



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:42 pm BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



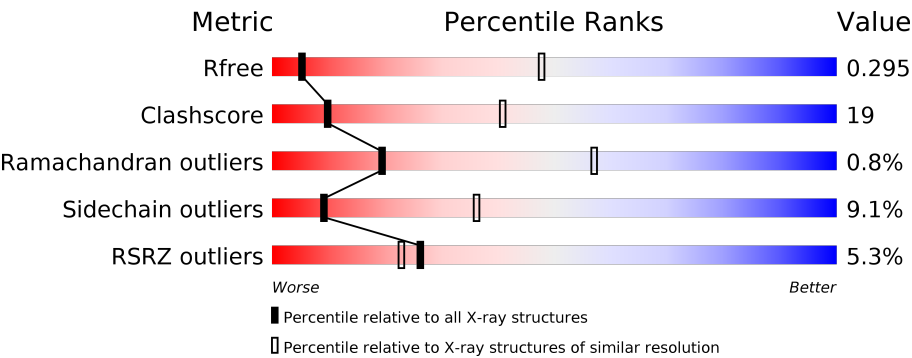
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div><div>0%</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
7	MG	J	1501	-	-	-	X
8	ZN	D	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.

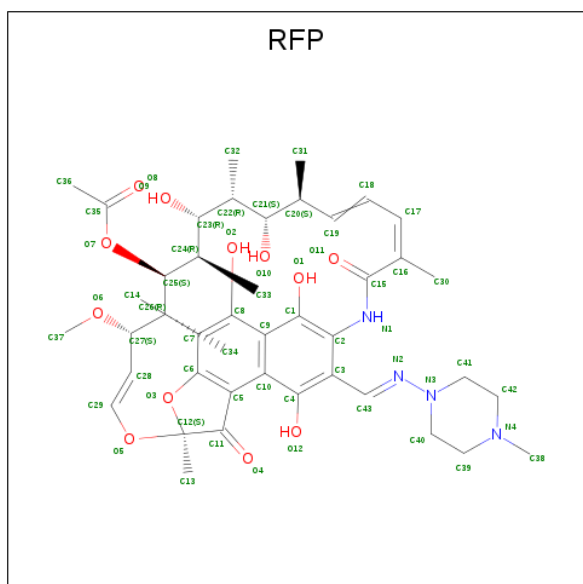
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			



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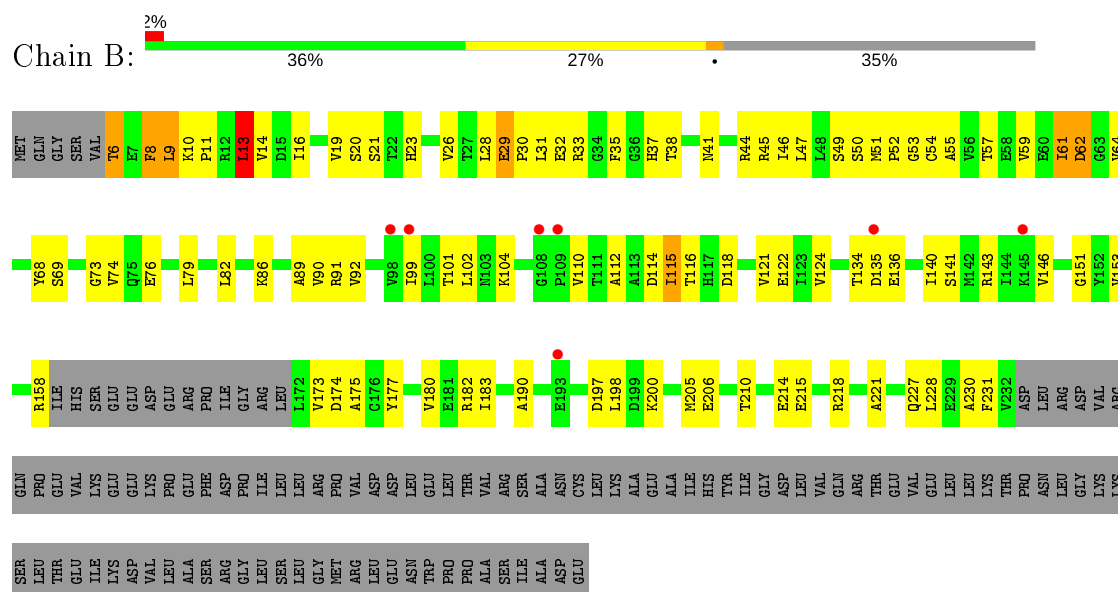
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		



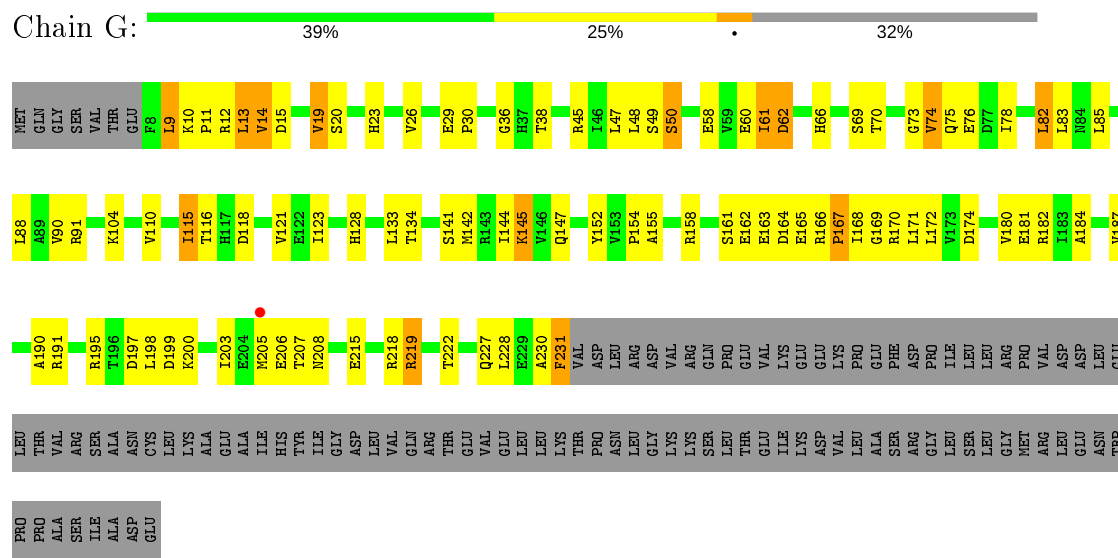


- Molecule 1: DNA-directed RNA polymerase subunit alpha

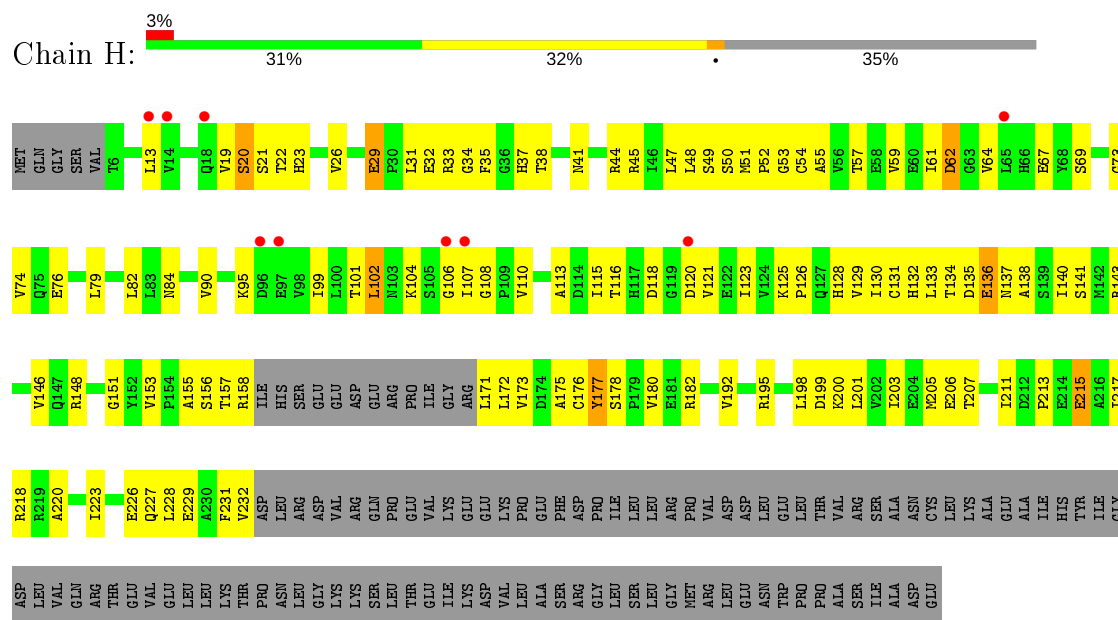




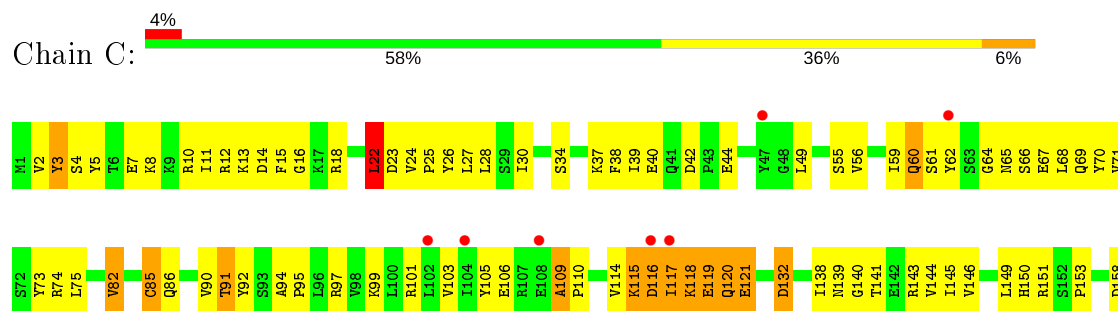
- Molecule 1: DNA-directed RNA polymerase subunit alpha



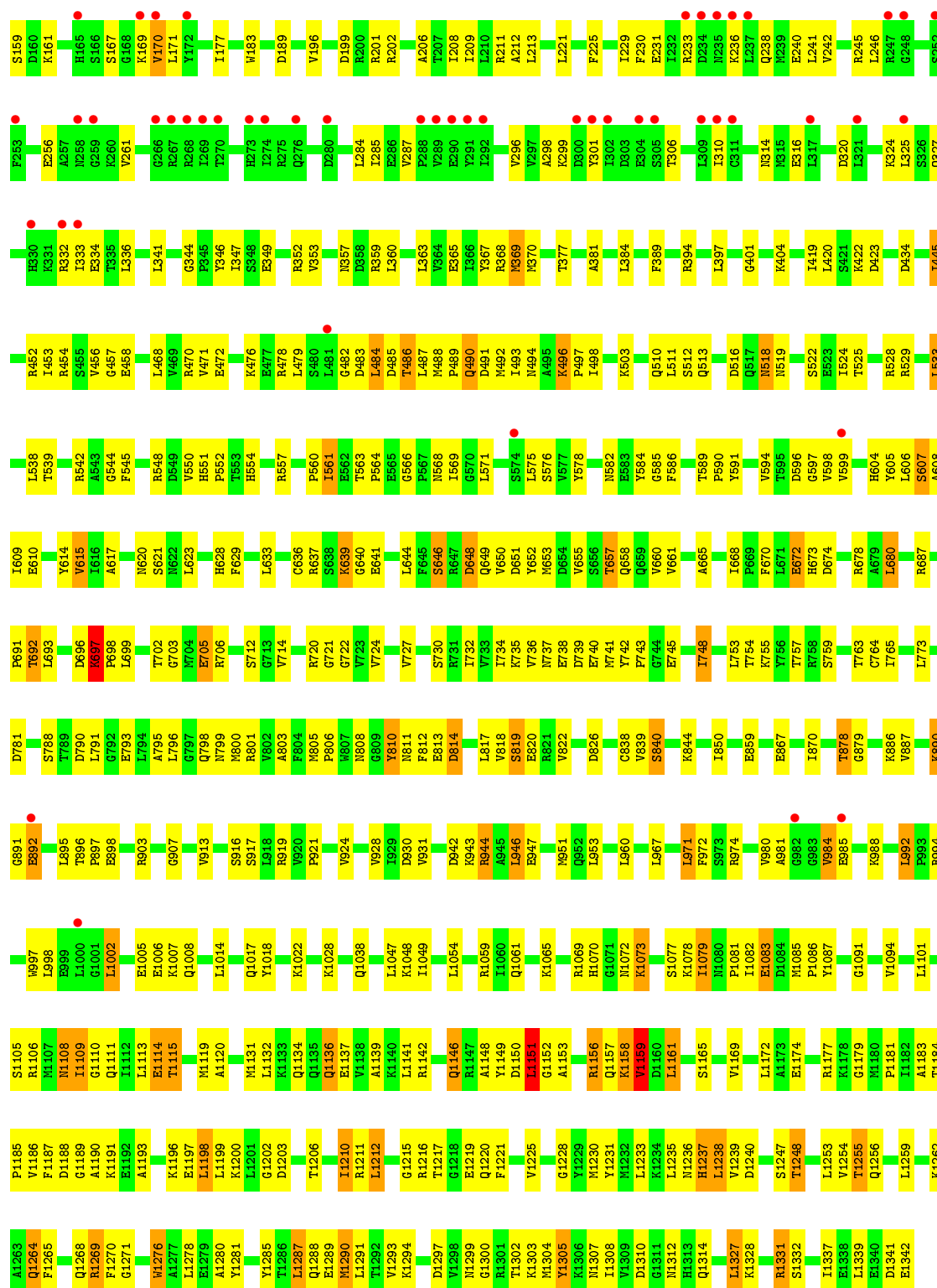
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta







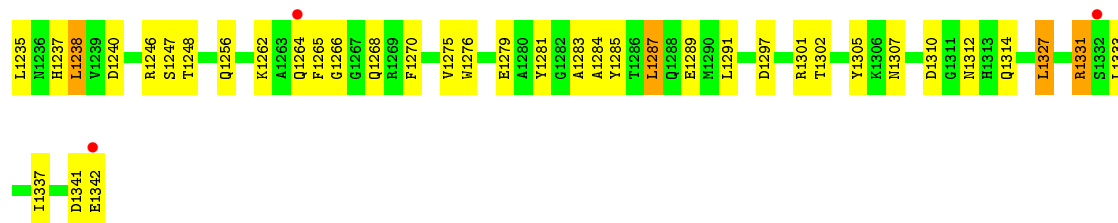
• Molecule 2: DNA-directed RNA polymerase subunit beta



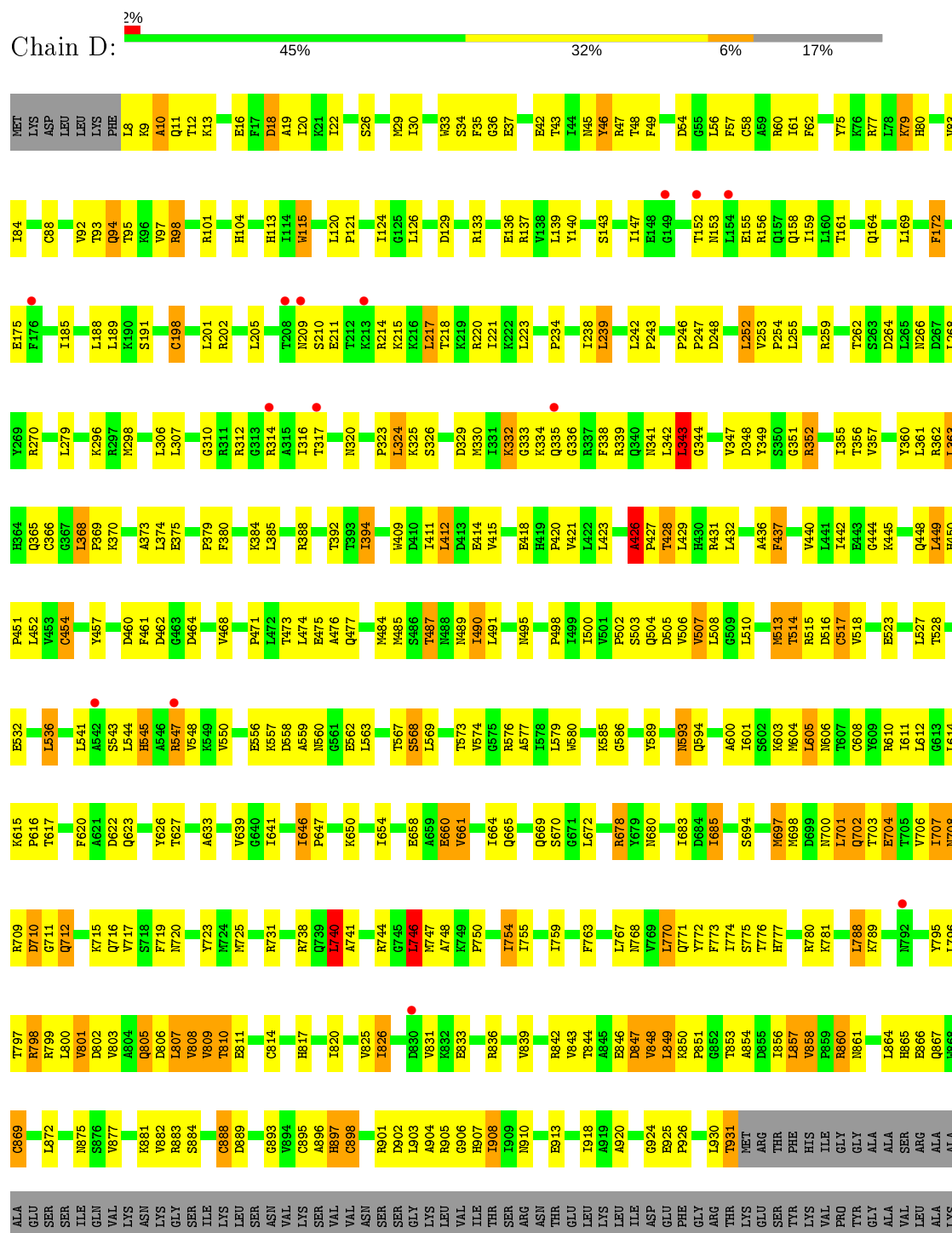


Y1155	I1076	L992	G879	L794	P898	E610	L538	I453	Y367	G266	S167	Y92	MET
R1156	P993	P993	R886	A795	L699	E610	T539	V456	R368	G266	G168	S93	VAL
Q1157	R994	R994	R886	L796	V700	V615	R540	V456	M369	R267	G169	A94	Y3
K1158	D995	D995	R886	G797	G701	I616	R540	V456	M370	R268	Y170	P95	S4
D1159	K996	K996	K996	Q798	G702	A617	R542	N462	G373	T270	L171	L96	Y5
L1161	N997	N997	E892	Q811	G703	Q618	V550	R465	E374	T270	L176	R97	T6
	L998	L998	E892	M800	M704	A619	V550	R466	E375	H273	I177	V98	
	E999	E999	E892	R801	E705	R620	T553	G467	P376	H273	I177	R99	R10
	L1000	L1000	L895	P806	V714	S621	T553	G467	P376	H273	I177	R99	R10
	G1001	G1001	S916	N807	A718	L623	H554	L468	P377	H273	I177	R99	R10
	P1002	P1002	S917	N808	K719	L623	H554	L468	P377	H273	I177	R99	R10
	T1003	T1003	N809	Y810	R720	H628	G556	R470	A381	H273	I177	R99	R10
	D1004	D1004	R811	R812	G721	F629	G556	R471	A381	H273	I177	R99	R10
	E1005	E1005	V920	V810	G721	F629	G556	R471	A381	H273	I177	R99	R10
	E1006	E1006	V920	V810	G721	F629	G556	R471	A381	H273	I177	R99	R10
	K1007	K1007	I929	N811	G721	F629	G556	R471	A381	H273	I177	R99	R10
	Q1008	Q1008	I929	N811	G721	F629	G556	R471	A381	H273	I177	R99	R10
	N1009	N1009	V931	D814	V724	L633	P560	R476	L388	F188	R107	R18	
	Q1010	Q1010	D942	L817	V724	L633	P560	R476	L388	F188	R107	R18	
	L1011	L1011	R943	V818	V724	L633	P560	R476	L388	F188	R107	R18	
	E1012	E1012	R943	V818	V724	L633	P560	R476	L388	F188	R107	R18	
	Q1013	Q1013	R944	E820	V733	T635	P564	R476	L388	F188	R107	R18	
	L1014	L1014	E820	V733	V733	T635	P564	R476	L388	F188	R107	R18	
	A1015	A1015	L946	Q824	K734	S646	P564	R476	L388	F188	R107	R18	
	E1016	E1016	E947	Q824	K734	S646	P564	R476	L388	F188	R107	R18	
	Q1017	Q1017	I948	E825	V736	Q649	P564	R476	L388	F188	R107	R18	
	L1018	L1018	R948	E825	V736	Q649	P564	R476	L388	F188	R107	R18	
	D1019	D1019	R948	E825	V736	Q649	P564	R476	L388	F188	R107	R18	
	E1020	E1020	M951	R827	E738	D650	P564	R476	L388	F188	R107	R18	
	Q1021	Q1021	R948	R827	E738	D650	P564	R476	L388	F188	R107	R18	
	L1022	L1022	L953	T829	E740	Y652	P564	R476	L388	F188	R107	R18	
	K1023	K1023	L953	T829	E740	Y652	P564	R476	L388	F188	R107	R18	
	E1030	E1030	L860	H832	M741	T657	P564	R476	L388	F188	R107	R18	
	R1033	R1033	E963	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	Q1038	Q1038	L967	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	G1039	G1039	E968	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	D1040	D1040	E970	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	G1045	G1045	F972	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	L1047	L1047	R974	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	K1048	K1048	R976	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	A1055	A1055	R976	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	R1058	R1058	R977	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	V1138	V1138	R978	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	A1139	A1139	R979	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	P1062	P1062	A981	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	K1065	K1065	G982	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	M1066	M1066	G983	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	R1069	R1069	G984	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	H1070	H1070	G985	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	G1071	G1071	G986	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	N1072	N1072	G987	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	D1150	D1150	G988	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	L1151	L1151	G989	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	A1152	A1152	G990	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	G1228	G1228	G991	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	Y1229	Y1229	G991	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	M1230	M1230	G991	E835	E745	Q658	P564	R476	L388	F188	R107	R18	
	K1234	K1234	G991	E835	E745	Q658	P564	R476	L388	F188	R107	R18	

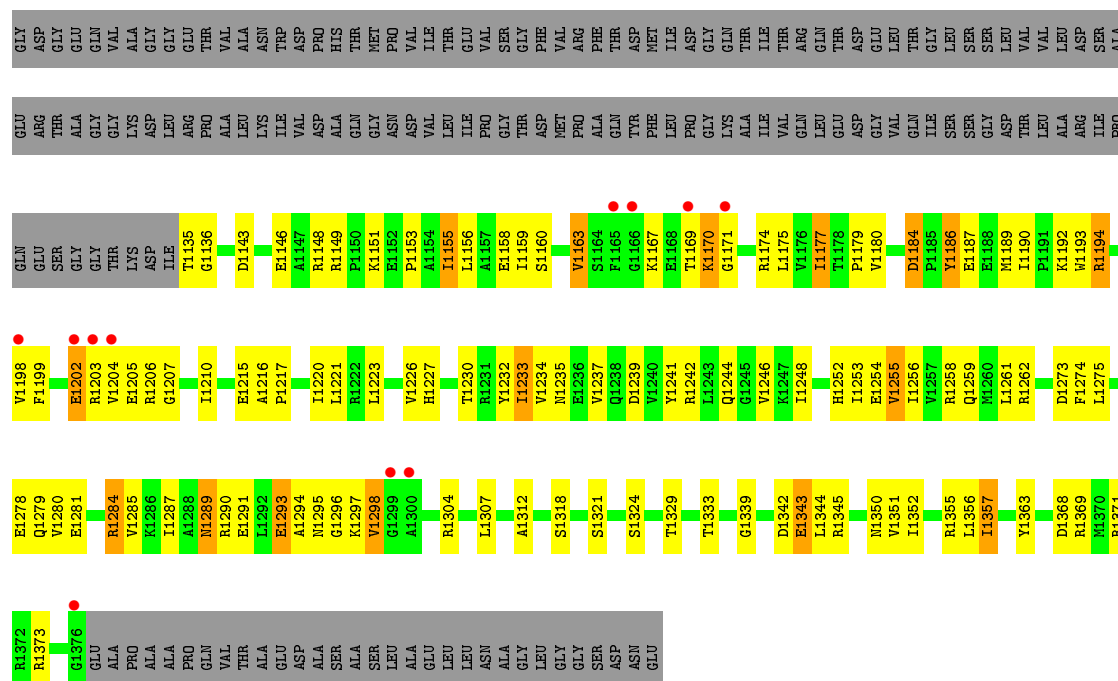




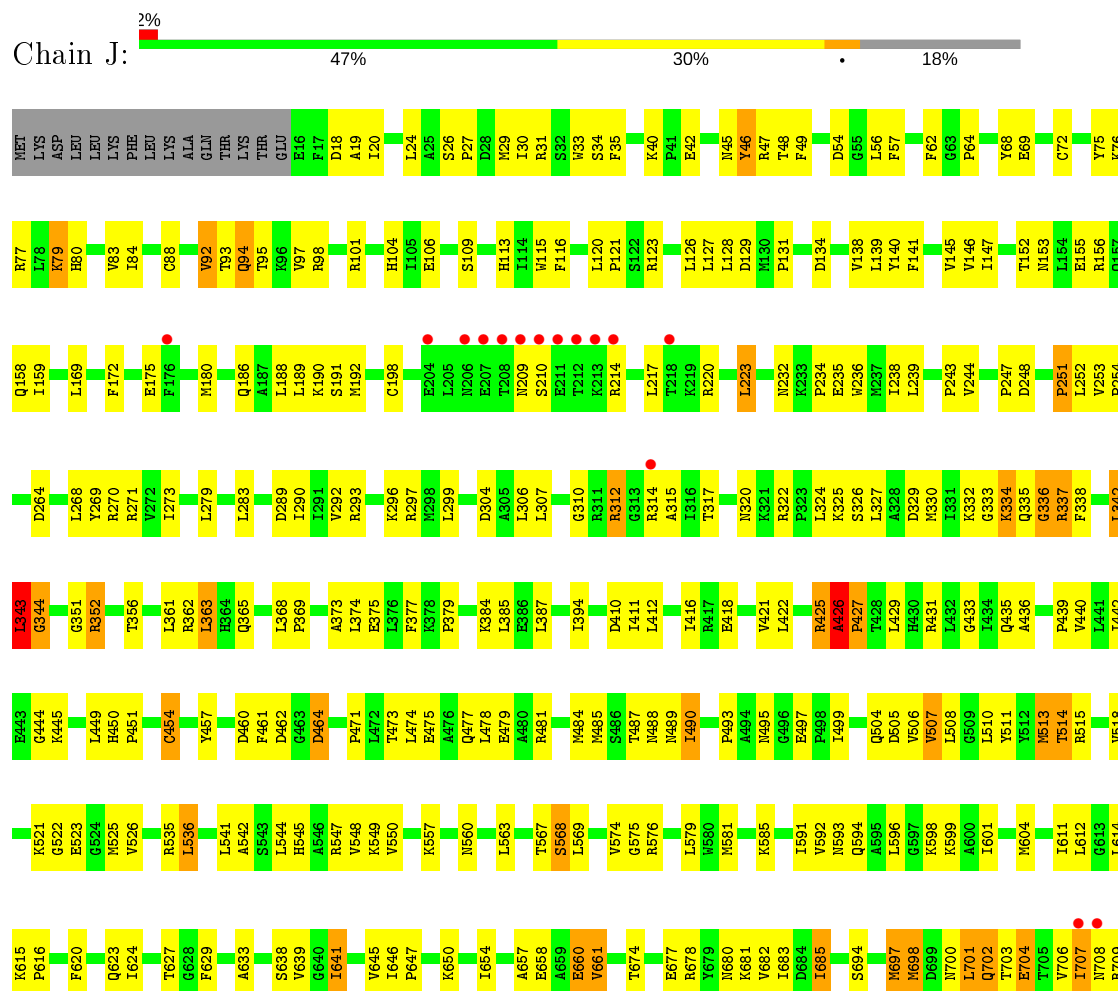
- Molecule 3: DNA-directed RNA polymerase subunit beta'



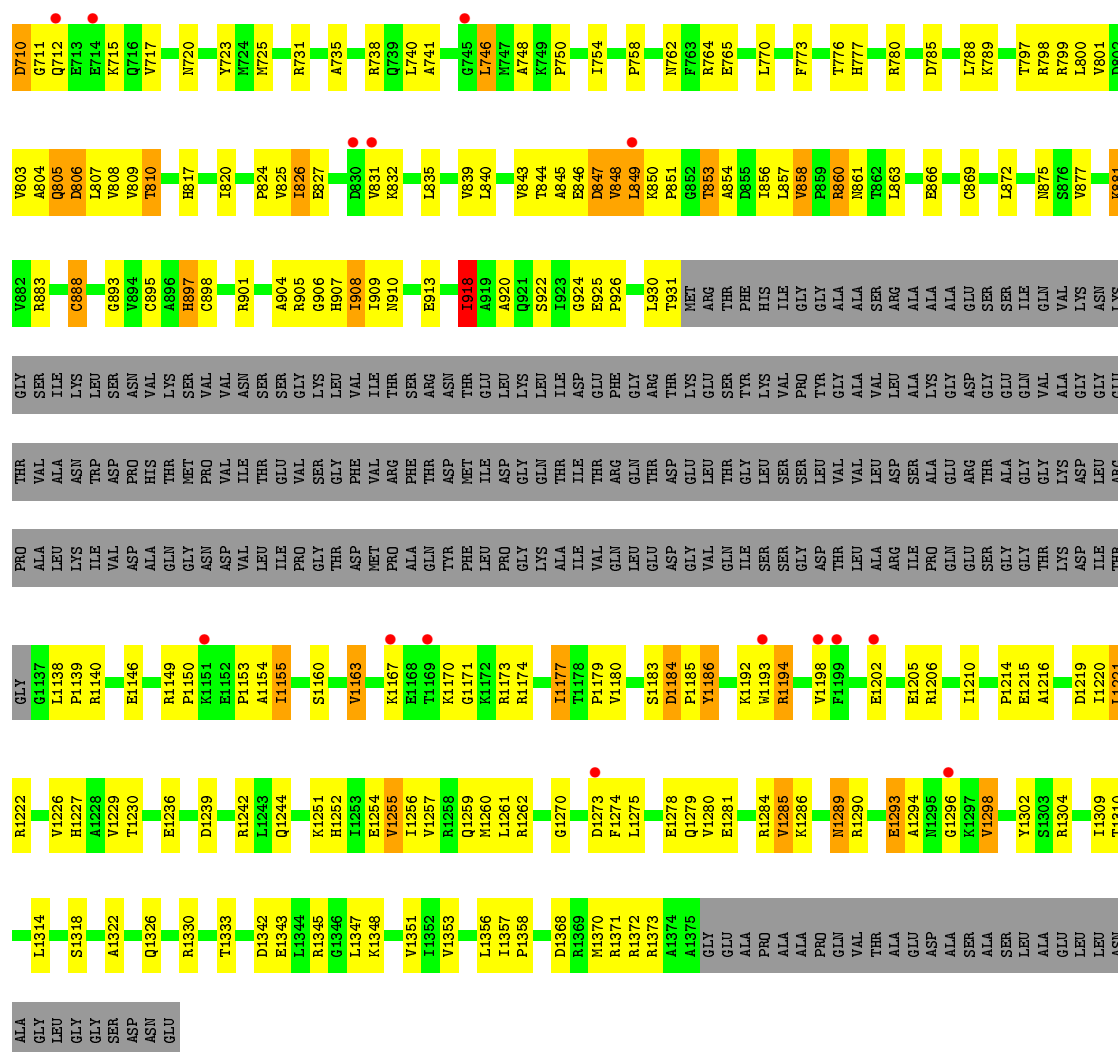




• Molecule 3: DNA-directed RNA polymerase subunit beta'

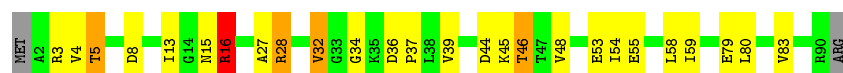






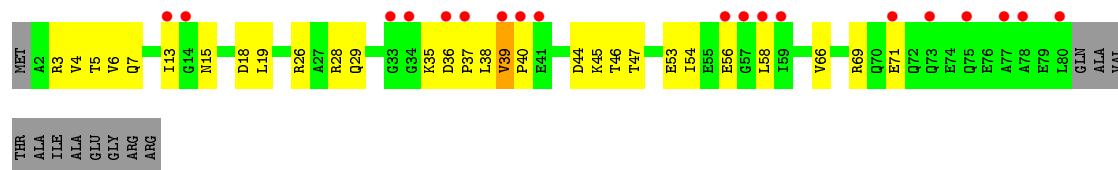
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  69% 23% . . .



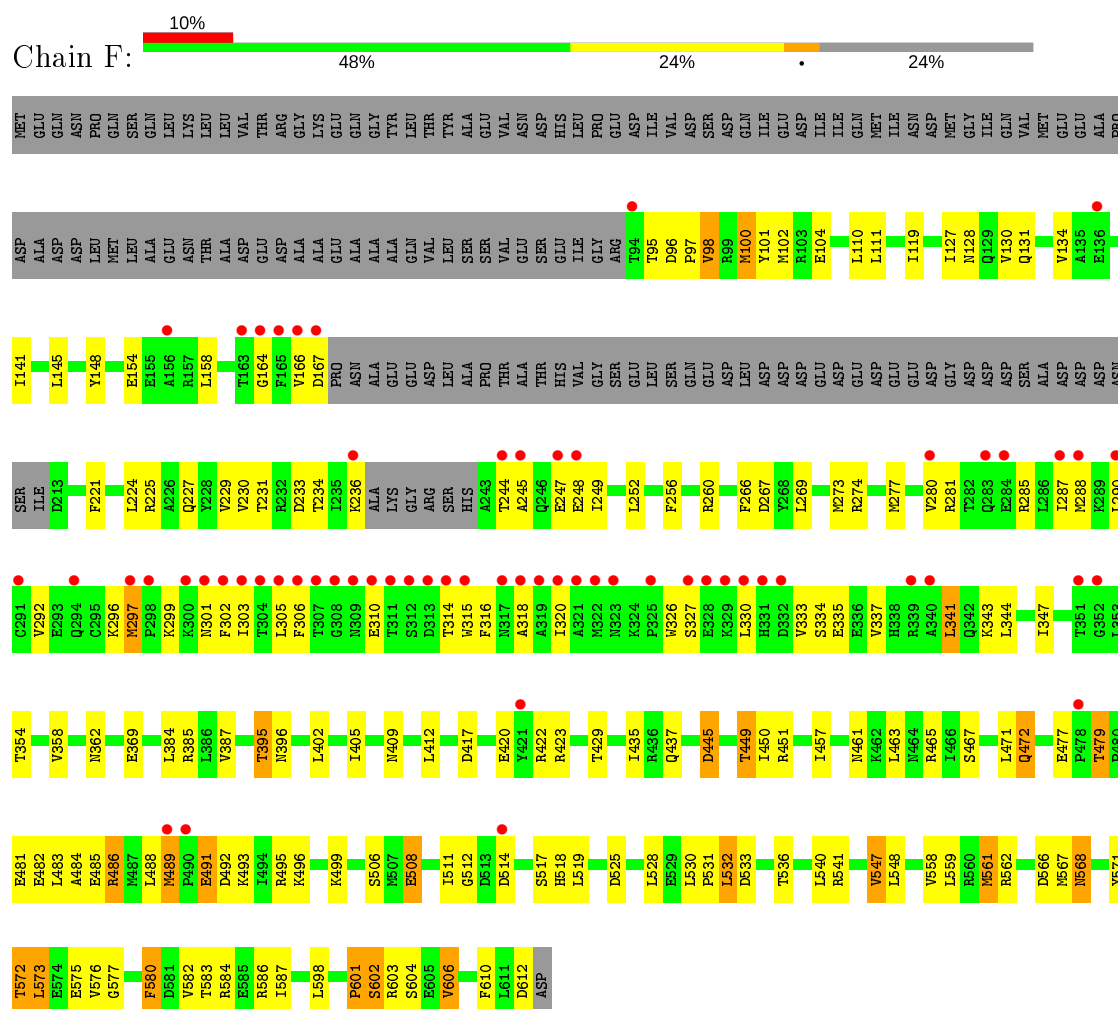
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 

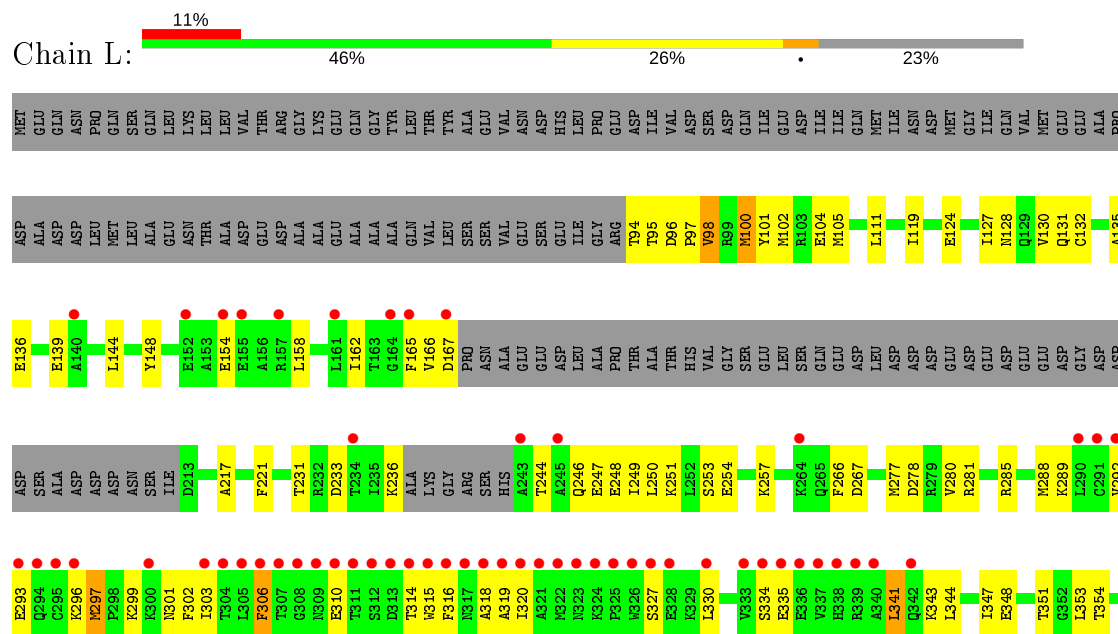


- Molecule 5: RNA polymerase sigma factor RpoD

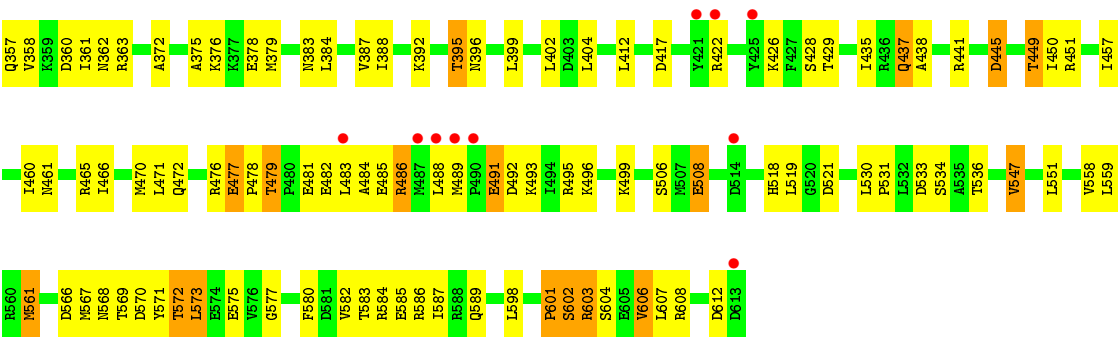




- Molecule 5: RNA polymerase sigma factor RpoD









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 3.75Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.248 , 0.295 0.248 , 0.295	Depositor DCC
$R_{free}$ test set	1991 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	159.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 102.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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:560:PRO:O	3:J:780:ARG:NH2	2.15	0.77
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.66	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:820:ILE:HG22	3:J:1227:HIS:ND1	2.06	0.71
3:J:343:LEU:CD2	3:J:343:LEU:CB	2.69	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:77:ARG:HG3	3:D:79:LYS:H	1.54	0.70
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.74	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:805:GLN:OE1	3:J:1348:LYS:HD3	1.92	0.69
3:J:384:LYS:HD2	3:J:387:LEU:HD23	1.74	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
3:J:426:ALA:HB1	3:J:427:PRO:HD3	1.72	0.69
2:I:808:ASN:H	3:J:633:ALA:HB2	1.57	0.69
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.27	0.68
2:C:1247:SER:HB3	3:D:375:GLU:O	1.94	0.68
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.75	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:1101:LEU:HD12	3:J:505:ASP:OD2	1.94	0.67
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.75	0.67
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1191:LYS:HD3	2:I:1193:ALA:H	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:94:GLN:O	3:J:97:VAL:HG23	1.95	0.67
3:J:98:ARG:HB3	3:J:248:ASP:OD2	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:91:THR:HG21	2:C:503:LYS:HZ3	1.61	0.65
2:C:703:GLY:N	2:C:705:GLU:OE2	2.28	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:270:ARG:HH21	5:F:449:THR:HG23	1.63	0.63
3:D:30:ILE:CG2	3:D:243:PRO:HG3	2.29	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:820:ILE:HG22	3:D:1227:HIS:ND1	2.13	0.63
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.79	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
2:C:1291:LEU:HD21	3:D:1351:VAL:HG13	1.82	0.62
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.33	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:60:GLN:HA	2:C:67:GLU:HA	1.82	0.62
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.35	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:674:ASP:OD2	2:C:1070:HIS:ND1	2.31	0.61
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.82	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:91:THR:HG21	2:C:503:LYS:NZ	2.17	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: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
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.51	0.58
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.84	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: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
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.40	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:20:SER:OG	1:H:21:SER:N	2.36	0.57
1:H:55:ALA:O	1:H:146:VAL:HG13	2.04	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
2:C:560:PRO:O	3:D:780:ARG:NH2	2.37	0.55
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.41	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:1087:TYR:HE1	2:I:1215:GLY:HA2	1.71	0.55
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.72	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:213:LEU:HB3	2:C:422:LYS:HD2	1.89	0.54
2:C:310:ILE:HG21	2:C:325:LEU:HB3	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:98:VAL:O	2:I:121:GLU:HA	2.07	0.53
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.72	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:661:VAL:HB	2:C:665:ALA:HB3	1.91	0.53
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.73	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: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
3:D:1291:GLU:HG2	3:J:1302:TYR:OH	2.09	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:819:SER:HB2	2:I:1085:MET:SD	2.50	0.52
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.90	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:12:ARG:HH21	2:C:793:GLU:CD	2.13	0.52
2:C:529:ARG:HH12	6:C:3001:RFP:C17	2.22	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:159:SER:HB2	2:I:442:VAL:HG21	1.92	0.52
2:I:818:VAL:O	2:I:1079:ILE:HD12	2.09	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: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
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.92	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: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:I:146:VAL:HG21	2:I:513:GLN:NE2	2.25	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:801:ARG:HG2	2:C:1094:VAL:HG23	1.91	0.51
2:C:698:PRO:HG3	2:C:1231:TYR:CE2	2.45	0.51
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.46	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:97:VAL:HG11	3:D:101:ARG:NH2	2.26	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
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:57:PHE:HB3	3:D:98:ARG:HH22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:622:ASP:HB3	3:D:626:TYR:HE2	1.76	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: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
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.10	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:930:LEU:HD23	3:J:1244:GLN:HG3	1.92	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
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:61:SER:HB3	2:C:479:LEU:HB3	1.93	0.50
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.11	0.50
2:C:898:GLU:OE2	5:F:541:ARG:NH1	2.44	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: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
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.92	0.50
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.58	0.50
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.76	0.50
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.23	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
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.27	0.50
3:J:270:ARG:NH2	5:L:449:THR:HG23	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:117:ILE:HD12	2:C:488:MET:HG2	1.94	0.49
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.30	0.49
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.93	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:566:GLY:H	2:I:569:ILE:CG1	2.24	0.49
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	1.94	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:362:ARG:H	3:J:365:GLN:NE2	2.09	0.49
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.47	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
3:D:1297:LYS:HD3	3:J:1302:TYR:CE1	2.47	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: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
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
3:D:79:LYS:HD3	5:F:568:ASN:HB3	1.94	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:314:ASN:O	2:C:352:ARG:NH1	2.41	0.48
2:C:149:LEU:HD13	2:C:453:ILE:CG1	2.44	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:244:THR:O	5:F:247:GLU:HG2	2.13	0.48
5:F:164:GLY:O	5:F:260:ARG:HB2	2.12	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
1:H:34:GLY:HA3	2:I:1083:GLU:OE1	2.14	0.47
2:I:593:LYS:HA	2:I:652:TYR:CD2	2.49	0.47
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.48	0.47
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.50	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:73:GLY:O	1:B:134:THR:HG22	2.15	0.47
1:B:29:GLU:HG3	1:B:30:PRO:CG	2.44	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:801:ARG:HD3	2:C:1094:VAL:HA	1.96	0.47
2:C:1337:ILE:O	2:C:1337:ILE:HG23	2.14	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:A:154:PRO:HB2	2:C:1059:ARG:HH21	1.79	0.47
1:B:89:ALA:O	1:B:124:VAL:HG12	2.14	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
1:H:182:ARG:NH1	3:J:581:MET:SD	2.88	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: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:688:GLN:HB2	2:I:1235:LEU:HD22	1.97	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
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:981:ALA:O	2:I:1002:LEU:HD11	2.15	0.46
2:I:556:GLY:HA2	2:I:659:GLN:O	2.16	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:801:ARG:O	2:I:1095:ASP:HB2	2.14	0.46
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.97	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:672:GLU:HG2	2:C:1187:PHE:HA	1.97	0.46
2:C:582:ASN:HB3	2:C:586:PHE:N	2.31	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:180:ARG:NH2	2:I:396:ASP:HB2	2.29	0.46
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.97	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:886:LYS:HE3	2:I:916:SER:HB3	1.97	0.46
2:I:844:LYS:HD3	3:J:49:PHE:CE2	2.50	0.46
3:J:709:ARG:O	3:J:711:GLY:N	2.45	0.46
3:J:488:ASN:ND2	4:K:6:VAL:HG22	2.31	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:254:PRO:C	3:D:255:LEU:HD22	2.36	0.45
3:D:252:LEU:HD23	3:D:262:THR:HB	1.97	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:489:ASN:HA	3:J:904:ALA:HB1	1.99	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
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: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:D:1226:VAL:HB	3:J:1293:GLU:H	1.81	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:818:VAL:O	2:C:1079:ILE:HD12	2.17	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: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:O	2:C:805:MET:HG3	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: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
2:I:818:VAL:HG22	2:I:1096:ILE:HG23	1.99	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:97:VAL:HG11	3:J:101:ARG:CZ	2.48	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
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: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
3:D:392:THR:HG21	5:F:606:VAL:HA	2.00	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:G:83:LEU:HD23	2:I:694:ARG:NH2	2.33	0.43
1:H:47:LEU:HD21	1:H:220:ALA:HB2	2.00	0.43
1:H:228:LEU:HD23	1:H:228:LEU:HA	1.62	0.43
2:I:12:ARG:HG2	2:I:1183:ALA:HB2	1.99	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:810:TYR:CE1	2:I:1078:LYS:HB2	2.53	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: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:905:ARG:HH21	3:J:907:HIS:HB3	1.81	0.43
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.99	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:860:ARG:HB3	3:D:861:ASN:H	1.70	0.43
3:D:9:LYS:HG2	3:D:10:ALA:N	2.34	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:796:LEU:O	2:C:1233:LEU:HD12	2.19	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
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: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
2:C:1270:PHE:C	3:D:343:LEU:HD11	2.39	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:34:SER:HB2	3:D:104:HIS:HB3	2.01	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
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:591:TYR:HD2	2:I:606:LEU:HD13	1.85	0.42
2:I:565:GLU:HB2	2:I:680:LEU:HD21	2.01	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:97:VAL:HG11	3:D:101:ARG:CZ	2.50	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
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:94:ALA:HB2	2:I:129:LEU:HD11	2.01	0.42
2:I:736:VAL:HG23	2:I:748:ILE:HA	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:62:PHE:O	3:J:101:ARG:HD2	2.20	0.42
3:J:1285:VAL:O	3:J:1289:ASN:HB3	2.20	0.42
3:J:513:MET:O	3:J:575:GLY:HA3	2.20	0.42
3:J:513:MET:HE3	3:J:579:LEU:HD22	2.01	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: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
2:I:149:LEU:HD13	2:I:453:ILE:HG12	2.02	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: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:I:1314:GLN:HG2	4:K:28:ARG:NH2	2.35	0.41
2:C:1339:LEU:H	2:C:1339:LEU:HD12	1.85	0.41
2:C:298:ALA:HB3	2:C:334:GLU:HB2	2.01	0.41
2:C:221:LEU:HB3	2:C:336:LEU:HD21	2.02	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:149:LEU:HD13	2:C:453:ILE:HG12	2.02	0.41
2:C:42:ASP:O	2:C:44:GLU:N	2.50	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:G:152:TYR:CD1	2:I:824:GLN:HG2	2.56	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
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:545:PHE:CZ	3:D:781:LYS:HA	2.55	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
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:71:VAL:HG21	2:C:118:LYS:HE2	2.01	0.41
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.84	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:610:ARG:HG2	3:D:866:GLU:CD	2.41	0.41
3:D:706:VAL:HG12	3:D:715:LYS:HB3	2.03	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:478:LEU:HD21	4:K:47:THR:O	2.21	0.41
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
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:11:PRO:HG3	1:B:28:LEU:HD21	2.02	0.41
1:B:118:ASP:HB2	1:B:121:VAL:CG2	2.51	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:1065:LYS:CD	2:C:1235:LEU:HD12	2.50	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:1318:SER:OG	3:D:1342:ASP:OD2	2.23	0.41
3:D:126:LEU:CD1	3:D:223:LEU:HD22	2.51	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:A:233:ASP:HA	1:B:218:ARG:HH11	1.86	0.41
1:B:118:ASP:HB2	1:B:121:VAL:HG23	2.02	0.41
2:C:71:VAL:HB	2:C:99:LYS:HB2	2.03	0.41
2:C:890:LYS:HE2	2:C:891:GLY:H	1.86	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:15:PHE:CG	2:C:1190:ALA:HB2	2.56	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: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:145:ILE:CG2	2:I:456:VAL:HG22	2.50	0.41
2:I:202:ARG:HH11	2:I:369:MET:CG	2.34	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
2:C:1285:TYR:CD1	3:D:475:GLU:HB3	2.56	0.41
3:D:370:LYS:HD3	3:D:409:TRP:CH2	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:479:THR:HG23	5:F:481:GLU:N	2.32	0.41
5:F:467:SER:HB2	5:F:483:LEU:HD21	2.03	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:410:ASP:N	3:J:410:ASP:OD2	2.54	0.41
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.21	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:598:VAL:HG22	2:C:628:HIS:CE1	2.56	0.40
2:C:590:PRO:HB2	2:C:655:VAL:HG21	2.03	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:70:THR:HG21	2:I:755:LYS:HE2	2.04	0.40
1:G:85:LEU:HA	1:G:85:LEU:HD23	1.89	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%)	8	42
1	B	210/329 (64%)	183 (87%)	22 (10%)	5 (2%)	6	37
1	G	222/329 (68%)	193 (87%)	25 (11%)	4 (2%)	8	42
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	4	32
2	C	1340/1342 (100%)	1233 (92%)	100 (8%)	7 (0%)	29	66
2	I	1338/1342 (100%)	1232 (92%)	101 (8%)	5 (0%)	34	70
3	D	1162/1407 (83%)	1072 (92%)	81 (7%)	9 (1%)	19	57
3	J	1151/1407 (82%)	1056 (92%)	80 (7%)	15 (1%)	12	48
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%)	47	79
5	L	463/613 (76%)	424 (92%)	38 (8%)	1 (0%)	47	79
All	All	6948/8222 (84%)	6354 (92%)	536 (8%)	58 (1%)	19	57

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%)	18	49
1	B	182/286 (64%)	172 (94%)	10 (6%)	21	53
1	G	191/286 (67%)	179 (94%)	12 (6%)	18	49
1	H	184/286 (64%)	177 (96%)	7 (4%)	33	61
2	C	1157/1157 (100%)	1051 (91%)	106 (9%)	9	35
2	I	1154/1157 (100%)	1050 (91%)	104 (9%)	9	37
3	D	970/1168 (83%)	873 (90%)	97 (10%)	7	32
3	J	960/1168 (82%)	860 (90%)	100 (10%)	7	30
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	29
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	50
5	F	417/540 (77%)	376 (90%)	41 (10%)	8	33
5	L	418/540 (77%)	376 (90%)	42 (10%)	7	32
All	All	5966/7024 (85%)	5423 (91%)	543 (9%)	9	36

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	-	63,63,63	2.49	21 (33%)	94,94,94	2.68	36 (38%)

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	-	-	15/60/85/85	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	9.15	1.55	1.37
6	C	3001	RFP	O7-C25	-8.17	1.32	1.44
6	C	3001	RFP	C12-C11	-5.59	1.32	1.54
6	C	3001	RFP	C15-N1	4.86	1.46	1.35
6	C	3001	RFP	C18-C17	4.05	1.56	1.43
6	C	3001	RFP	O6-C27	-3.52	1.34	1.43
6	C	3001	RFP	C3-C43	3.47	1.53	1.46
6	C	3001	RFP	C6-C7	-3.29	1.34	1.39
6	C	3001	RFP	C34-C26	-3.00	1.47	1.53
6	C	3001	RFP	O9-C23	-2.95	1.36	1.43
6	C	3001	RFP	O10-C21	-2.89	1.36	1.43
6	C	3001	RFP	C26-C25	-2.84	1.46	1.54
6	C	3001	RFP	C24-C23	-2.63	1.47	1.54
6	C	3001	RFP	C40-N3	-2.50	1.40	1.46
6	C	3001	RFP	C31-C20	-2.39	1.47	1.53
6	C	3001	RFP	C29-C28	2.38	1.43	1.30
6	C	3001	RFP	C32-C22	-2.36	1.48	1.53
6	C	3001	RFP	C22-C21	-2.25	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	C17-C16	2.24	1.41	1.34
6	C	3001	RFP	C5-C10	-2.08	1.38	1.43
6	C	3001	RFP	C3-C2	-2.01	1.37	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C32-C22-C23	-7.21	96.82	111.39
6	C	3001	RFP	C33-C24-C23	-6.90	97.45	111.39
6	C	3001	RFP	C38-N4-C42	6.63	120.58	110.66
6	C	3001	RFP	O7-C25-C26	-6.57	92.21	107.50
6	C	3001	RFP	O4-C11-C5	-5.55	121.23	131.81
6	C	3001	RFP	C12-C11-C5	5.35	117.78	107.30
6	C	3001	RFP	C34-C26-C25	-5.31	101.87	111.40
6	C	3001	RFP	C41-N3-N2	5.27	141.05	113.86
6	C	3001	RFP	C13-C12-C11	-5.19	101.03	113.90
6	C	3001	RFP	C38-N4-C39	5.15	118.37	110.66
6	C	3001	RFP	C31-C20-C19	-5.13	97.59	109.99
6	C	3001	RFP	C2-C3-C43	-4.29	119.81	124.17
6	C	3001	RFP	C41-C42-N4	-4.04	106.24	110.80
6	C	3001	RFP	O7-C35-C36	3.51	117.55	111.09
6	C	3001	RFP	C40-N3-N2	-3.51	95.73	113.86
6	C	3001	RFP	C26-C25-C24	-3.34	107.87	114.68
6	C	3001	RFP	C17-C18-C19	-3.32	116.47	124.53
6	C	3001	RFP	C32-C22-C21	-3.27	104.79	111.39
6	C	3001	RFP	O5-C12-C13	3.26	115.52	106.99
6	C	3001	RFP	C4-C3-C43	3.25	120.40	116.52
6	C	3001	RFP	C25-O7-C35	3.23	122.72	117.72
6	C	3001	RFP	O7-C35-O8	-3.09	116.82	122.96
6	C	3001	RFP	C12-O3-C6	-3.03	102.58	107.68
6	C	3001	RFP	C40-C39-N4	-3.01	107.40	110.80
6	C	3001	RFP	C41-N3-C40	2.99	121.53	113.74
6	C	3001	RFP	O6-C27-C26	-2.94	101.85	107.98
6	C	3001	RFP	O1-C1-C2	2.83	124.89	119.26
6	C	3001	RFP	C3-C2-N1	-2.82	114.56	119.25
6	C	3001	RFP	C5-C10-C9	-2.54	115.03	119.66
6	C	3001	RFP	O9-C23-C22	-2.47	104.00	109.49
6	C	3001	RFP	C12-O5-C29	2.40	123.78	117.84
6	C	3001	RFP	O10-C21-C22	-2.40	104.14	109.49
6	C	3001	RFP	C42-C41-N3	-2.35	106.69	110.51
6	C	3001	RFP	C26-C27-C28	2.21	116.95	112.13
6	C	3001	RFP	O3-C6-C7	2.19	124.90	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C24-C23-C22	2.17	119.06	115.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C19-C20-C21-O10
6	C	3001	RFP	O6-C27-C28-C29
6	C	3001	RFP	C43-N2-N3-C40
6	C	3001	RFP	C43-N2-N3-C41
6	C	3001	RFP	C19-C20-C21-C22
6	C	3001	RFP	C16-C17-C18-C19
6	C	3001	RFP	C31-C20-C21-O10
6	C	3001	RFP	C1-C2-N1-C15
6	C	3001	RFP	C18-C19-C20-C31
6	C	3001	RFP	C30-C16-C17-C18
6	C	3001	RFP	C26-C27-C28-C29
6	C	3001	RFP	C26-C25-O7-C35
6	C	3001	RFP	C33-C24-C25-O7

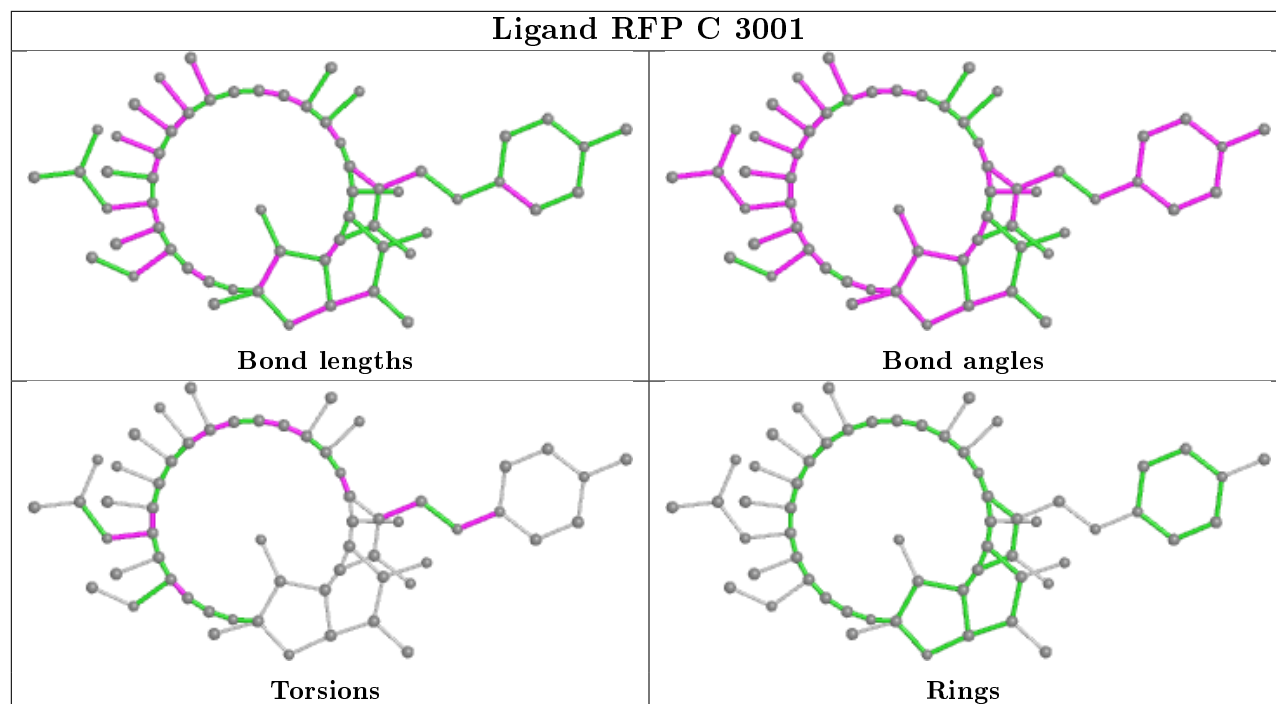
There are no ring outliers.

1 monomer is involved in 14 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/329 (68%)	-0.20	4 (1%) 68 61	128, 159, 207, 262	0
1	B	214/329 (65%)	0.12	7 (3%) 46 38	115, 179, 246, 259	0
1	G	224/329 (68%)	-0.20	1 (0%) 92 89	162, 193, 225, 245	0
1	H	215/329 (65%)	0.10	9 (4%) 36 30	165, 218, 246, 265	0
2	C	1342/1342 (100%)	-0.04	57 (4%) 36 30	96, 152, 303, 368	0
2	I	1340/1342 (99%)	0.24	90 (6%) 17 14	129, 200, 287, 371	0
3	D	1166/1407 (82%)	-0.14	25 (2%) 63 55	94, 140, 215, 278	0
3	J	1155/1407 (82%)	-0.07	30 (2%) 56 47	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%)	1.01	19 (24%) 0 0	221, 276, 310, 318	0
5	F	468/613 (76%)	0.50	62 (13%) 3 3	139, 216, 432, 522	0
5	L	469/613 (76%)	0.71	67 (14%) 2 3	144, 239, 458, 518	0
All	All	6988/8222 (84%)	0.09	371 (5%) 26 23	94, 176, 295, 522	0

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	318	ALA	14.7
5	L	319	ALA	13.8
5	L	321	ALA	13.7
5	F	312	SER	13.5
5	L	327	SER	12.4
5	L	311	THR	11.9
5	F	304	THR	11.7
2	I	980	VAL	11.4
5	L	325	PRO	11.3
5	F	305	LEU	10.7
5	L	312	SER	10.6

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Mol	Chain	Res	Type	RSRZ
2	I	979	LEU	9.5
2	I	1017	GLN	9.4
5	F	328	GLU	9.3
5	L	314	THR	9.2
5	L	313	ASP	8.7
5	L	328	GLU	8.6
5	L	167	ASP	8.5
5	L	326	TRP	8.4
5	L	309	ASN	8.3
5	L	315	TRP	7.9
5	L	310	GLU	7.9
2	C	236	LYS	7.9
2	I	978	VAL	7.7
5	L	308	GLY	7.7
5	F	167	ASP	7.6
5	F	306	PHE	7.6
2	I	976	ARG	7.4
5	F	319	ALA	7.2
2	I	1018	TYR	7.0
2	I	977	ALA	6.9
2	I	107	ARG	6.7
2	I	266	GLY	6.7
2	I	986	ALA	6.4
2	I	1016	GLU	6.4
5	F	329	LYS	6.4
5	L	320	ILE	6.3
5	L	337	VAL	6.3
2	I	1009	ASN	6.3
5	F	314	THR	6.3
3	D	1166	GLY	6.2
5	F	313	ASP	6.2
5	L	291	CYS	6.1
5	F	331	HIS	6.1
2	I	970	GLY	6.1
5	L	323	ASN	6.1
2	I	999	GLU	6.0
5	F	327	SER	6.0
5	L	322	MET	5.9
2	I	1013	GLN	5.7
5	L	333	VAL	5.7
2	I	1010	GLN	5.6
2	I	984	VAL	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	K	57	GLY	5.6
5	F	308	GLY	5.5
5	L	290	LEU	5.4
2	I	998	LEU	5.3
5	L	336	GLU	5.3
5	F	294	GLN	5.2
2	C	321	LEU	5.2
2	I	1005	GLU	5.1
2	I	1015	ALA	5.1
5	F	332	ASP	5.1
2	I	1021	LEU	5.1
5	F	317	ASN	5.1
5	F	323	ASN	5.1
5	F	315	TRP	5.0
2	C	273	HIS	5.0
3	D	1299	GLY	5.0
5	F	300	LYS	5.0
2	I	987	GLU	5.0
5	L	613	ASP	5.0
2	C	274	ILE	4.9
5	F	330	LEU	4.9
2	C	311	CYS	4.9
2	I	60	GLN	4.9
2	I	1006	GLU	4.8
2	I	1000	LEU	4.8
5	F	244	THR	4.7
2	I	1007	LYS	4.7
2	C	301	TYR	4.7
5	L	317	ASN	4.7
2	I	1022	LYS	4.5
2	C	252	SER	4.5
2	C	325	LEU	4.5
5	L	294	GLN	4.5
3	J	207	GLU	4.4
5	F	287	ILE	4.4
5	F	320	ILE	4.4
2	C	309	LEU	4.4
2	C	290	GLU	4.4
2	I	108	GLU	4.3
2	I	1004	ASP	4.3
2	I	981	ALA	4.3
2	C	268	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	259	GLY	4.2
2	I	983	GLY	4.2
2	I	1008	GLN	4.2
2	C	276	GLN	4.1
2	C	108	GLU	4.1
3	J	314	ARG	4.1
2	I	997	TRP	4.1
2	C	302	ILE	4.0
5	F	310	GLU	3.9
2	I	634	VAL	3.9
4	K	58	LEU	3.9
3	J	708	ASN	3.9
5	F	284	GLU	3.9
5	F	245	ALA	3.8
5	L	295	CYS	3.8
4	K	75	GLN	3.8
3	D	1204	VAL	3.8
5	F	301	ASN	3.8
5	F	283	GLN	3.8
5	F	280	VAL	3.7
2	C	62	TYR	3.7
1	B	98	VAL	3.7
5	L	296	LYS	3.7
5	L	307	THR	3.7
3	J	714	GLU	3.7
4	K	59	ILE	3.7
5	F	156	ALA	3.7
1	B	135	ASP	3.7
4	K	56	GLU	3.7
2	C	333	ILE	3.7
2	C	253	PHE	3.7
2	I	415	GLU	3.7
5	L	165	PHE	3.6
3	J	218	THR	3.6
2	C	233	ARG	3.6
3	J	1273	ASP	3.6
1	H	14	VAL	3.6
5	L	161	LEU	3.6
5	L	324	LYS	3.6
5	F	290	LEU	3.6
3	D	154	LEU	3.5
1	H	96	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
4	K	37	PRO	3.5
2	C	982	GLY	3.5
5	L	487	MET	3.5
4	K	71	GLU	3.5
3	D	1198	VAL	3.5
5	F	309	ASN	3.5
2	C	116	ASP	3.5
3	J	1151	LYS	3.5
5	L	243	ALA	3.4
2	I	487	LEU	3.4
2	I	1020	GLU	3.4
5	F	303	ILE	3.4
5	F	164	GLY	3.4
5	F	298	PRO	3.4
5	L	293	GLU	3.4
3	J	212	THR	3.4
5	L	340	ALA	3.4
5	F	490	PRO	3.3
2	I	1012	GLU	3.3
5	F	351	THR	3.3
2	I	985	GLU	3.3
4	K	36	ASP	3.3
1	B	99	ILE	3.2
5	L	490	PRO	3.2
2	C	269	ILE	3.2
2	I	318	SER	3.2
3	D	1376	GLY	3.2
2	C	165	HIS	3.2
5	F	322	MET	3.2
2	C	300	ASP	3.2
2	I	650	VAL	3.2
2	I	248	GLY	3.2
3	J	830	ASP	3.1
5	L	164	GLY	3.1
2	C	985	GLU	3.1
2	C	247	ARG	3.1
3	D	208	THR	3.1
2	C	117	ILE	3.1
4	K	39	VAL	3.1
2	I	982	GLY	3.1
5	L	488	LEU	3.1
2	C	172	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	109	PRO	3.0
3	J	1169	THR	3.0
5	F	307	THR	3.0
2	I	268	ARG	3.0
5	F	318	ALA	3.0
2	I	67	GLU	3.0
5	F	297	MET	3.0
2	C	330	HIS	3.0
2	C	291	TYR	3.0
2	I	250	THR	3.0
5	F	311	THR	3.0
2	C	104	ILE	3.0
2	I	106	GLU	3.0
5	L	154	GLU	3.0
5	L	157	ARG	3.0
2	C	234	ASP	2.9
5	L	304	THR	2.9
3	J	176	PHE	2.9
2	I	165	HIS	2.9
5	F	288	MET	2.9
1	H	106	GLY	2.9
2	I	481	LEU	2.9
2	I	231	GLU	2.9
2	C	266	GLY	2.9
3	D	213	LYS	2.9
3	J	1198	VAL	2.9
4	K	13	ILE	2.9
3	D	209	ASN	2.9
2	C	169	LYS	2.9
5	L	489	MET	2.9
3	D	1203	ARG	2.8
3	D	314	ARG	2.8
5	L	339	ARG	2.8
2	I	1019	ASP	2.8
5	F	340	ALA	2.8
2	I	117	ILE	2.8
1	H	13	LEU	2.8
3	J	712	GLN	2.8
2	I	333	ILE	2.8
2	I	115	LYS	2.8
4	K	78	ALA	2.8
1	H	65	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	235	ASN	2.7
2	C	305	SER	2.7
5	L	421	TYR	2.7
5	L	303	ILE	2.7
5	L	155	GLU	2.7
5	F	421	TYR	2.7
3	J	849	LEU	2.7
5	F	302	PHE	2.7
3	J	214	ARG	2.7
5	L	264	LYS	2.7
2	C	280	ASP	2.7
2	I	59	ILE	2.7
5	F	94	THR	2.7
5	L	334	SER	2.7
3	D	542	ALA	2.7
2	I	1003	THR	2.7
5	F	291	CYS	2.7
5	L	514	ASP	2.6
1	A	164	ASP	2.6
2	I	252	SER	2.6
3	D	1165	PHE	2.6
5	F	165	PHE	2.6
2	I	270	THR	2.6
2	I	311	CYS	2.6
2	C	258	ASN	2.6
1	B	145	LYS	2.6
5	L	234	THR	2.6
2	I	969	ALA	2.6
3	D	1169	THR	2.6
3	J	206	ASN	2.6
1	A	160	HIS	2.6
3	J	213	LYS	2.6
2	C	102	LEU	2.6
2	C	270	THR	2.6
2	C	304	GLU	2.6
4	K	34	GLY	2.6
3	J	208	THR	2.5
5	L	305	LEU	2.5
2	C	574	SER	2.5
4	K	33	GLY	2.5
5	F	321	ALA	2.5
2	I	154	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
5	L	342	GLN	2.5
2	C	310	ILE	2.5
3	D	792	ASN	2.5
5	F	489	MET	2.5
4	K	14	GLY	2.5
2	C	267	ARG	2.5
2	C	599	VAL	2.5
2	I	247	ARG	2.5
2	I	1332	SER	2.4
1	H	18	GLN	2.4
5	F	339	ARG	2.4
3	J	1202	GLU	2.4
2	C	292	ILE	2.4
4	K	40	PRO	2.4
2	C	237	LEU	2.4
5	L	330	LEU	2.4
2	I	601	ASP	2.4
5	F	247	GLU	2.4
2	I	105	TYR	2.4
3	J	707	ILE	2.4
3	D	1300	ALA	2.4
3	J	204	GLU	2.4
2	I	104	ILE	2.4
2	I	331	LYS	2.4
2	I	1264	GLN	2.4
5	F	478	PRO	2.3
3	D	152	THR	2.3
2	I	414	ILE	2.3
2	I	652	TYR	2.3
4	K	41	GLU	2.3
1	B	108	GLY	2.3
3	D	335	GLN	2.3
3	J	1296	GLY	2.3
3	D	317	THR	2.3
2	C	1000	LEU	2.3
2	I	725	GLN	2.3
5	F	163	THR	2.3
3	J	209	ASN	2.3
4	K	73	GLN	2.3
2	I	413	GLU	2.3
4	K	80	LEU	2.3
5	F	352	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	298	ALA	2.3
5	L	422	ARG	2.2
5	L	483	LEU	2.2
2	I	163	LYS	2.2
2	I	633	LEU	2.2
5	F	166	VAL	2.2
5	L	292	VAL	2.2
2	C	332	ARG	2.2
2	I	439	LYS	2.2
3	J	745	GLY	2.2
2	I	375	PRO	2.2
3	J	210	SER	2.2
3	D	149	GLY	2.2
2	I	245	ARG	2.2
5	L	425	TYR	2.2
2	I	1342	GLU	2.2
3	D	176	PHE	2.2
2	I	492	MET	2.2
2	C	317	LEU	2.2
5	L	300	LYS	2.2
5	L	335	GLU	2.2
3	D	1202	GLU	2.2
5	F	248	GLU	2.2
1	A	25	LYS	2.1
3	D	1171	GLY	2.1
2	C	170	VAL	2.1
2	C	289	VAL	2.1
2	I	273	HIS	2.1
5	F	325	PRO	2.1
1	A	193	GLU	2.1
5	L	152	GLU	2.1
2	I	734	ILE	2.1
3	J	1193	TRP	2.1
2	I	975	ILE	2.1
1	B	193	GLU	2.1
3	J	1167	LYS	2.1
5	F	236	LYS	2.1
1	H	97	GLU	2.1
2	C	47	TYR	2.1
1	H	120	ASP	2.1
2	I	367	TYR	2.1
3	J	1199	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	830	ASP	2.1
5	L	306	PHE	2.0
1	G	205	MET	2.0
1	H	107	ILE	2.0
2	C	288	PRO	2.0
4	K	77	ALA	2.0
2	C	481	LEU	2.0
2	I	483	ASP	2.0
2	I	594	VAL	2.0
2	I	753	LEU	2.0
5	L	338	HIS	2.0
3	D	547	ARG	2.0
2	I	571	LEU	2.0
5	L	316	PHE	2.0
3	J	211	GLU	2.0
5	F	136	GLU	2.0
2	I	167	SER	2.0
5	F	514	ASP	2.0
5	L	140	ALA	2.0
3	J	831	VAL	2.0
2	I	392	GLU	2.0
5	L	245	ALA	2.0
2	C	248	GLY	2.0
2	C	892	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.

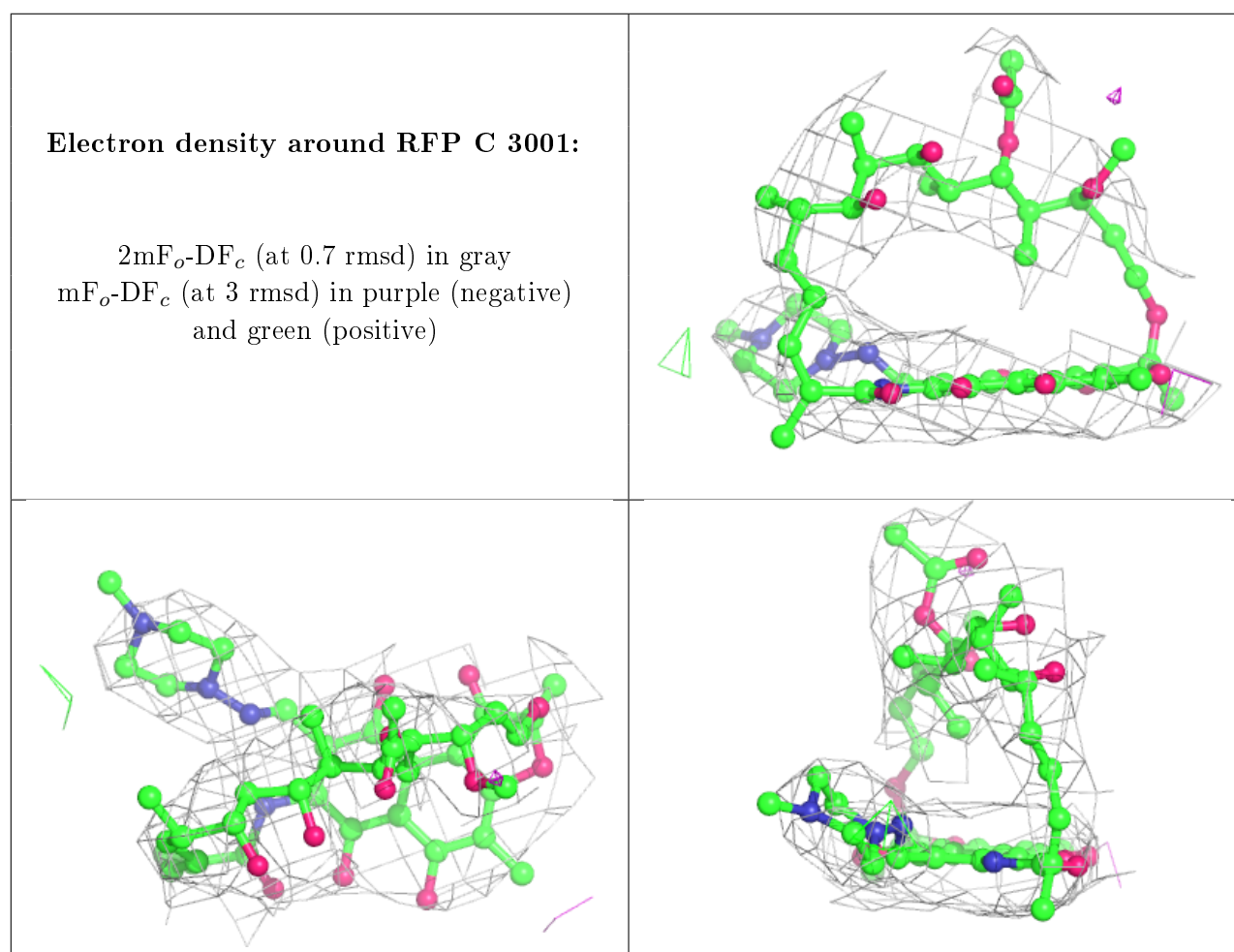
## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	J	1501	1/1	0.51	0.51	290,290,290,290	0
8	ZN	D	1502	1/1	0.58	0.25	324,324,324,324	0
8	ZN	J	1502	1/1	0.61	0.18	322,322,322,322	0
8	ZN	D	1503	1/1	0.71	0.37	274,274,274,274	0
7	MG	D	1501	1/1	0.80	0.41	264,264,264,264	0
8	ZN	J	1503	1/1	0.86	0.42	281,281,281,281	0
6	RFP	C	3001	59/59	0.92	0.22	88,136,160,162	0

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.