THR:CG2	2.27	0.47
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.97	0.47
3:J:682:VAL:O	3:J:685:ILE:HG12	2.15	0.47
3:J:827:GLU:CG	3:J:832:LYS:HD2	2.44	0.47
1:B:153:VAL:H	1:B:175:ALA:HB3	1.79	0.47
2:C:22:LEU:HD22	2:C:22:LEU:HA	1.55	0.47
3:D:1174:ARG:HG2	3:D:1189:MET:SD	2.55	0.47
3:D:1206:ARG:HB2	3:D:1223:LEU:HD12	1.96	0.47
3:D:461:PHE:HA	3:D:461:PHE:HD2	1.60	0.47
3:D:563:LEU:HD12	3:D:563:LEU:H	1.79	0.47
3:D:896:ALA:O	3:D:908:ILE:HD11	2.15	0.47
1:G:181:GLU:HB3	1:G:206:GLU:HG3	1.95	0.47
3:J:1270:GLY:HA3	3:J:1298:VAL:HG22	1.95	0.47
1:B:29:GLU:HG3	1:B:30:PRO:N	2.30	0.47
2:C:74:ARG:NH2	2:C:97:ARG:HG3	2.30	0.47
4:E:15:ASN:O	4:E:16:ARG:HB3	2.15	0.47
1:H:156:SER:C	1:H:158:ARG:H	2.18	0.47
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.47	0.47
2:I:718:ALA:HB3	2:I:781:ASP:H	1.79	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.97	0.47
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.75	0.47
1:A:172:LEU:H	1:A:172:LEU:HD12	1.79	0.47
2:C:62:TYR:C	2:C:64:GLY:H	2.17	0.47
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.96	0.47
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.97	0.47
5:L:144:LEU:HG	5:L:221:PHE:HE1	1.78	0.47
1:B:57:THR:O	1:B:173:VAL:HG22	2.14	0.47
3:D:1259:GLN:NE2	3:D:1262:ARG:HH12	2.13	0.47
3:D:1344:LEU:HB3	3:D:1350:ASN:HD21	1.79	0.47
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.96	0.47
2:I:980:VAL:O	2:I:984:VAL:HB	2.15	0.47
1:B:89:ALA:O	1:B:124:VAL:HG12	2.14	0.47
1:A:154:PRO:HB2	2:C:1059:ARG:HH21	1.79	0.47
2:C:359:ARG:CZ	2:C:363:LEU:HD11	2.44	0.47
2:C:566:GLY:H	2:C:569:ILE:HD11	1.80	0.47
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.97	0.47
2:I:106:GLU:OE1	2:I:114:VAL:HG22	2.14	0.47
2:I:466:VAL:O	2:I:469:VAL:HG22	2.15	0.47
2:I:836:LEU:HD12	2:I:836:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.39	0.47
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	1.96	0.47
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.80	0.47
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.45	0.47
1:G:19:VAL:HG13	1:G:20:SER:H	1.79	0.47
2:I:211:ARG:NH1	2:I:357:ASN:O	2.48	0.47
2:I:685:MET:HA	2:I:688:GLN:HE21	1.80	0.47
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.30	0.47
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.96	0.47
1:H:182:ARG:NH1	3:J:581:MET:SD	2.88	0.47
1:B:151:GLY:O	1:B:177:TYR:HB2	2.14	0.46
3:D:420:PRO:HA	3:D:437:PHE:O	2.15	0.46
1:G:164:ASP:C	1:G:166:ARG:H	2.18	0.46
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.80	0.46
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.45	0.46
2:I:696:ASP:OD2	2:I:827:ARG:NH2	2.48	0.46
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.19	0.46
3:J:623:GLN:O	3:J:627:THR:HG22	2.15	0.46
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.50	0.46
1:B:11:PRO:HB3	1:B:28:LEU:HD21	1.97	0.46
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.95	0.46
2:C:24:VAL:HG12	2:C:25:PRO:O	2.15	0.46
2:C:62:TYR:O	2:C:64:GLY:N	2.49	0.46
3:D:129:ASP:HB2	3:D:220:ARG:NE	2.29	0.46
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.97	0.46
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.49	0.46
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.69	0.46
2:I:246:LEU:HB3	2:I:269:ILE:HG21	1.97	0.46
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	1.97	0.46
1:A:233:ASP:O	1:A:234:LEU:HD22	2.14	0.46
1:B:19:VAL:O	1:B:20:SER:HB3	2.14	0.46
6:C:3001:RFP:H342	6:C:3001:RFP:H24C	1.67	0.46
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.97	0.46
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.16	0.46
3:D:848:VAL:CG2	3:D:858:VAL:HG13	2.45	0.46
2:I:518:ASN:N	2:I:518:ASN:OD1	2.48	0.46
2:I:530:ILE:O	2:I:572:ILE:HA	2.15	0.46
5:L:246:GLN:HE21	5:L:249:ILE:HD12	1.79	0.46
5:L:372:ALA:O	5:L:376:LYS:HG3	2.16	0.46
2:C:1018:TYR:OH	2:C:1022:LYS:NZ	2.33	0.46
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.16	0.46
2:C:1287:LEU:HD21	3:D:1351:VAL:HG22	1.97	0.46
3:D:255:LEU:HA	3:D:255:LEU:HD13	1.73	0.46
3:D:614:LEU:O	3:D:615:LYS:C	2.52	0.46
1:H:130:ILE:HG22	1:H:131:CYS:SG	2.55	0.46
1:H:172:LEU:H	1:H:172:LEU:HD12	1.80	0.46
1:H:64:VAL:HG11	1:H:69:SER:CB	2.45	0.46
2:I:1132:LEU:HD22	2:I:1177:ARG:CZ	2.46	0.46
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.79	0.46
3:J:657:ALA:O	3:J:661:VAL:HG12	2.15	0.46
3:J:847:ASP:HB3	3:J:856:ILE:HG23	1.98	0.46
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.50	0.46
2:C:158:ASP:OD1	2:C:159:SER:N	2.46	0.46
2:C:596:ASP:O	2:C:648:ASP:OD1	2.33	0.46
3:D:339:ARG:O	3:D:344:GLY:HA2	2.16	0.46
2:I:556:GLY:HA2	2:I:659:GLN:O	2.16	0.46
2:I:981:ALA:O	2:I:1002:LEU:HD11	2.15	0.46
3:J:1160:SER:OG	3:J:1205:GLU:HA	2.15	0.46
3:J:363:LEU:HG	3:J:363:LEU:O	2.15	0.46
3:J:514:THR:CB	3:J:576:ARG:HG2	2.46	0.46
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.98	0.46
1:G:9:LEU:HD21	1:G:195:ARG:NH2	2.31	0.46
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.97	0.46
2:I:801:ARG:O	2:I:1095:ASP:HB2	2.14	0.46
2:I:976:ARG:HB2	2:I:997:TRP:HZ3	1.80	0.46
3:J:1262:ARG:HD2	3:J:1279:GLN:OE1	2.15	0.46
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.97	0.46
3:J:481:ARG:NH1	4:K:3:ARG:O	2.49	0.46
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.42	0.46
2:C:582:ASN:HB3	2:C:586:PHE:N	2.31	0.46
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.97	0.46
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.16	0.46
3:D:1227:HIS:O	3:D:1230:THR:HG22	2.15	0.46
3:D:279:LEU:HD23	3:D:279:LEU:O	2.15	0.46
3:D:362:ARG:H	3:D:365:GLN:NE2	2.12	0.46
3:D:518:VAL:O	3:D:547:ARG:NH1	2.48	0.46
3:D:605:LEU:HA	3:D:605:LEU:HD23	1.49	0.46
3:D:770:LEU:HD12	3:D:770:LEU:HA	1.73	0.46
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.98	0.46
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.97	0.46
2:I:180:ARG:NH2	2:I:396:ASP:HB2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:808:VAL:HG12	3:J:809:VAL:N	2.31	0.46
1:B:11:PRO:HB2	1:B:28:LEU:CG	2.45	0.46
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.97	0.46
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.30	0.46
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.96	0.46
3:D:755:ILE:HD12	3:D:774:ILE:CG2	2.46	0.46
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.65	0.46
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.50	0.46
1:B:11:PRO:CG	1:B:28:LEU:HD21	2.45	0.46
2:C:301:TYR:OH	2:C:333:ILE:HA	2.16	0.46
2:C:557:ARG:O	2:C:576:SER:OG	2.32	0.46
2:C:981:ALA:HB1	2:C:1007:LYS:HZ3	1.81	0.46
3:D:369:PRO:HB3	3:D:444:GLY:O	2.15	0.46
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.50	0.46
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.98	0.46
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.71	0.46
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.56	0.46
2:I:844:LYS:HD3	3:J:49:PHE:CE2	2.50	0.46
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.97	0.46
3:J:488:ASN:ND2	4:K:6:VAL:HG22	2.31	0.46
3:J:709:ARG:O	3:J:711:GLY:N	2.45	0.46
5:L:124:GLU:O	5:L:127:ILE:HG13	2.16	0.46
5:L:470:MET:CE	5:L:478:PRO:HB3	2.46	0.46
1:B:59:VAL:HG12	1:B:61:ILE:HD13	1.96	0.46
3:D:384:LYS:O	3:D:388:ARG:HG3	2.15	0.46
3:D:808:VAL:HG12	3:D:809:VAL:N	2.31	0.46
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.31	0.46
1:H:47:LEU:HA	1:H:47:LEU:HD23	1.78	0.46
2:I:1268:GLN:OE1	3:J:352:ARG:HG2	2.15	0.46
3:J:385:LEU:HA	3:J:385:LEU:HD23	1.66	0.46
3:J:461:PHE:HD2	3:J:461:PHE:HA	1.61	0.46
5:L:585:GLU:O	5:L:589:GLN:HG3	2.16	0.46
1:B:11:PRO:HB2	1:B:28:LEU:CD1	2.44	0.45
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.45	0.45
2:C:61:SER:N	2:C:66:SER:O	2.45	0.45
3:D:1184:ASP:O	3:D:1186:TYR:N	2.49	0.45
5:F:511:ILE:HG23	5:F:511:ILE:O	2.16	0.45
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.98	0.45
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.97	0.45
2:I:136:PHE:O	2:I:143:ARG:N	2.40	0.45
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1328:LYS:O	2:C:1332:SER:N	2.49	0.45
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	1.98	0.45
3:D:185:ILE:HG23	3:D:185:ILE:HD12	1.66	0.45
3:D:252:LEU:HD23	3:D:262:THR:HB	1.97	0.45
3:D:254:PRO:C	3:D:255:LEU:HD22	2.36	0.45
3:D:755:ILE:HD12	3:D:774:ILE:HG23	1.99	0.45
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.98	0.45
1:G:145:LYS:HB3	1:G:145:LYS:HE3	1.73	0.45
1:G:74:VAL:HG22	1:G:76:GLU:H	1.82	0.45
1:H:108:GLY:O	1:H:133:LEU:HB2	2.16	0.45
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.98	0.45
2:I:17:LYS:CE	2:I:1154:ASP:HB3	2.45	0.45
2:I:1238:LEU:HD12	2:I:1238:LEU:N	2.31	0.45
3:J:369:PRO:HB3	3:J:444:GLY:O	2.17	0.45
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.23	0.45
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.81	0.45
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	1.97	0.45
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.45
3:D:1203:ARG:HH22	3:D:1205:GLU:CG	2.28	0.45
3:D:355:ILE:HG21	3:D:355:ILE:HD13	1.73	0.45
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.98	0.45
1:H:90:VAL:HG22	1:H:123:ILE:HD13	1.98	0.45
1:H:22:THR:OG1	1:H:207:THR:O	2.34	0.45
3:J:325:LYS:HG3	3:J:329:ASP:CB	2.45	0.45
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.99	0.45
3:J:785:ASP:O	3:J:789:LYS:HG3	2.17	0.45
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.99	0.45
1:B:28:LEU:HD23	1:B:31:LEU:HD21	1.98	0.45
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.17	0.45
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.82	0.45
2:C:1264:GLN:O	2:C:1264:GLN:HG2	2.16	0.45
2:C:571:LEU:HA	2:C:571:LEU:HD23	1.79	0.45
3:D:351:GLY:O	3:D:352:ARG:HB3	2.16	0.45
3:D:513:MET:HE3	3:D:579:LEU:HD22	1.99	0.45
3:D:708:ASN:N	3:D:708:ASN:OD1	2.45	0.45
3:D:825:VAL:C	3:D:826:ILE:HG13	2.37	0.45
3:D:43:THR:OG1	5:F:449:THR:O	2.29	0.45
1:H:84:ASN:ND2	1:H:129:VAL:O	2.45	0.45
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.51	0.45
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.98	0.45
2:I:312:ALA:HB3	2:I:315:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:577:VAL:HG23	2:I:661:VAL:O	2.16	0.45
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.98	0.45
3:J:849:LEU:HD13	3:J:849:LEU:H	1.81	0.45
5:L:461:ASN:O	5:L:465:ARG:HG2	2.16	0.45
5:L:561:MET:HA	5:L:567:MET:HE1	1.98	0.45
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.32	0.45
2:C:212:ALA:HA	2:C:359:ARG:HG3	1.98	0.45
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.36	0.45
2:C:972:PHE:HB2	2:C:994:ARG:HH21	1.82	0.45
3:D:255:LEU:N	3:D:259:ARG:O	2.48	0.45
3:D:559:ALA:CB	3:D:562:GLU:HB3	2.46	0.45
2:I:1088:ASP:OD1	2:I:1088:ASP:N	2.48	0.45
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.99	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.17	0.45
2:C:796:LEU:HD12	2:C:796:LEU:N	2.32	0.45
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	1.98	0.45
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.81	0.45
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.97	0.45
5:F:299:LYS:O	5:F:303:ILE:HG12	2.16	0.45
5:F:489:MET:CE	5:F:493:LYS:HD2	2.46	0.45
5:F:517:SER:O	5:F:518:HIS:HD2	2.00	0.45
2:I:74:ARG:HG2	2:I:75:LEU:N	2.32	0.45
3:J:1184:ASP:O	3:J:1186:TYR:N	2.50	0.45
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.43	0.45
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.98	0.45
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.75	0.45
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.16	0.45
2:I:564:PRO:CD	2:I:572:ILE:HB	2.47	0.45
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.98	0.45
3:J:860:ARG:HB3	3:J:861:ASN:H	1.67	0.45
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.35	0.45
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.62	0.45
5:L:399:LEU:HB3	5:L:404:LEU:HD21	1.99	0.45
1:B:228:LEU:HA	1:B:228:LEU:HD23	1.43	0.45
2:C:468:LEU:HA	2:C:468:LEU:HD23	1.62	0.45
2:C:468:LEU:O	2:C:471:VAL:HG12	2.16	0.45
2:C:639:LYS:O	2:C:641:GLU:N	2.50	0.45
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.61	0.45
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.99	0.45
1:G:169:GLY:O	1:G:171:LEU:HD22	2.17	0.45
1:H:51:MET:HG3	1:H:52:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:TYR:HD2	2:I:778:GLU:N	2.14	0.45
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.82	0.45
2:I:960:LEU:HD13	2:I:960:LEU:HA	1.82	0.45
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.99	0.45
3:J:701:LEU:CD1	3:J:723:TYR:HB2	2.47	0.45
5:L:233:ASP:O	5:L:236:LYS:HE2	2.17	0.45
5:L:296:LYS:HA	5:L:296:LYS:HD3	1.82	0.45
5:L:375:ALA:O	5:L:378:GLU:HB3	2.16	0.45
2:C:139:ASN:O	2:C:141:THR:N	2.50	0.45
2:C:158:ASP:CG	2:C:159:SER:H	2.21	0.45
2:C:38:PHE:HB2	2:C:457:GLY:HA2	1.99	0.45
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.81	0.45
3:D:429:LEU:HD13	3:D:429:LEU:HA	1.68	0.45
3:D:646:ILE:HG22	3:D:647:PRO:HD2	1.97	0.45
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.31	0.45
1:H:113:ALA:HB2	1:H:126:PRO:HB3	1.99	0.45
2:I:316:GLU:CD	2:I:316:GLU:H	2.20	0.45
2:I:445:ILE:HG22	2:I:446:ASP:OD1	2.17	0.45
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.97	0.45
2:I:761:GLN:O	2:I:762:ASN:HB2	2.17	0.45
3:J:269:TYR:O	3:J:273:ILE:HG13	2.17	0.45
3:J:490:ILE:HG13	3:J:490:ILE:O	2.17	0.45
5:L:603:ARG:H	5:L:603:ARG:HG2	1.45	0.45
2:C:754:THR:O	2:C:755:LYS:HD2	2.17	0.45
3:D:557:LYS:HA	3:D:563:LEU:HA	1.97	0.45
5:F:489:MET:HE3	5:F:493:LYS:HD2	1.98	0.45
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.98	0.45
1:G:45:ARG:NE	2:I:1083:GLU:HB3	2.32	0.45
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.17	0.45
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.98	0.45
2:I:737:ASN:HB3	2:I:739:ASP:OD1	2.15	0.45
2:I:860:ALA:O	2:I:863:SER:OG	2.18	0.45
3:J:232:ASN:HA	3:J:236:TRP:HZ3	1.81	0.45
3:J:93:THR:HG22	3:J:94:GLN:N	2.31	0.45
5:L:132:CYS:O	5:L:136:GLU:HG3	2.17	0.45
1:B:104:LYS:NZ	1:B:114:ASP:OD2	2.30	0.44
1:B:51:MET:HG3	1:B:52:PRO:HD2	1.99	0.44
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.98	0.44
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.52	0.44
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.50	0.44
3:D:93:THR:HG22	3:D:94:GLN:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:ALA:HB3	1:G:231:PHE:CD2	2.51	0.44
2:I:1079:ILE:HG23	2:I:1079:ILE:O	2.17	0.44
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.17	0.44
2:I:596:ASP:OD2	2:I:598:VAL:HG23	2.16	0.44
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.98	0.44
3:J:289:ASP:HA	3:J:292:VAL:HG22	1.99	0.44
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.98	0.44
5:L:476:ARG:HG3	5:L:477:GLU:HG2	1.99	0.44
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.32	0.44
1:A:65:LEU:N	1:A:65:LEU:HD22	2.32	0.44
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.98	0.44
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.98	0.44
3:D:440:VAL:O	3:D:442:ILE:HG12	2.18	0.44
3:D:489:ASN:HA	3:D:904:ALA:HB1	2.00	0.44
2:I:10:ARG:CZ	2:I:697:LYS:HD3	2.47	0.44
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.99	0.44
5:L:292:VAL:HG21	5:L:299:LYS:HG2	1.99	0.44
5:L:518:HIS:O	5:L:521:ASP:N	2.44	0.44
1:A:61:ILE:HB	1:A:64:VAL:HG23	1.99	0.44
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.18	0.44
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.17	0.44
2:C:49:LEU:HD12	2:C:73:TYR:CE2	2.51	0.44
2:C:818:VAL:O	2:C:1079:ILE:HD12	2.17	0.44
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.32	0.44
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.99	0.44
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.16	0.44
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.53	0.44
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.82	0.44
3:D:543:SER:OG	3:D:544:LEU:N	2.51	0.44
1:H:79:LEU:O	1:H:82:LEU:HB2	2.17	0.44
2:I:159:SER:HB2	2:I:442:VAL:HG11	1.98	0.44
2:I:739:ASP:N	2:I:739:ASP:OD1	2.51	0.44
2:C:66:SER:HB2	2:C:479:LEU:HB3	1.98	0.44
2:C:886:LYS:CE	2:C:916:SER:HB3	2.44	0.44
3:D:211:GLU:OE2	3:D:214:ARG:NH1	2.50	0.44
3:D:516:ASP:OD1	3:D:516:ASP:N	2.50	0.44
5:F:148:TYR:HB2	5:F:221:PHE:CE1	2.53	0.44
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.82	0.44
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.99	0.44
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.98	0.44
1:A:195:ARG:HG2	1:A:198:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1005:GLU:OE1	2:C:1007:LYS:HD2	2.17	0.44
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.81	0.44
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.73	0.44
3:D:239:LEU:HD23	3:D:239:LEU:HA	1.77	0.44
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.52	0.44
3:D:528:THR:HG22	3:D:532:GLU:OE1	2.18	0.44
1:G:191:ARG:NH1	1:G:197:ASP:HA	2.32	0.44
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.99	0.44
2:I:1059:ARG:O	2:I:1234:LYS:NZ	2.51	0.44
3:J:334:LYS:HA	3:J:335:GLN:HA	1.64	0.44
3:J:681:LYS:O	3:J:685:ILE:HG23	2.17	0.44
3:J:845:ALA:CB	3:J:881:LYS:HD2	2.48	0.44
5:L:348:GLU:HA	5:L:353:LEU:O	2.18	0.44
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.99	0.44
2:C:1236:ASN:C	2:C:1237:HIS:HD1	2.16	0.44
2:C:1290:MET:SD	2:C:1294:LYS:HE3	2.57	0.44
2:C:805:MET:HG3	2:C:805:MET:O	2.17	0.44
2:C:985:GLU:HB3	2:C:988:LYS:HD2	2.00	0.44
3:D:1280:VAL:CG2	3:D:1304:ARG:HE	2.23	0.44
3:D:514:THR:OG1	3:D:594:GLN:O	2.36	0.44
3:D:650:LYS:HE2	3:D:654:ILE:HD11	2.00	0.44
4:E:53:GLU:OE1	4:E:59:ILE:HG13	2.17	0.44
1:H:182:ARG:H	1:H:206:GLU:HB2	1.82	0.44
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.47	0.44
2:I:1142:ARG:HD3	2:I:1161:LEU:CD1	2.47	0.44
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.18	0.44
2:I:5:TYR:CD2	2:I:778:GLU:HB2	2.53	0.44
3:J:19:ALA:O	3:J:20:ILE:HG13	2.17	0.44
3:J:839:VAL:HG12	3:J:839:VAL:O	2.16	0.44
2:C:891:GLY:O	2:C:892:GLU:HG3	2.18	0.44
3:D:1175:LEU:HA	3:D:1175:LEU:HD12	1.91	0.44
3:D:495:ASN:OD1	3:D:495:ASN:N	2.48	0.44
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.70	0.44
5:F:512:GLY:O	5:F:514:ASP:N	2.51	0.44
2:I:1038:GLN:HG3	2:I:1038:GLN:O	2.17	0.44
2:I:818:VAL:HG22	2:I:1096:ILE:HG23	1.99	0.44
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.99	0.44
2:I:593:LYS:HD3	2:I:652:TYR:CZ	2.52	0.44
3:J:239:LEU:HD23	3:J:239:LEU:HA	1.79	0.44
3:J:411:ILE:HG23	3:J:411:ILE:HD12	1.65	0.44
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASP:HB3	1:A:121:VAL:HG23	2.00	0.44
1:B:46:ILE:HD13	1:B:46:ILE:HG21	1.71	0.44
2:C:138:ILE:O	2:C:139:ASN:ND2	2.51	0.44
2:C:518:ASN:O	2:C:691:PRO:HD3	2.18	0.44
2:C:722:GLY:HA2	2:C:737:ASN:OD1	2.18	0.44
3:D:746:LEU:HD22	3:D:754:ILE:HD11	2.00	0.44
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.00	0.44
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.47	0.44
1:G:182:ARG:H	1:G:206:GLU:HB3	1.83	0.44
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.32	0.44
2:I:169:LYS:HE2	2:I:190:PRO:O	2.18	0.44
2:I:720:ARG:HH21	2:I:736:VAL:HG11	1.82	0.44
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	2.30	0.44
3:J:361:LEU:HD22	3:J:365:GLN:HG3	2.00	0.44
3:J:698:MET:O	3:J:702:GLN:HB3	2.18	0.44
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.32	0.44
3:J:97:VAL:HG11	3:J:101:ARG:CZ	2.48	0.44
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.98	0.44
3:J:487:THR:OG1	4:K:4:VAL:O	2.24	0.44
3:J:42:GLU:HG3	5:L:451:ARG:HE	1.83	0.44
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.99	0.44
3:D:1155:ILE:HD13	3:D:1190:ILE:HD13	1.99	0.44
3:D:268:LEU:HG	3:D:324:LEU:HD22	2.00	0.44
3:D:334:LYS:HA	3:D:335:GLN:HA	1.58	0.44
3:D:568:SER:OG	3:D:569:LEU:N	2.51	0.44
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.99	0.44
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.83	0.44
2:I:62:TYR:CZ	2:I:476:LYS:HB3	2.53	0.44
3:J:248:ASP:O	3:J:251:PRO:HG3	2.18	0.44
3:J:481:ARG:O	3:J:485:MET:HB2	2.17	0.44
3:J:557:LYS:HA	3:J:563:LEU:HA	1.99	0.44
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.98	0.44
3:J:79:LYS:HB3	5:L:569:THR:HB	2.00	0.44
2:C:985:GLU:HB3	2:C:988:LYS:HB2	2.00	0.43
3:D:333:GLY:HA3	3:D:338:PHE:CZ	2.53	0.43
3:D:392:THR:HG21	5:F:606:VAL:HA	2.00	0.43
3:D:740:LEU:HD12	3:D:740:LEU:HA	1.40	0.43
3:D:810:THR:HG23	3:D:811:GLU:H	1.82	0.43
4:E:59:ILE:HD13	4:E:59:ILE:HA	1.81	0.43
5:F:288:MET:HA	5:F:302:PHE:CZ	2.53	0.43
2:I:301:TYR:CE2	2:I:333:ILE:HA	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:ASP:OD2	2:I:44:GLU:HG2	2.18	0.43
3:J:351:GLY:O	3:J:352:ARG:HB3	2.18	0.43
1:A:77:ASP:O	1:A:80:GLU:N	2.51	0.43
1:A:86:LYS:HB2	1:A:86:LYS:HE3	1.77	0.43
2:C:668:ILE:HD13	2:C:668:ILE:HG21	1.64	0.43
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.18	0.43
3:D:612:LEU:HB3	3:D:616:PRO:HG2	2.00	0.43
3:D:708:ASN:HB3	3:D:712:GLN:O	2.18	0.43
3:D:805:GLN:O	3:D:807:LEU:N	2.51	0.43
1:G:154:PRO:HA	1:G:174:ASP:HB3	2.01	0.43
1:H:228:LEU:HD23	1:H:228:LEU:HA	1.62	0.43
1:H:47:LEU:HD21	1:H:220:ALA:HB2	2.00	0.43
2:I:12:ARG:HG2	2:I:1183:ALA:HB2	1.99	0.43
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.33	0.43
3:J:1347:LEU:HD12	3:J:1358:PRO:HG2	2.00	0.43
3:J:140:TYR:O	3:J:297:ARG:NH1	2.47	0.43
3:J:146:VAL:HG23	3:J:158:GLN:O	2.18	0.43
3:J:805:GLN:O	3:J:807:LEU:N	2.50	0.43
1:B:140:ILE:HG23	1:B:140:ILE:O	2.18	0.43
1:B:49:SER:O	1:B:151:GLY:HA2	2.17	0.43
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.53	0.43
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	1.99	0.43
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	2.00	0.43
3:D:1262:ARG:HD2	3:D:1279:GLN:NE2	2.34	0.43
3:D:355:ILE:HD12	3:D:449:LEU:HD23	2.00	0.43
3:D:45:ASN:O	3:D:46:TYR:HD2	2.01	0.43
1:G:231:PHE:HB3	1:H:218:ARG:NH1	2.18	0.43
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.80	0.43
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.34	0.43
2:I:810:TYR:CE1	2:I:1078:LYS:HB2	2.53	0.43
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.33	0.43
3:J:377:PHE:CD2	3:J:416:ILE:HD11	2.53	0.43
3:J:514:THR:HG23	3:J:596:LEU:HB2	2.00	0.43
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.49	0.43
3:J:518:VAL:HG11	3:J:707:ILE:HD13	2.00	0.43
1:A:90:VAL:HG22	1:A:91:ARG:H	1.83	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.99	0.43
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.00	0.43
2:C:397:LEU:HD12	2:C:397:LEU:N	2.33	0.43
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.99	0.43
3:D:1290:ARG:HD3	3:D:1294:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:484:ALA:HB1	5:F:491:GLU:HG3	2.00	0.43
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.53	0.43
1:G:166:ARG:O	1:G:168:ILE:HG23	2.19	0.43
2:I:448:LEU:HG	2:I:553:THR:OG1	2.19	0.43
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.00	0.43
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.99	0.43
3:J:905:ARG:HH21	3:J:907:HIS:HB3	1.81	0.43
1:B:47:LEU:O	1:B:180:VAL:HG21	2.19	0.43
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	2.01	0.43
2:C:208:ILE:HD11	2:C:365:GLU:HB3	2.00	0.43
2:C:82:VAL:HG22	2:C:92:TYR:CZ	2.53	0.43
3:D:1179:PRO:CD	3:D:1184:ASP:HA	2.48	0.43
3:D:18:ASP:HB2	3:D:1373:ARG:CZ	2.47	0.43
3:D:384:LYS:NZ	3:D:414:GLU:OE1	2.51	0.43
3:D:670:SER:HB2	3:D:672:LEU:HD13	1.99	0.43
2:I:1077:SER:HA	3:J:356:THR:OG1	2.18	0.43
2:I:384:LEU:O	2:I:388:LEU:HG	2.19	0.43
2:I:494:ASN:HB3	2:I:497:PRO:HD2	2.00	0.43
3:J:536:LEU:HD12	3:J:542:ALA:HB2	2.00	0.43
5:L:353:LEU:HD13	5:L:361:ILE:HD12	2.00	0.43
5:L:388:ILE:O	5:L:392:LYS:HG3	2.18	0.43
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.99	0.43
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.50	0.43
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.00	0.43
2:C:735:LYS:HA	2:C:748:ILE:HG22	2.00	0.43
2:C:738:GLU:HG2	2:C:741:MET:CE	2.48	0.43
3:D:9:LYS:HG2	3:D:10:ALA:N	2.34	0.43
3:D:860:ARG:HB3	3:D:861:ASN:H	1.70	0.43
5:F:145:LEU:HD13	5:F:225:ARG:NH2	2.33	0.43
5:F:333:VAL:HG13	5:F:337:VAL:HG23	2.00	0.43
1:H:95:LYS:HG3	1:H:120:ASP:OD2	2.18	0.43
2:I:197:ARG:NH1	2:I:201:ARG:O	2.43	0.43
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.46	0.43
2:I:854:ILE:O	2:I:857:VAL:HG22	2.18	0.43
3:J:138:VAL:HG21	3:J:145:VAL:HB	2.00	0.43
2:I:1283:ALA:HB1	3:J:479:GLU:OE2	2.19	0.43
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.52	0.43
2:C:1299:ASN:O	2:C:1300:GLY:C	2.56	0.43
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.54	0.43
2:C:796:LEU:O	2:C:1233:LEU:HD12	2.19	0.43
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:297:MET:HG3	5:F:326:TRP:HB2	2.01	0.43
1:G:161:SER:O	1:G:163:GLU:HG3	2.18	0.43
1:G:38:THR:OG1	1:H:45:ARG:HD3	2.19	0.43
1:G:82:LEU:HD23	1:G:82:LEU:HA	1.64	0.43
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	2.01	0.43
2:I:115:LYS:HE3	2:I:116:ASP:H	1.84	0.43
3:J:317:THR:CG2	3:J:320:ASN:HB3	2.48	0.43
3:J:475:GLU:OE1	4:K:28:ARG:NH1	2.50	0.43
5:L:482:GLU:O	5:L:486:ARG:NH2	2.52	0.43
5:L:606:VAL:HG13	5:L:607:LEU:HD12	2.00	0.43
1:A:102:LEU:HD23	1:A:115:ILE:HA	2.00	0.43
1:A:115:ILE:HG22	1:A:116:THR:H	1.84	0.43
2:C:1270:PHE:C	3:D:343:LEU:HD11	2.39	0.43
2:C:2:VAL:HG13	2:C:1158:LYS:HZ1	1.84	0.43
2:C:903:ARG:O	2:C:907:GLY:N	2.51	0.43
2:C:943:LYS:HG2	2:C:947:GLU:OE1	2.18	0.43
3:D:368:LEU:HD22	3:D:373:ALA:HB2	2.01	0.43
3:D:856:ILE:HG21	3:D:856:ILE:HD13	1.72	0.43
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.19	0.43
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.66	0.43
1:G:75:GLN:HA	2:I:729:ALA:N	2.34	0.43
2:I:619:ALA:HB1	2:I:657:THR:HA	1.99	0.43
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.34	0.43
3:J:368:LEU:HD22	3:J:373:ALA:HB2	2.01	0.43
3:J:440:VAL:O	3:J:442:ILE:HG12	2.19	0.43
3:J:641:ILE:O	3:J:641:ILE:HD13	2.18	0.43
1:A:10:LYS:HA	1:B:227:GLN:HE22	1.81	0.43
1:B:118:ASP:H	1:B:121:VAL:HB	1.83	0.43
1:B:182:ARG:H	1:B:206:GLU:HB2	1.83	0.43
2:C:28:LEU:HA	2:C:28:LEU:HD23	1.65	0.43
2:C:389:PHE:HB3	2:C:420:LEU:HD12	2.00	0.43
2:C:960:LEU:HD11	2:C:1028:LYS:HE2	2.01	0.43
3:D:872:LEU:HD22	3:D:877:VAL:HG11	2.01	0.43
3:D:901:ARG:HD2	3:D:906:GLY:O	2.18	0.43
1:H:125:LYS:HE2	1:H:128:HIS:HB2	2.01	0.43
1:H:22:THR:O	1:H:213:PRO:HG3	2.19	0.43
2:I:806:PRO:HD3	2:I:1100:PRO:HG2	2.01	0.43
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.19	0.43
3:J:521:LYS:HE3	3:J:541:LEU:O	2.19	0.43
3:J:526:VAL:HA	3:J:549:LYS:O	2.19	0.43
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.79	0.43
2:C:644:LEU:HD13	2:C:644:LEU:HA	1.79	0.43
2:C:75:LEU:HD13	2:C:75:LEU:HA	1.84	0.43
3:D:1230:THR:O	3:D:1234:VAL:HG22	2.18	0.43
3:D:930:LEU:CD2	3:D:1244:GLN:HG3	2.42	0.43
3:D:341:ASN:O	3:D:343:LEU:HA	2.19	0.43
3:D:500:ILE:O	3:D:500:ILE:HG22	2.19	0.43
3:D:744:ARG:O	3:D:759:ILE:HB	2.18	0.43
1:G:172:LEU:N	1:G:172:LEU:HD12	2.34	0.43
1:H:74:VAL:HG22	1:H:132:HIS:O	2.19	0.43
2:I:1137:GLU:HG3	2:I:1139:ALA:H	1.83	0.43
3:J:425:ARG:HG2	3:J:426:ALA:N	2.33	0.43
3:J:369:PRO:HA	3:J:442:ILE:O	2.19	0.43
3:J:69:GLU:HG3	3:J:76:LYS:HA	2.00	0.43
3:J:801:VAL:O	3:J:805:GLN:HB2	2.19	0.43
5:L:354:THR:N	5:L:357:GLN:OE1	2.51	0.43
5:L:360:ASP:O	5:L:363:ARG:HB3	2.18	0.43
2:C:145:ILE:CG2	2:C:456:VAL:HG22	2.48	0.42
2:C:233:ARG:HH12	2:C:332:ARG:HH12	1.66	0.42
2:C:533:LEU:HA	2:C:533:LEU:HD23	1.75	0.42
2:C:980:VAL:HA	2:C:984:VAL:HA	2.01	0.42
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.60	0.42
3:D:412:LEU:HA	3:D:415:VAL:HG22	2.00	0.42
3:D:559:ALA:HB3	3:D:562:GLU:O	2.19	0.42
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.52	0.42
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.01	0.42
2:I:1333:LEU:HD22	3:J:307:LEU:HD22	2.01	0.42
5:L:584:ARG:NH1	5:L:584:ARG:HA	2.34	0.42
1:A:185:TYR:HE1	2:C:1087:TYR:HH	1.67	0.42
2:C:169:LYS:O	2:C:169:LYS:HG2	2.19	0.42
6:C:3001:RFP:O4	6:C:3001:RFP:O12	2.37	0.42
2:C:544:GLY:O	2:C:548:ARG:HG3	2.19	0.42
3:D:1280:VAL:HG21	3:D:1304:ARG:CD	2.49	0.42
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.52	0.42
3:D:34:SER:HB2	3:D:104:HIS:HB3	2.01	0.42
5:F:134:VAL:HG12	5:F:256:PHE:CE2	2.54	0.42
2:I:1066:MET:HE1	2:I:1076:ILE:HB	2.01	0.42
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.84	0.42
2:C:1132:LEU:HD22	2:C:1177:ARG:CZ	2.48	0.42
2:C:132:ASP:N	2:C:132:ASP:OD1	2.34	0.42
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:HD22	1:H:173:VAL:CG1	2.50	0.42
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.01	0.42
3:J:1150:PRO:HG2	3:J:1153:PRO:HG3	2.02	0.42
3:J:1322:ALA:HB1	3:J:1326:GLN:NE2	2.34	0.42
3:J:804:ALA:O	3:J:806:ASP:N	2.52	0.42
1:B:44:ARG:HG3	1:B:183:ILE:HG22	2.00	0.42
1:B:64:VAL:HG11	1:B:69:SER:CB	2.47	0.42
2:C:702:THR:HA	2:C:1184:THR:O	2.18	0.42
3:D:1256:ILE:HD13	3:D:1256:ILE:HA	1.77	0.42
3:D:153:ASN:HB2	3:D:172:PHE:CZ	2.55	0.42
3:D:601:ILE:HG21	3:D:601:ILE:HD13	1.66	0.42
5:F:457:ILE:H	5:F:457:ILE:HG13	1.64	0.42
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.52	0.42
2:I:68:LEU:HD11	2:I:100:LEU:HB3	2.00	0.42
2:I:968:GLU:CG	2:I:1018:TYR:HE1	2.31	0.42
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.54	0.42
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.94	0.42
2:I:565:GLU:HB2	2:I:680:LEU:HD21	2.01	0.42
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.85	0.42
2:I:1281:TYR:CZ	3:J:431:ARG:O	2.72	0.42
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	2.01	0.42
3:J:474:LEU:HA	3:J:477:GLN:HG3	2.01	0.42
1:A:196:THR:OG1	1:A:197:ASP:N	2.52	0.42
1:B:153:VAL:HB	1:B:175:ALA:CB	2.50	0.42
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	2.00	0.42
2:C:341:LEU:HD23	2:C:341:LEU:HA	1.83	0.42
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.49	0.42
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.54	0.42
3:D:1357:ILE:HG21	3:D:1357:ILE:HD13	1.63	0.42
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.55	0.42
3:D:475:GLU:N	3:D:475:GLU:OE1	2.45	0.42
3:D:702:GLN:HG2	3:D:703:THR:N	2.30	0.42
3:D:808:VAL:HG13	3:D:913:GLU:O	2.19	0.42
2:I:1136:GLN:O	2:I:1137:GLU:HB3	2.19	0.42
2:I:122:VAL:HG11	2:I:493:ILE:HG21	2.02	0.42
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.65	0.42
2:I:607:SER:N	2:I:610:GLU:OE1	2.48	0.42
3:J:418:GLU:HG3	4:K:45:LYS:N	2.25	0.42
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.49	0.42
5:L:289:LYS:HA	5:L:293:GLU:OE1	2.20	0.42
1:B:112:ALA:O	1:B:115:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:3001:RFP:H22C	6:C:3001:RFP:H333	1.89	0.42
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.85	0.42
3:D:875:ASN:OD1	3:D:875:ASN:N	2.52	0.42
2:I:65:ASN:HB3	2:I:105:TYR:HD2	1.84	0.42
2:I:1211:ARG:HD3	2:I:1213:TYR:OH	2.19	0.42
2:I:1248:THR:HG21	5:L:531:PRO:CG	2.49	0.42
3:J:1167:LYS:HD3	3:J:1174:ARG:HH11	1.84	0.42
5:L:357:GLN:HG3	5:L:357:GLN:H	1.67	0.42
2:C:1220:GLN:HG2	2:C:1221:PHE:H	1.84	0.42
3:D:139:LEU:HD23	3:D:139:LEU:HA	1.79	0.42
3:D:574:VAL:O	3:D:577:ALA:HB3	2.20	0.42
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.50	0.42
4:E:36:ASP:HB2	4:E:37:PRO:HD2	2.02	0.42
5:F:110:LEU:HD21	5:F:385:ARG:HD2	2.02	0.42
5:F:111:LEU:HD11	5:F:119:ILE:HD12	2.01	0.42
5:F:481:GLU:O	5:F:484:ALA:HB3	2.20	0.42
1:G:29:GLU:OE1	1:G:200:LYS:HE2	2.19	0.42
1:H:47:LEU:HD22	1:H:180:VAL:HG11	2.01	0.42
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.55	0.42
2:I:736:VAL:HG23	2:I:748:ILE:HA	2.01	0.42
2:I:94:ALA:HB2	2:I:129:LEU:HD11	2.01	0.42
2:I:985:GLU:HG2	2:I:988:LYS:HD2	2.00	0.42
3:J:510:LEU:HA	3:J:513:MET:HB2	2.02	0.42
3:J:810:THR:HG22	3:J:893:GLY:HA3	2.01	0.42
5:L:320:ILE:HG23	5:L:327:SER:O	2.19	0.42
5:L:383:ASN:HB2	5:L:412:LEU:HD21	2.01	0.42
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.71	0.42
2:C:161:LYS:HA	2:C:170:VAL:HA	2.02	0.42
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.55	0.42
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.84	0.42
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	2.01	0.42
3:D:185:ILE:HA	3:D:185:ILE:HD13	1.84	0.42
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.02	0.42
3:D:600:ALA:O	3:D:603:LYS:HG2	2.20	0.42
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.59	0.42
2:I:98:VAL:C	2:I:121:GLU:HA	2.40	0.42
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.79	0.42
3:J:493:PRO:O	3:J:1252:HIS:NE2	2.43	0.42
5:L:288:MET:HA	5:L:302:PHE:CZ	2.55	0.42
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.81	0.42
2:C:557:ARG:HH21	2:C:608:ALA:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.35	0.42
3:D:279:LEU:HD11	3:D:296:LYS:CG	2.49	0.42
3:D:332:LYS:HG2	3:D:333:GLY:H	1.84	0.42
3:D:356:THR:OG1	3:D:357:VAL:N	2.51	0.42
3:D:412:LEU:HA	3:D:415:VAL:CG2	2.50	0.42
5:F:525:ASP:OD2	5:F:528:LEU:HG	2.19	0.42
1:H:116:THR:HG23	1:H:116:THR:O	2.19	0.42
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	2.02	0.42
2:I:344:GLY:HA3	2:I:346:TYR:CE2	2.55	0.42
3:J:1285:VAL:O	3:J:1289:ASN:HB3	2.20	0.42
3:J:513:MET:HE3	3:J:579:LEU:HD22	2.01	0.42
3:J:513:MET:O	3:J:575:GLY:HA3	2.20	0.42
3:J:62:PHE:O	3:J:101:ARG:HD2	2.20	0.42
3:J:824:PRO:HD3	3:J:835:LEU:HD13	2.02	0.42
1:B:205:MET:HG2	1:B:206:GLU:N	2.34	0.42
2:C:1256:GLN:OE1	5:F:528:LEU:HD11	2.20	0.42
2:C:22:LEU:HD13	2:C:23:ASP:N	2.35	0.42
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.50	0.42
3:D:846:GLU:HA	3:D:860:ARG:CD	2.50	0.42
3:D:842:ARG:HD3	3:D:882:VAL:HG11	2.02	0.42
1:G:167:PRO:HB2	1:G:170:ARG:HB2	2.01	0.42
2:I:1069:ARG:HH21	2:I:1114:GLU:CD	2.23	0.42
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.19	0.42
2:I:149:LEU:HD13	2:I:453:ILE:HG12	2.02	0.42
2:I:405:PHE:CZ	2:I:424:ASP:HB3	2.55	0.42
2:I:149:LEU:HD13	2:I:453:ILE:CG1	2.50	0.42
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.86	0.42
4:K:26:ARG:NH1	4:K:35:LYS:HD2	2.35	0.42
1:B:79:LEU:O	1:B:82:LEU:HB2	2.19	0.41
2:C:1077:SER:OG	2:C:1078:LYS:N	2.52	0.41
2:C:513:GLN:HB2	6:C:3001:RFP:O9	2.19	0.41
2:C:211:ARG:HD3	2:C:357:ASN:O	2.20	0.41
2:C:617:ALA:HB3	2:C:653:MET:CB	2.50	0.41
3:D:238:ILE:HD13	3:D:238:ILE:HA	1.82	0.41
3:D:491:LEU:HD23	3:D:498:PRO:HA	2.01	0.41
3:D:701:LEU:HD22	3:D:701:LEU:HA	1.83	0.41
3:D:796:LEU:HA	3:D:796:LEU:HD12	1.71	0.41
5:F:233:ASP:O	5:F:236:LYS:HE2	2.20	0.41
5:F:445:ASP:OD2	5:F:451:ARG:HD2	2.20	0.41
1:G:73:GLY:C	1:G:134:THR:HG22	2.40	0.41
1:G:36:GLY:C	1:G:187:VAL:HG11	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:593:LYS:HB3	2:I:602:GLU:CG	2.50	0.41
1:H:33:ARG:NH2	2:I:820:GLU:OE2	2.52	0.41
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	2.02	0.41
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.75	0.41
3:J:433:GLY:O	3:J:457:TYR:HE1	2.03	0.41
1:A:208:ASN:N	1:A:208:ASN:OD1	2.52	0.41
1:B:47:LEU:HD13	1:B:183:ILE:HG12	2.03	0.41
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.85	0.41
2:C:141:THR:O	2:C:143:ARG:HG3	2.20	0.41
3:D:1256:ILE:HD12	3:D:1256:ILE:HG23	1.70	0.41
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.20	0.41
3:D:541:LEU:HA	3:D:541:LEU:HD23	1.84	0.41
3:D:616:PRO:O	3:D:620:PHE:HB2	2.19	0.41
5:F:499:LYS:HE3	5:F:499:LYS:HB2	1.89	0.41
1:G:207:THR:HG22	1:G:208:ASN:N	2.35	0.41
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.35	0.41
2:I:1314:GLN:HG2	4:K:28:ARG:NH2	2.35	0.41
2:I:27:LEU:HD23	2:I:27:LEU:HA	1.87	0.41
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.01	0.41
2:C:1339:LEU:H	2:C:1339:LEU:HD12	1.85	0.41
2:C:221:LEU:HB3	2:C:336:LEU:HD21	2.02	0.41
2:C:298:ALA:HB3	2:C:334:GLU:HB2	2.01	0.41
2:C:867:GLU:H	2:C:867:GLU:HG3	1.69	0.41
3:D:694:SER:OG	3:D:738:ARG:NE	2.50	0.41
3:D:768:ASN:OD1	3:D:771:GLN:HG3	2.21	0.41
3:D:800:LEU:O	3:D:803:VAL:HG12	2.21	0.41
3:D:88:CYS:O	3:D:88:CYS:SG	2.79	0.41
2:I:692:THR:OG1	2:I:693:LEU:N	2.52	0.41
2:I:850:ILE:O	2:I:850:ILE:HG22	2.20	0.41
3:J:1154:ALA:N	3:J:1214:PRO:O	2.44	0.41
3:J:536:LEU:HD13	3:J:541:LEU:HB2	2.01	0.41
4:K:29:GLN:CD	4:K:35:LYS:HE2	2.40	0.41
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.50	0.41
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.35	0.41
2:C:814:ASP:CG	2:C:1106:ARG:HH12	2.19	0.41
2:C:1248:THR:HB	5:F:532:LEU:CD1	2.50	0.41
2:C:42:ASP:O	2:C:44:GLU:N	2.50	0.41
2:C:149:LEU:HD13	2:C:453:ILE:HG12	2.02	0.41
2:C:820:GLU:HA	2:C:1079:ILE:HD11	2.02	0.41
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.01	0.41
3:D:16:GLU:HG3	3:D:1369:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.02	0.41
3:D:788:LEU:HA	3:D:788:LEU:HD12	1.83	0.41
3:D:905:ARG:HH21	3:D:907:HIS:CG	2.38	0.41
5:F:341:LEU:HD23	5:F:344:LEU:HD23	2.02	0.41
5:F:580:PHE:HD1	5:F:580:PHE:HA	1.69	0.41
1:H:31:LEU:HB2	1:H:199:ASP:O	2.20	0.41
2:I:557:ARG:HH21	2:I:607:SER:C	2.23	0.41
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.56	0.41
2:I:992:LEU:HD23	2:I:992:LEU:H	1.85	0.41
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	2.02	0.41
3:J:139:LEU:HD23	3:J:139:LEU:HA	1.86	0.41
2:C:13:LYS:HD2	2:C:14:ASP:N	2.36	0.41
2:C:569:ILE:HD13	2:C:569:ILE:HG21	1.84	0.41
2:C:59:ILE:O	2:C:68:LEU:N	2.32	0.41
3:D:1151:LYS:C	3:D:1153:PRO:HD3	2.41	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.86	0.41
3:D:279:LEU:HD23	3:D:279:LEU:C	2.41	0.41
3:D:42:GLU:HG3	5:F:451:ARG:HE	1.85	0.41
2:C:545:PHE:CZ	3:D:781:LYS:HA	2.55	0.41
1:G:69:SER:O	1:G:78:ILE:HG12	2.21	0.41
2:I:819:SER:HB2	2:I:1085:MET:CG	2.50	0.41
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.01	0.41
3:J:34:SER:OG	3:J:104:HIS:ND1	2.30	0.41
3:J:1198:VAL:HB	3:J:1210:ILE:HA	2.03	0.41
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.18	0.41
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.35	0.41
3:J:141:PHE:HA	3:J:180:MET:HE2	2.02	0.41
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.55	0.41
3:J:429:LEU:HD13	3:J:429:LEU:HA	1.87	0.41
3:J:647:PRO:HG3	3:J:697:MET:N	2.36	0.41
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.56	0.41
1:A:207:THR:HG22	1:A:208:ASN:N	2.35	0.41
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.84	0.41
2:C:71:VAL:HG21	2:C:118:LYS:HE2	2.01	0.41
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.01	0.41
3:D:124:ILE:HG13	3:D:124:ILE:H	1.72	0.41
3:D:706:VAL:HG12	3:D:715:LYS:HB3	2.03	0.41
3:D:610:ARG:HG2	3:D:866:GLU:CD	2.41	0.41
5:F:512:GLY:C	5:F:514:ASP:H	2.24	0.41
1:G:142:MET:SD	1:G:144:ILE:HD11	2.61	0.41
1:G:47:LEU:HD23	1:G:47:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:585:LYS:HD3	3:J:585:LYS:HA	1.84	0.41
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.55	0.41
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.21	0.41
3:J:478:LEU:HD21	4:K:47:THR:O	2.21	0.41
5:L:316:PHE:O	5:L:320:ILE:HG13	2.20	0.41
5:L:343:LYS:O	5:L:347:ILE:HG13	2.21	0.41
1:B:118:ASP:HB2	1:B:121:VAL:CG2	2.51	0.41
1:B:11:PRO:HG3	1:B:28:LEU:HD21	2.02	0.41
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.50	0.41
2:C:119:GLU:HB2	2:C:489:PRO:HB2	2.01	0.41
2:C:1217:THR:OG1	2:C:1219:GLU:HG2	2.20	0.41
2:C:1271:GLY:HA2	3:D:343:LEU:HG	2.02	0.41
2:C:34:SER:O	2:C:37:LYS:N	2.54	0.41
3:D:126:LEU:CD1	3:D:223:LEU:HD22	2.51	0.41
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.23	0.41
3:D:560:ASN:ND2	3:D:560:ASN:O	2.54	0.41
3:D:709:ARG:HA	3:D:709:ARG:HD2	1.90	0.41
5:F:269:LEU:O	5:F:273:MET:HG3	2.20	0.41
5:F:384:LEU:HD22	5:F:409:ASN:HD21	1.84	0.41
2:I:1291:LEU:CD2	3:J:1351:VAL:HG13	2.50	0.41
3:J:1353:VAL:O	3:J:1353:VAL:HG22	2.20	0.41
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.56	0.41
1:B:118:ASP:HB2	1:B:121:VAL:HG23	2.02	0.41
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.86	0.41
2:C:890:LYS:HE2	2:C:891:GLY:H	1.86	0.41
2:C:71:VAL:HB	2:C:99:LYS:HB2	2.03	0.41
3:D:113:HIS:ND1	3:D:115:TRP:HB2	2.36	0.41
3:D:58:CYS:SG	3:D:60:ARG:N	2.93	0.41
5:F:316:PHE:CZ	5:F:337:VAL:HB	2.55	0.41
5:F:603:ARG:HG2	5:F:603:ARG:H	1.52	0.41
1:G:61:ILE:HG23	1:G:142:MET:HB3	2.03	0.41
1:G:190:ALA:H	1:G:199:ASP:HA	1.85	0.41
1:H:118:ASP:H	1:H:121:VAL:HB	1.86	0.41
1:H:211:ILE:HD11	1:H:215:GLU:HB3	2.02	0.41
2:I:1178:LYS:HA	2:I:1178:LYS:HD3	1.93	0.41
2:I:18:ARG:HG2	2:I:18:ARG:H	1.68	0.41
2:I:540:ARG:H	2:I:540:ARG:HG3	1.56	0.41
2:I:720:ARG:NE	2:I:736:VAL:HG11	2.35	0.41
2:I:953:LEU:HD12	2:I:953:LEU:HA	1.84	0.41
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.01	0.41
3:J:1221:LEU:HB2	3:J:1229:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1251:LYS:O	3:J:1254:GLU:N	2.53	0.41
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.16	0.41
3:J:190:LYS:HD3	3:J:235:GLU:HG2	2.02	0.41
3:J:596:LEU:HD13	3:J:596:LEU:HA	1.80	0.41
5:L:303:ILE:HA	5:L:306:PHE:HB2	2.02	0.41
5:L:426:LYS:HE2	5:L:428:SER:OG	2.21	0.41
5:L:585:GLU:O	5:L:586:ARG:C	2.59	0.41
5:L:598:LEU:O	5:L:604:SER:OG	2.39	0.41
5:L:602:SER:OG	5:L:603:ARG:HG2	2.21	0.41
1:A:9:LEU:HD21	1:A:195:ARG:HH21	1.85	0.41
1:A:76:GLU:HB3	1:A:81:ILE:HG12	2.03	0.41
1:B:29:GLU:HG3	1:B:30:PRO:CD	2.51	0.41
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.54	0.41
2:C:153:PRO:HA	2:C:177:ILE:O	2.21	0.41
2:C:518:ASN:OD1	2:C:518:ASN:N	2.46	0.41
2:C:850:ILE:HG23	2:C:850:ILE:HD12	1.73	0.41
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.35	0.41
3:D:1352:ILE:HG23	3:D:1352:ILE:HD12	1.79	0.41
3:D:348:ASP:O	3:D:349:TYR:C	2.59	0.41
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	2.02	0.41
5:F:100:MET:O	5:F:104:GLU:HB2	2.20	0.41
2:I:1275:VAL:HG13	2:I:1287:LEU:CD1	2.48	0.41
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.50	0.41
2:I:758:ARG:NH1	2:I:835:GLU:OE1	2.54	0.41
2:I:75:LEU:HD13	2:I:96:LEU:HA	2.02	0.41
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.50	0.41
3:J:127:LEU:HA	3:J:127:LEU:HD12	1.80	0.41
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.86	0.41
3:J:45:ASN:O	3:J:46:TYR:HD2	2.03	0.41
5:L:354:THR:O	5:L:358:VAL:HG23	2.20	0.41
5:L:533:ASP:O	5:L:534:SER:C	2.59	0.41
5:L:601:PRO:CA	5:L:604:SER:HB2	2.50	0.41
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.36	0.41
1:A:233:ASP:HB2	1:A:234:LEU:H	1.77	0.41
1:A:11:PRO:HD3	1:B:227:GLN:CD	2.42	0.41
2:C:1172:LEU:HD22	2:C:1172:LEU:O	2.21	0.41
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.86	0.41
2:C:1339:LEU:N	2:C:1339:LEU:HD12	2.35	0.41
2:C:15:PHE:CG	2:C:1190:ALA:HB2	2.56	0.41
2:C:231:GLU:HG2	2:C:332:ARG:HD3	2.02	0.41
2:C:233:ARG:HH12	2:C:332:ARG:NH1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.86	0.41
5:F:548:LEU:HD23	5:F:548:LEU:HA	1.85	0.41
1:H:54:CYS:SG	1:H:148:ARG:HG3	2.61	0.41
2:I:202:ARG:HH11	2:I:369:MET:CG	2.34	0.41
2:I:145:ILE:CG2	2:I:456:VAL:HG22	2.50	0.41
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.41
2:I:684:ASN:HA	2:I:687:ARG:NH1	2.35	0.41
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.79	0.41
3:J:310:GLY:HA2	3:J:314:ARG:HD2	2.03	0.41
3:J:495:ASN:O	3:J:497:GLU:N	2.54	0.41
3:J:522:GLY:O	3:J:525:MET:HG2	2.20	0.41
3:J:544:LEU:O	3:J:574:VAL:HB	2.21	0.41
5:L:315:TRP:O	5:L:319:ALA:HB3	2.21	0.41
3:D:370:LYS:HD3	3:D:409:TRP:CH2	2.56	0.41
2:C:1285:TYR:CD1	3:D:475:GLU:HB3	2.56	0.41
3:D:622:ASP:HB3	3:D:626:TYR:CE2	2.55	0.41
3:D:75:TYR:CD1	3:D:75:TYR:N	2.89	0.41
3:D:842:ARG:NH2	3:D:884:SER:HA	2.36	0.41
5:F:467:SER:HB2	5:F:483:LEU:HD21	2.03	0.41
5:F:479:THR:HG23	5:F:481:GLU:N	2.32	0.41
5:F:602:SER:OG	5:F:603:ARG:N	2.52	0.41
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	2.02	0.41
2:I:22:LEU:HD22	2:I:22:LEU:HA	1.88	0.41
2:I:581:THR:HG22	2:I:582:ASN:O	2.21	0.41
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.67	0.41
2:I:878:THR:O	2:I:920:VAL:HB	2.21	0.41
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.21	0.41
3:J:410:ASP:N	3:J:410:ASP:OD2	2.54	0.41
3:J:499:ILE:HD12	3:J:499:ILE:HA	1.93	0.41
5:L:292:VAL:HG11	5:L:299:LYS:HG3	2.02	0.41
5:L:320:ILE:HG12	5:L:330:LEU:HD12	2.02	0.41
5:L:341:LEU:HD23	5:L:344:LEU:HD23	2.03	0.41
5:L:518:HIS:O	5:L:519:LEU:C	2.58	0.41
1:B:89:ALA:HB1	1:B:210:THR:HG23	2.02	0.40
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.21	0.40
2:C:349:GLU:O	2:C:353:VAL:HG23	2.21	0.40
2:C:640:GLY:O	2:C:641:GLU:HG3	2.20	0.40
3:D:20:ILE:HG21	3:D:20:ILE:HD13	1.84	0.40
3:D:795:TYR:CE2	3:D:799:ARG:NE	2.89	0.40
3:D:79:LYS:HG3	3:D:80:HIS:N	2.35	0.40
5:F:225:ARG:O	5:F:229:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:LEU:HD23	1:H:48:LEU:HA	1.79	0.40
2:I:1172:LEU:O	2:I:1176:LEU:HG	2.21	0.40
2:I:1120:ALA:HB2	2:I:1199:LEU:HG	2.03	0.40
2:I:699:LEU:HA	2:I:699:LEU:HD23	1.63	0.40
2:I:738:GLU:HG2	2:I:741:MET:CE	2.51	0.40
2:I:819:SER:HB2	2:I:1085:MET:HG3	2.03	0.40
3:J:1345:ARG:HD2	3:J:1370:MET:CE	2.52	0.40
3:J:279:LEU:O	3:J:283:LEU:HG	2.21	0.40
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.18	0.40
3:J:808:VAL:HG13	3:J:913:GLU:O	2.21	0.40
5:L:601:PRO:HB3	5:L:608:ARG:NH2	2.36	0.40
1:A:181:GLU:HB3	1:A:206:GLU:CG	2.52	0.40
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	2.03	0.40
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.86	0.40
2:C:40:GLU:O	2:C:73:TYR:OH	2.35	0.40
2:C:732:ILE:HG21	2:C:732:ILE:HD13	1.76	0.40
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	2.03	0.40
3:D:746:LEU:N	3:D:746:LEU:HD12	2.37	0.40
5:F:230:VAL:O	5:F:234:THR:HG23	2.21	0.40
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.88	0.40
1:H:213:PRO:O	1:H:217:ILE:HG13	2.21	0.40
2:I:1096:ILE:HD13	2:I:1096:ILE:HG21	1.83	0.40
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.56	0.40
2:I:26:TYR:HB3	2:I:29:SER:OG	2.21	0.40
3:J:77:ARG:HD2	3:J:77:ARG:HA	1.91	0.40
5:L:289:LYS:HB3	5:L:289:LYS:HE2	1.95	0.40
1:A:164:ASP:C	1:A:166:ARG:H	2.25	0.40
1:A:187:VAL:HG23	1:A:187:VAL:O	2.22	0.40
1:A:78:ILE:HD12	1:A:78:ILE:HG23	1.80	0.40
1:B:197:ASP:N	1:B:197:ASP:OD1	2.52	0.40
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.22	0.40
2:C:921:PRO:O	2:C:924:VAL:HG22	2.22	0.40
3:D:9:LYS:CE	3:D:11:GLN:HA	2.51	0.40
3:D:1234:VAL:HG23	3:D:1235:ASN:N	2.36	0.40
3:D:298:MET:SD	5:F:402:LEU:HB3	2.61	0.40
3:D:47:ARG:HA	3:D:47:ARG:HD2	1.87	0.40
3:D:825:VAL:HG11	3:D:833:GLU:HB3	2.03	0.40
4:E:27:ALA:HB1	4:E:46:THR:OG1	2.21	0.40
5:F:230:VAL:HG13	5:F:231:THR:H	1.87	0.40
5:F:277:MET:HG3	5:F:362:ASN:CG	2.42	0.40
1:G:88:LEU:HD13	1:G:128:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:ALA:HB2	1:H:173:VAL:C	2.41	0.40
1:H:201:LEU:HG	1:H:203:ILE:HG13	2.03	0.40
2:I:168:GLY:C	2:I:170:VAL:N	2.74	0.40
2:I:202:ARG:H	2:I:202:ARG:HG3	1.71	0.40
3:J:1256:ILE:HG23	3:J:1256:ILE:HD12	1.77	0.40
3:J:306:LEU:O	3:J:326:SER:HB2	2.21	0.40
3:J:425:ARG:HH11	3:J:425:ARG:HD2	1.64	0.40
3:J:560:ASN:O	3:J:560:ASN:ND2	2.55	0.40
5:L:253:SER:O	5:L:257:LYS:HG3	2.21	0.40
1:B:29:GLU:OE1	1:B:200:LYS:HE2	2.21	0.40
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.51	0.40
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.57	0.40
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.24	0.40
2:C:149:LEU:HD13	2:C:453:ILE:HG13	2.03	0.40
2:C:590:PRO:HB2	2:C:655:VAL:HG21	2.03	0.40
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.56	0.40
2:C:998:LEU:N	2:C:998:LEU:HD12	2.36	0.40
3:D:12:THR:HB	3:D:13:LYS:HZ3	1.87	0.40
3:D:161:THR:HG22	3:D:164:GLN:CD	2.42	0.40
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.56	0.40
1:G:58:GLU:HB2	1:G:145:LYS:HB3	2.03	0.40
1:G:85:LEU:HA	1:G:85:LEU:HD23	1.89	0.40
1:G:70:THR:HG21	2:I:755:LYS:HE2	2.04	0.40
3:J:544:LEU:HD12	3:J:544:LEU:HA	1.86	0.40
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.37	0.40
3:J:846:GLU:OE1	3:J:881:LYS:HE2	2.21	0.40
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.87	0.40
2:C:94:ALA:HA	2:C:95:PRO:HD3	1.93	0.40
2:C:960:LEU:HD13	2:C:960:LEU:HA	1.81	0.40
3:D:394:ILE:HG22	3:D:394:ILE:H	1.53	0.40
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.04	0.40
3:D:604:MET:HB2	3:D:604:MET:HE3	1.98	0.40
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.57	0.40
4:E:80:LEU:HD12	4:E:80:LEU:HA	1.90	0.40
2:I:138:ILE:HG22	2:I:139:ASN:N	2.35	0.40
2:I:462:ASN:O	2:I:465:ARG:HB3	2.21	0.40
2:I:696:ASP:O	2:I:697:LYS:HB3	2.22	0.40
3:J:442:ILE:HA	3:J:442:ILE:HD13	1.89	0.40
3:J:825:VAL:O	3:J:826:ILE:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	196 (87%)	25 (11%)	4 (2%)	11	55
1	B	210/329 (64%)	183 (87%)	22 (10%)	5 (2%)	7	50
1	G	222/329 (68%)	193 (87%)	25 (11%)	4 (2%)	11	55
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	5	43
2	C	1340/1342 (100%)	1233 (92%)	100 (8%)	7 (0%)	34	77
2	I	1338/1342 (100%)	1232 (92%)	101 (8%)	5 (0%)	39	80
3	D	1162/1407 (83%)	1072 (92%)	81 (7%)	9 (1%)	24	70
3	J	1151/1407 (82%)	1056 (92%)	80 (7%)	15 (1%)	15	61
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	422 (91%)	39 (8%)	1 (0%)	52	86
5	L	463/613 (76%)	424 (92%)	38 (8%)	1 (0%)	52	86
All	All	6948/8222 (84%)	6354 (92%)	536 (8%)	58 (1%)	24	70

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	167	PRO
1	B	13	LEU
2	C	1159	VAL
3	D	10	ALA
3	D	332	LYS
1	H	135	ASP
2	I	1159	VAL
3	J	332	LYS
3	J	426	ALA
1	B	135	ASP
1	B	136	GLU

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Mol	Chain	Res	Type
2	C	3	TYR
2	C	170	VAL
2	C	697	LYS
1	G	162	GLU
1	G	167	PRO
1	H	136	GLU
1	H	177	TYR
2	I	170	VAL
3	J	334	LYS
3	J	427	PRO
1	H	157	THR
2	I	697	LYS
3	J	337	ARG
2	C	484	LEU
2	C	1158	LYS
3	D	710	ASP
3	D	806	ASP
1	G	14	VAL
1	G	62	ASP
1	H	20	SER
3	J	338	PHE
3	J	342	LEU
3	J	344	GLY
3	J	710	ASP
3	J	806	ASP
1	A	14	VAL
1	A	62	ASP
1	B	62	ASP
3	D	428	THR
1	H	62	ASP
1	H	138	ALA
2	I	484	LEU
3	J	333	GLY
1	B	14	VAL
3	D	426	ALA
3	D	831	VAL
5	F	477	GLU
3	J	831	VAL
2	C	1186	VAL
2	I	1186	VAL
3	D	1180	VAL
3	J	826	ILE

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Mol	Chain	Res	Type
3	J	1180	VAL
5	L	477	GLU
3	D	826	ILE
3	J	336	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/286 (68%)	182 (94%)	12 (6%)	23	64
1	B	182/286 (64%)	172 (94%)	10 (6%)	27	68
1	G	191/286 (67%)	179 (94%)	12 (6%)	22	63
1	H	184/286 (64%)	177 (96%)	7 (4%)	40	76
2	C	1157/1157 (100%)	1051 (91%)	106 (9%)	11	48
2	I	1154/1157 (100%)	1050 (91%)	104 (9%)	12	49
3	D	970/1168 (83%)	873 (90%)	97 (10%)	9	43
3	J	960/1168 (82%)	860 (90%)	100 (10%)	9	42
4	E	72/75 (96%)	64 (89%)	8 (11%)	8	39
4	K	67/75 (89%)	63 (94%)	4 (6%)	24	65
5	F	417/540 (77%)	376 (90%)	41 (10%)	10	44
5	L	418/540 (77%)	376 (90%)	42 (10%)	9	43
All	All	5966/7024 (85%)	5423 (91%)	543 (9%)	12	48

All (543) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	50	SER
1	A	61	ILE
1	A	74	VAL
1	A	115	ILE

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Mol	Chain	Res	Type
1	A	133	LEU
1	A	145	LYS
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	A	233	ASP
1	B	6	THR
1	B	8	PHE
1	B	9	LEU
1	B	10	LYS
1	B	13	LEU
1	B	50	SER
1	B	61	ILE
1	B	115	ILE
1	B	215	GLU
1	B	231	PHE
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	60	GLN
2	C	70	TYR
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	189	ASP
2	C	285	ILE
2	C	299	LYS
2	C	306	THR
2	C	320	ASP
2	C	360	LEU
2	C	369	MET
2	C	377	THR

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Mol	Chain	Res	Type
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	518	ASN
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
2	C	554	HIS
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	800	MET
2	C	814	ASP
2	C	817	LEU
2	C	819	SER
2	C	826	ASP

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Mol	Chain	Res	Type
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	944	ARG
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1073	LYS
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU
3	D	18	ASP
3	D	26	SER
3	D	29	MET
3	D	46	TYR

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Mol	Chain	Res	Type
3	D	54	ASP
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	98	ARG
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	217	LEU
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	343	LEU
3	D	352	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	454	CYS
3	D	490	ILE
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET

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Mol	Chain	Res	Type
3	D	701	LEU
3	D	702	GLN
3	D	704	GLU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	805	GLN
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU

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Mol	Chain	Res	Type
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1333	THR
3	D	1343	GLU
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	154	GLU
5	F	266	PHE
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	422	ARG
5	F	429	THR
5	F	437	GLN
5	F	445	ASP
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	485	GLU
5	F	486	ARG

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Mol	Chain	Res	Type
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	587	ILE
5	F	606	VAL
5	F	612	ASP
1	G	9	LEU
1	G	13	LEU
1	G	19	VAL
1	G	50	SER
1	G	61	ILE
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	13	LEU
1	H	19	VAL
1	H	26	VAL
1	H	50	SER
1	H	61	ILE
1	H	115	ILE
1	H	215	GLU
2	I	4	SER
2	I	11	ILE
2	I	22	LEU
2	I	60	GLN
2	I	70	TYR
2	I	82	VAL
2	I	85	CYS

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Mol	Chain	Res	Type
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	189	ASP
2	I	285	ILE
2	I	299	LYS
2	I	306	THR
2	I	320	ASP
2	I	360	LEU
2	I	369	MET
2	I	377	THR
2	I	394	ARG
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
2	I	554	HIS
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS

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Mol	Chain	Res	Type
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	817	LEU
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	944	ARG
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	984	VAL
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1040	ASP
2	I	1073	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1151	LEU

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Mol	Chain	Res	Type
2	I	1156	ARG
2	I	1159	VAL
2	I	1198	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1238	LEU
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	26	SER
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	159	ILE
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	217	LEU
3	J	251	PRO
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	343	LEU
3	J	352	ARG
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	454	CYS
3	J	490	ILE
3	J	506	VAL
3	J	507	VAL

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Mol	Chain	Res	Type
3	J	513	MET
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	704	GLU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	764	ARG
3	J	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	803	VAL
3	J	805	GLN
3	J	810	THR
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR

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Mol	Chain	Res	Type
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	931	THR
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	154	GLU
5	L	266	PHE
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	306	PHE

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Mol	Chain	Res	Type
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	422	ARG
5	L	429	THR
5	L	437	GLN
5	L	445	ASP
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL
5	L	612	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	B	66	HIS
1	B	128	HIS
2	C	31	GLN
2	C	69	GLN

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Mol	Chain	Res	Type
2	C	120	GLN
2	C	139	ASN
2	C	494	ASN
2	C	510	GLN
2	C	513	GLN
2	C	573	ASN
2	C	620	ASN
2	C	628	HIS
2	C	1116	HIS
2	C	1136	GLN
2	C	1146	GLN
2	C	1288	GLN
2	C	1299	ASN
3	D	94	GLN
3	D	200	GLN
3	D	294	ASN
3	D	365	GLN
3	D	450	HIS
3	D	477	GLN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1259	GLN
3	D	1366	HIS
5	F	131	GLN
5	F	362	ASN
5	F	383	ASN
5	F	446	GLN
5	F	455	HIS
5	F	472	GLN
5	F	518	HIS
1	G	103	ASN
1	H	66	HIS
2	I	69	GLN
2	I	86	GLN
2	I	139	ASN
2	I	343	HIS
2	I	513	GLN
2	I	628	HIS

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Mol	Chain	Res	Type
2	I	688	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1288	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	365	GLN
3	J	669	GLN
3	J	702	GLN
3	J	716	GLN
3	J	817	HIS
3	J	861	ASN
3	J	910	ASN
3	J	1218	HIS
3	J	1259	GLN
5	L	131	GLN
5	L	246	GLN
5	L	362	ASN
5	L	383	ASN
5	L	446	GLN
5	L	455	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	RFP	C	3001	-	62,63,63	2.81	26 (41%)	76,94,94	2.82	32 (42%)

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

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O7-C25	-8.23	1.32	1.44
6	C	3001	RFP	C12-C11	-7.88	1.32	1.54
6	C	3001	RFP	O6-C27	-4.15	1.34	1.43
6	C	3001	RFP	C26-C25	-3.29	1.46	1.53
6	C	3001	RFP	C6-C7	-3.17	1.34	1.39
6	C	3001	RFP	C34-C26	-2.97	1.47	1.53
6	C	3001	RFP	C24-C23	-2.95	1.47	1.54
6	C	3001	RFP	O9-C23	-2.94	1.36	1.43
6	C	3001	RFP	O10-C21	-2.89	1.36	1.43
6	C	3001	RFP	O3-C12	-2.53	1.40	1.45
6	C	3001	RFP	C22-C21	-2.52	1.48	1.54
6	C	3001	RFP	C4-C10	-2.44	1.37	1.43
6	C	3001	RFP	C40-N3	-2.38	1.40	1.46
6	C	3001	RFP	C32-C22	-2.33	1.48	1.53
6	C	3001	RFP	C3-C4	-2.31	1.37	1.40
6	C	3001	RFP	C31-C20	-2.30	1.47	1.53
6	C	3001	RFP	C5-C10	-2.09	1.38	1.43
6	C	3001	RFP	C22-C23	-2.09	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	C18-C19	2.02	1.40	1.33
6	C	3001	RFP	C29-C28	2.15	1.43	1.30
6	C	3001	RFP	C43-N2	2.31	1.32	1.27
6	C	3001	RFP	C17-C16	2.69	1.41	1.34
6	C	3001	RFP	C3-C43	3.89	1.53	1.46
6	C	3001	RFP	C18-C17	4.26	1.56	1.43
6	C	3001	RFP	C15-N1	4.90	1.46	1.35
6	C	3001	RFP	O3-C6	10.93	1.55	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C32-C22-C23	-7.00	96.82	111.25
6	C	3001	RFP	C33-C24-C23	-6.69	97.45	111.25
6	C	3001	RFP	C13-C12-C11	-5.78	101.03	113.94
6	C	3001	RFP	O7-C25-C26	-5.71	92.21	107.72
6	C	3001	RFP	C34-C26-C25	-5.16	101.87	111.45
6	C	3001	RFP	O4-C11-C5	-5.10	121.23	131.67
6	C	3001	RFP	C31-C20-C19	-4.98	97.59	110.16
6	C	3001	RFP	C12-O3-C6	-4.58	102.58	107.86
6	C	3001	RFP	C41-C42-N4	-4.16	106.24	110.76
6	C	3001	RFP	C40-N3-N2	-3.57	95.73	113.51
6	C	3001	RFP	C26-C25-C24	-3.48	107.87	114.72
6	C	3001	RFP	C17-C18-C19	-3.27	116.47	124.06
6	C	3001	RFP	C32-C22-C21	-3.14	104.79	111.25
6	C	3001	RFP	C40-C39-N4	-3.09	107.40	110.76
6	C	3001	RFP	O7-C35-O8	-3.00	116.82	122.92
6	C	3001	RFP	C42-C41-N3	-2.75	106.69	110.38
6	C	3001	RFP	O6-C27-C26	-2.71	101.85	108.31
6	C	3001	RFP	O9-C23-C22	-2.69	104.00	109.67
6	C	3001	RFP	O10-C21-C22	-2.62	104.14	109.67
6	C	3001	RFP	C2-C3-C43	-2.51	119.81	123.33
6	C	3001	RFP	C5-C10-C9	-2.31	115.03	119.83
6	C	3001	RFP	O2-C8-C9	2.25	123.76	118.59
6	C	3001	RFP	C26-C27-C28	2.37	116.95	112.12
6	C	3001	RFP	C24-C23-C22	2.46	119.06	115.46
6	C	3001	RFP	C41-N3-C40	2.60	121.53	114.22
6	C	3001	RFP	C12-O5-C29	2.91	123.78	117.07
6	C	3001	RFP	C25-O7-C35	3.20	122.72	117.71
6	C	3001	RFP	O7-C35-C36	3.39	117.55	111.09
6	C	3001	RFP	C38-N4-C39	4.82	118.37	110.68
6	C	3001	RFP	O5-C12-C13	5.06	115.52	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C41-N3-N2	5.54	141.05	113.51
6	C	3001	RFP	C38-N4-C42	6.20	120.58	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	14	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/329 (68%)	-0.20	3 (1%) 79 65	128, 159, 207, 262	0
1	B	214/329 (65%)	0.11	7 (3%) 50 34	115, 179, 246, 259	0
1	G	224/329 (68%)	-0.20	1 (0%) 93 87	162, 193, 225, 245	0
1	H	215/329 (65%)	0.10	10 (4%) 35 23	165, 218, 246, 265	0
2	C	1342/1342 (100%)	-0.04	55 (4%) 41 27	96, 152, 303, 368	0
2	I	1340/1342 (99%)	0.23	89 (6%) 22 12	129, 200, 287, 371	0
3	D	1166/1407 (82%)	-0.14	25 (2%) 67 51	94, 140, 215, 278	0
3	J	1155/1407 (82%)	-0.07	28 (2%) 62 46	118, 164, 225, 300	0
4	E	89/91 (97%)	-0.16	0 100 100	131, 170, 200, 214	0
4	K	79/91 (86%)	1.00	18 (22%) 1 1	221, 276, 310, 318	0
5	F	468/613 (76%)	0.49	62 (13%) 4 4	139, 216, 432, 522	0
5	L	469/613 (76%)	0.71	66 (14%) 4 3	144, 239, 458, 518	0
All	All	6988/8222 (84%)	0.09	364 (5%) 31 21	94, 176, 295, 522	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	318	ALA	14.6
5	L	321	ALA	13.9
5	L	319	ALA	13.9
5	F	312	SER	13.4
5	L	327	SER	12.4
5	F	304	THR	12.0
5	L	311	THR	11.7
2	I	980	VAL	11.4
5	L	325	PRO	11.2
5	F	305	LEU	10.7
5	L	312	SER	10.4

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Mol	Chain	Res	Type	RSRZ
2	I	979	LEU	9.6
2	I	1017	GLN	9.3
5	F	328	GLU	9.2
5	L	314	THR	8.9
5	L	328	GLU	8.8
5	L	167	ASP	8.7
5	L	326	TRP	8.6
5	L	313	ASP	8.5
5	L	309	ASN	8.1
2	C	236	LYS	7.9
5	L	310	GLU	7.8
5	L	315	TRP	7.8
2	I	978	VAL	7.8
5	L	308	GLY	7.7
2	I	976	ARG	7.6
5	F	306	PHE	7.6
5	F	167	ASP	7.6
5	F	319	ALA	7.3
2	I	977	ALA	7.1
2	I	1018	TYR	7.0
2	I	107	ARG	6.7
2	I	266	GLY	6.7
5	L	320	ILE	6.5
2	I	986	ALA	6.5
2	I	1016	GLU	6.4
5	L	337	VAL	6.3
2	I	1009	ASN	6.3
5	L	291	CYS	6.2
3	D	1166	GLY	6.2
5	F	331	HIS	6.1
5	F	329	LYS	6.1
5	L	323	ASN	6.1
5	F	314	THR	6.1
5	F	313	ASP	6.0
2	I	970	GLY	6.0
5	L	322	MET	6.0
2	I	999	GLU	6.0
5	F	327	SER	6.0
2	I	1013	GLN	5.7
5	L	333	VAL	5.7
4	K	57	GLY	5.7
2	I	1010	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
2	I	984	VAL	5.6
5	L	290	LEU	5.6
5	F	308	GLY	5.4
5	L	336	GLU	5.3
2	I	998	LEU	5.2
5	F	294	GLN	5.2
2	C	321	LEU	5.2
2	I	1005	GLU	5.1
5	F	332	ASP	5.1
5	F	323	ASN	5.1
2	C	273	HIS	5.1
5	F	317	ASN	5.1
2	I	1015	ALA	5.1
5	F	300	LYS	5.0
3	D	1299	GLY	5.0
2	C	274	ILE	5.0
5	F	315	TRP	5.0
2	I	987	GLU	5.0
2	I	1021	LEU	5.0
5	L	613	ASP	5.0
2	I	1006	GLU	4.9
2	C	311	CYS	4.9
5	F	330	LEU	4.8
2	I	1007	LYS	4.8
2	I	60	GLN	4.7
2	I	1000	LEU	4.7
5	F	244	THR	4.7
5	L	317	ASN	4.7
5	F	320	ILE	4.6
2	C	301	TYR	4.5
2	C	325	LEU	4.5
2	C	290	GLU	4.4
5	F	287	ILE	4.4
2	C	252	SER	4.4
5	L	294	GLN	4.4
2	I	1022	LYS	4.4
2	C	309	LEU	4.4
3	J	207	GLU	4.4
2	I	1004	ASP	4.3
2	I	981	ALA	4.2
2	I	108	GLU	4.2
2	I	1008	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	268	ARG	4.2
2	C	259	GLY	4.2
3	J	314	ARG	4.1
4	K	58	LEU	4.1
2	C	276	GLN	4.1
2	I	983	GLY	4.0
2	I	997	TRP	4.0
2	C	108	GLU	4.0
5	F	284	GLU	4.0
3	J	708	ASN	3.9
5	F	310	GLU	3.9
5	F	283	GLN	3.9
5	F	301	ASN	3.9
2	I	634	VAL	3.9
3	D	1204	VAL	3.8
2	C	302	ILE	3.8
5	F	245	ALA	3.8
5	L	295	CYS	3.8
2	C	62	TYR	3.8
5	L	307	THR	3.8
2	C	333	ILE	3.8
4	K	59	ILE	3.8
4	K	56	GLU	3.8
1	B	98	VAL	3.8
4	K	75	GLN	3.8
5	F	280	VAL	3.7
5	L	165	PHE	3.7
3	J	714	GLU	3.7
3	J	1273	ASP	3.7
2	C	253	PHE	3.6
1	H	14	VAL	3.6
1	B	135	ASP	3.6
3	J	218	THR	3.6
2	I	415	GLU	3.6
5	F	156	ALA	3.6
5	L	296	LYS	3.6
5	L	487	MET	3.5
1	H	96	ASP	3.5
2	C	233	ARG	3.5
5	F	290	LEU	3.5
5	L	161	LEU	3.5
4	K	37	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
5	L	324	LYS	3.5
3	J	1151	LYS	3.5
3	D	154	LEU	3.5
2	C	116	ASP	3.5
2	C	982	GLY	3.5
2	I	487	LEU	3.5
4	K	71	GLU	3.5
3	D	1198	VAL	3.5
5	L	340	ALA	3.5
5	F	309	ASN	3.4
5	L	243	ALA	3.4
2	I	1020	GLU	3.4
5	F	303	ILE	3.4
2	I	1012	GLU	3.3
3	J	212	THR	3.3
5	F	490	PRO	3.3
1	B	99	ILE	3.3
4	K	36	ASP	3.3
5	F	164	GLY	3.3
2	I	318	SER	3.3
5	F	298	PRO	3.3
5	L	293	GLU	3.3
5	L	490	PRO	3.3
2	I	985	GLU	3.3
5	F	351	THR	3.3
5	F	322	MET	3.2
2	I	650	VAL	3.2
2	C	269	ILE	3.2
2	I	248	GLY	3.2
2	C	300	ASP	3.2
3	D	1376	GLY	3.2
2	C	165	HIS	3.1
5	L	488	LEU	3.1
2	C	247	ARG	3.1
2	C	117	ILE	3.1
3	J	830	ASP	3.1
5	L	304	THR	3.1
5	L	164	GLY	3.1
2	C	985	GLU	3.1
3	D	208	THR	3.1
5	L	154	GLU	3.1
4	K	39	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	109	PRO	3.0
2	I	982	GLY	3.0
2	C	330	HIS	3.0
2	C	291	TYR	3.0
5	F	307	THR	3.0
5	F	318	ALA	3.0
2	C	172	TYR	3.0
2	C	104	ILE	3.0
3	J	1169	THR	3.0
2	I	67	GLU	3.0
2	I	250	THR	3.0
2	I	268	ARG	3.0
2	I	481	LEU	3.0
5	F	297	MET	3.0
5	L	157	ARG	3.0
1	H	106	GLY	3.0
5	F	311	THR	3.0
3	J	1198	VAL	2.9
3	J	176	PHE	2.9
5	F	288	MET	2.9
5	L	303	ILE	2.9
5	L	339	ARG	2.9
2	I	106	GLU	2.9
2	I	231	GLU	2.9
5	L	489	MET	2.9
1	H	13	LEU	2.9
2	C	169	LYS	2.9
2	I	165	HIS	2.9
4	K	13	ILE	2.9
2	I	115	LYS	2.8
3	D	1203	ARG	2.8
3	D	213	LYS	2.8
5	F	340	ALA	2.8
3	D	314	ARG	2.8
2	I	117	ILE	2.8
2	C	234	ASP	2.8
2	I	1019	ASP	2.8
3	J	712	GLN	2.8
2	C	266	GLY	2.8
5	F	302	PHE	2.8
4	K	78	ALA	2.8
3	D	209	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	I	252	SER	2.7
2	I	333	ILE	2.7
5	L	334	SER	2.7
5	L	155	GLU	2.7
3	D	542	ALA	2.7
5	F	94	THR	2.7
2	C	235	ASN	2.7
1	H	65	LEU	2.7
5	L	421	TYR	2.7
2	C	280	ASP	2.7
3	J	849	LEU	2.7
2	I	1003	THR	2.7
3	J	214	ARG	2.7
5	F	421	TYR	2.7
3	D	1165	PHE	2.7
2	I	59	ILE	2.7
5	L	264	LYS	2.7
2	I	270	THR	2.7
1	A	164	ASP	2.6
2	I	311	CYS	2.6
5	L	514	ASP	2.6
1	A	160	HIS	2.6
2	C	305	SER	2.6
5	L	234	THR	2.6
5	F	165	PHE	2.6
2	C	102	LEU	2.6
5	F	291	CYS	2.6
2	C	270	THR	2.6
4	K	34	GLY	2.6
1	B	145	LYS	2.6
2	I	969	ALA	2.6
3	D	1169	THR	2.6
3	D	792	ASN	2.6
3	J	208	THR	2.6
5	L	305	LEU	2.5
4	K	14	GLY	2.5
3	J	206	ASN	2.5
5	F	321	ALA	2.5
2	I	154	GLY	2.5
3	J	213	LYS	2.5
5	L	342	GLN	2.5
4	K	33	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	258	ASN	2.5
2	C	310	ILE	2.5
2	C	574	SER	2.5
2	C	292	ILE	2.5
2	C	599	VAL	2.5
2	I	601	ASP	2.5
5	F	489	MET	2.5
5	L	330	LEU	2.4
2	C	267	ARG	2.4
5	F	339	ARG	2.4
2	I	247	ARG	2.4
1	H	18	GLN	2.4
4	K	40	PRO	2.4
2	I	1332	SER	2.4
3	J	1202	GLU	2.4
2	C	237	LEU	2.4
2	C	304	GLU	2.4
3	J	707	ILE	2.4
5	F	247	GLU	2.4
3	J	204	GLU	2.3
1	B	108	GLY	2.3
4	K	80	LEU	2.3
2	I	414	ILE	2.3
2	I	1264	GLN	2.3
3	J	1296	GLY	2.3
3	D	1300	ALA	2.3
2	I	725	GLN	2.3
5	F	478	PRO	2.3
2	I	104	ILE	2.3
2	C	1000	LEU	2.3
2	I	105	TYR	2.3
5	L	292	VAL	2.3
2	C	332	ARG	2.3
2	I	633	LEU	2.3
3	J	209	ASN	2.3
3	D	317	THR	2.3
2	I	331	LYS	2.3
3	D	335	GLN	2.3
4	K	41	GLU	2.3
5	F	166	VAL	2.3
2	I	298	ALA	2.3
3	D	152	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	413	GLU	2.2
2	I	245	ARG	2.2
3	J	745	GLY	2.2
4	K	73	GLN	2.2
2	I	652	TYR	2.2
5	L	422	ARG	2.2
5	F	163	THR	2.2
5	L	335	GLU	2.2
5	L	483	LEU	2.2
5	F	352	GLY	2.2
2	C	317	LEU	2.2
2	I	492	MET	2.2
3	D	149	GLY	2.2
2	I	163	LYS	2.2
3	J	210	SER	2.2
2	I	439	LYS	2.2
3	D	1171	GLY	2.2
1	A	25	LYS	2.2
3	D	1202	GLU	2.2
5	L	306	PHE	2.2
5	L	316	PHE	2.1
3	D	176	PHE	2.1
2	C	289	VAL	2.1
5	L	425	TYR	2.1
1	B	193	GLU	2.1
2	I	1342	GLU	2.1
2	I	734	ILE	2.1
2	I	975	ILE	2.1
2	I	273	HIS	2.1
2	C	170	VAL	2.1
2	I	483	ASP	2.1
2	I	375	PRO	2.1
5	L	152	GLU	2.1
5	L	300	LYS	2.1
2	C	47	TYR	2.1
3	D	830	ASP	2.1
5	F	136	GLU	2.1
1	H	97	GLU	2.1
5	F	248	GLU	2.1
5	L	338	HIS	2.1
1	G	205	MET	2.1
2	C	288	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	1199	PHE	2.1
2	I	167	SER	2.0
3	J	1193	TRP	2.0
5	F	236	LYS	2.0
3	D	547	ARG	2.0
1	H	107	ILE	2.0
1	H	120	ASP	2.0
3	J	1167	LYS	2.0
5	F	422	ARG	2.0
2	I	571	LEU	2.0
2	I	594	VAL	2.0
1	H	58	GLU	2.0
5	F	514	ASP	2.0
5	L	245	ALA	2.0
2	I	118	LYS	2.0
2	I	753	LEU	2.0
2	C	67	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	ZN	J	1503	1/1	0.86	0.42	3.25	281,281,281,281	0
8	ZN	D	1503	1/1	0.71	0.37	1.35	274,274,274,274	0
8	ZN	D	1502	1/1	0.58	0.25	0.23	324,324,324,324	0
6	RFP	C	3001	59/59	0.92	0.22	-0.50	88,136,160,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	ZN	J	1502	1/1	0.61	0.18	-0.94	322,322,322,322	0
7	MG	D	1501	1/1	0.80	0.41	-	264,264,264,264	0
7	MG	J	1501	1/1	0.52	0.51	-	290,290,290,290	0

6.5 Other polymers [i](#)

There are no such residues in this entry.