



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:38 PM UTC

PDB ID : 4KN7 / pdb_00004kn7
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Benzoxazinorifamycin-2c
Authors : Murakami, K.S.
Deposited on : 2013-05-08
Resolution : 3.69 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

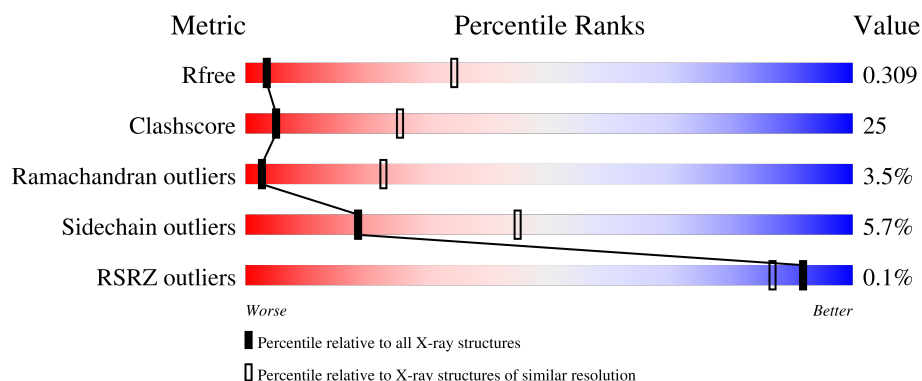
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

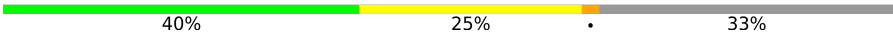
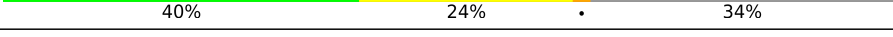
The reported resolution of this entry is 3.69 Å.

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



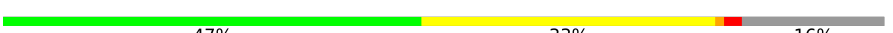
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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

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

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Mol	Chain	Length	Quality of chain
2	H	1342	 54% 39% 6% .
3	D	1407	 38% 40% 5% 18%
3	I	1407	 40% 38% . 18%
4	E	91	 63% 33% ...
4	J	91	 47% 33% .. 16%
5	X	613	 48% 32% . 16%
5	Y	613	 43% 29% . 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56331 atoms, of which 117 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	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

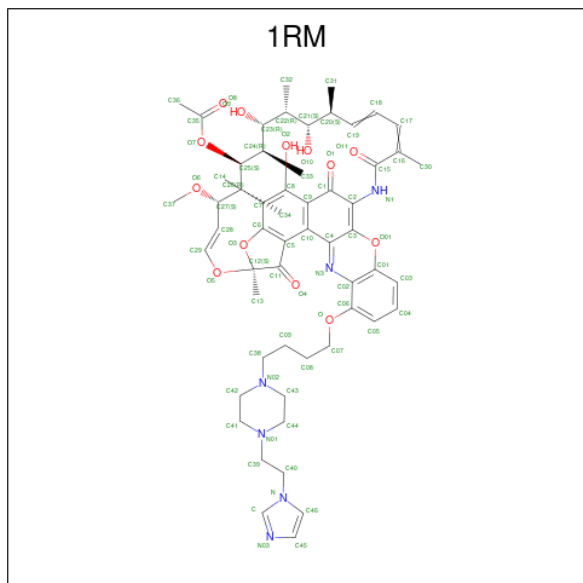
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is Benzoxazinorifamycin-2c (CCD ID: 1RM) (formula: C₅₆H₇₀N₆O₁₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			145	56	70	6	13		
6	H	1	Total	C	H	N	O	0	0
			105	43	47	2	13		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	I	2	Total	Zn	0	0
			2	2		

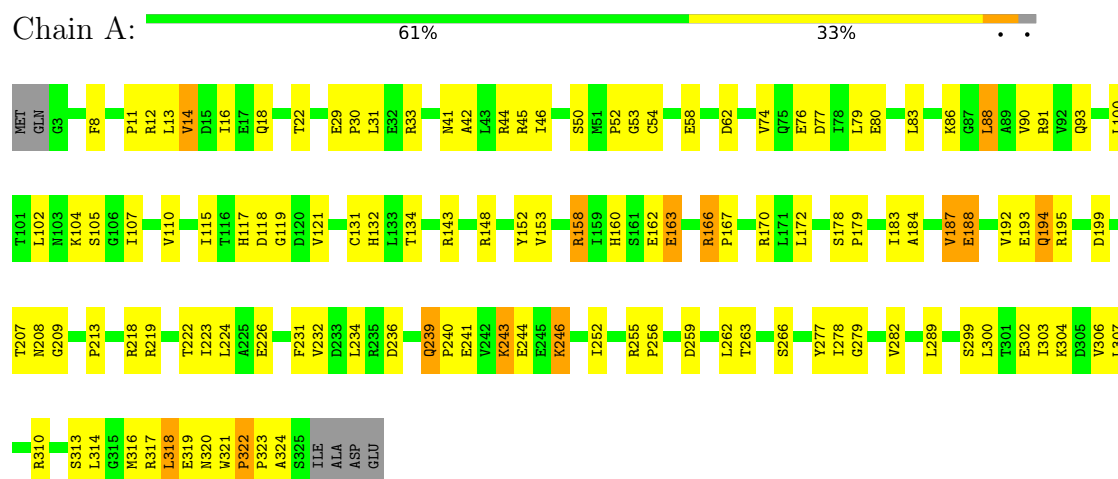
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	Mg 1	0	0
8	I	1	Total 1	Mg 1	0	0

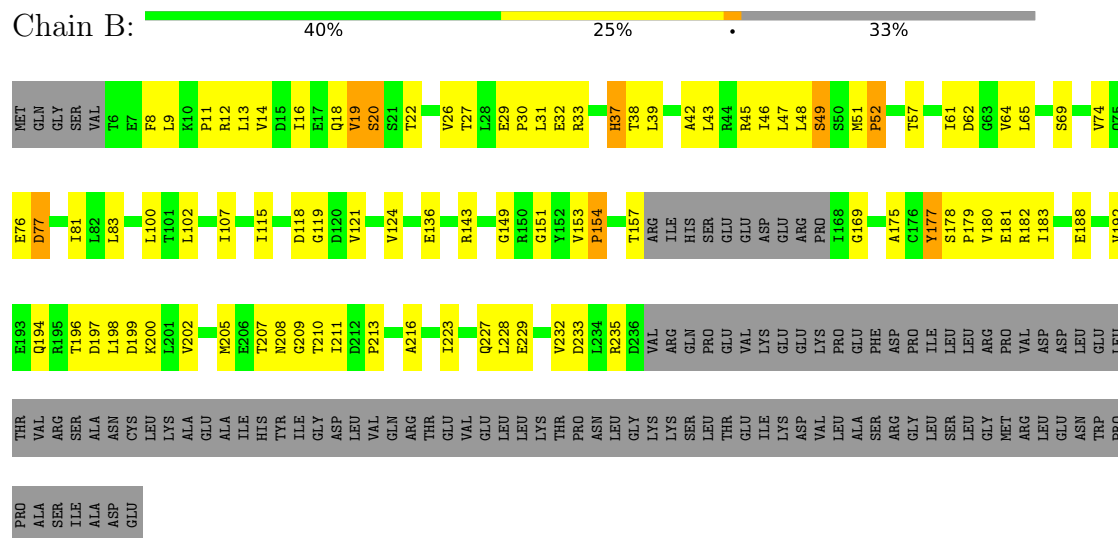
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

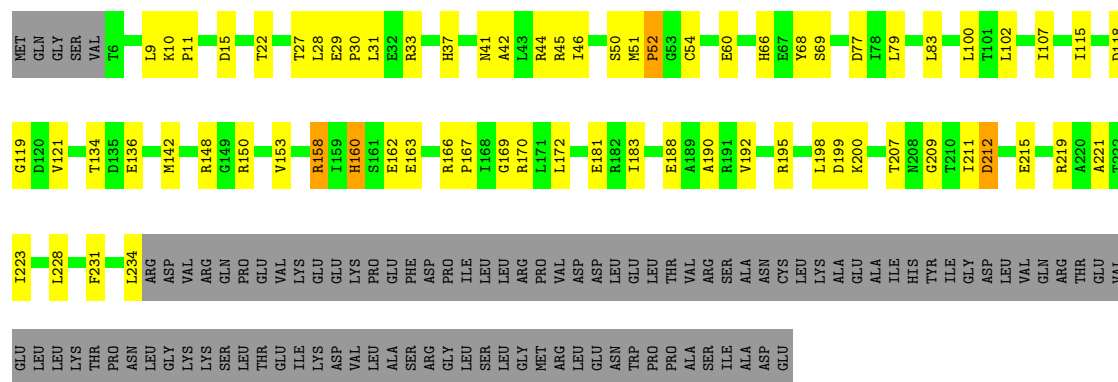


• Molecule 1: DNA-directed RNA polymerase subunit alpha

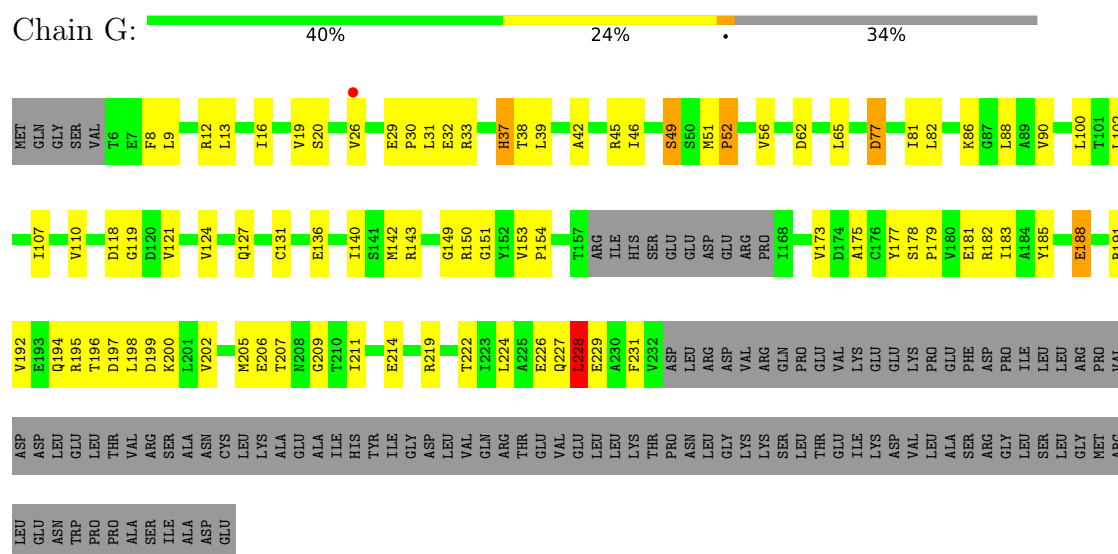


• Molecule 1: DNA-directed RNA polymerase subunit alpha

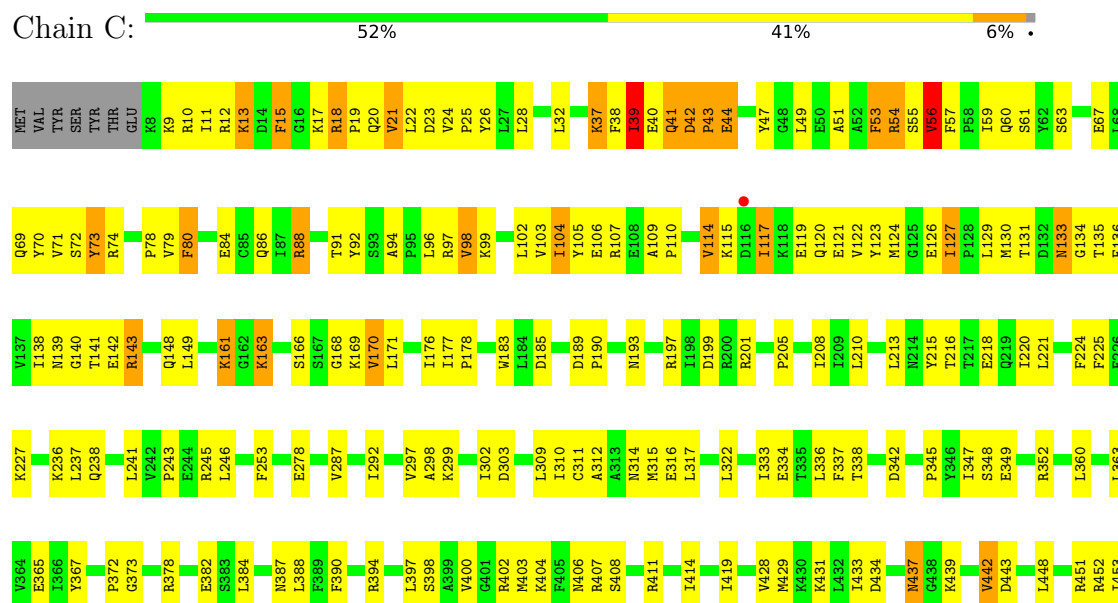


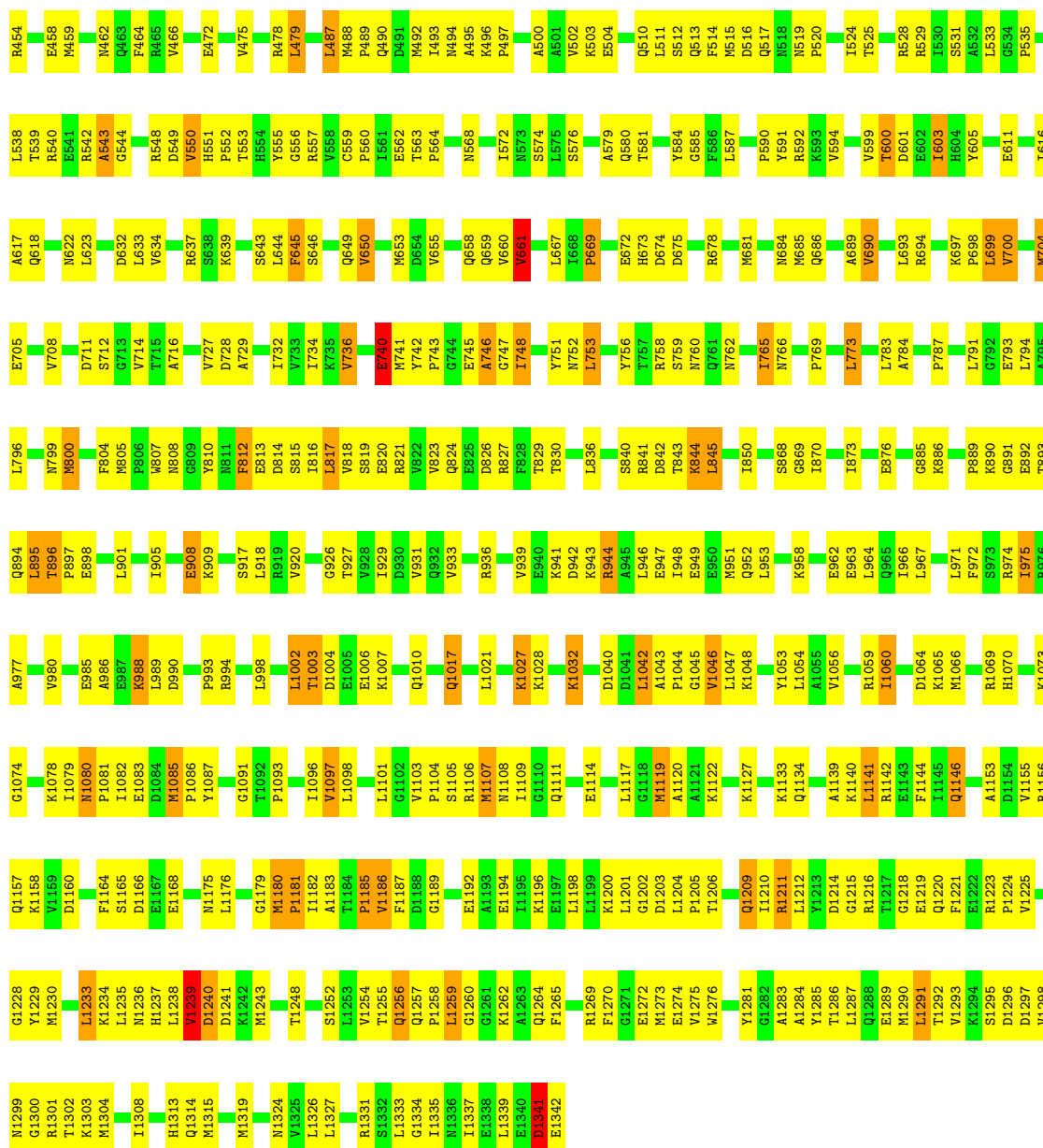


• Molecule 1: DNA-directed RNA polymerase subunit alpha



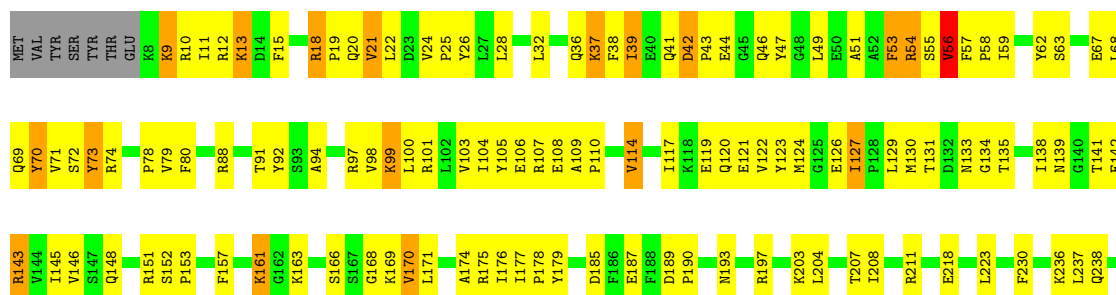
• Molecule 2: DNA-directed RNA polymerase subunit beta



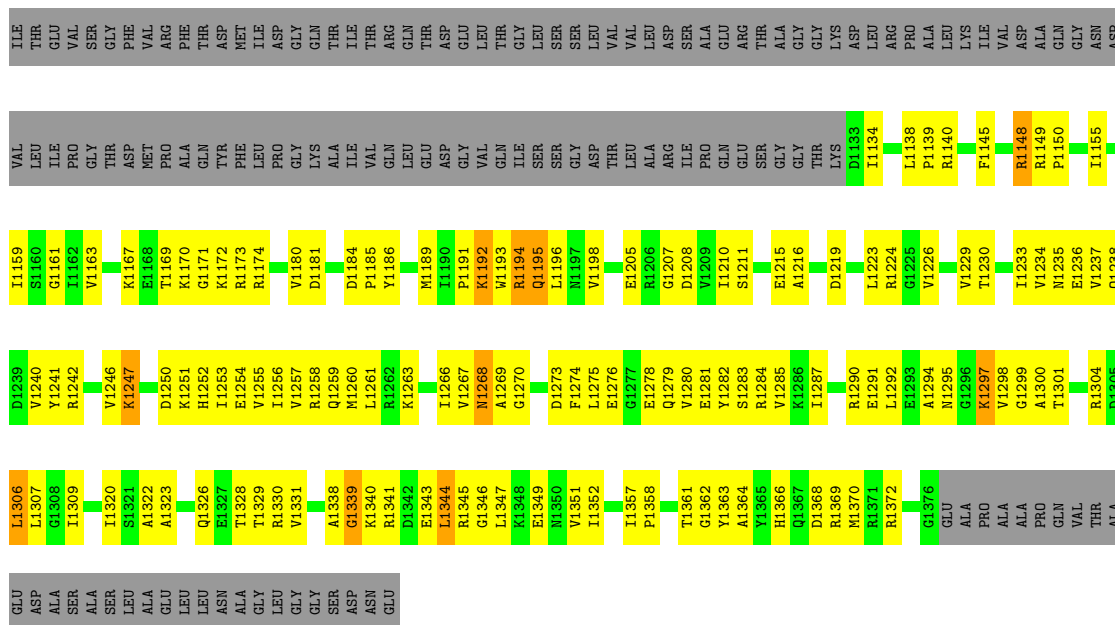


• Molecule 2: DNA-directed RNA polymerase subunit beta

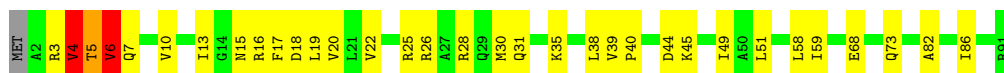
Chain H: 54% 39% 6%



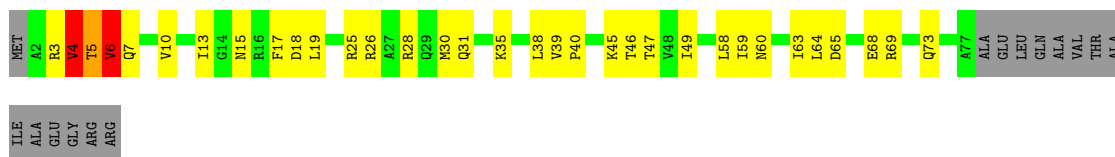
Q1195	ASP	THR	G852	L767	C608	R535	D462	F380	K222	E148	K79
L1196	GLY	LYS	T853	N768	Y609	R538	G463	I381	L223	G149	I84
N1197	VAL	GLU	A854	Y769	R610	S539	D464	Y382	G150	C85	C85
V1198	GLN	THR	D855	L770	L611	S539	Q465	L307	M151	T152	
E1205	ILE	TYR	T856	Q771	L612	G540	M466	L387	M153	G89	C88
E1206	SER	LYS	L857	Y772	G613	L541	H469	R388	L154	E155	V90
D1208	SER	VAL	V858	F773	L614	A542		C389	E156	V92	
V1209	GLY	PRO	P859		K615			R312	L157		
I1210	THR	THR	L863	T776	P616	H545	L472	R390	Q158		V97
S1211	THR	GLY	L864	H777	L617	A546	L473	G313	L159		R98
A1216	LEU	ALA	H865	Y778	G618	R547	L474	T392	L160		R99
A1216	LEU	VAL	H865	R780	G619	V548	E475	A315	L161		E100
I1220	ASP	LEU	E866	F773	P620	K549	A476	I316	L162		M102
L1221	SER	ALA	Q867			V550	Q477	T317			G103
L1221	PRO	ALA	E873	K789	Q623	R551	L478	G318			H104
G1225	GLN	LYS	D873	T797	M625	T553	E479	S319			I105
V1226	GLY	ASP	V880	L800	G626	E554	A480	N320	Y165		L166
V1229	GLY	GLY	K881	V801	T627	Y555	R481	R322	L167		D167
T1230	THR	GLN	V882	D802	G628		A482	P323	A168		L169
I1233	LYS	VAL	S884	V803	F629	D588	M484	L324	E170		E171
I1233	GLY	ALA	V885	L807		A559	M485	K325	E171		A108
I1234	LEU	ASN	V886	V808	A633	K570	T487	G333	F172		A112
N1235	ARG	LYS	S887	T819	G636	D571		GLN	G173		H113
E1236	PRO	THR	C888	T810	G637	T572	R417	GLY	D174		I114
V1237	ALA	VAL		D811	A637	T573		PHE	E175		M115
Q1238	LYS	ALA	G893	E812	S638			ARG	A178		F116
A1242	ILE	ASN	A896	D813	G640	R576	L500	GLN	K179		L117
V1240	VAL	ASP		T816		A577	P502	ASN	M180		K118
I1241	ASP	PRO	V899	H817	D643	L578	S503	LEU	G181		L120
R1242	ALA	HIS	G900	E818	M644	M581	Q504	G344	I185		P121
R1246	GLN	THR	R901	H819	V645	L582	T428	K345	Q186		S122
K1247	GLY	MET	D902	T822	L646	V583	V507	R346	A187		R123
	ASN	PRO	L903	T823	P647	V583	L429	R347	L188		I124
	VAL	VAL	A904	P824	E648	P584	L508	V347	L189		G125
	ASN	ILE	R905	V825		K585		D348	Y269		L126
K1251	LEU	THR	G906	I826	S655	G586	Y512	Y349			L127
I1253	ILE	GLU	H907	E327	E658	L587	M513	I355	M192		L128
V1254	PRO	VAL	L908	G828	E659	P588	T514	T356	L273		D129
I1255	GLY	SER	V909	G831	E660	Y589	R515	E197	E197		M130
V1256	THR	GLY	R910	V831	V661	S590	V518	V357	R275		P131
V1257	ASP	PHE	K911	K832	V662	T591	M519	R362	L201		L132
R1258	MET	VAL	G912		A662	V592	K521	L363	R202		R133
Q1259	PRO	ARG	E913	R836	E663	M593	A520	L364	L205		D134
M1260	ALA	PHE	A914	D837	T664	Q594	G522	H364	N206		I135
L1261	GLN	THR	I915	R838	L746	A595	G522	G367	A287		E136
R1262	ASP	ASP	V839	V839	Q667	L596	E523	G367	P288		R137
K1263	PHE	MET	T918	L840	P668	G597	G524	L368	S210		V138
A1264	LEU	ILE	A919	G841		K598	R525	P369	I291		L139
I1265	PRO	ASP	A920	R842	R678	K599	V526	K370	V292		Y140
V1266	GLY	GLY	Q921	V843	V679	A600	L442	K371	R293		F141
N1268	LYS	GLN	S922		M690	I601	T528	M372	K215		E142
A1269	THR	THR	I923	E846	V682	S602	G529	A373	K216		S143
I1269	ILE	ILE	G924	K847	K681	K603	P530	L374	L217		Y144
P1191	VAL	THR	E925	V848	L683	M684	K531	Y457	T218		K219
K1192	GLN	ARG	P926	L349	D684	L605	E532	M458	K220		V145
W1193	LEU	GLN		E785	G685	N606	A533	K378	R220		L147
R1194	THR	THR	L930	P851	V686	T607	E534	P379	I221		



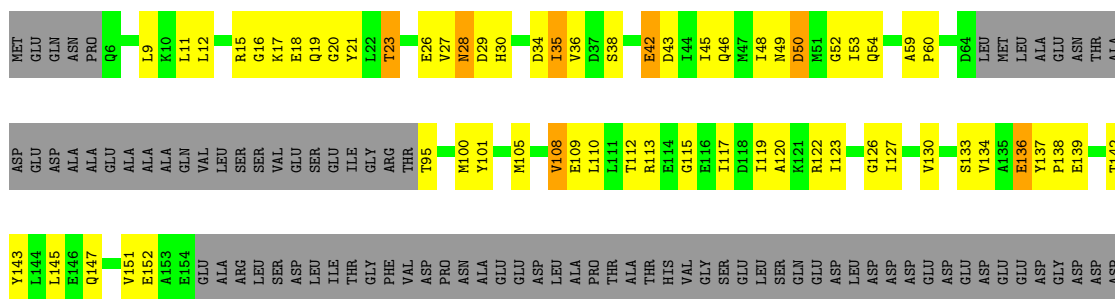
- Molecule 4: DNA-directed RNA polymerase subunit omega

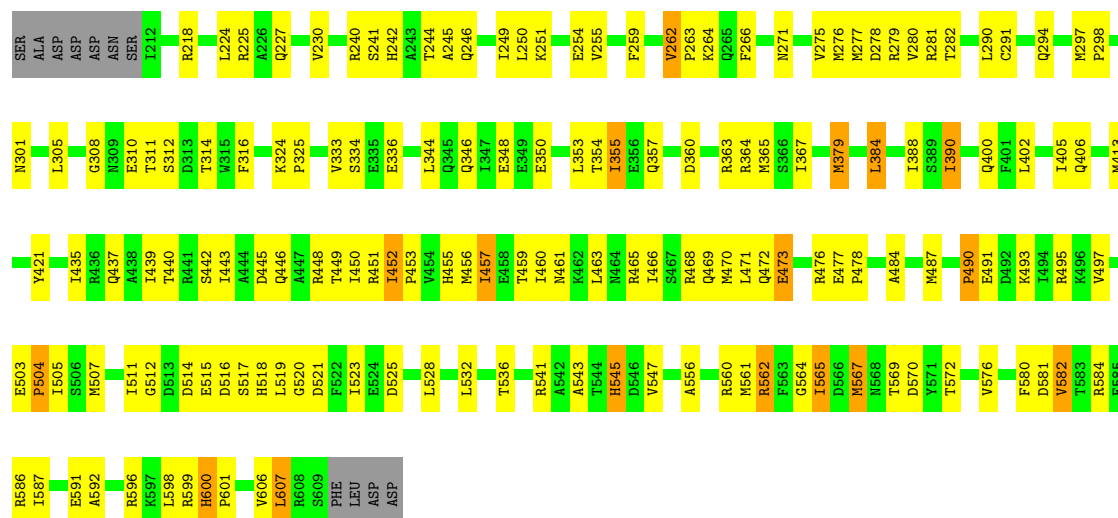


- Molecule 4: DNA-directed RNA polymerase subunit omega

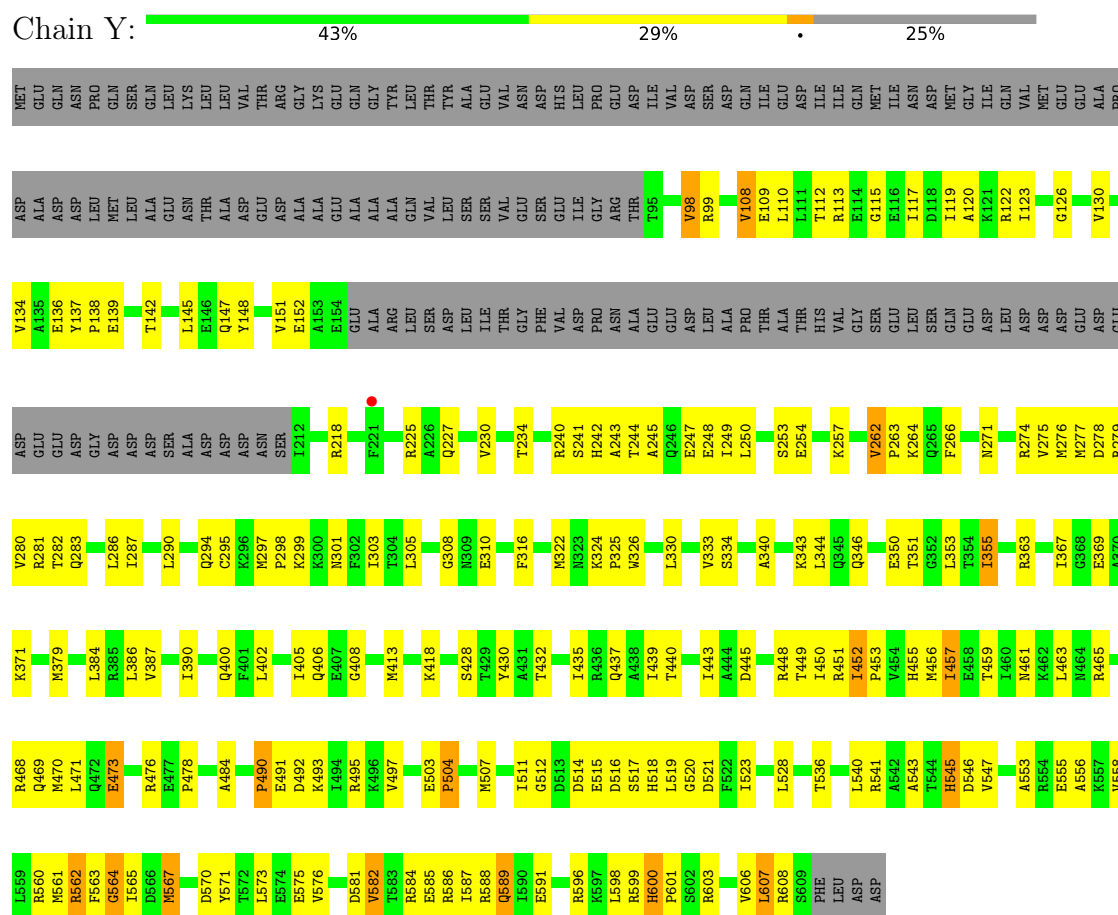


- Molecule 5: RNA polymerase sigma factor RpoD





- Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.83Å 204.58Å 308.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.69 29.88 – 3.69	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.88-3.69) 86.8 (29.88-3.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.252 , 0.309 0.252 , 0.309	Depositor DCC
R_{free} test set	5907 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	120.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	56331	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 1RM

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	0.25	0/2548	0.71	1/3454 (0.0%)
1	B	0.25	0/1725	0.72	0/2337
1	F	0.26	0/1797	0.76	2/2436 (0.1%)
1	G	0.26	0/1690	0.72	0/2290
2	C	0.25	0/10690	0.73	8/14423 (0.1%)
2	H	0.25	0/10690	0.73	8/14423 (0.1%)
3	D	0.26	0/9198	0.74	6/12413 (0.0%)
3	I	0.25	0/9198	0.75	7/12413 (0.1%)
4	E	0.25	0/710	0.69	0/956
4	J	0.24	0/607	0.71	0/817
5	X	0.24	0/4253	0.71	0/5719
5	Y	0.24	0/3783	0.70	0/5083
All	All	0.25	0/56889	0.73	32/76764 (0.0%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	120	LEU	CA-C-N	-7.64	111.50	120.13
3	D	120	LEU	C-N-CA	-7.64	111.50	120.13
3	I	120	LEU	CA-C-N	-7.45	111.71	120.13
3	I	120	LEU	C-N-CA	-7.45	111.71	120.13
2	C	42	ASP	CA-C-N	7.13	128.75	119.84
2	C	42	ASP	C-N-CA	7.13	128.75	119.84
3	I	529	GLY	CA-C-N	6.15	126.33	119.32
3	I	529	GLY	C-N-CA	6.15	126.33	119.32
3	I	854	ALA	CB-CA-C	-6.01	109.66	116.63
3	D	854	ALA	CB-CA-C	-5.96	109.71	116.63
2	H	986	ALA	CB-CA-C	-5.87	109.79	116.54
2	C	1085	MET	CA-C-N	5.78	127.06	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1085	MET	C-N-CA	5.78	127.06	119.84
1	F	212	ASP	CA-C-N	5.67	125.51	119.28
1	F	212	ASP	C-N-CA	5.67	125.51	119.28
2	C	986	ALA	CB-CA-C	-5.61	110.09	116.54
3	D	904	ALA	N-CA-C	-5.41	106.18	112.89
2	H	1184	THR	CA-C-N	5.40	126.59	119.84
2	H	1184	THR	C-N-CA	5.40	126.59	119.84
1	A	241	GLU	CB-CA-C	-5.22	110.13	117.23
3	I	827	GLU	N-CA-C	-5.22	106.69	113.16
3	D	529	GLY	CA-C-N	5.21	125.26	119.32
3	D	529	GLY	C-N-CA	5.21	125.26	119.32
2	C	54	ARG	N-CA-C	5.11	120.91	114.31
2	H	242	VAL	CA-C-N	5.08	125.11	119.32
2	H	242	VAL	C-N-CA	5.08	125.11	119.32
2	H	54	ARG	N-CA-C	5.07	120.85	114.31
2	C	896	THR	CA-C-N	5.05	126.16	119.84
2	C	896	THR	C-N-CA	5.05	126.16	119.84
2	H	896	THR	CA-C-N	5.03	126.12	119.84
2	H	896	THR	C-N-CA	5.03	126.12	119.84
3	I	904	ALA	N-CA-C	-5.00	106.69	112.89

There are no chirality outliers.

There are no planarity outliers.

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	2514	0	2566	103	0
1	B	1706	0	1738	88	0
1	F	1775	0	1800	66	0
1	G	1671	0	1706	81	0
2	C	10523	0	10546	585	0
2	H	10523	0	10546	556	0
3	D	9060	0	9257	615	0
3	I	9060	0	9256	553	0
4	E	708	0	719	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	605	0	612	31	0
5	X	4198	0	4250	192	0
5	Y	3732	0	3809	148	0
6	C	75	70	70	10	0
6	H	58	47	46	8	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56214	117	56921	2821	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 25.

All (2821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.26	1.17
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.28	1.14
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.22	1.13
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.31	1.10
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.29	1.09
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.35	1.08
2:H:488:MET:HB2	2:H:490:GLN:H	1.11	1.08
2:H:54:ARG:H	2:H:55:SER:HB2	1.20	1.06
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.36	1.04
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.40	1.03
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.40	1.03
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.40	1.00
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.43	0.99
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.44	0.99
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.45	0.98
2:C:54:ARG:H	2:C:55:SER:HB2	1.23	0.97
2:H:487:LEU:HB3	2:H:488:MET:HA	1.46	0.97
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.43	0.97
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.46	0.96
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.45	0.96
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.47	0.94
1:B:12:ARG:H	1:B:30:PRO:HG2	1.33	0.93
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.49	0.92
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.51	0.92
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.53	0.91
2:H:488:MET:HB2	2:H:490:GLN:N	1.84	0.90
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.52	0.90
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.35	0.90
3:D:546:ALA:H	3:D:547:ARG:HA	1.37	0.89
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.53	0.89
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.54	0.89
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.55	0.88
2:H:908:GLU:HG2	2:H:909:LYS:H	1.36	0.88
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.03	0.88
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.55	0.88
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.54	0.88
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.52	0.88
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.55	0.88
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.55	0.88
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.54	0.88
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.56	0.88
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.03	0.87
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.57	0.87
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.55	0.87
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.40	0.87
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.55	0.86
3:I:546:ALA:H	3:I:547:ARG:HA	1.40	0.86
3:I:1297:LYS:HZ3	3:I:1297:LYS:HA	1.41	0.86
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.57	0.86
6:H:1401:1RM:H23	6:H:1401:1RM:H26	1.55	0.86
2:H:487:LEU:CB	2:H:488:MET:HA	2.04	0.86
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.56	0.85
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.57	0.85
4:E:5:THR:HA	4:E:6:VAL:CB	2.04	0.85
2:C:131:THR:HG21	2:C:135:THR:HG22	1.58	0.85
2:H:488:MET:CB	2:H:490:GLN:H	1.89	0.85
4:J:5:THR:HA	4:J:6:VAL:CB	2.05	0.85
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.59	0.84
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.43	0.84
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.59	0.84
2:H:488:MET:HE3	2:H:489:PRO:HA	1.58	0.84
5:X:35:ILE:HG13	5:X:36:VAL:H	1.40	0.83
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.59	0.83
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.60	0.83
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.60	0.83
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.60	0.83
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.59	0.83
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.58	0.83
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.43	0.83
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.60	0.83
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.44	0.83
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.60	0.82
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.61	0.82
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.62	0.82
2:H:800:MET:HA	2:H:800:MET:HE3	1.60	0.82
4:J:5:THR:HA	4:J:6:VAL:HB	1.62	0.82
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.62	0.81
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.61	0.81
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.61	0.81
3:D:643:ASP:O	3:D:720:ASN:ND2	2.12	0.81
2:C:170:VAL:HG23	2:C:171:LEU:H	1.45	0.81
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.61	0.81
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.62	0.81
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.06	0.81
3:D:512:TYR:HD2	3:D:724:MET:HE1	1.45	0.80
3:D:828:GLY:HA2	3:D:832:LYS:H	1.45	0.80
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.64	0.80
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.62	0.80
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.64	0.80
2:C:800:MET:HE1	2:C:827:ARG:HD3	1.64	0.80
2:H:487:LEU:HB3	2:H:488:MET:CA	2.11	0.80
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	1.62	0.80
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.63	0.80
4:E:5:THR:HA	4:E:6:VAL:HB	1.64	0.80
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.47	0.80
2:H:54:ARG:N	2:H:55:SER:HB2	1.96	0.79
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.45	0.79
2:C:131:THR:CG2	2:C:135:THR:HG22	2.13	0.79
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.63	0.79
2:H:660:VAL:HG22	2:H:661:VAL:H	1.47	0.79
2:C:660:VAL:HG22	2:C:661:VAL:H	1.47	0.79
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.63	0.79
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.45	0.79
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:316:ILE:HG23	3:D:317:THR:H	1.47	0.79
5:X:240:ARG:HD3	5:X:244:THR:HB	1.65	0.79
3:D:230:SER:HB2	3:D:1339:GLY:H	1.47	0.78
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.47	0.78
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.18	0.78
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.64	0.78
4:E:5:THR:HA	4:E:6:VAL:CG1	2.14	0.78
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.65	0.78
1:F:11:PRO:HG2	1:G:228:LEU:H	1.49	0.78
2:H:163:LYS:H	2:H:163:LYS:HD3	1.48	0.78
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.78
3:I:850:LYS:O	3:I:852:GLY:N	2.17	0.78
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.66	0.78
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.64	0.78
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.66	0.78
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.48	0.78
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.64	0.78
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.66	0.77
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.67	0.77
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.64	0.77
2:C:54:ARG:N	2:C:55:SER:HB2	1.99	0.77
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.66	0.77
4:E:5:THR:HA	4:E:6:VAL:HG12	1.66	0.77
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.49	0.77
6:C:1401:1RM:H23	6:C:1401:1RM:H26	1.65	0.77
2:H:131:THR:HG21	2:H:135:THR:HG22	1.66	0.77
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.66	0.77
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	1.66	0.77
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.66	0.77
5:X:511:ILE:HG23	5:X:512:GLY:H	1.49	0.77
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.67	0.76
2:H:142:GLU:HG2	2:H:515:MET:SD	2.25	0.76
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.66	0.76
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.50	0.76
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.66	0.76
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.67	0.76
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.51	0.76
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.68	0.76
3:D:546:ALA:H	3:D:547:ARG:CA	1.99	0.76
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.65	0.76
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:THR:CG2	2:H:135:THR:HG22	2.16	0.75
3:I:643:ASP:O	3:I:720:ASN:ND2	2.14	0.75
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.67	0.75
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.51	0.75
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.50	0.75
3:I:230:SER:HB2	3:I:1339:GLY:H	1.49	0.75
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.67	0.75
4:J:15:ASN:HD22	4:J:18:ASP:H	1.34	0.75
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.69	0.75
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.67	0.75
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.69	0.75
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.02	0.75
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.68	0.75
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.67	0.75
2:H:1042:LEU:HD13	2:H:1042:LEU:H	1.50	0.75
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.68	0.74
3:I:828:GLY:HA2	3:I:832:LYS:H	1.51	0.74
2:H:1101:LEU:HD21	3:I:508:LEU:HD12	1.69	0.74
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.70	0.74
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.70	0.74
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.69	0.74
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.68	0.74
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.23	0.74
2:C:1211:ARG:NE	2:C:1211:ARG:O	2.20	0.74
3:D:142:GLU:HA	3:D:180:MET:HE2	1.70	0.73
3:D:1149:ARG:HD3	3:D:1149:ARG:H	1.52	0.73
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.70	0.73
2:C:562:GLU:HG2	2:C:574:SER:CB	2.19	0.73
3:D:822:MET:SD	3:D:838:ARG:NH1	2.61	0.73
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.70	0.73
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.70	0.73
2:H:21:VAL:HG13	2:H:22:LEU:H	1.54	0.73
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.71	0.73
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.71	0.73
5:X:139:GLU:HA	5:X:142:THR:HG22	1.69	0.73
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.71	0.73
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.53	0.73
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.53	0.73
4:J:5:THR:HA	4:J:6:VAL:CG1	2.19	0.73
3:D:850:LYS:O	3:D:852:GLY:N	2.21	0.73
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ARG:O	3:I:538:ARG:NH2	2.22	0.73
5:X:457:ILE:O	5:X:461:ASN:ND2	2.22	0.73
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.70	0.73
3:D:128:LEU:HA	3:D:192:MET:HE1	1.71	0.73
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.54	0.73
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.71	0.72
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.69	0.72
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.71	0.72
3:D:546:ALA:N	3:D:547:ARG:HA	2.03	0.72
2:C:309:LEU:HD23	2:C:309:LEU:H	1.54	0.72
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.19	0.72
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.71	0.72
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.71	0.72
2:H:127:ILE:H	2:H:127:ILE:HD13	1.54	0.72
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.72	0.72
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.70	0.72
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.71	0.72
3:I:546:ALA:H	3:I:547:ARG:CA	2.02	0.72
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.88	0.72
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.69	0.72
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.24	0.72
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.72	0.71
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.70	0.71
3:I:828:GLY:HA2	3:I:832:LYS:N	2.05	0.71
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.70	0.71
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.71	0.71
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.20	0.71
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.73	0.71
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.73	0.71
2:H:131:THR:HG23	2:H:133:ASN:H	1.54	0.71
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.71	0.71
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.71	0.71
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.73	0.71
3:I:822:MET:SD	3:I:838:ARG:NH1	2.64	0.71
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.56	0.71
1:B:29:GLU:HA	1:B:200:LYS:CB	2.20	0.71
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.72	0.71
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.56	0.70
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.73	0.70
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.24	0.70
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.70
4:J:5:THR:HA	4:J:6:VAL:HG12	1.72	0.70
3:I:546:ALA:N	3:I:547:ARG:HA	2.04	0.70
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.73	0.70
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.72	0.70
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.72	0.70
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.74	0.70
2:C:714:VAL:HG23	2:C:787:PRO:HD2	1.73	0.70
3:D:828:GLY:HA2	3:D:832:LYS:N	2.07	0.70
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.74	0.70
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.39	0.70
3:I:1173:ARG:HG2	3:I:1189:MET:HE1	1.74	0.70
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.73	0.70
4:J:5:THR:CA	4:J:6:VAL:HB	2.21	0.70
2:C:131:THR:HG23	2:C:133:ASN:H	1.56	0.70
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.27	0.70
5:X:108:VAL:HG23	5:X:109:GLU:H	1.57	0.70
3:D:836:ARG:HH12	3:D:839:VAL:HB	1.57	0.69
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.55	0.69
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.06	0.69
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.27	0.69
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.74	0.69
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.21	0.69
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.21	0.69
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.75	0.69
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.74	0.69
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.25	0.69
2:C:1042:LEU:HD13	2:C:1042:LEU:H	1.58	0.69
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.27	0.69
3:D:1260:MET:HE2	3:D:1306:LEU:HD11	1.74	0.69
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.74	0.69
3:D:932:MET:O	3:D:933:ARG:HG3	1.91	0.69
2:H:170:VAL:HG23	2:H:171:LEU:H	1.57	0.69
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.74	0.69
2:C:189:ASP:OD1	2:C:193:ASN:N	2.21	0.69
2:C:568:ASN:HB3	2:C:572:ILE:HD12	1.75	0.69
1:G:65:LEU:HD23	1:G:65:LEU:H	1.56	0.69
2:H:664:GLY:O	2:H:686:GLN:NE2	2.25	0.69
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.75	0.69
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.27	0.69
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:517:GLN:HE21	2:C:760:ASN:H	1.40	0.69
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.28	0.69
2:H:55:SER:CB	2:H:56:VAL:HG22	2.23	0.69
2:H:309:LEU:HD23	2:H:309:LEU:H	1.55	0.69
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.29	0.69
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.75	0.68
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.75	0.68
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.93	0.68
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.58	0.68
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.23	0.68
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.57	0.68
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.75	0.68
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.76	0.68
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.24	0.68
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.59	0.68
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.57	0.68
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.76	0.68
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.28	0.68
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.76	0.68
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.26	0.68
2:H:637:ARG:HE	3:I:770:LEU:HD23	1.59	0.68
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.74	0.68
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.75	0.68
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.27	0.68
1:G:49:SER:OG	3:I:538:ARG:NH2	2.27	0.68
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.74	0.68
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.27	0.68
5:X:476:ARG:H	5:X:476:ARG:HD2	1.59	0.68
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.29	0.68
2:H:510:GLN:O	2:H:513:GLN:NE2	2.27	0.68
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.76	0.68
3:D:711:GLY:O	3:D:712:GLN:HG2	1.93	0.68
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.58	0.68
3:D:259:ARG:HH21	5:X:504:PRO:HB2	1.58	0.67
2:H:1252:SER:OG	2:H:1255:THR:O	2.12	0.67
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.27	0.67
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.77	0.67
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.76	0.67
2:C:37:LYS:HA	2:C:37:LYS:HE3	1.76	0.67
3:D:151:MET:SD	3:D:151:MET:N	2.68	0.67
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:133:ARG:O	3:I:133:ARG:NH2	2.26	0.67
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.76	0.67
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.28	0.67
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.75	0.67
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.59	0.67
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.77	0.67
2:C:55:SER:CB	2:C:56:VAL:HG22	2.25	0.67
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.77	0.67
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.77	0.67
1:F:11:PRO:CG	1:G:228:LEU:H	2.07	0.67
2:C:127:ILE:H	2:C:127:ILE:HD13	1.60	0.67
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.76	0.67
3:I:1297:LYS:HA	3:I:1297:LYS:NZ	2.09	0.67
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.25	0.67
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.60	0.67
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.77	0.67
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.76	0.66
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.77	0.66
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.60	0.66
3:D:56:LEU:HB3	3:D:250:ARG:HH21	1.59	0.66
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.28	0.66
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.59	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.29	0.66
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.60	0.66
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.23	0.66
5:X:442:SER:OG	5:X:446:GLN:NE2	2.28	0.66
3:I:145:VAL:HG22	3:I:180:MET:SD	2.35	0.66
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.76	0.66
3:D:405:GLU:O	3:D:407:VAL:N	2.29	0.66
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.77	0.66
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.60	0.66
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.77	0.66
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.78	0.66
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.60	0.66
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.77	0.66
3:D:245:LEU:O	3:D:250:ARG:NH1	2.29	0.66
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.10	0.66
3:D:1362:GLY:O	3:D:1364:ALA:N	2.29	0.66
2:H:54:ARG:H	2:H:55:SER:CB	2.04	0.66
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.76	0.66
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.78	0.66
2:C:20:GLN:O	2:C:22:LEU:N	2.29	0.66
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.77	0.66
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.77	0.66
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.78	0.66
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.77	0.66
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.61	0.66
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.77	0.65
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.76	0.65
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.26	0.65
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.79	0.65
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.77	0.65
2:H:143:ARG:NH1	2:H:512:SER:O	2.29	0.65
2:C:488:MET:N	2:C:489:PRO:HD3	2.11	0.65
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.77	0.65
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.78	0.65
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.60	0.65
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.76	0.65
3:D:720:ASN:O	3:D:722:ILE:N	2.29	0.65
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.78	0.65
2:H:660:VAL:O	2:H:661:VAL:HG22	1.95	0.65
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.78	0.65
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.79	0.65
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.79	0.65
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.79	0.65
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.79	0.65
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.79	0.65
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.25	0.65
2:C:845:LEU:HD13	2:C:845:LEU:H	1.62	0.65
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.79	0.65
3:D:589:TYR:O	3:D:591:ILE:N	2.28	0.65
2:C:634:VAL:H	2:C:645:PHE:HE2	1.45	0.65
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.12	0.65
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.26	0.65
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.12	0.65
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.77	0.65
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.60	0.65
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.30	0.65
2:H:908:GLU:HG2	2:H:909:LYS:N	2.11	0.65
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.26	0.65
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.12	0.65
2:H:99:LYS:HD3	2:H:99:LYS:N	2.12	0.65
3:I:827:GLU:O	3:I:831:VAL:HG12	1.96	0.65
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.77	0.65
2:C:660:VAL:O	2:C:661:VAL:HG22	1.97	0.65
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.79	0.65
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.78	0.65
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.60	0.65
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.78	0.65
3:I:720:ASN:O	3:I:722:ILE:N	2.30	0.65
3:I:858:VAL:HB	3:I:859:PRO:CD	2.24	0.65
3:D:1254:GLU:O	3:D:1257:VAL:HG12	1.97	0.64
5:X:517:SER:O	5:X:518:HIS:ND1	2.30	0.64
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.79	0.64
2:C:1304:MET:HE1	3:D:472:LEU:HD13	1.78	0.64
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.08	0.64
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.80	0.64
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.62	0.64
3:D:154:LEU:HD21	3:D:160:LEU:HD21	1.80	0.64
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.80	0.64
3:I:151:MET:SD	3:I:151:MET:N	2.70	0.64
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.79	0.64
3:I:711:GLY:O	3:I:712:GLN:HG2	1.97	0.64
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.78	0.64
2:C:1239:VAL:O	2:C:1241:ASP:N	2.29	0.64
2:H:255:ILE:HD12	2:H:263:VAL:HB	1.79	0.64
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.31	0.64
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.80	0.64
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.63	0.64
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.80	0.64
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.62	0.64
2:C:1200:LYS:O	2:C:1202:GLY:N	2.31	0.64
4:E:5:THR:HB	4:E:7:GLN:HB2	1.80	0.64
5:X:112:THR:HG22	5:X:113:ARG:H	1.62	0.64
3:I:541:LEU:HD23	3:I:541:LEU:H	1.61	0.64
1:B:227:GLN:O	1:B:228:LEU:HG	1.97	0.64
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.80	0.64
2:C:142:GLU:HG2	2:C:515:MET:SD	2.38	0.64
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.80	0.64
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.30	0.64
2:C:568:ASN:HB3	2:C:572:ILE:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.99	0.63
2:C:1243:MET:HE3	3:D:372:MET:HB2	1.79	0.63
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.79	0.63
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.31	0.63
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.79	0.63
3:D:316:ILE:HG23	3:D:317:THR:N	2.13	0.63
1:A:318:LEU:O	1:A:320:ASN:N	2.31	0.63
2:C:94:ALA:N	2:C:126:GLU:OE2	2.24	0.63
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.79	0.63
4:E:5:THR:CA	4:E:6:VAL:HB	2.28	0.63
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.28	0.63
5:X:514:ASP:C	5:X:516:ASP:HA	2.24	0.63
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.80	0.63
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.63	0.63
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.80	0.63
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.63
2:C:54:ARG:HG2	2:C:55:SER:CB	2.29	0.63
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.31	0.63
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.26	0.63
2:H:1176:LEU:HD22	2:H:1180:MET:O	1.99	0.63
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.14	0.63
2:H:568:ASN:HB3	2:H:572:ILE:CD1	2.29	0.63
3:I:139:LEU:HD13	3:I:140:TYR:N	2.14	0.63
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.81	0.63
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.81	0.63
5:X:264:LYS:H	5:X:264:LYS:HD2	1.64	0.62
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.80	0.62
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.29	0.62
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.81	0.62
2:C:529:ARG:HB2	2:C:529:ARG:HH11	1.64	0.62
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.81	0.62
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.64	0.62
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.81	0.62
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.14	0.62
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.81	0.62
2:H:618:GLN:OE1	3:I:770:LEU:HB2	1.99	0.62
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.99	0.62
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.26	0.62
3:I:1260:MET:HE2	3:I:1306:LEU:HD11	1.81	0.62
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.24	0.62
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.62
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.34	0.62
3:I:1338:ALA:O	3:I:1340:LYS:N	2.33	0.62
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.14	0.62
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.82	0.62
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.82	0.62
2:H:1288:GLN:HA	2:H:1288:GLN:HE21	1.65	0.62
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.82	0.62
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.32	0.62
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.33	0.62
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.81	0.62
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.80	0.62
2:C:1255:THR:O	2:C:1257:GLN:N	2.33	0.61
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.81	0.61
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.82	0.61
3:D:1338:ALA:O	3:D:1340:LYS:N	2.33	0.61
2:H:55:SER:HB3	2:H:56:VAL:CB	2.30	0.61
2:H:94:ALA:N	2:H:126:GLU:OE2	2.25	0.61
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.82	0.61
5:X:240:ARG:O	5:X:242:HIS:N	2.33	0.61
2:H:845:LEU:HD13	2:H:845:LEU:H	1.64	0.61
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.30	0.61
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.30	0.61
2:C:302:ILE:HA	2:C:309:LEU:HA	1.81	0.61
3:D:77:ARG:HG3	3:D:78:LEU:H	1.63	0.61
3:D:139:LEU:HD13	3:D:140:TYR:N	2.16	0.61
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.65	0.61
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.81	0.61
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.82	0.61
2:C:681:MET:O	2:C:685:MET:HG2	2.00	0.61
2:C:1252:SER:OG	2:C:1255:THR:O	2.18	0.61
2:H:800:MET:HE1	2:H:827:ARG:HD3	1.82	0.61
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.01	0.61
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.30	0.61
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.35	0.61
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.81	0.61
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.83	0.61
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.31	0.61
3:I:50:LYS:HB3	3:I:50:LYS:NZ	2.15	0.61
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.83	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.66	0.61
3:D:1191:PRO:O	3:D:1193:TRP:N	2.31	0.61
2:H:590:PRO:O	2:H:659:GLN:NE2	2.34	0.61
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.66	0.61
2:C:403:MET:HG3	2:C:414:ILE:HB	1.83	0.61
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.83	0.61
2:C:898:GLU:OE1	2:C:898:GLU:N	2.31	0.61
2:H:510:GLN:NE2	2:H:534:GLY:HA2	2.15	0.61
3:I:422:LEU:HA	3:I:436:ALA:HA	1.83	0.61
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.83	0.61
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.36	0.61
3:I:1362:GLY:O	3:I:1364:ALA:N	2.33	0.61
1:A:282:VAL:CG2	1:A:316:MET:HE2	2.30	0.61
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.81	0.61
2:C:901:LEU:O	2:C:905:ILE:HG13	2.01	0.61
3:D:500:ILE:H	3:D:500:ILE:HD13	1.66	0.61
2:H:459:MET:SD	2:H:511:LEU:HD22	2.40	0.61
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.66	0.61
2:H:1200:LYS:O	2:H:1202:GLY:N	2.33	0.61
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.16	0.61
3:I:514:THR:HG23	3:I:576:ARG:HE	1.66	0.61
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.81	0.61
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.36	0.61
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.16	0.61
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.82	0.61
5:X:445:ASP:OD1	5:X:445:ASP:N	2.34	0.61
5:X:448:ARG:HD3	5:X:450:ILE:HG13	1.83	0.61
1:F:221:ALA:HB1	1:G:228:LEU:HD12	1.83	0.61
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.82	0.61
3:I:88:CYS:O	3:I:90:VAL:N	2.34	0.61
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.83	0.61
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.82	0.60
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.82	0.60
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.34	0.60
1:B:49:SER:HA	1:B:151:GLY:HA2	1.83	0.60
2:C:166:SER:O	2:C:168:GLY:N	2.33	0.60
2:H:146:VAL:HG13	2:H:513:GLN:HG3	1.83	0.60
2:H:528:ARG:NH2	2:H:576:SER:O	2.34	0.60
3:I:512:TYR:HD2	3:I:724:MET:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.65	0.60
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.00	0.60
2:C:163:LYS:H	2:C:163:LYS:HD3	1.64	0.60
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.26	0.60
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.83	0.60
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.83	0.60
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.30	0.60
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.22	0.60
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.31	0.60
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.31	0.60
2:C:106:GLU:N	2:C:107:ARG:HA	2.14	0.60
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.33	0.60
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.82	0.60
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.83	0.60
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.83	0.60
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.16	0.60
3:D:389:GLY:O	3:D:391:ALA:N	2.35	0.60
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.66	0.60
3:D:858:VAL:HB	3:D:859:PRO:CD	2.24	0.60
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.66	0.60
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.83	0.60
1:B:227:GLN:O	1:B:229:GLU:N	2.29	0.60
2:C:21:VAL:HG13	2:C:22:LEU:H	1.66	0.60
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.64	0.60
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.84	0.60
3:I:245:LEU:O	3:I:250:ARG:NH1	2.34	0.60
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.83	0.60
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.31	0.60
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.83	0.60
2:H:20:GLN:O	2:H:22:LEU:N	2.34	0.60
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.83	0.60
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.16	0.60
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.32	0.60
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.66	0.60
2:H:1304:MET:HE1	3:I:472:LEU:HD13	1.83	0.60
3:I:213:LYS:O	3:I:217:LEU:HG	2.01	0.60
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.31	0.60
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.02	0.60
2:C:808:ASN:H	3:D:633:ALA:HB2	1.67	0.60
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.01	0.60
3:D:1173:ARG:HG2	3:D:1189:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:CB	2:H:56:VAL:HG13	2.28	0.60
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.84	0.60
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.35	0.60
2:C:402:ARG:NH2	2:C:419:ILE:O	2.35	0.60
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.84	0.60
2:C:572:ILE:HD13	6:C:1401:1RM:O1	2.02	0.60
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.33	0.60
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.84	0.60
2:H:106:GLU:N	2:H:107:ARG:HA	2.16	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.34	0.60
2:H:898:GLU:OE1	2:H:898:GLU:N	2.33	0.60
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.67	0.60
2:H:1255:THR:O	2:H:1257:GLN:N	2.35	0.60
3:I:768:ASN:O	3:I:771:GLN:NE2	2.35	0.60
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.17	0.59
2:C:487:LEU:CD1	2:C:488:MET:H	2.15	0.59
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.84	0.59
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.02	0.59
2:C:408:SER:O	2:C:431:LYS:NZ	2.28	0.59
3:D:29:MET:HA	3:D:29:MET:HE3	1.84	0.59
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.67	0.59
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.83	0.59
3:I:824:PRO:O	3:I:826:ILE:HG13	2.03	0.59
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.33	0.59
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.31	0.59
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.84	0.59
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.35	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.02	0.59
3:D:703:THR:HA	3:D:717:VAL:HA	1.82	0.59
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.83	0.59
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.38	0.59
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.17	0.59
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.84	0.59
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.66	0.59
5:X:28:ASN:HD22	5:X:29:ASP:N	2.00	0.59
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.35	0.59
2:H:1239:VAL:O	2:H:1241:ASP:N	2.35	0.59
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.34	0.59
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.83	0.59
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.84	0.59
2:H:568:ASN:HB3	2:H:572:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.84	0.59
5:Y:277:MET:HE3	5:Y:281:ARG:HG3	1.82	0.59
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.85	0.59
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.85	0.59
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.37	0.59
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.67	0.59
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.85	0.59
2:C:55:SER:CB	2:C:56:VAL:HG13	2.31	0.59
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.32	0.59
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.02	0.59
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.85	0.59
3:D:608:CYS:O	3:D:612:LEU:HB2	2.03	0.59
5:X:379:MET:HE2	5:X:379:MET:HA	1.85	0.59
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.33	0.59
1:B:179:PRO:O	1:B:207:THR:OG1	2.16	0.59
2:C:542:ARG:O	2:C:544:GLY:N	2.32	0.59
2:C:550:VAL:HG11	3:D:776:THR:HG23	1.84	0.59
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.32	0.59
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.68	0.59
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.84	0.59
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.85	0.59
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.85	0.59
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.84	0.58
2:C:1273:MET:HB3	3:D:428:THR:HB	1.85	0.58
5:X:108:VAL:HB	5:X:110:LEU:HG	1.84	0.58
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.85	0.58
1:B:65:LEU:HD23	1:B:65:LEU:H	1.67	0.58
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.84	0.58
2:C:41:GLN:CD	2:C:42:ASP:H	2.10	0.58
2:C:54:ARG:H	2:C:55:SER:CB	2.07	0.58
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.33	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.85	0.58
5:X:561:MET:HA	5:X:567:MET:SD	2.43	0.58
2:C:55:SER:HB3	2:C:56:VAL:CB	2.34	0.58
3:D:768:ASN:O	3:D:771:GLN:NE2	2.36	0.58
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.58
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.86	0.58
4:J:26:ARG:HE	4:J:30:MET:HE3	1.67	0.58
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.36	0.58
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.33	0.58
3:I:125:GLY:O	3:I:129:ASP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:264:LYS:HD2	5:Y:264:LYS:H	1.69	0.58
4:E:3:ARG:NH2	4:E:44:ASP:OD2	2.31	0.58
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.68	0.58
3:I:77:ARG:HG3	3:I:78:LEU:H	1.68	0.58
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.86	0.58
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.85	0.58
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.84	0.58
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.84	0.58
4:E:26:ARG:HE	4:E:30:MET:HE3	1.68	0.58
2:H:1283:ALA:HB1	2:H:1286:THR:HB	1.84	0.58
3:I:405:GLU:O	3:I:407:VAL:N	2.36	0.58
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.37	0.58
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.69	0.58
2:C:752:ASN:O	2:C:753:LEU:HG	2.03	0.58
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.67	0.58
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.39	0.58
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.03	0.58
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.36	0.58
2:C:163:LYS:H	2:C:163:LYS:CD	2.16	0.58
3:D:125:GLY:O	3:D:129:ASP:N	2.37	0.58
2:H:600:THR:HG22	2:H:601:ASP:H	1.68	0.58
2:H:634:VAL:H	2:H:645:PHE:HE2	1.52	0.58
2:H:747:GLY:O	2:H:748:ILE:HG13	2.03	0.58
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.86	0.58
3:D:120:LEU:CB	3:D:121:PRO:CD	2.80	0.58
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.18	0.58
2:H:753:LEU:HD12	2:H:753:LEU:O	2.04	0.58
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.02	0.57
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.85	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.86	0.57
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.86	0.57
2:H:1141:LEU:H	2:H:1141:LEU:CD1	2.17	0.57
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.85	0.57
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.57
2:H:54:ARG:HG2	2:H:55:SER:CB	2.34	0.57
2:H:985:GLU:HG2	2:H:989:LEU:HD13	1.86	0.57
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.38	0.57
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.84	0.57
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.37	0.57
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.34	0.57
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.68	0.57
1:B:64:VAL:HG13	1:B:69:SER:OG	2.04	0.57
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.40	0.57
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.39	0.57
3:I:29:MET:HA	3:I:29:MET:HE3	1.85	0.57
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.04	0.57
2:C:528:ARG:NH2	2:C:576:SER:O	2.38	0.57
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.87	0.57
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.86	0.57
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.17	0.57
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.18	0.57
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.03	0.57
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.34	0.57
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.69	0.57
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.29	0.57
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.86	0.57
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.86	0.57
1:G:29:GLU:HA	1:G:200:LYS:CB	2.35	0.57
3:I:481:ARG:HA	3:I:485:MET:HE2	1.87	0.57
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.34	0.57
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.05	0.57
3:D:213:LYS:O	3:D:217:LEU:HG	2.04	0.57
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.25	0.57
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.37	0.57
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.87	0.57
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.03	0.57
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.39	0.57
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.86	0.57
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.37	0.57
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.87	0.57
5:X:363:ARG:O	5:X:367:ILE:HG12	2.05	0.57
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.40	0.57
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.87	0.57
2:C:829:THR:HG22	2:C:1059:ARG:HG2	1.87	0.57
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.34	0.57
3:D:136:GLU:HA	3:D:139:LEU:HD12	1.87	0.57
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.86	0.57
2:H:951:MET:HA	2:H:951:MET:HE3	1.86	0.57
3:I:128:LEU:HD13	3:I:189:LEU:HD23	1.87	0.57
3:I:389:GLY:O	3:I:391:ALA:N	2.38	0.57
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.40	0.56
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.68	0.56
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.31	0.56
2:H:504:GLU:O	2:H:508:SER:HB3	2.05	0.56
2:C:704:MET:HE3	2:C:704:MET:HA	1.87	0.56
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.40	0.56
3:D:85:CYS:HB3	3:D:88:CYS:O	2.05	0.56
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.87	0.56
3:D:423:LEU:CD2	3:D:447:ILE:HD11	2.35	0.56
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.88	0.56
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.87	0.56
4:E:45:LYS:O	4:E:49:ILE:HG12	2.06	0.56
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.86	0.56
2:H:516:ASP:HB2	6:H:1401:1RM:H10	1.86	0.56
2:H:531:SER:OG	6:H:1401:1RM:O2	2.14	0.56
2:H:901:LEU:O	2:H:905:ILE:HG13	2.05	0.56
3:I:85:CYS:HB3	3:I:88:CYS:O	2.04	0.56
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.87	0.56
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.70	0.56
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.87	0.56
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.20	0.56
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.69	0.56
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.87	0.56
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.38	0.56
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.86	0.56
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.86	0.56
3:I:128:LEU:HD12	3:I:192:MET:CE	2.35	0.56
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.88	0.56
3:I:704:GLU:HB2	3:I:718:SER:OG	2.06	0.56
3:D:173:GLY:O	3:D:175:GLU:HG3	2.06	0.56
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.35	0.56
5:X:515:GLU:N	5:X:516:ASP:HA	2.20	0.56
2:H:73:TYR:HD2	2:H:74:ARG:H	1.53	0.56
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.34	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.06	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.06	0.56
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.86	0.56
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.14	0.56
3:I:122:SER:HB2	3:I:132:LEU:HD22	1.87	0.56
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.87	0.56
2:C:143:ARG:NH1	2:C:512:SER:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.69	0.56
3:D:51:PRO:HB3	3:D:57:PHE:O	2.06	0.56
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.40	0.56
3:D:591:ILE:HD12	3:D:592:VAL:N	2.21	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.05	0.56
2:H:704:MET:HA	2:H:704:MET:HE3	1.88	0.56
3:I:644:MET:O	3:I:764:ARG:NH1	2.39	0.56
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.86	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.88	0.56
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.41	0.56
2:H:9:LYS:HD3	2:H:9:LYS:N	2.19	0.56
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.70	0.56
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.21	0.56
5:Y:514:ASP:C	5:Y:516:ASP:HA	2.30	0.56
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.87	0.56
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.36	0.56
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.88	0.56
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.88	0.56
2:C:42:ASP:O	2:C:44:GLU:HG2	2.06	0.56
2:C:897:PRO:HB3	5:X:564:GLY:O	2.06	0.56
3:D:107:LEU:H	3:D:107:LEU:HD12	1.70	0.56
3:D:589:TYR:O	3:D:591:ILE:HG13	2.06	0.56
5:X:503:GLU:N	5:X:504:PRO:HA	2.21	0.56
1:G:33:ARG:HE	1:G:197:ASP:HB2	1.71	0.56
1:G:42:ALA:O	1:G:46:ILE:HG12	2.06	0.56
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.88	0.56
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.41	0.56
3:I:919:ALA:O	3:I:923:ILE:HG12	2.06	0.56
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.88	0.56
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.88	0.56
1:B:49:SER:OG	3:D:538:ARG:NH2	2.39	0.56
2:C:572:ILE:HD13	6:C:1401:1RM:C1	2.35	0.56
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.39	0.56
3:I:107:LEU:H	3:I:107:LEU:HD12	1.70	0.56
1:A:219:ARG:O	1:A:223:ILE:HG13	2.07	0.55
2:C:149:LEU:HD12	2:C:452:ARG:O	2.06	0.55
1:F:44:ARG:HG3	1:F:183:ILE:HG22	1.88	0.55
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.88	0.55
2:H:1268:GLN:O	3:I:346:ARG:HA	2.06	0.55
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.39	0.55
3:I:412:LEU:O	3:I:416:ILE:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.88	0.55
3:I:589:TYR:O	3:I:591:ILE:N	2.35	0.55
5:Y:476:ARG:H	5:Y:476:ARG:HD2	1.71	0.55
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.21	0.55
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.05	0.55
2:C:747:GLY:O	2:C:748:ILE:HG13	2.05	0.55
2:C:951:MET:HA	2:C:951:MET:HE3	1.89	0.55
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.87	0.55
3:D:809:VAL:HG13	3:D:912:GLY:H	1.71	0.55
4:E:5:THR:CA	4:E:6:VAL:CB	2.83	0.55
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.06	0.55
1:G:49:SER:HA	1:G:151:GLY:HA2	1.88	0.55
2:H:487:LEU:HB3	2:H:488:MET:CG	2.36	0.55
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.34	0.55
3:I:832:LYS:HZ1	3:I:832:LYS:HA	1.69	0.55
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.71	0.55
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.05	0.55
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.88	0.55
2:C:9:LYS:N	2:C:9:LYS:HD3	2.20	0.55
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.70	0.55
2:C:104:ILE:HD11	2:C:115:LYS:HB2	1.88	0.55
2:C:127:ILE:HG22	2:C:502:VAL:HG11	1.88	0.55
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.89	0.55
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.88	0.55
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.36	0.55
3:I:640:GLY:N	3:I:643:ASP:OD2	2.39	0.55
2:C:106:GLU:HG2	2:C:109:ALA:H	1.72	0.55
2:C:131:THR:HG22	2:C:135:THR:N	2.22	0.55
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.88	0.55
3:D:179:LYS:H	3:D:179:LYS:HD3	1.69	0.55
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.30	0.55
2:H:800:MET:HA	2:H:800:MET:CE	2.36	0.55
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.88	0.55
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.89	0.55
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.41	0.55
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.22	0.55
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.89	0.55
2:H:484:LEU:H	2:H:484:LEU:HD22	1.70	0.55
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.20	0.55
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.41	0.55
5:Y:279:ARG:NH2	5:Y:350:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:120:LEU:HG	5:X:46:GLN:CB	2.36	0.55
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.40	0.55
5:X:584:ARG:O	5:X:587:ILE:HG22	2.07	0.55
3:D:932:MET:SD	3:D:932:MET:N	2.70	0.55
1:A:104:LYS:HD3	1:A:105:SER:N	2.22	0.55
2:C:600:THR:HG22	2:C:601:ASP:H	1.70	0.55
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.42	0.55
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.88	0.55
2:H:660:VAL:HG22	2:H:661:VAL:N	2.20	0.55
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.36	0.55
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.89	0.55
2:C:841:ARG:HH12	3:D:256:ASP:HB3	1.72	0.55
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.89	0.55
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.70	0.55
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.88	0.55
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.87	0.55
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.54	0.55
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.72	0.55
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.06	0.55
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.27	0.55
3:D:1347:LEU:HD22	3:D:1357:ILE:CG2	2.37	0.55
2:H:496:LYS:N	2:H:497:PRO:HD2	2.22	0.55
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.37	0.55
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.22	0.54
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.88	0.54
3:D:422:LEU:HA	3:D:436:ALA:HA	1.89	0.54
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.88	0.54
2:H:582:ASN:HB2	2:H:588:GLU:HG3	1.88	0.54
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.72	0.54
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.43	0.54
3:D:56:LEU:O	3:D:250:ARG:NH2	2.34	0.54
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.89	0.54
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.41	0.54
3:D:474:LEU:HD13	3:D:478:LEU:HD13	1.90	0.54
2:H:505:PHE:O	2:H:512:SER:OG	2.24	0.54
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.25	0.54
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.71	0.54
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.36	0.54
2:C:1141:LEU:CD1	2:C:1141:LEU:H	2.19	0.54
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.88	0.54
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.90	0.54
1:G:118:ASP:OD1	1:G:119:GLY:N	2.41	0.54
2:H:747:GLY:C	2:H:748:ILE:HG13	2.32	0.54
2:H:808:ASN:H	3:I:633:ALA:HB2	1.70	0.54
3:I:252:LEU:H	3:I:252:LEU:HD23	1.71	0.54
3:I:591:ILE:HD12	3:I:592:VAL:N	2.21	0.54
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.73	0.54
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.72	0.54
3:D:515:ARG:HH22	3:D:717:VAL:C	2.15	0.54
2:H:21:VAL:HG13	2:H:22:LEU:N	2.21	0.54
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.88	0.54
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.88	0.54
2:C:660:VAL:HG22	2:C:661:VAL:N	2.20	0.54
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.90	0.54
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.72	0.54
3:D:27:PRO:O	3:D:31:ARG:HD3	2.07	0.54
3:D:573:THR:HG22	3:D:576:ARG:CG	2.37	0.54
3:D:827:GLU:O	3:D:831:VAL:HG12	2.08	0.54
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.08	0.54
5:X:17:LYS:N	5:X:18:GLU:HA	2.22	0.54
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.88	0.54
1:B:42:ALA:O	1:B:46:ILE:HG12	2.07	0.54
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	0.54
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.41	0.54
3:I:120:LEU:CB	3:I:121:PRO:CD	2.86	0.54
3:I:491:LEU:HB2	3:I:904:ALA:HA	1.90	0.54
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	1.90	0.54
1:A:282:VAL:HG22	1:A:316:MET:HE2	1.88	0.54
2:C:311:CYS:SG	2:C:315:MET:HB2	2.48	0.54
2:C:843:THR:HG22	2:C:844:LYS:H	1.72	0.54
2:C:894:GLN:O	2:C:895:LEU:HB2	2.07	0.54
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.08	0.54
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.43	0.54
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.53	0.54
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.54
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.90	0.54
3:I:292:VAL:HG22	3:I:296:LYS:HE3	1.90	0.54
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.89	0.54
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.08	0.54
2:C:843:THR:HB	2:C:845:LEU:HD22	1.89	0.54
2:C:873:ILE:HD11	2:C:931:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.43	0.54
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.07	0.54
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.30	0.54
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.36	0.54
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.90	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.41	0.54
3:D:118:LYS:NZ	5:X:43:ASP:OD2	2.41	0.54
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.33	0.54
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.42	0.54
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.89	0.54
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.90	0.54
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.38	0.54
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.38	0.54
1:G:31:LEU:HB2	1:G:199:ASP:O	2.08	0.54
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.73	0.54
1:A:263:THR:HG23	1:A:266:SER:H	1.74	0.53
3:D:316:ILE:HG13	3:D:317:THR:N	2.24	0.53
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.73	0.53
5:X:466:ILE:HD12	5:X:487:MET:HE2	1.88	0.53
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.40	0.53
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.53
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.90	0.53
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.90	0.53
3:I:546:ALA:HB3	3:I:547:ARG:O	2.07	0.53
3:I:733:SER:O	3:I:737:ILE:HG12	2.08	0.53
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.89	0.53
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.73	0.53
2:C:487:LEU:HD13	2:C:488:MET:H	1.72	0.53
1:F:118:ASP:OD1	1:F:119:GLY:N	2.41	0.53
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.88	0.53
4:J:5:THR:HB	4:J:7:GLN:HB2	1.91	0.53
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.42	0.53
1:B:77:ASP:O	1:B:81:ILE:HG13	2.08	0.53
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.43	0.53
3:D:412:LEU:O	3:D:416:ILE:HG23	2.07	0.53
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.91	0.53
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.33	0.53
2:H:1085:MET:HE2	2:H:1094:VAL:HG23	1.90	0.53
3:I:508:LEU:O	3:I:508:LEU:HD23	2.08	0.53
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.91	0.53
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:747:GLY:C	2:C:748:ILE:HG13	2.33	0.53
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.38	0.53
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.89	0.53
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.38	0.53
3:I:809:VAL:HG13	3:I:912:GLY:H	1.74	0.53
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.90	0.53
4:J:45:LYS:O	4:J:49:ILE:HG12	2.08	0.53
1:B:18:GLN:C	1:B:20:SER:H	2.16	0.53
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.38	0.53
1:G:56:VAL:HG12	1:G:173:VAL:HG11	1.89	0.53
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.90	0.53
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.09	0.53
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.24	0.53
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.43	0.53
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.39	0.53
3:I:1266:ILE:HG13	3:I:1274:PHE:O	2.09	0.53
2:C:12:ARG:O	2:C:13:LYS:HG2	2.09	0.53
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.89	0.53
2:C:590:PRO:O	2:C:659:GLN:NE2	2.41	0.53
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.33	0.53
3:D:541:LEU:HD23	3:D:541:LEU:H	1.74	0.53
3:D:640:GLY:N	3:D:643:ASP:OD2	2.42	0.53
5:X:402:LEU:HD13	5:X:405:ILE:HD11	1.90	0.53
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.24	0.53
5:X:355:ILE:O	5:X:355:ILE:HD13	2.07	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.39	0.53
2:H:844:LYS:HB2	2:H:844:LYS:NZ	2.24	0.53
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.90	0.53
4:J:4:VAL:O	4:J:5:THR:OG1	2.23	0.53
1:A:192:VAL:O	1:A:194:GLN:N	2.40	0.53
2:C:496:LYS:N	2:C:497:PRO:HD2	2.23	0.53
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.08	0.53
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.53
5:X:143:TYR:O	5:X:147:GLN:HG2	2.09	0.53
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.43	0.53
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.74	0.53
3:I:482:ALA:C	3:I:483:LEU:HD12	2.34	0.53
3:D:252:LEU:HD23	3:D:252:LEU:H	1.73	0.53
5:X:301:ASN:O	5:X:305:LEU:HD13	2.09	0.53
5:X:598:LEU:O	5:X:599:ARG:HD2	2.07	0.53
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.90	0.53
3:I:546:ALA:N	3:I:547:ARG:CA	2.68	0.53
3:I:1287:ILE:HG22	3:I:1290:ARG:HE	1.73	0.53
1:B:118:ASP:OD1	1:B:119:GLY:N	2.42	0.53
2:C:728:ASP:OD2	2:C:729:ALA:N	2.42	0.53
3:D:202:ARG:O	3:D:206:ASN:ND2	2.42	0.53
3:D:546:ALA:N	3:D:547:ARG:CA	2.67	0.53
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.91	0.53
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.91	0.53
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.38	0.53
3:I:918:ILE:HD13	3:I:919:ALA:N	2.23	0.53
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.91	0.52
2:C:946:LEU:O	2:C:949:GLU:HG3	2.09	0.52
2:C:1119:MET:HG2	2:C:1228:GLY:CA	2.22	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.09	0.52
5:X:115:GLY:O	5:X:119:ILE:HG12	2.09	0.52
1:G:16:ILE:HG12	1:G:26:VAL:HG22	1.90	0.52
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.55	0.52
2:H:384:LEU:O	2:H:388:LEU:HG	2.10	0.52
2:H:843:THR:HG22	2:H:844:LYS:H	1.74	0.52
2:H:892:GLU:O	2:H:893:THR:OG1	2.18	0.52
3:I:222:LYS:HZ1	3:I:1276:GLU:HB2	1.74	0.52
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.91	0.52
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.74	0.52
2:C:131:THR:HG22	2:C:135:THR:H	1.73	0.52
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.52
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.09	0.52
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.73	0.52
3:I:709:ARG:O	3:I:711:GLY:N	2.42	0.52
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.34	0.52
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.75	0.52
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.74	0.52
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.91	0.52
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.91	0.52
1:A:256:PRO:HA	1:A:277:TYR:HA	1.90	0.52
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.91	0.52
2:C:516:ASP:HB2	6:C:1401:1RM:H10	1.90	0.52
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.22	0.52
3:I:305:ALA:O	3:I:309:ASN:ND2	2.43	0.52
2:C:51:ALA:C	2:C:53:PHE:H	2.17	0.52
2:C:59:ILE:CG2	2:C:479:LEU:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:HG22	2:C:139:ASN:H	1.74	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.42	0.52
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.90	0.52
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.09	0.52
2:H:728:ASP:OD2	2:H:729:ALA:N	2.42	0.52
2:H:838:CYS:HB2	2:H:918:LEU:HB2	1.92	0.52
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.09	0.52
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.23	0.52
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.35	0.52
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.91	0.52
2:C:130:MET:HE3	2:C:136:PHE:CZ	2.44	0.52
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.42	0.52
2:C:314:ASN:HD21	2:C:348:SER:HA	1.74	0.52
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.91	0.52
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.75	0.52
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.90	0.52
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.44	0.52
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.75	0.52
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.44	0.52
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.25	0.52
1:A:42:ALA:O	1:A:46:ILE:HG12	2.09	0.52
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.92	0.52
2:C:533:LEU:HG	6:C:1401:1RM:H05	1.90	0.52
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.08	0.52
3:D:185:ILE:HG22	3:D:238:ILE:HD13	1.91	0.52
3:D:527:LEU:HD13	3:D:531:LYS:CB	2.40	0.52
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.92	0.52
5:X:278:ASP:O	5:X:282:THR:OG1	2.22	0.52
1:F:9:LEU:O	1:G:227:GLN:NE2	2.43	0.52
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.91	0.52
2:H:453:ILE:HG22	2:H:585:GLY:O	2.09	0.52
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.45	0.52
2:H:752:ASN:O	2:H:753:LEU:HG	2.10	0.52
2:H:843:THR:HB	2:H:845:LEU:HD22	1.91	0.52
3:I:316:ILE:HD13	3:I:316:ILE:H	1.74	0.52
3:I:646:ILE:HG22	3:I:741:ALA:O	2.10	0.52
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.25	0.52
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.38	0.52
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.25	0.52
3:D:137:ARG:NH1	5:X:95:THR:HG23	2.24	0.52
1:F:42:ALA:O	1:F:46:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:ARG:O	2:H:13:LYS:HG2	2.10	0.52
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.92	0.52
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.91	0.52
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.92	0.52
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.45	0.52
2:C:818:VAL:HG22	2:C:819:SER:H	1.75	0.52
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.92	0.52
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.91	0.52
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.44	0.52
2:H:36:GLN:O	2:H:39:ILE:HG22	2.10	0.52
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.92	0.52
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.74	0.52
3:I:534:GLU:O	3:I:538:ARG:HB2	2.10	0.52
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.40	0.52
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.45	0.52
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.90	0.52
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.92	0.52
2:H:106:GLU:HG2	2:H:109:ALA:H	1.75	0.52
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.92	0.52
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.09	0.52
5:Y:278:ASP:O	5:Y:282:THR:OG1	2.25	0.52
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.92	0.51
2:C:740:GLU:OE2	2:C:974:ARG:NH2	2.43	0.51
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.09	0.51
2:H:59:ILE:HB	2:H:480:SER:OG	2.10	0.51
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	1.93	0.51
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.92	0.51
3:I:552:ILE:HD13	3:I:570:LYS:HB2	1.92	0.51
3:I:800:LEU:O	3:I:803:VAL:HG12	2.10	0.51
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.10	0.51
1:B:45:ARG:O	3:D:538:ARG:NH2	2.42	0.51
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.92	0.51
1:B:227:GLN:C	1:B:229:GLU:H	2.18	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.45	0.51
2:C:1111:GLN:HE21	2:C:1230:MET:HE1	1.75	0.51
3:D:316:ILE:O	3:D:317:THR:OG1	2.25	0.51
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.25	0.51
3:D:552:ILE:HD13	3:D:570:LYS:HB2	1.91	0.51
5:X:27:VAL:HA	5:X:30:HIS:HD2	1.75	0.51
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.26	0.51
2:H:360:LEU:HD13	2:H:378:ARG:NH1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.57	0.51
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	1.91	0.51
1:A:58:GLU:HG2	1:A:172:LEU:HD23	1.92	0.51
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.92	0.51
3:D:646:ILE:HG22	3:D:741:ALA:O	2.10	0.51
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.92	0.51
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.91	0.51
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.93	0.51
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.76	0.51
2:H:91:THR:HG22	2:H:139:ASN:H	1.76	0.51
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.75	0.51
3:I:807:LEU:HD12	3:I:807:LEU:O	2.11	0.51
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.91	0.51
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.26	0.51
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.76	0.51
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.22	0.51
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.45	0.51
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.35	0.51
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.91	0.51
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.25	0.51
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.92	0.51
5:X:379:MET:HA	5:X:379:MET:CE	2.40	0.51
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.51
2:H:628:HIS:HB3	2:H:647:ARG:HH22	1.74	0.51
2:H:741:MET:SD	2:H:741:MET:N	2.82	0.51
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.40	0.51
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.92	0.51
2:C:21:VAL:HG13	2:C:22:LEU:N	2.25	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.93	0.51
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.92	0.51
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.92	0.51
3:D:152:THR:O	3:D:154:LEU:N	2.41	0.51
3:D:260:PHE:O	5:X:504:PRO:HG2	2.11	0.51
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.11	0.51
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.92	0.51
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.10	0.51
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.51
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.40	0.51
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.91	0.51
3:I:500:ILE:HD13	3:I:500:ILE:H	1.75	0.51
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:O	1:B:20:SER:HB3	2.10	0.51
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.26	0.51
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.92	0.51
3:D:141:PHE:O	3:D:297:ARG:HD3	2.10	0.51
3:D:647:PRO:HG3	3:D:697:MET:HA	1.92	0.51
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.75	0.51
1:G:179:PRO:O	1:G:207:THR:OG1	2.20	0.51
2:H:145:ILE:CG2	2:H:456:VAL:HG22	2.40	0.51
2:H:637:ARG:NE	3:I:770:LEU:HD23	2.24	0.51
3:I:197:GLU:O	3:I:201:LEU:HD23	2.10	0.51
3:I:513:MET:O	3:I:575:GLY:HA3	2.11	0.51
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.92	0.51
4:J:60:ASN:H	4:J:63:ILE:HB	1.76	0.51
1:A:134:THR:HG21	2:C:727:VAL:O	2.10	0.51
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.26	0.51
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.40	0.51
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.92	0.51
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.92	0.51
3:D:810:THR:OG1	3:D:811:GLU:N	2.42	0.51
1:F:68:TYR:HB3	2:H:756:TYR:CD1	2.46	0.51
2:H:11:ILE:HG21	2:H:697:LYS:HZ2	1.74	0.51
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.45	0.51
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.10	0.51
2:C:106:GLU:H	2:C:107:ARG:HA	1.76	0.51
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.93	0.51
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.41	0.51
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.76	0.51
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.36	0.51
1:G:227:GLN:C	1:G:228:LEU:HD23	2.36	0.51
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.93	0.51
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.46	0.51
1:A:44:ARG:HG3	1:A:183:ILE:CG2	2.41	0.51
1:A:79:LEU:O	1:A:83:LEU:HD13	2.11	0.51
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.93	0.51
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.11	0.51
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.25	0.51
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.76	0.51
1:F:52:PRO:HG2	1:F:219:ARG:NH2	2.25	0.51
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.46	0.51
2:H:119:GLU:HG2	2:H:120:GLN:N	2.25	0.51
2:H:189:ASP:OD1	2:H:193:ASN:N	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:494:ASN:OD1	2:H:495:ALA:N	2.43	0.51
3:I:56:LEU:HB3	3:I:250:ARG:NH2	2.26	0.51
3:I:543:SER:O	3:I:574:VAL:HB	2.11	0.51
3:I:707:ILE:HG22	3:I:708:ASN:H	1.75	0.51
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.92	0.51
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.46	0.51
2:C:699:LEU:H	2:C:799:ASN:HD21	1.58	0.51
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.11	0.51
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.92	0.51
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.45	0.51
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.10	0.51
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.93	0.50
2:C:517:GLN:HG3	2:C:759:SER:OG	2.10	0.50
2:C:975:ILE:O	2:C:975:ILE:HD13	2.11	0.50
5:X:493:LYS:O	5:X:497:VAL:HG23	2.11	0.50
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.47	0.50
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.92	0.50
2:H:1006:GLU:H	2:H:1006:GLU:CD	2.19	0.50
3:I:316:ILE:HD13	3:I:316:ILE:N	2.26	0.50
3:I:766:GLY:C	3:I:767:LEU:HD22	2.36	0.50
1:A:300:LEU:CD1	1:A:304:LYS:HE2	2.41	0.50
2:C:539:THR:O	2:C:540:ARG:HG3	2.11	0.50
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.47	0.50
3:D:648:GLU:N	3:D:648:GLU:OE2	2.43	0.50
3:D:1284:ARG:HH22	3:I:1292:LEU:HD21	1.75	0.50
5:X:35:ILE:HG13	5:X:36:VAL:N	2.20	0.50
2:H:18:ARG:HD3	2:H:619:ALA:O	2.11	0.50
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.12	0.50
2:C:72:SER:O	2:C:98:VAL:HG23	2.11	0.50
2:C:685:MET:CE	2:C:1235:LEU:HD11	2.41	0.50
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.94	0.50
3:D:704:GLU:HB2	3:D:718:SER:OG	2.12	0.50
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.11	0.50
5:X:600:HIS:H	5:X:601:PRO:HD2	1.76	0.50
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.47	0.50
2:H:572:ILE:HD13	6:H:1401:1RM:O1	2.11	0.50
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.93	0.50
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.92	0.50
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.93	0.50
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.39	0.50
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:482:ALA:C	3:D:483:LEU:HD12	2.35	0.50
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.46	0.50
3:I:515:ARG:HH22	3:I:717:VAL:C	2.18	0.50
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.11	0.50
4:J:3:ARG:O	4:J:4:VAL:HG13	2.10	0.50
3:D:395:LYS:NZ	5:X:607:LEU:O	2.45	0.50
3:D:746:LEU:H	3:D:746:LEU:HD22	1.76	0.50
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.12	0.50
5:X:35:ILE:HG23	5:X:36:VAL:N	2.26	0.50
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.75	0.50
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.93	0.50
3:I:746:LEU:H	3:I:746:LEU:HD22	1.76	0.50
3:I:1195:GLN:OE1	3:I:1195:GLN:N	2.45	0.50
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.36	0.50
2:H:403:MET:HG3	2:H:414:ILE:HB	1.93	0.50
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.92	0.50
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.44	0.50
3:I:152:THR:O	3:I:154:LEU:N	2.40	0.50
3:I:221:ILE:HG13	3:I:222:LYS:N	2.27	0.50
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.94	0.50
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.12	0.50
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.11	0.50
3:D:899:TYR:CZ	3:D:915:ILE:HD12	2.47	0.50
3:D:1320:ILE:HG22	3:D:1352:ILE:CD1	2.42	0.50
2:H:127:ILE:O	2:H:127:ILE:HG12	2.11	0.50
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.40	0.50
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.76	0.50
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.75	0.50
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.44	0.50
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.11	0.50
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.12	0.50
1:F:79:LEU:O	1:F:83:LEU:HD13	2.12	0.50
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.93	0.50
2:H:51:ALA:C	2:H:53:PHE:H	2.19	0.50
2:H:898:GLU:HB2	5:Y:540:LEU:HD21	1.94	0.50
2:H:908:GLU:H	2:H:908:GLU:CD	2.20	0.50
3:I:450:HIS:NE2	3:I:625:MET:SD	2.84	0.50
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.11	0.50
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.92	0.50
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.26	0.50
2:C:127:ILE:HD13	2:C:127:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:221:LEU:HD21	2:C:314:ASN:HD22	1.76	0.50
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.94	0.50
2:C:1274:GLU:OE1	2:C:1274:GLU:N	2.44	0.50
3:D:394:ILE:HG21	5:X:536:THR:HA	1.93	0.50
5:X:311:THR:HG21	5:X:348:GLU:CD	2.37	0.50
3:I:147:ILE:HG23	3:I:156:ARG:C	2.37	0.50
3:I:279:LEU:HD23	3:I:295:GLU:HB3	1.94	0.50
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.75	0.50
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.44	0.49
2:C:98:VAL:HG11	2:C:124:MET:SD	2.52	0.49
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.47	0.49
2:C:807:TRP:HE1	2:C:1086:PRO:HD3	1.77	0.49
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.60	0.49
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.47	0.49
1:F:158:ARG:NH2	1:F:158:ARG:HB2	2.27	0.49
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	0.49
2:H:511:LEU:HA	2:H:513:GLN:HE21	1.76	0.49
3:I:510:LEU:HD12	3:I:601:ILE:HD11	1.94	0.49
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.11	0.49
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.12	0.49
2:C:756:TYR:H	2:C:766:ASN:HB3	1.78	0.49
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.26	0.49
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.36	0.49
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.12	0.49
5:X:264:LYS:HD2	5:X:264:LYS:N	2.28	0.49
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.77	0.49
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.93	0.49
2:H:1122:LYS:HG2	2:H:1229:TYR:CE2	2.47	0.49
3:D:263:SER:HB2	5:X:507:MET:HE2	1.93	0.49
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.49
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.47	0.49
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.11	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.12	0.49
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.28	0.49
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.94	0.49
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.49
1:A:207:THR:OG1	1:A:208:ASN:N	2.42	0.49
2:C:452:ARG:HH22	2:C:458:GLU:CD	2.20	0.49
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.93	0.49
2:C:756:TYR:H	2:C:766:ASN:CB	2.25	0.49
2:C:842:ASP:HB2	2:C:1046:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.28	0.49
3:D:50:LYS:HB3	3:D:50:LYS:HZ2	1.75	0.49
3:D:807:LEU:HD12	3:D:807:LEU:O	2.12	0.49
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.43	0.49
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.42	0.49
2:H:127:ILE:HD13	2:H:127:ILE:N	2.26	0.49
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.78	0.49
2:H:510:GLN:HE22	2:H:534:GLY:HA2	1.75	0.49
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.95	0.49
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.94	0.49
3:I:648:GLU:OE2	3:I:648:GLU:N	2.43	0.49
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.93	0.49
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.94	0.49
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	1.94	0.49
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.94	0.49
3:D:221:ILE:HG13	3:D:222:LYS:N	2.27	0.49
5:X:511:ILE:HG23	5:X:512:GLY:N	2.25	0.49
1:G:51:MET:HE1	1:G:219:ARG:HG2	1.95	0.49
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.40	0.49
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.94	0.49
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.77	0.49
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.93	0.49
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.33	0.49
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.95	0.49
2:C:556:GLY:O	2:C:579:ALA:HB2	2.13	0.49
2:C:893:THR:O	2:C:895:LEU:N	2.40	0.49
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.27	0.49
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.94	0.49
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.28	0.49
5:X:126:GLY:O	5:X:130:VAL:HG23	2.12	0.49
5:X:580:PHE:O	5:X:582:VAL:N	2.46	0.49
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.13	0.49
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.27	0.49
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.93	0.49
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.26	0.49
3:I:515:ARG:NH2	3:I:718:SER:O	2.46	0.49
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.12	0.49
1:A:118:ASP:OD1	1:A:119:GLY:N	2.45	0.49
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.47	0.49
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.78	0.49
3:D:539:SER:OG	3:D:540:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.12	0.49
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.48	0.49
2:H:453:ILE:O	2:H:453:ILE:HG23	2.13	0.49
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.13	0.49
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.95	0.49
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.13	0.49
3:I:504:GLN:HA	3:I:730:ALA:HA	1.92	0.49
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.13	0.49
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.12	0.49
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.28	0.49
2:C:845:LEU:HD13	2:C:845:LEU:N	2.28	0.49
2:C:1066:MET:HG3	2:C:1234:LYS:HA	1.95	0.49
3:D:481:ARG:HA	3:D:485:MET:HE2	1.95	0.49
4:E:6:VAL:HG23	4:E:51:LEU:HD13	1.95	0.49
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.46	0.49
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.77	0.49
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.27	0.49
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.95	0.49
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.12	0.49
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.25	0.49
2:C:91:THR:HG22	2:C:138:ILE:HA	1.95	0.49
2:C:453:ILE:HG23	2:C:453:ILE:O	2.13	0.49
2:C:891:GLY:O	2:C:893:THR:HG23	2.13	0.49
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.48	0.49
3:D:1171:GLY:N	3:D:1172:LYS:O	2.44	0.49
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.93	0.49
2:H:38:PHE:O	2:H:39:ILE:HB	2.12	0.49
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.12	0.49
2:H:176:ILE:HD11	2:H:428:VAL:HG21	1.94	0.49
2:H:488:MET:HB2	2:H:489:PRO:CA	2.43	0.49
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.95	0.49
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.48	0.49
2:H:678:ARG:HD3	2:H:681:MET:HG3	1.94	0.49
2:H:756:TYR:H	2:H:766:ASN:HB3	1.78	0.49
2:H:1156:ARG:HH11	2:H:1157:GLN:H	1.59	0.49
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.46	0.49
3:I:428:THR:HG23	3:I:433:GLY:HA3	1.93	0.49
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.95	0.49
3:I:810:THR:OG1	3:I:811:GLU:N	2.42	0.49
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.46	0.49
2:C:513:GLN:HG2	6:C:1401:1RM:C34	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:ILE:HG22	5:X:450:ILE:HG22	1.94	0.49
3:D:355:ILE:HG12	3:D:464:ASP:O	2.13	0.49
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.13	0.49
3:D:919:ALA:O	3:D:923:ILE:HG12	2.12	0.49
2:H:735:LYS:HA	2:H:748:ILE:HA	1.95	0.49
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.28	0.49
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.77	0.49
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.13	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.28	0.48
2:C:493:ILE:O	5:X:472:GLN:NE2	2.45	0.48
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.43	0.48
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.24	0.48
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.95	0.48
1:F:207:THR:HG23	1:F:209:GLY:H	1.77	0.48
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.41	0.48
3:I:161:THR:HG22	3:I:162:GLU:H	1.78	0.48
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.95	0.48
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.13	0.48
2:C:119:GLU:HG2	2:C:120:GLN:N	2.28	0.48
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.48	0.48
2:C:812:PHE:H	2:C:815:SER:HB2	1.77	0.48
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.20	0.48
6:C:1401:1RM:O9	6:C:1401:1RM:O10	2.18	0.48
3:D:50:LYS:HD3	3:D:71:LEU:HD11	1.93	0.48
3:D:138:VAL:O	3:D:143:SER:HB3	2.12	0.48
3:D:609:TYR:HA	3:D:617:THR:OG1	2.13	0.48
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.12	0.48
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.95	0.48
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.28	0.48
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.43	0.48
3:I:238:ILE:HG13	3:I:238:ILE:O	2.14	0.48
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.13	0.48
2:C:510:GLN:O	2:C:511:LEU:HB2	2.13	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.12	0.48
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.96	0.48
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.46	0.48
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.93	0.48
2:H:812:PHE:H	2:H:815:SER:HB2	1.78	0.48
2:H:888:THR:O	2:H:914:LYS:N	2.40	0.48
3:I:202:ARG:O	3:I:206:ASN:ND2	2.41	0.48
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:514:PHE:HB2	6:C:1401:IRM:O8	2.12	0.48
2:C:1106:ARG:O	2:C:1108:ASN:N	2.43	0.48
5:X:384:LEU:O	5:X:384:LEU:HD13	2.13	0.48
5:Y:297:MET:HE2	5:Y:326:TRP:CZ3	2.48	0.48
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.28	0.48
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.35	0.48
2:C:667:LEU:O	2:C:1069:ARG:NH2	2.46	0.48
2:C:1104:PRO:HG3	3:D:725:MET:SD	2.53	0.48
3:D:646:ILE:HD12	3:D:646:ILE:O	2.14	0.48
3:D:1284:ARG:NH2	3:I:1292:LEU:HD11	2.27	0.48
4:E:44:ASP:HB2	4:E:49:ILE:HD11	1.96	0.48
5:X:582:VAL:HG11	5:X:586:ARG:HG2	1.94	0.48
5:X:600:HIS:H	5:X:601:PRO:CD	2.26	0.48
1:G:86:LYS:NZ	3:I:526:VAL:O	2.47	0.48
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.37	0.48
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.95	0.48
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.95	0.48
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.94	0.48
3:I:589:TYR:O	3:I:591:ILE:HG13	2.14	0.48
3:I:608:CYS:O	3:I:612:LEU:HB2	2.13	0.48
3:I:856:ILE:HG13	3:I:857:LEU:O	2.13	0.48
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.95	0.48
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.49	0.48
2:C:453:ILE:HG22	2:C:585:GLY:O	2.13	0.48
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.33	0.48
2:C:1272:GLU:HA	2:C:1275:VAL:HG22	1.95	0.48
3:D:546:ALA:H	3:D:547:ARG:C	2.21	0.48
3:D:800:LEU:O	3:D:803:VAL:HG12	2.12	0.48
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.35	0.48
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.94	0.48
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.28	0.48
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.13	0.48
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.14	0.48
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.49	0.48
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.96	0.48
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.96	0.48
3:D:253:VAL:HG11	5:X:523:ILE:HG21	1.95	0.48
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.48	0.48
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.13	0.48
2:H:106:GLU:CB	2:H:107:ARG:HA	2.43	0.48
2:H:223:LEU:HD13	2:H:426:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.95	0.48
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.14	0.48
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.13	0.48
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.95	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.14	0.48
5:Y:558:VAL:O	5:Y:562:ARG:HB2	2.14	0.48
2:C:91:THR:HG22	2:C:139:ASN:N	2.29	0.48
2:C:963:GLU:O	2:C:967:LEU:HD13	2.13	0.48
3:D:515:ARG:NH2	3:D:718:SER:O	2.47	0.48
3:D:1297:LYS:HA	3:D:1297:LYS:NZ	2.28	0.48
5:X:133:SER:OG	5:X:365:MET:HB2	2.13	0.48
2:H:839:VAL:O	2:H:886:LYS:NZ	2.32	0.48
2:H:843:THR:HB	2:H:845:LEU:CD2	2.44	0.48
6:H:1401:1RM:H26	6:H:1401:1RM:C31	2.35	0.48
3:I:136:GLU:HA	3:I:139:LEU:HD12	1.95	0.48
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.96	0.48
2:C:348:SER:O	2:C:352:ARG:HG3	2.13	0.48
2:C:434:ASP:HB3	2:C:439:LYS:HB2	1.96	0.48
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.95	0.48
2:C:842:ASP:CB	2:C:1046:VAL:HG21	2.44	0.48
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.94	0.48
3:D:856:ILE:HG13	3:D:857:LEU:O	2.13	0.48
3:D:918:ILE:HD11	3:D:1252:HIS:HE2	1.77	0.48
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.79	0.48
2:H:963:GLU:O	2:H:967:LEU:HD13	2.13	0.48
3:I:619:ILE:O	3:I:623:GLN:HG2	2.14	0.48
3:I:700:ASN:O	3:I:704:GLU:HG2	2.14	0.48
5:Y:316:PHE:HZ	5:Y:334:SER:HA	1.79	0.48
1:A:317:ARG:C	1:A:318:LEU:HD13	2.39	0.48
2:C:494:ASN:OD1	2:C:495:ALA:N	2.46	0.48
2:C:639:LYS:HE2	2:C:639:LYS:HA	1.96	0.48
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.14	0.48
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.13	0.48
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.96	0.48
2:H:989:LEU:HG	2:H:990:ASP:H	1.79	0.48
3:I:394:ILE:CG2	5:Y:536:THR:HG22	2.44	0.48
3:I:413:ASP:HA	3:I:416:ILE:HD12	1.95	0.48
3:I:546:ALA:H	3:I:547:ARG:C	2.21	0.48
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.78	0.48
1:B:151:GLY:O	1:B:177:TYR:HB2	2.14	0.47
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.95	0.47
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.29	0.47
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.29	0.47
3:D:412:LEU:O	3:D:416:ILE:HD12	2.13	0.47
4:E:82:ALA:O	4:E:86:ILE:HG13	2.13	0.47
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.96	0.47
1:G:12:ARG:H	1:G:30:PRO:HG2	1.79	0.47
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.49	0.47
2:H:442:VAL:HG12	2:H:443:ASP:H	1.79	0.47
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.39	0.47
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.95	0.47
2:C:943:LYS:O	2:C:947:GLU:HG2	2.13	0.47
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.14	0.47
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.43	0.47
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.48	0.47
3:D:840:LEU:HD12	3:D:840:LEU:O	2.14	0.47
1:F:134:THR:HG21	2:H:727:VAL:O	2.14	0.47
1:G:227:GLN:C	1:G:229:GLU:H	2.22	0.47
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.44	0.47
3:I:660:GLU:O	3:I:664:ILE:HG12	2.13	0.47
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.43	0.47
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.96	0.47
5:Y:546:ASP:HB3	5:Y:603:ARG:NH2	2.28	0.47
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.29	0.47
3:D:238:ILE:HG13	3:D:238:ILE:O	2.13	0.47
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.96	0.47
2:H:71:VAL:O	2:H:72:SER:OG	2.25	0.47
2:H:639:LYS:HA	2:H:639:LYS:HE2	1.95	0.47
3:I:840:LEU:HD12	3:I:840:LEU:O	2.15	0.47
3:I:1170:LYS:C	3:I:1173:ARG:HD2	2.39	0.47
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.95	0.47
2:C:442:VAL:HG12	2:C:443:ASP:H	1.79	0.47
2:C:529:ARG:HB2	2:C:529:ARG:NH1	2.27	0.47
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.44	0.47
1:G:29:GLU:HA	1:G:200:LYS:HB2	1.96	0.47
2:H:163:LYS:H	2:H:163:LYS:CD	2.24	0.47
2:H:365:GLU:OE2	2:H:368:ARG:NH2	2.48	0.47
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.50	0.47
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.48	0.47
2:H:975:ILE:HD13	2:H:975:ILE:O	2.13	0.47
1:A:318:LEU:HD13	1:A:318:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:748:ILE:C	2:C:748:ILE:HD12	2.40	0.47
2:C:989:LEU:HG	2:C:990:ASP:H	1.79	0.47
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.95	0.47
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.96	0.47
3:D:1170:LYS:C	3:D:1173:ARG:HD2	2.39	0.47
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	1.96	0.47
2:H:868:SER:OG	2:H:942:ASP:OD1	2.28	0.47
2:H:924:VAL:HG12	2:H:1058:ARG:HH22	1.80	0.47
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.54	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
1:B:118:ASP:HB3	1:B:121:VAL:HB	1.96	0.47
2:C:131:THR:HG23	2:C:133:ASN:N	2.28	0.47
2:C:510:GLN:HG3	2:C:535:PRO:HD3	1.96	0.47
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.97	0.47
3:D:697:MET:HE1	3:D:738:ARG:HA	1.97	0.47
5:X:45:ILE:C	5:X:45:ILE:HD12	2.40	0.47
2:H:130:MET:HG3	2:H:134:GLY:HA2	1.97	0.47
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.48	0.47
3:I:425:ARG:NH2	3:I:464:ASP:OD2	2.47	0.47
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.43	0.47
3:I:773:PHE:O	3:I:776:THR:HG22	2.13	0.47
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.14	0.47
2:C:59:ILE:HD13	2:C:479:LEU:HD22	1.96	0.47
2:C:91:THR:HB	2:C:138:ILE:HD13	1.96	0.47
2:C:127:ILE:O	2:C:127:ILE:HG12	2.14	0.47
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.96	0.47
2:C:843:THR:HB	2:C:845:LEU:CD2	2.45	0.47
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.50	0.47
6:C:1401:1RM:H	5:X:515:GLU:HB2	1.95	0.47
3:D:63:GLY:O	3:D:98:ARG:NH2	2.47	0.47
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.44	0.47
3:D:451:PRO:HG2	3:D:625:MET:SD	2.54	0.47
5:X:277:MET:HE3	5:X:281:ARG:HG3	1.96	0.47
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.95	0.47
1:F:60:GLU:HG3	1:F:169:GLY:O	2.14	0.47
2:H:578:TYR:CD2	2:H:659:GLN:HA	2.49	0.47
2:H:699:LEU:H	2:H:799:ASN:HD21	1.62	0.47
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.45	0.47
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.97	0.47
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.97	0.47
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.49	0.47
3:I:194:LEU:O	3:I:198:CYS:HB2	2.15	0.47
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.97	0.47
3:I:393:THR:HG23	3:I:396:ALA:H	1.79	0.47
3:I:473:THR:HB	3:I:476:ALA:HB2	1.97	0.47
3:I:797:THR:O	3:I:801:VAL:HG23	2.14	0.47
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.44	0.47
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.47
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.47	0.47
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.80	0.47
3:D:914:ALA:O	3:D:918:ILE:HG22	2.15	0.47
2:H:748:ILE:C	2:H:748:ILE:HD12	2.40	0.47
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.14	0.47
3:I:288:PRO:HG2	5:Y:413:MET:HE2	1.97	0.47
3:I:292:VAL:O	3:I:296:LYS:HG3	2.15	0.47
3:I:512:TYR:CD2	3:I:724:MET:HE1	2.47	0.47
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.97	0.47
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.15	0.47
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.97	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.50	0.47
3:D:275:ARG:HD2	3:D:302:ALA:HB2	1.97	0.47
3:D:533:ALA:HB2	3:D:578:ILE:HD13	1.96	0.47
3:D:700:ASN:O	3:D:704:GLU:HG2	2.15	0.47
3:D:824:PRO:O	3:D:826:ILE:HG13	2.14	0.47
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.80	0.47
2:H:488:MET:H	2:H:489:PRO:HA	1.79	0.47
3:I:646:ILE:HD12	3:I:646:ILE:O	2.14	0.47
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.79	0.47
2:C:102:LEU:HB3	2:C:117:ILE:HD11	1.97	0.47
3:D:139:LEU:O	3:D:139:LEU:HD22	2.15	0.47
3:D:620:PHE:O	3:D:624:ILE:HG23	2.14	0.47
3:D:655:SER:O	3:D:658:GLU:HG2	2.14	0.47
3:D:918:ILE:HD11	3:D:1252:HIS:NE2	2.30	0.47
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.45	0.47
3:D:1287:ILE:HA	3:D:1290:ARG:HG2	1.96	0.47
2:H:500:ALA:O	2:H:504:GLU:HB2	2.15	0.47
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.97	0.47
3:I:166:LEU:HD12	3:I:167:ASP:N	2.29	0.47
3:I:205:LEU:HB3	3:I:217:LEU:HB3	1.97	0.47
3:I:481:ARG:HG2	4:J:6:VAL:HG21	1.96	0.47
3:I:1215:GLU:OE1	3:I:1224:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.14	0.47
5:Y:428:SER:O	5:Y:432:THR:OG1	2.27	0.47
2:C:71:VAL:O	2:C:72:SER:OG	2.28	0.46
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.80	0.46
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.97	0.46
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.97	0.46
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.46
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.30	0.46
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.97	0.46
3:I:217:LEU:O	3:I:221:ILE:HG12	2.14	0.46
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.49	0.46
2:C:510:GLN:C	2:C:512:SER:H	2.24	0.46
3:D:166:LEU:HD12	3:D:167:ASP:N	2.31	0.46
3:D:377:PHE:O	3:D:381:ILE:HG13	2.15	0.46
3:D:704:GLU:HB2	3:D:718:SER:HG	1.79	0.46
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.98	0.46
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.45	0.46
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.97	0.46
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.30	0.46
3:I:390:LEU:HD21	3:I:407:VAL:HG11	1.97	0.46
1:A:107:ILE:HG12	1:A:134:THR:O	2.16	0.46
2:C:97:ARG:HA	2:C:122:VAL:O	2.15	0.46
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.80	0.46
4:E:4:VAL:O	4:E:5:THR:OG1	2.22	0.46
5:X:448:ARG:NH1	5:X:452:ILE:HD12	2.31	0.46
5:X:459:THR:O	5:X:463:LEU:HD13	2.15	0.46
2:H:514:PHE:HB2	6:H:1401:1RM:O8	2.14	0.46
2:H:632:ASP:O	2:H:633:LEU:HD23	2.16	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.50	0.46
2:H:771:VAL:HG23	2:H:775:GLU:CD	2.40	0.46
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.98	0.46
1:B:31:LEU:HB2	1:B:199:ASP:O	2.15	0.46
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.50	0.46
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.16	0.46
3:D:362:ARG:HD2	3:D:364:HIS:HE1	1.81	0.46
2:H:106:GLU:H	2:H:107:ARG:HA	1.81	0.46
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.96	0.46
3:I:141:PHE:O	3:I:297:ARG:HD3	2.15	0.46
3:I:596:LEU:N	3:I:596:LEU:HD23	2.30	0.46
5:Y:448:ARG:HD2	5:Y:452:ILE:HD12	1.98	0.46
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.97	0.46
1:A:321:TRP:HA	1:A:322:PRO:HA	1.67	0.46
1:B:74:VAL:HG12	1:B:76:GLU:H	1.81	0.46
2:C:43:PRO:HD3	2:C:47:TYR:CE2	2.50	0.46
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.98	0.46
2:C:1166:ASP:C	2:C:1168:GLU:H	2.23	0.46
3:D:514:THR:HG21	3:D:595:ALA:O	2.15	0.46
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.97	0.46
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.46
3:D:766:GLY:C	3:D:767:LEU:HD22	2.41	0.46
3:D:1369:ARG:HB3	3:D:1369:ARG:HH11	1.80	0.46
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.51	0.46
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.97	0.46
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	1.98	0.46
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.30	0.46
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.97	0.46
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.49	0.46
3:D:161:THR:HG22	3:D:162:GLU:H	1.79	0.46
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.46
3:D:909:ILE:HD12	3:D:909:ILE:O	2.16	0.46
3:D:1297:LYS:HE3	3:I:1267:VAL:HB	1.97	0.46
5:X:316:PHE:CZ	5:X:334:SER:HA	2.51	0.46
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.96	0.46
2:H:91:THR:HG22	2:H:139:ASN:N	2.30	0.46
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.46
2:H:756:TYR:H	2:H:766:ASN:CB	2.27	0.46
2:H:998:LEU:O	2:H:998:LEU:HD13	2.16	0.46
3:I:8:LEU:HD23	3:I:8:LEU:N	2.31	0.46
3:I:265:LEU:HD11	3:I:330:MET:SD	2.56	0.46
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.80	0.46
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.15	0.46
1:A:11:PRO:HA	1:A:30:PRO:O	2.16	0.46
1:A:218:ARG:NH1	1:B:233:ASP:OD2	2.48	0.46
2:C:15:PHE:CD2	2:C:1182:ILE:HD11	2.51	0.46
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.98	0.46
2:C:740:GLU:HB2	2:C:741:MET:SD	2.56	0.46
2:C:804:PHE:O	3:D:638:SER:OG	2.30	0.46
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.15	0.46
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.80	0.46
3:D:8:LEU:HD23	3:D:8:LEU:N	2.30	0.46
3:D:122:SER:HB2	3:D:132:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:143:SER:HB2	5:X:100:MET:HE2	1.96	0.46
3:D:286:ALA:HB3	5:X:413:MET:SD	2.55	0.46
3:D:292:VAL:HG22	3:D:296:LYS:HE3	1.97	0.46
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.46	0.46
5:X:119:ILE:O	5:X:123:ILE:HG13	2.15	0.46
5:X:465:ARG:O	5:X:468:ARG:HG2	2.15	0.46
3:I:139:LEU:O	3:I:139:LEU:HD22	2.15	0.46
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.40	0.46
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.16	0.46
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.51	0.46
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.46	0.46
3:D:707:ILE:HD11	3:D:716:GLN:CD	2.40	0.46
5:X:346:GLN:O	5:X:350:GLU:HG3	2.15	0.46
1:F:190:ALA:HB2	1:F:200:LYS:CB	2.46	0.46
3:I:492:SER:HB2	3:I:499:ILE:HB	1.97	0.46
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.51	0.46
5:Y:286:LEU:HD23	5:Y:340:ALA:HB2	1.96	0.46
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.16	0.46
5:Y:546:ASP:HB3	5:Y:603:ARG:HH22	1.79	0.46
1:B:180:VAL:HG11	1:B:183:ILE:HG12	1.98	0.46
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.46	0.46
2:C:11:ILE:HD11	2:C:1181:PRO:HD3	1.98	0.46
2:C:892:GLU:C	2:C:894:GLN:H	2.24	0.46
2:C:1223:ARG:HD2	3:D:637:ALA:HA	1.97	0.46
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.29	0.46
5:X:250:LEU:O	5:X:254:GLU:HG2	2.15	0.46
1:G:9:LEU:HD23	1:G:9:LEU:H	1.81	0.46
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.31	0.46
2:H:999:GLU:HG2	2:H:1000:LEU:H	1.81	0.46
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.16	0.46
3:I:522:GLY:HA2	3:I:545:HIS:CD2	2.51	0.46
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.98	0.46
3:I:1171:GLY:N	3:I:1172:LYS:O	2.48	0.46
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.97	0.46
2:C:337:PHE:O	2:C:338:THR:OG1	2.27	0.46
2:C:1214:ASP:HA	2:C:1221:PHE:CZ	2.51	0.46
3:D:508:LEU:O	3:D:508:LEU:HD22	2.16	0.46
2:H:91:THR:HB	2:H:138:ILE:HD13	1.98	0.46
2:H:122:VAL:HG13	2:H:124:MET:HG3	1.98	0.46
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.51	0.46
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:149:GLY:HA2	3:I:156:ARG:HG2	1.98	0.46
3:I:260:PHE:O	5:Y:504:PRO:HG2	2.16	0.46
3:I:377:PHE:O	3:I:381:ILE:HG13	2.16	0.46
3:I:909:ILE:HD12	3:I:909:ILE:O	2.16	0.46
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.16	0.46
1:A:12:ARG:HB2	1:A:30:PRO:HG2	1.98	0.45
1:A:300:LEU:O	1:A:300:LEU:HD13	2.16	0.45
1:B:16:ILE:HG12	1:B:26:VAL:HG22	1.98	0.45
1:B:61:ILE:HB	1:B:64:VAL:HB	1.98	0.45
2:C:170:VAL:O	2:C:171:LEU:HB2	2.15	0.45
2:C:560:PRO:HB2	3:D:776:THR:OG1	2.16	0.45
3:D:145:VAL:HG22	3:D:180:MET:SD	2.57	0.45
3:D:619:ILE:O	3:D:623:GLN:HG2	2.15	0.45
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.51	0.45
5:X:9:LEU:HD22	5:X:60:PRO:HB3	1.98	0.45
5:X:123:ILE:O	5:X:127:ILE:HG12	2.17	0.45
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.98	0.45
2:H:848:GLU:CD	2:H:888:THR:HG22	2.41	0.45
2:H:902:LEU:HD11	5:Y:608:ARG:HA	1.97	0.45
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.51	0.45
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.71	0.45
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.50	0.45
3:D:526:VAL:HG12	3:D:549:LYS:O	2.15	0.45
2:H:607:SER:H	2:H:610:GLU:HB2	1.81	0.45
2:H:766:ASN:H	2:H:787:PRO:HG3	1.80	0.45
2:H:840:SER:HB3	2:H:850:ILE:HD11	1.98	0.45
2:H:869:GLY:C	2:H:870:ILE:HD12	2.41	0.45
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.30	0.45
3:I:264:ASP:OD2	3:I:324:LEU:HD12	2.17	0.45
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.80	0.45
1:B:22:THR:HG22	1:B:208:ASN:O	2.16	0.45
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.51	0.45
2:C:216:THR:O	2:C:220:ILE:HG13	2.16	0.45
3:D:77:ARG:HA	3:D:77:ARG:HD2	1.73	0.45
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.98	0.45
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.16	0.45
5:X:310:GLU:O	5:X:344:LEU:HD23	2.16	0.45
2:H:994:ARG:HD3	2:H:994:ARG:N	2.30	0.45
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.15	0.45
2:H:1243:MET:HE3	3:I:372:MET:HB2	1.98	0.45
3:I:275:ARG:HD3	3:I:298:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:886:VAL:HG13	3:I:1230:THR:HG21	1.98	0.45
4:J:65:ASP:O	4:J:69:ARG:HG3	2.16	0.45
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.16	0.45
5:Y:561:MET:HA	5:Y:567:MET:SD	2.57	0.45
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.45
2:C:130:MET:CG	2:C:134:GLY:HA2	2.47	0.45
2:C:590:PRO:HB3	2:C:605:TYR:CE1	2.51	0.45
3:D:227:PHE:O	3:D:230:SER:OG	2.24	0.45
3:D:512:TYR:CD2	3:D:724:MET:HE1	2.36	0.45
3:D:915:ILE:O	3:D:918:ILE:HG23	2.15	0.45
5:X:242:HIS:HA	5:X:245:ALA:HB3	1.98	0.45
1:G:227:GLN:O	1:G:229:GLU:N	2.50	0.45
2:H:706:ARG:HA	2:H:793:GLU:HA	1.99	0.45
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.42	0.45
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.31	0.45
1:A:222:THR:O	1:A:226:GLU:HG3	2.17	0.45
2:C:92:TYR:HD1	2:C:129:LEU:HB2	1.80	0.45
3:D:217:LEU:O	3:D:221:ILE:HG12	2.15	0.45
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.99	0.45
5:X:271:ASN:O	5:X:275:VAL:HG23	2.16	0.45
2:H:946:LEU:O	2:H:949:GLU:HG3	2.15	0.45
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.48	0.45
2:H:1287:LEU:HD23	3:I:1357:ILE:HG12	1.98	0.45
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.16	0.45
3:I:313:GLY:O	3:I:314:ARG:HB2	2.16	0.45
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.25	0.45
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.23	0.45
4:J:15:ASN:ND2	4:J:18:ASP:H	2.09	0.45
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.24	0.45
1:B:232:VAL:O	1:B:233:ASP:HB2	2.16	0.45
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.45
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.98	0.45
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.47	0.45
3:D:112:ALA:HA	3:D:238:ILE:HG22	1.98	0.45
3:D:133:ARG:HB2	3:D:133:ARG:NH2	2.32	0.45
3:D:291:ILE:HD11	5:X:384:LEU:HD21	1.98	0.45
3:D:527:LEU:HB2	3:D:535:ARG:CZ	2.47	0.45
3:D:678:ARG:HD2	3:D:678:ARG:C	2.41	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.32	0.45
2:H:131:THR:HG23	2:H:133:ASN:N	2.27	0.45
2:H:549:ASP:OD1	2:H:550:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:572:ILE:HD13	6:H:1401:1RM:C1	2.47	0.45
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.47	0.45
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.32	0.45
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.56	0.45
5:Y:596:ARG:HA	5:Y:596:ARG:HE	1.81	0.45
1:A:289:LEU:HD11	1:A:314:LEU:HD11	1.98	0.45
2:C:197:ARG:NH1	2:C:201:ARG:O	2.49	0.45
2:C:805:MET:HE1	2:C:1221:PHE:CZ	2.51	0.45
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.45
2:C:929:ILE:HG12	2:C:1053:TYR:O	2.17	0.45
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.31	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.52	0.45
3:D:120:LEU:CD2	3:D:1330:ARG:HD2	2.46	0.45
3:D:155:GLU:H	3:D:155:GLU:CD	2.24	0.45
3:D:697:MET:SD	3:D:741:ALA:HB3	2.56	0.45
5:X:543:ALA:O	5:X:547:VAL:HG23	2.16	0.45
2:H:489:PRO:HB2	2:H:492:MET:CB	2.40	0.45
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	1.99	0.45
3:I:56:LEU:HB3	3:I:250:ARG:HH21	1.80	0.45
3:I:139:LEU:HD22	3:I:139:LEU:C	2.42	0.45
3:I:147:ILE:HD12	3:I:178:ALA:CB	2.46	0.45
3:I:412:LEU:O	3:I:415:VAL:HG22	2.17	0.45
3:I:697:MET:SD	3:I:741:ALA:HB3	2.57	0.45
3:I:1194:ARG:N	3:I:1194:ARG:HD2	2.32	0.45
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.17	0.45
3:I:1287:ILE:HA	3:I:1290:ARG:HG2	1.99	0.45
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.98	0.45
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.98	0.45
3:D:573:THR:HG23	3:D:576:ARG:H	1.81	0.45
3:D:905:ARG:HH12	4:E:10:VAL:HG12	1.81	0.45
5:X:357:GLN:NE2	5:X:360:ASP:OD2	2.50	0.45
2:H:170:VAL:O	2:H:171:LEU:HB2	2.17	0.45
2:H:892:GLU:C	2:H:894:GLN:H	2.25	0.45
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.98	0.45
3:I:194:LEU:HD21	3:I:234:PRO:HG3	1.98	0.45
3:I:370:LYS:HG3	3:I:371:LYS:H	1.82	0.45
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.52	0.45
1:A:158:ARG:HB2	1:A:158:ARG:HH21	1.82	0.45
1:A:184:ALA:HB2	2:C:1091:GLY:N	2.32	0.45
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.51	0.45
2:C:773:LEU:C	2:C:773:LEU:HD22	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:269:TYR:CG	3:D:306:LEU:HD11	2.52	0.45
2:H:1254:VAL:O	3:I:99:ARG:NH1	2.48	0.45
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.29	0.45
3:I:1269:ALA:H	3:I:1300:ALA:HB2	1.81	0.45
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.16	0.45
2:C:752:ASN:C	2:C:753:LEU:HG	2.42	0.45
3:D:368:LEU:HG	3:D:373:ALA:HB2	1.99	0.45
3:D:424:ASN:HB2	3:D:434:ILE:HG13	1.99	0.45
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.99	0.45
2:H:42:ASP:HB2	2:H:47:TYR:CG	2.51	0.45
2:H:53:PHE:HA	2:H:56:VAL:HG23	1.99	0.45
2:H:207:THR:O	2:H:211:ARG:HG3	2.17	0.45
3:I:539:SER:OG	3:I:540:GLY:N	2.47	0.45
1:A:90:VAL:HG13	1:A:121:VAL:HG13	2.00	0.44
2:C:170:VAL:HG23	2:C:171:LEU:N	2.24	0.44
2:C:1284:ALA:HA	3:D:1357:ILE:HD13	1.99	0.44
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	1.98	0.44
3:D:139:LEU:HD22	3:D:139:LEU:C	2.43	0.44
3:D:596:LEU:N	3:D:596:LEU:HD23	2.32	0.44
3:D:703:THR:O	3:D:718:SER:N	2.50	0.44
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.81	0.44
1:G:179:PRO:HB2	1:G:211:ILE:HG22	1.99	0.44
2:H:67:GLU:HG2	2:H:103:VAL:HG12	1.99	0.44
2:H:97:ARG:HA	2:H:122:VAL:O	2.17	0.44
2:H:469:VAL:O	2:H:472:GLU:HB3	2.17	0.44
2:H:1233:LEU:HD12	2:H:1233:LEU:O	2.17	0.44
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.29	0.44
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.52	0.44
3:I:26:SER:O	3:I:30:ILE:HG12	2.17	0.44
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.98	0.44
5:Y:585:GLU:O	5:Y:589:GLN:N	2.45	0.44
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.32	0.44
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.82	0.44
2:C:841:ARG:HA	2:C:1046:VAL:CG1	2.47	0.44
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.17	0.44
2:C:1272:GLU:HG3	2:C:1276:TRP:CE2	2.53	0.44
3:D:316:ILE:HD11	3:D:320:ASN:O	2.17	0.44
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.47	0.44
5:X:242:HIS:O	5:X:246:GLN:HB2	2.18	0.44
5:X:470:MET:HB2	5:X:478:PRO:HB3	1.99	0.44
2:H:546:GLU:O	2:H:548:ARG:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:943:LYS:O	2:H:947:GLU:HG2	2.16	0.44
2:H:1166:ASP:C	2:H:1168:GLU:H	2.25	0.44
2:H:1276:TRP:HA	2:H:1276:TRP:HE3	1.82	0.44
2:H:1333:LEU:HB2	2:H:1335:ILE:HG22	1.99	0.44
3:I:681:LYS:O	3:I:685:ILE:HG13	2.18	0.44
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.99	0.44
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.99	0.44
1:A:102:LEU:HD12	1:A:115:ILE:HG12	1.99	0.44
2:C:201:ARG:HH12	5:X:36:VAL:HG11	1.82	0.44
2:C:475:VAL:O	2:C:479:LEU:HB2	2.17	0.44
2:C:533:LEU:HD23	2:C:533:LEU:H	1.82	0.44
2:C:741:MET:SD	2:C:741:MET:N	2.90	0.44
2:C:816:ILE:HG13	2:C:1098:LEU:CD2	2.38	0.44
2:C:819:SER:HB2	2:C:1085:MET:SD	2.57	0.44
2:C:826:ASP:HA	2:C:829:THR:HG23	1.99	0.44
3:D:122:SER:CB	3:D:132:LEU:HD13	2.48	0.44
3:D:355:ILE:HA	3:D:447:ILE:HG23	1.98	0.44
3:D:644:MET:HE2	3:D:644:MET:HB3	1.94	0.44
3:D:706:VAL:C	3:D:707:ILE:HG13	2.42	0.44
4:E:16:ARG:O	4:E:20:VAL:HG23	2.17	0.44
5:X:449:THR:HG23	5:X:503:GLU:OE1	2.18	0.44
1:F:45:ARG:HG2	2:H:1083:GLU:HB2	1.99	0.44
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.52	0.44
2:H:517:GLN:HE21	2:H:760:ASN:H	1.65	0.44
2:H:1065:LYS:HG2	2:H:1235:LEU:HD12	1.99	0.44
3:I:12:THR:O	3:I:13:LYS:HD2	2.17	0.44
3:I:138:VAL:O	3:I:143:SER:HB3	2.17	0.44
5:Y:264:LYS:HD2	5:Y:264:LYS:N	2.30	0.44
1:A:178:SER:HA	1:A:179:PRO:HD3	1.79	0.44
2:C:429:MET:O	2:C:433:ILE:HG13	2.18	0.44
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.46	0.44
2:C:1319:MET:HE3	2:C:1324:ASN:HB2	1.99	0.44
3:D:298:MET:HE3	5:X:402:LEU:HB3	2.00	0.44
3:D:313:GLY:O	3:D:314:ARG:HB2	2.17	0.44
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.73	0.44
2:H:582:ASN:HD22	2:H:588:GLU:CD	2.24	0.44
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.99	0.44
3:I:124:ILE:HG13	3:I:189:LEU:HD11	1.98	0.44
3:I:384:LYS:HA	3:I:384:LYS:HD2	1.84	0.44
3:I:1290:ARG:HD2	3:I:1299:GLY:HA3	2.00	0.44
1:B:182:ARG:HD3	3:D:581:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.51	0.44
2:C:818:VAL:HG22	2:C:819:SER:N	2.33	0.44
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.16	0.44
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.47	0.44
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.98	0.44
3:D:746:LEU:HD22	3:D:746:LEU:N	2.33	0.44
4:E:15:ASN:OD1	4:E:17:PHE:HB2	2.17	0.44
2:H:130:MET:SD	2:H:134:GLY:HA2	2.57	0.44
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.17	0.44
1:A:14:VAL:HG21	1:A:29:GLU:HB2	1.98	0.44
1:B:9:LEU:H	1:B:9:LEU:HD23	1.83	0.44
1:B:192:VAL:HG21	1:B:198:LEU:CD1	2.34	0.44
3:D:116:PHE:HB3	3:D:237:MET:CE	2.48	0.44
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.99	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.79	0.44
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.18	0.44
5:X:52:GLY:O	5:X:53:ILE:HB	2.18	0.44
5:X:519:LEU:O	5:X:519:LEU:HD13	2.18	0.44
1:G:110:VAL:HG11	1:G:140:ILE:HD11	1.99	0.44
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.83	0.44
2:H:478:ARG:CD	2:H:492:MET:HG3	2.47	0.44
2:H:818:VAL:HG22	2:H:819:SER:N	2.33	0.44
3:I:413:ASP:HA	3:I:416:ILE:CD1	2.46	0.44
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.48	0.44
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.99	0.44
5:Y:386:LEU:O	5:Y:390:ILE:HG23	2.18	0.44
1:A:310:ARG:NE	1:A:310:ARG:HA	2.33	0.44
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.52	0.44
3:D:531:LYS:HB3	3:D:531:LYS:NZ	2.33	0.44
3:D:1341:ARG:HH21	3:D:1343:GLU:CD	2.26	0.44
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.82	0.44
2:H:773:LEU:C	2:H:773:LEU:HD22	2.42	0.44
2:H:1204:LEU:CD2	2:H:1205:PRO:HD2	2.48	0.44
2:H:1214:ASP:HB3	2:H:1218:GLY:H	1.83	0.44
3:I:50:LYS:HB3	3:I:50:LYS:HZ3	1.83	0.44
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.75	0.44
3:I:510:LEU:HD12	3:I:601:ILE:CD1	2.47	0.44
3:I:1357:ILE:HD12	3:I:1357:ILE:N	2.33	0.44
5:Y:234:THR:HG21	5:Y:248:GLU:OE2	2.17	0.44
5:Y:305:LEU:HD21	5:Y:322:MET:HE1	1.99	0.44
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:563:THR:HG21	3:D:780:ARG:CZ	2.48	0.44
2:C:591:TYR:CE1	2:C:616:ILE:HG23	2.53	0.44
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.17	0.44
2:C:1204:LEU:CD2	2:C:1205:PRO:HD2	2.48	0.44
3:D:72:CYS:SG	3:D:73:GLY:N	2.91	0.44
3:D:165:TYR:O	3:D:169:LEU:HB2	2.17	0.44
3:D:217:LEU:O	3:D:221:ILE:HG23	2.17	0.44
3:D:704:GLU:O	3:D:705:THR:OG1	2.28	0.44
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.32	0.44
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.99	0.44
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.81	0.44
2:H:54:ARG:N	2:H:55:SER:CB	2.75	0.44
2:H:54:ARG:N	2:H:55:SER:C	2.76	0.44
2:H:122:VAL:HG22	2:H:123:TYR:N	2.32	0.44
2:H:170:VAL:HG23	2:H:171:LEU:N	2.29	0.44
2:H:555:TYR:HE2	2:H:616:ILE:HD13	1.83	0.44
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.32	0.44
3:I:555:TYR:HD1	3:I:589:TYR:HE2	1.66	0.44
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.48	0.44
3:I:720:ASN:ND2	3:I:720:ASN:O	2.51	0.44
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.99	0.44
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.31	0.44
1:B:153:VAL:O	1:B:175:ALA:N	2.50	0.44
2:C:998:LEU:HD13	2:C:998:LEU:O	2.18	0.44
2:C:1042:LEU:HB2	2:C:1043:ALA:H	1.68	0.44
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.44	0.44
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.47	0.44
3:D:318:GLY:C	3:D:320:ASN:H	2.26	0.44
3:D:664:ILE:HG21	3:D:681:LYS:HD2	2.00	0.44
5:X:130:VAL:O	5:X:134:VAL:HG23	2.18	0.44
5:X:245:ALA:O	5:X:249:ILE:HG13	2.18	0.44
1:F:11:PRO:CD	1:G:227:GLN:HG3	2.48	0.44
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.53	0.44
2:H:342:ASP:OD1	2:H:342:ASP:N	2.46	0.44
2:H:511:LEU:HA	2:H:513:GLN:NE2	2.33	0.44
2:H:697:LYS:HG3	2:H:698:PRO:HD2	2.00	0.44
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.49	0.44
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.47	0.44
1:A:299:SER:O	1:A:303:ILE:HG12	2.18	0.43
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.45	0.43
2:C:130:MET:HG3	2:C:134:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:ILE:O	2:C:311:CYS:HB3	2.18	0.43
2:C:559:CYS:SG	2:C:661:VAL:HA	2.57	0.43
2:C:646:SER:HB2	2:C:649:GLN:HG3	2.00	0.43
2:C:985:GLU:HG3	2:C:988:LYS:HB2	2.00	0.43
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.48	0.43
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.53	0.43
3:D:504:GLN:HA	3:D:730:ALA:HA	2.00	0.43
3:D:588:PRO:HG2	3:D:591:ILE:HD11	2.00	0.43
3:D:1247:LYS:H	3:D:1247:LYS:CD	2.24	0.43
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.47	0.43
5:X:291:CYS:O	5:X:297:MET:HB3	2.18	0.43
2:H:59:ILE:HG22	2:H:476:LYS:HA	2.00	0.43
2:H:157:PHE:CZ	2:H:431:LYS:HD3	2.53	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.33	0.43
2:H:1269:ARG:HD3	2:H:1269:ARG:N	2.33	0.43
2:H:1332:SER:O	3:I:243:PRO:HG2	2.18	0.43
3:I:44:ILE:HG22	5:Y:450:ILE:HG22	2.00	0.43
3:I:390:LEU:N	3:I:390:LEU:HD12	2.32	0.43
5:Y:596:ARG:HH21	5:Y:599:ARG:CZ	2.31	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.53	0.43
2:C:54:ARG:HG2	2:C:55:SER:OG	2.18	0.43
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.83	0.43
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.83	0.43
2:C:1141:LEU:H	2:C:1141:LEU:HD13	1.83	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:HG12	2.00	0.43
3:D:452:LEU:HG	3:D:625:MET:SD	2.58	0.43
1:F:200:LYS:HG3	1:F:200:LYS:O	2.19	0.43
1:G:178:SER:HA	1:G:179:PRO:HD3	1.88	0.43
5:Y:240:ARG:O	5:Y:242:HIS:N	2.52	0.43
2:C:49:LEU:HD11	2:C:464:PHE:CG	2.53	0.43
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.99	0.43
2:C:617:ALA:HB2	2:C:650:VAL:CG2	2.46	0.43
2:C:843:THR:HG22	2:C:844:LYS:N	2.32	0.43
2:C:985:GLU:HG2	2:C:989:LEU:HD13	2.00	0.43
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.33	0.43
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.82	0.43
5:X:592:ALA:O	5:X:596:ARG:HG2	2.18	0.43
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.98	0.43
2:H:73:TYR:O	2:H:74:ARG:HB2	2.17	0.43
2:H:106:GLU:HG3	2:H:108:GLU:N	2.34	0.43
2:H:505:PHE:O	2:H:509:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	2.00	0.43
3:I:31:ARG:HD2	3:I:104:HIS:CD2	2.54	0.43
3:I:33:TRP:O	3:I:102:MET:HB2	2.18	0.43
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.48	0.43
3:I:703:THR:O	3:I:718:SER:N	2.52	0.43
2:C:243:PRO:HB2	2:C:278:GLU:HG3	2.00	0.43
2:C:312:ALA:HB3	2:C:315:MET:HE3	2.00	0.43
2:C:511:LEU:HD13	2:C:535:PRO:HD3	2.00	0.43
2:C:580:GLN:HG2	2:C:581:THR:N	2.34	0.43
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.48	0.43
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	2.00	0.43
3:D:120:LEU:HA	5:X:46:GLN:CD	2.43	0.43
3:D:413:ASP:HA	3:D:416:ILE:CD1	2.48	0.43
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.99	0.43
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.18	0.43
5:X:514:ASP:HB2	5:X:517:SER:OG	2.18	0.43
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.87	0.43
2:H:69:GLN:HE22	2:H:101:ARG:NH2	2.16	0.43
2:H:468:LEU:O	2:H:471:VAL:HG22	2.18	0.43
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.51	0.43
3:I:72:CYS:SG	3:I:73:GLY:N	2.90	0.43
3:I:165:TYR:O	3:I:169:LEU:HB2	2.18	0.43
3:I:531:LYS:HB3	3:I:531:LYS:NZ	2.33	0.43
3:I:611:ILE:HG13	3:I:612:LEU:HD23	2.00	0.43
3:I:647:PRO:HG3	3:I:697:MET:HA	1.99	0.43
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.37	0.43
3:I:1307:LEU:N	3:I:1307:LEU:HD23	2.33	0.43
5:Y:130:VAL:O	5:Y:134:VAL:HG23	2.18	0.43
1:B:22:THR:HB	1:B:207:THR:O	2.19	0.43
2:C:130:MET:SD	2:C:134:GLY:HA2	2.59	0.43
2:C:205:PRO:O	2:C:208:ILE:HG22	2.19	0.43
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.00	0.43
2:C:519:ASN:ND2	2:C:689:ALA:O	2.52	0.43
2:C:734:ILE:O	2:C:748:ILE:HA	2.18	0.43
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	2.01	0.43
2:C:1314:GLN:O	3:D:473:THR:HG23	2.18	0.43
3:D:395:LYS:HD3	5:X:607:LEU:HD13	2.01	0.43
3:D:720:ASN:ND2	3:D:720:ASN:O	2.51	0.43
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.43	0.43
5:X:437:GLN:HA	5:X:440:THR:HG22	1.99	0.43
1:F:41:ASN:HD21	2:H:1218:GLY:CA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.84	0.43
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.54	0.43
2:H:131:THR:HG22	2:H:135:THR:N	2.34	0.43
2:H:966:ILE:HG23	2:H:967:LEU:HD12	2.01	0.43
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.99	0.43
3:I:161:THR:HG22	3:I:162:GLU:N	2.34	0.43
3:I:165:TYR:CE1	3:I:169:LEU:HD23	2.54	0.43
3:I:522:GLY:HA2	3:I:545:HIS:CG	2.53	0.43
1:A:131:CYS:O	1:A:132:HIS:ND1	2.52	0.43
1:A:320:ASN:O	1:A:323:PRO:HD3	2.19	0.43
2:C:705:GLU:H	2:C:705:GLU:CD	2.27	0.43
2:C:892:GLU:O	2:C:893:THR:OG1	2.21	0.43
3:D:390:LEU:N	3:D:390:LEU:HD12	2.33	0.43
1:G:195:ARG:HH21	1:G:198:LEU:HD21	1.84	0.43
2:H:519:ASN:ND2	2:H:689:ALA:O	2.51	0.43
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.51	0.43
2:H:972:PHE:HA	2:H:975:ILE:HG22	1.99	0.43
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.84	0.43
3:I:12:THR:C	3:I:13:LYS:HD2	2.43	0.43
3:I:185:ILE:HD12	3:I:185:ILE:HA	1.92	0.43
3:I:205:LEU:HB3	3:I:217:LEU:HD13	2.00	0.43
3:I:412:LEU:HA	3:I:415:VAL:HG22	1.99	0.43
3:I:678:ARG:O	3:I:681:LYS:HG3	2.18	0.43
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.43	0.43
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.18	0.43
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	2.00	0.43
1:A:252:ILE:HG22	1:A:278:ILE:HD11	2.00	0.43
1:B:179:PRO:HB3	1:B:210:THR:HB	2.00	0.43
2:C:169:LYS:HD3	2:C:169:LYS:HA	1.73	0.43
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.33	0.43
2:C:740:GLU:CD	2:C:740:GLU:H	2.27	0.43
2:C:886:LYS:H	2:C:917:SER:HB3	1.82	0.43
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.53	0.43
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.58	0.43
3:D:126:LEU:HD21	3:D:223:LEU:HD13	2.00	0.43
3:D:205:LEU:HD13	3:D:217:LEU:HD22	2.00	0.43
3:D:313:GLY:H	5:X:38:SER:HB3	1.81	0.43
3:D:393:THR:HG23	3:D:396:ALA:H	1.83	0.43
3:D:505:ASP:HB3	3:D:629:PHE:HE2	1.83	0.43
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.43
5:X:290:LEU:HD13	5:X:336:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:525:ASP:OD1	5:X:528:LEU:HG	2.19	0.43
1:G:19:VAL:O	1:G:20:SER:OG	2.19	0.43
1:G:191:ARG:NH2	3:I:441:LEU:O	2.51	0.43
2:H:1042:LEU:HD13	2:H:1042:LEU:N	2.25	0.43
2:H:1106:ARG:O	2:H:1108:ASN:N	2.45	0.43
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.84	0.43
1:B:183:ILE:HD11	1:B:205:MET:HE2	2.00	0.43
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	1.99	0.43
3:D:268:LEU:HD22	3:D:324:LEU:HD23	2.01	0.43
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.33	0.43
5:X:224:LEU:HB2	5:X:259:PHE:CE1	2.53	0.43
5:X:556:ALA:O	5:X:560:ARG:HB2	2.18	0.43
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.43
1:G:185:TYR:HA	1:G:202:VAL:O	2.19	0.43
2:H:170:VAL:CG2	2:H:171:LEU:H	2.23	0.43
2:H:481:LEU:HD13	2:H:481:LEU:C	2.44	0.43
2:H:591:TYR:HD2	2:H:606:LEU:HD23	1.84	0.43
2:H:681:MET:O	2:H:685:MET:HG2	2.19	0.43
2:H:752:ASN:C	2:H:753:LEU:HG	2.44	0.43
2:H:923:GLY:HA2	3:I:371:LYS:HE3	2.01	0.43
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.99	0.43
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.18	0.43
3:I:1270:GLY:HA3	3:I:1299:GLY:HA2	2.01	0.43
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.18	0.43
2:C:73:TYR:N	2:C:73:TYR:CD2	2.87	0.43
3:D:97:VAL:O	3:D:101:ARG:HG2	2.18	0.43
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.85	0.43
3:D:413:ASP:HA	3:D:416:ILE:HD12	2.00	0.43
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.18	0.43
3:D:773:PHE:O	3:D:776:THR:HG22	2.19	0.43
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.83	0.43
3:D:1234:VAL:HG13	3:D:1235:ASN:N	2.34	0.43
1:F:51:MET:HA	1:F:52:PRO:HD3	1.83	0.43
2:H:73:TYR:N	2:H:73:TYR:CD2	2.87	0.43
2:H:807:TRP:HE1	2:H:1086:PRO:CD	2.30	0.43
2:H:866:ASP:HA	2:H:872:TYR:OH	2.19	0.43
3:I:1196:LEU:HG	3:I:1210:ILE:HD11	2.01	0.43
3:I:1281:GLU:O	3:I:1285:VAL:HG13	2.19	0.43
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.19	0.43
1:A:45:ARG:NE	1:B:38:THR:OG1	2.45	0.43
1:A:236:ASP:HA	1:B:14:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:HD3	1:A:246:LYS:N	2.34	0.43
2:C:56:VAL:HB	2:C:57:PHE:H	1.52	0.43
2:C:1141:LEU:O	2:C:1141:LEU:HD22	2.18	0.43
3:D:905:ARG:HG2	3:D:907:HIS:H	1.84	0.43
3:D:1171:GLY:CA	3:D:1172:LYS:C	2.92	0.43
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	2.00	0.43
5:X:439:ILE:O	5:X:443:ILE:HG13	2.19	0.43
5:X:477:GLU:CD	5:X:477:GLU:H	2.27	0.43
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.01	0.43
2:H:578:TYR:HD2	2:H:659:GLN:HA	1.84	0.43
2:H:582:ASN:HB3	2:H:586:PHE:C	2.44	0.43
2:H:734:ILE:HG23	2:H:749:ASP:HB2	2.01	0.43
2:H:759:SER:HB3	2:H:763:THR:H	1.83	0.43
2:H:1314:GLN:O	3:I:473:THR:HG23	2.18	0.43
3:I:142:GLU:HA	3:I:180:MET:HE2	2.00	0.43
3:I:235:GLU:OE1	3:I:235:GLU:N	2.52	0.43
3:I:363:LEU:O	3:I:486:SER:OG	2.25	0.43
3:I:746:LEU:HD22	3:I:746:LEU:N	2.34	0.43
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	1.99	0.43
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.54	0.42
2:C:73:TYR:O	2:C:74:ARG:HB2	2.18	0.42
2:C:138:ILE:O	2:C:141:THR:OG1	2.34	0.42
2:C:177:ILE:N	2:C:177:ILE:HD12	2.35	0.42
2:C:185:ASP:HB2	2:C:197:ARG:HB2	2.00	0.42
3:D:12:THR:C	3:D:13:LYS:HD2	2.44	0.42
3:D:26:SER:O	3:D:30:ILE:HG12	2.19	0.42
3:D:42:GLU:HG3	5:X:451:ARG:HH21	1.84	0.42
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.48	0.42
3:D:246:PRO:HB2	3:D:249:LEU:HD13	2.01	0.42
3:D:325:LYS:HE2	3:D:325:LYS:HB3	1.90	0.42
3:D:771:GLN:HE21	3:D:772:TYR:N	2.17	0.42
3:D:843:VAL:HG12	3:D:883:ARG:HD3	2.00	0.42
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.83	0.42
5:X:117:ILE:HG13	5:X:421:TYR:HB2	2.01	0.42
5:X:484:ALA:HB1	5:X:490:PRO:O	2.17	0.42
5:X:532:LEU:O	5:X:536:THR:HG23	2.19	0.42
1:F:45:ARG:NE	1:G:38:THR:OG1	2.49	0.42
2:H:106:GLU:CB	2:H:107:ARG:CA	2.96	0.42
2:H:820:GLU:O	2:H:824:GLN:HG3	2.19	0.42
2:H:999:GLU:HG2	2:H:1000:LEU:N	2.34	0.42
3:I:51:PRO:HB3	3:I:57:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:161:THR:H	3:I:164:GLN:CD	2.27	0.42
3:I:524:GLY:HA2	3:I:548:VAL:HG23	2.01	0.42
3:I:586:GLY:O	3:I:587:LEU:HB2	2.19	0.42
3:I:661:VAL:O	3:I:665:GLN:HG3	2.19	0.42
3:I:697:MET:HE1	3:I:738:ARG:HA	2.01	0.42
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.34	0.42
1:A:91:ARG:NH2	1:A:209:GLY:O	2.52	0.42
1:B:57:THR:HG21	1:B:177:TYR:OH	2.19	0.42
2:C:345:PRO:O	2:C:349:GLU:HG2	2.19	0.42
2:C:524:ILE:HD11	2:C:712:SER:HB2	2.00	0.42
2:C:727:VAL:CG2	2:C:773:LEU:HB3	2.44	0.42
2:C:745:GLU:HA	2:C:1017:GLN:OE1	2.19	0.42
2:C:805:MET:HE1	2:C:1221:PHE:CE1	2.54	0.42
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.33	0.42
2:C:1335:ILE:CD1	3:D:22:ILE:HD11	2.47	0.42
3:D:595:ALA:HB1	3:D:596:LEU:HD23	2.01	0.42
5:X:48:ILE:HG13	5:X:49:ASN:H	1.84	0.42
1:F:54:CYS:SG	1:F:148:ARG:HD3	2.58	0.42
1:G:82:LEU:O	1:G:86:LYS:HG3	2.19	0.42
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.43	0.42
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.18	0.42
2:H:429:MET:O	2:H:433:ILE:HG13	2.19	0.42
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	2.01	0.42
1:A:22:THR:HB	1:A:207:THR:O	2.19	0.42
2:C:42:ASP:HB3	2:C:43:PRO:CD	2.28	0.42
2:C:462:ASN:O	2:C:466:VAL:HG23	2.20	0.42
2:C:557:ARG:HH12	2:C:611:GLU:CD	2.24	0.42
2:C:850:ILE:HG23	2:C:885:GLY:O	2.20	0.42
2:C:948:ILE:O	2:C:952:GLN:HG3	2.19	0.42
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.53	0.42
3:D:22:ILE:HG12	3:D:1336:ALA:HA	2.02	0.42
3:D:66:LYS:HB2	3:D:69:GLU:HG2	2.00	0.42
3:D:355:ILE:HA	3:D:447:ILE:O	2.19	0.42
3:D:701:LEU:HD21	3:D:723:TYR:HB2	2.02	0.42
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.47	0.42
5:X:276:MET:O	5:X:280:VAL:HG23	2.20	0.42
1:G:153:VAL:HA	1:G:154:PRO:HD3	1.85	0.42
2:H:99:LYS:HD3	2:H:99:LYS:H	1.80	0.42
2:H:977:ALA:O	2:H:980:VAL:HG12	2.19	0.42
2:H:1270:PHE:HB3	2:H:1271:GLY:H	1.58	0.42
2:H:1339:LEU:HD12	2:H:1339:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:252:LEU:HG	3:I:252:LEU:O	2.20	0.42
3:I:326:SER:O	3:I:330:MET:HG3	2.18	0.42
3:I:613:GLY:O	3:I:617:THR:OG1	2.30	0.42
3:I:1140:ARG:HH21	3:I:1236:GLU:CG	2.32	0.42
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.32	0.42
1:B:179:PRO:HB2	1:B:211:ILE:HG22	2.00	0.42
2:C:660:VAL:C	2:C:661:VAL:HG13	2.44	0.42
3:D:161:THR:HG22	3:D:162:GLU:N	2.34	0.42
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.48	0.42
3:D:295:GLU:OE1	5:X:406:GLN:HG2	2.19	0.42
3:D:678:ARG:O	3:D:681:LYS:HG3	2.20	0.42
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.48	0.42
1:F:44:ARG:HG3	1:F:183:ILE:CG2	2.49	0.42
1:G:181:GLU:HB2	1:G:206:GLU:O	2.19	0.42
2:H:138:ILE:O	2:H:141:THR:OG1	2.30	0.42
2:H:576:SER:HB3	2:H:579:ALA:HB2	2.02	0.42
2:H:705:GLU:H	2:H:705:GLU:CD	2.27	0.42
2:H:1045:GLY:O	2:H:1046:VAL:HB	2.18	0.42
3:I:155:GLU:CD	3:I:155:GLU:H	2.24	0.42
3:I:412:LEU:O	3:I:416:ILE:HD12	2.19	0.42
3:I:771:GLN:HE21	3:I:772:TYR:N	2.17	0.42
3:I:856:ILE:HD12	3:I:857:LEU:N	2.35	0.42
3:I:1247:LYS:H	3:I:1247:LYS:CD	2.20	0.42
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.44	0.42
2:C:53:PHE:HD1	2:C:57:PHE:CD2	2.36	0.42
2:C:1043:ALA:C	2:C:1045:GLY:H	2.27	0.42
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.83	0.42
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.50	0.42
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.19	0.42
3:D:306:LEU:C	3:D:306:LEU:HD23	2.43	0.42
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.18	0.42
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	2.02	0.42
1:F:102:LEU:HB3	1:F:142:MET:HG2	2.02	0.42
2:H:310:ILE:HG21	2:H:324:LYS:HB2	2.01	0.42
2:H:948:ILE:O	2:H:952:GLN:HG3	2.19	0.42
2:H:1259:LEU:HD12	2:H:1259:LEU:O	2.19	0.42
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.33	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.34	0.42
2:C:603:ILE:HD12	2:C:603:ILE:O	2.19	0.42
2:C:1027:LYS:HB2	2:C:1027:LYS:NZ	2.35	0.42
3:D:79:LYS:HE3	5:X:569:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.99	0.42
3:D:521:LYS:HB2	3:D:542:ALA:HB2	2.00	0.42
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.50	0.42
3:D:607:THR:O	3:D:611:ILE:HG12	2.19	0.42
4:E:5:THR:HB	4:E:7:GLN:H	1.84	0.42
1:F:28:LEU:HD13	1:G:231:PHE:CE2	2.55	0.42
1:F:41:ASN:CG	2:H:1218:GLY:HA3	2.44	0.42
2:H:105:TYR:HA	2:H:106:GLU:HA	1.89	0.42
2:H:153:PRO:HD2	2:H:452:ARG:HD3	2.01	0.42
2:H:1192:GLU:O	2:H:1196:LYS:HD3	2.20	0.42
2:H:1273:MET:HB3	3:I:428:THR:HB	2.00	0.42
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.49	0.42
3:I:1216:ALA:HB3	3:I:1219:ASP:OD1	2.20	0.42
3:I:1234:VAL:HA	3:I:1253:ILE:HG21	2.02	0.42
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.20	0.42
1:B:213:PRO:HA	1:B:216:ALA:HB3	2.01	0.42
2:C:57:PHE:HE1	2:C:472:GLU:HA	1.84	0.42
2:C:384:LEU:O	2:C:388:LEU:HG	2.20	0.42
2:C:490:GLN:O	5:X:472:GLN:HG3	2.20	0.42
3:D:130:MET:HA	3:D:131:PRO:HD3	1.95	0.42
3:D:147:ILE:HG13	3:D:148:GLU:N	2.34	0.42
3:D:252:LEU:HA	3:D:261:ALA:O	2.19	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.55	0.42
3:D:1141:VAL:HG22	3:D:1240:VAL:HG21	2.01	0.42
3:D:1171:GLY:HA3	3:D:1172:LYS:C	2.44	0.42
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.19	0.42
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.34	0.42
4:E:5:THR:HB	4:E:7:GLN:N	2.35	0.42
5:X:528:LEU:C	5:X:528:LEU:HD12	2.44	0.42
5:X:560:ARG:HG2	5:X:565:ILE:HG23	2.01	0.42
2:H:24:VAL:HG11	2:H:704:MET:HE1	2.01	0.42
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.37	0.42
2:H:148:GLN:HB2	2:H:511:LEU:HD21	2.02	0.42
2:H:177:ILE:N	2:H:177:ILE:HD12	2.34	0.42
2:H:475:VAL:O	2:H:479:LEU:HB2	2.19	0.42
2:H:768:MET:O	2:H:785:ASP:N	2.46	0.42
2:H:850:ILE:HG23	2:H:885:GLY:O	2.19	0.42
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.85	0.42
6:H:1401:1RM:O2	6:H:1401:1RM:O1	2.37	0.42
3:I:120:LEU:N	3:I:120:LEU:HD12	2.35	0.42
3:I:269:TYR:HA	3:I:272:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:513:MET:HE2	3:I:513:MET:HB3	1.97	0.42
3:I:844:THR:CG2	3:I:848:VAL:HG23	2.50	0.42
3:I:1140:ARG:HH21	3:I:1236:GLU:HG2	1.85	0.42
5:Y:148:TYR:OH	5:Y:218:ARG:HG2	2.20	0.42
5:Y:540:LEU:HD13	5:Y:607:LEU:HD22	2.01	0.42
1:A:74:VAL:HG12	1:A:76:GLU:O	2.20	0.42
1:B:19:VAL:O	1:B:19:VAL:HG12	2.20	0.42
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.34	0.42
2:C:106:GLU:CB	2:C:107:ARG:HA	2.49	0.42
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.01	0.42
2:C:531:SER:OG	6:C:1401:1RM:O2	2.19	0.42
2:C:812:PHE:HB2	3:D:357:VAL:HG21	2.02	0.42
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.33	0.42
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	2.01	0.42
5:X:227:GLN:O	5:X:230:VAL:HG12	2.20	0.42
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.85	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
2:H:993:PRO:HB2	2:H:994:ARG:H	1.60	0.42
2:H:1108:ASN:ND2	2:H:1108:ASN:O	2.50	0.42
3:I:1171:GLY:HA3	3:I:1172:LYS:C	2.44	0.42
3:I:1230:THR:O	3:I:1234:VAL:HG12	2.20	0.42
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.26	0.42
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.34	0.42
2:C:92:TYR:CE1	2:C:129:LEU:HB2	2.55	0.42
2:C:342:ASP:O	2:C:437:ASN:ND2	2.53	0.42
2:C:538:LEU:HD12	2:C:538:LEU:N	2.35	0.42
2:C:958:LYS:O	2:C:962:GLU:HG2	2.20	0.42
3:D:33:TRP:O	3:D:102:MET:HB2	2.19	0.42
3:D:167:ASP:O	3:D:171:GLU:HG2	2.20	0.42
3:D:185:ILE:HD12	3:D:185:ILE:HA	1.92	0.42
3:D:286:ALA:C	3:D:288:PRO:HD3	2.44	0.42
3:D:681:LYS:O	3:D:685:ILE:HG13	2.19	0.42
3:D:841:GLY:HA3	3:D:901:ARG:HD3	2.02	0.42
1:G:33:ARG:NE	1:G:197:ASP:HB2	2.33	0.42
2:H:704:MET:HE2	2:H:707:ALA:HB3	2.01	0.42
3:I:911:LYS:HD2	3:I:911:LYS:O	2.20	0.42
5:Y:553:ALA:C	5:Y:555:GLU:H	2.27	0.42
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.53	0.42
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.50	0.42
2:C:59:ILE:HD11	2:C:63:SER:OG	2.20	0.42
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:SER:OG	3:D:132:LEU:HD13	2.19	0.42
2:H:37:LYS:HA	2:H:37:LYS:HE3	2.01	0.42
2:H:133:ASN:O	2:H:527:LYS:NZ	2.43	0.42
2:H:241:LEU:HD22	2:H:285:ILE:HD13	2.02	0.42
2:H:333:ILE:N	2:H:333:ILE:HD12	2.35	0.42
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.42
2:H:1054:LEU:O	2:H:1054:LEU:HD12	2.20	0.42
2:H:1120:ALA:HB2	2:H:1199:LEU:HD23	2.02	0.42
2:H:1259:LEU:HD12	2:H:1259:LEU:C	2.45	0.42
3:I:1234:VAL:HG13	3:I:1235:ASN:N	2.35	0.42
1:A:102:LEU:HD23	1:A:102:LEU:C	2.45	0.41
1:A:110:VAL:HB	1:A:131:CYS:HB2	2.01	0.41
1:A:303:ILE:O	1:A:307:LEU:HD13	2.20	0.41
2:C:60:GLN:O	2:C:61:SER:OG	2.33	0.41
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.49	0.41
2:C:210:LEU:O	2:C:215:TYR:HB2	2.19	0.41
2:C:1002:LEU:HD13	2:C:1003:THR:H	1.85	0.41
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.02	0.41
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	2.02	0.41
3:D:288:PRO:O	3:D:292:VAL:HG12	2.20	0.41
3:D:356:THR:O	3:D:448:GLN:HA	2.19	0.41
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.20	0.41
4:E:19:LEU:HD13	4:E:19:LEU:C	2.45	0.41
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.52	0.41
2:H:1027:LYS:HB2	2:H:1027:LYS:NZ	2.35	0.41
2:H:1117:LEU:HD11	2:H:1182:ILE:HD13	2.01	0.41
3:I:41:PRO:HB3	3:I:270:ARG:HG3	2.01	0.41
3:I:709:ARG:HD2	3:I:714:GLU:HB2	2.02	0.41
3:I:909:ILE:H	3:I:909:ILE:HG13	1.55	0.41
5:Y:99:ARG:O	5:Y:99:ARG:HD3	2.20	0.41
1:A:104:LYS:HD2	1:A:110:VAL:HG22	2.01	0.41
1:A:302:GLU:O	1:A:306:VAL:HG22	2.19	0.41
1:B:51:MET:HA	1:B:52:PRO:HD3	1.86	0.41
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.35	0.41
2:C:812:PHE:N	2:C:815:SER:HB2	2.35	0.41
3:D:159:ILE:N	3:D:159:ILE:HD12	2.35	0.41
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.02	0.41
3:D:846:GLU:O	3:D:847:ASP:C	2.63	0.41
5:X:147:GLN:O	5:X:151:VAL:HG23	2.20	0.41
1:F:22:THR:HB	1:F:207:THR:O	2.21	0.41
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:506:VAL:HG23	3:I:628:GLY:HA3	2.01	0.41
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.92	0.41
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.41
1:A:234:LEU:N	1:A:234:LEU:HD12	2.35	0.41
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.41
2:C:17:LYS:N	2:C:17:LYS:HD2	2.35	0.41
2:C:622:ASN:OD1	2:C:623:LEU:N	2.53	0.41
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.50	0.41
2:C:823:VAL:HG22	2:C:1060:ILE:HG13	2.01	0.41
2:C:868:SER:OG	2:C:942:ASP:OD1	2.25	0.41
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.20	0.41
2:C:1287:LEU:O	2:C:1291:LEU:HB2	2.20	0.41
3:D:522:GLY:O	3:D:523:GLU:HG2	2.21	0.41
3:D:644:MET:O	3:D:764:ARG:NH1	2.52	0.41
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.19	0.41
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.55	0.41
2:H:338:THR:OG1	2:H:345:PRO:HG3	2.21	0.41
3:I:311:ARG:HH21	3:I:1329:THR:HG21	1.85	0.41
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.50	0.41
3:I:1161:GLY:HA2	3:I:1181:ASP:HB2	2.02	0.41
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.20	0.41
5:Y:400:GLN:H	5:Y:400:GLN:CD	2.28	0.41
5:Y:437:GLN:HA	5:Y:440:THR:HG22	2.01	0.41
5:Y:528:LEU:HD12	5:Y:528:LEU:O	2.21	0.41
2:C:96:LEU:HD22	2:C:127:ILE:HD12	2.03	0.41
2:C:971:LEU:C	2:C:971:LEU:HD13	2.45	0.41
3:D:118:LYS:HZ2	5:X:42:GLU:CD	2.28	0.41
3:D:502:PRO:HB3	3:D:506:VAL:HG11	2.03	0.41
3:D:646:ILE:H	3:D:646:ILE:HG13	1.64	0.41
3:D:660:GLU:O	3:D:664:ILE:HG12	2.20	0.41
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.20	0.41
3:D:1290:ARG:HD2	3:D:1299:GLY:HA3	2.02	0.41
4:E:18:ASP:O	4:E:22:VAL:HG12	2.20	0.41
5:X:532:LEU:C	5:X:532:LEU:HD13	2.45	0.41
2:H:58:PRO:O	2:H:476:LYS:HE3	2.21	0.41
2:H:92:TYR:HE1	2:H:129:LEU:HD12	1.85	0.41
2:H:130:MET:CG	2:H:134:GLY:HA2	2.50	0.41
2:H:734:ILE:O	2:H:749:ASP:N	2.53	0.41
2:H:866:ASP:HA	2:H:872:TYR:CZ	2.56	0.41
3:I:147:ILE:HG13	3:I:148:GLU:N	2.34	0.41
3:I:355:ILE:HG12	3:I:464:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:605:LEU:O	3:I:605:LEU:HD13	2.20	0.41
3:I:706:VAL:C	3:I:707:ILE:HG13	2.46	0.41
3:I:735:ALA:O	3:I:739:GLN:HG3	2.20	0.41
3:I:1171:GLY:CA	3:I:1172:LYS:C	2.94	0.41
4:J:26:ARG:HD3	4:J:64:LEU:HD21	2.01	0.41
5:Y:492:ASP:HA	5:Y:495:ARG:HG3	2.01	0.41
2:C:397:LEU:O	2:C:398:SER:OG	2.31	0.41
2:C:406:ASN:HB3	2:C:411:ARG:HB2	2.01	0.41
2:C:1004:ASP:OD1	2:C:1004:ASP:N	2.54	0.41
2:C:1196:LYS:HG3	2:C:1206:THR:OG1	2.20	0.41
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.80	0.41
3:D:252:LEU:HG	3:D:252:LEU:O	2.20	0.41
3:D:442:ILE:HD12	3:D:448:GLN:CD	2.46	0.41
5:X:528:LEU:HD12	5:X:528:LEU:O	2.18	0.41
2:H:705:GLU:HG2	2:H:793:GLU:HG3	2.02	0.41
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.20	0.41
2:H:944:ARG:HD3	2:H:944:ARG:O	2.21	0.41
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	2.02	0.41
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.50	0.41
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.21	0.41
2:C:80:PHE:O	2:C:84:GLU:HB3	2.19	0.41
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.85	0.41
2:C:1258:PRO:HG2	3:D:346:ARG:CB	2.50	0.41
2:C:1272:GLU:HG3	2:C:1276:TRP:CZ2	2.56	0.41
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.68	0.41
3:D:77:ARG:CG	3:D:78:LEU:H	2.33	0.41
3:D:205:LEU:HB3	3:D:217:LEU:HB3	2.02	0.41
3:D:423:LEU:HB3	3:D:466:MET:HE2	2.03	0.41
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.91	0.41
3:D:501:VAL:HA	3:D:502:PRO:HD3	1.97	0.41
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.03	0.41
3:D:918:ILE:HD13	3:D:919:ALA:N	2.36	0.41
5:X:262:VAL:HG12	5:X:264:LYS:H	1.85	0.41
5:X:456:MET:O	5:X:460:ILE:HG13	2.20	0.41
5:X:514:ASP:HB3	5:X:515:GLU:H	1.65	0.41
2:H:120:GLN:HG3	2:H:121:GLU:N	2.36	0.41
2:H:157:PHE:HD2	2:H:174:ALA:HB2	1.85	0.41
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.55	0.41
2:H:1111:GLN:HE21	2:H:1230:MET:HE1	1.84	0.41
3:I:128:LEU:HA	3:I:192:MET:HE1	2.03	0.41
3:I:271:ARG:NH1	3:I:317:THR:HG21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.54	0.41
3:I:368:LEU:HG	3:I:373:ALA:HB2	2.02	0.41
3:I:591:ILE:HD12	3:I:592:VAL:HG13	2.02	0.41
3:I:1297:LYS:HA	3:I:1297:LYS:CE	2.50	0.41
5:Y:562:ARG:HG3	5:Y:591:GLU:OE1	2.19	0.41
2:C:977:ALA:O	2:C:980:VAL:HG12	2.20	0.41
3:D:19:ALA:HB2	3:D:1343:GLU:CB	2.48	0.41
3:D:66:LYS:NZ	3:D:66:LYS:HB3	2.36	0.41
3:D:126:LEU:HD21	3:D:223:LEU:CD1	2.50	0.41
3:D:412:LEU:O	3:D:415:VAL:HG22	2.21	0.41
3:D:473:THR:HB	3:D:476:ALA:HB2	2.01	0.41
3:D:586:GLY:O	3:D:587:LEU:HB2	2.20	0.41
5:X:23:THR:HG22	5:X:26:GLU:HG2	2.03	0.41
2:H:161:LYS:NZ	2:H:161:LYS:HB3	2.36	0.41
2:H:488:MET:HB2	2:H:489:PRO:HA	2.02	0.41
2:H:773:LEU:CD1	2:H:773:LEU:H	2.32	0.41
2:H:886:LYS:HD3	2:H:916:SER:O	2.20	0.41
3:I:179:LYS:HD3	3:I:179:LYS:N	2.36	0.41
3:I:210:SER:O	3:I:214:ARG:HG3	2.21	0.41
3:I:306:LEU:C	3:I:306:LEU:HD23	2.45	0.41
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.31	0.41
3:I:492:SER:HA	3:I:493:PRO:HD3	1.95	0.41
3:I:579:LEU:O	3:I:579:LEU:HD13	2.19	0.41
3:I:905:ARG:HG2	3:I:907:HIS:H	1.85	0.41
4:J:26:ARG:HB2	4:J:64:LEU:HD11	2.01	0.41
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.85	0.41
5:Y:276:MET:O	5:Y:280:VAL:HG23	2.21	0.41
5:Y:587:ILE:HD12	5:Y:587:ILE:HA	1.95	0.41
1:A:207:THR:HG23	1:A:209:GLY:H	1.85	0.41
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.02	0.41
2:C:658:GLN:HB3	2:C:1186:VAL:HG11	2.02	0.41
2:C:758:ARG:NH1	2:C:762:ASN:OD1	2.54	0.41
3:D:62:PHE:O	3:D:101:ARG:HG3	2.20	0.41
3:D:84:ILE:H	3:D:84:ILE:HG13	1.78	0.41
3:D:490:ILE:HG23	3:D:500:ILE:HD11	2.03	0.41
3:D:527:LEU:H	3:D:550:VAL:HG12	1.85	0.41
3:D:905:ARG:HH12	4:E:10:VAL:CG1	2.32	0.41
5:X:290:LEU:O	5:X:294:GLN:HB3	2.21	0.41
5:X:453:PRO:HB2	5:X:455:HIS:CE1	2.55	0.41
1:F:11:PRO:HD2	1:G:227:GLN:HA	2.02	0.41
1:F:31:LEU:HB2	1:F:199:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:GLU:OE2	2:H:203:LYS:HD3	2.20	0.41
2:H:699:LEU:HB2	2:H:799:ASN:ND2	2.36	0.41
2:H:843:THR:HG22	2:H:844:LYS:N	2.36	0.41
2:H:1043:ALA:C	2:H:1045:GLY:H	2.29	0.41
3:I:526:VAL:CG1	3:I:549:LYS:HB2	2.47	0.41
3:I:532:GLU:OE2	3:I:574:VAL:HG13	2.19	0.41
3:I:1368:ASP:O	3:I:1372:ARG:HB2	2.20	0.41
4:J:26:ARG:NE	4:J:30:MET:HE3	2.35	0.41
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.81	0.41
2:C:22:LEU:HD13	2:C:23:ASP:O	2.21	0.41
2:C:548:ARG:O	3:D:780:ARG:NH1	2.54	0.41
2:C:800:MET:HA	2:C:800:MET:HE3	2.02	0.41
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.21	0.41
2:C:817:LEU:HD21	2:C:1080:ASN:HB2	2.03	0.41
2:C:966:ILE:HG23	2:C:967:LEU:HD12	2.03	0.41
2:C:1211:ARG:HB2	2:C:1220:GLN:HE21	1.85	0.41
2:C:1225:VAL:HG12	3:D:636:GLY:O	2.21	0.41
2:C:1333:LEU:HB2	2:C:1335:ILE:HG22	2.03	0.41
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	2.03	0.41
3:D:215:LYS:O	3:D:219:LYS:HG3	2.21	0.41
3:D:789:LYS:HD2	3:D:932:MET:SD	2.61	0.41
3:D:886:VAL:HG13	3:D:1230:THR:HG21	2.02	0.41
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.84	0.41
5:X:469:GLN:HE21	5:X:473:GLU:HG3	1.85	0.41
5:X:572:THR:O	5:X:576:VAL:HG23	2.21	0.41
1:G:222:THR:O	1:G:226:GLU:HG2	2.21	0.41
2:H:10:ARG:CZ	2:H:1171:ARG:HH21	2.33	0.41
2:H:138:ILE:HB	2:H:143:ARG:HD2	2.03	0.41
2:H:157:PHE:CD2	2:H:174:ALA:HB2	2.56	0.41
2:H:603:ILE:HD12	2:H:603:ILE:O	2.21	0.41
2:H:707:ALA:O	2:H:710:VAL:HG12	2.21	0.41
2:H:1101:LEU:O	2:H:1104:PRO:HD2	2.21	0.41
2:H:1264:GLN:HE21	2:H:1264:GLN:HB3	1.72	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.51	0.41
3:I:40:LYS:HE3	3:I:42:GLU:HG3	2.02	0.41
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.85	0.41
3:I:230:SER:CB	3:I:1339:GLY:H	2.28	0.41
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.85	0.41
3:I:286:ALA:C	3:I:288:PRO:HD3	2.45	0.41
3:I:421:VAL:HB	3:I:439:PRO:HG3	2.03	0.41
3:I:501:VAL:HG21	3:I:602:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:587:LEU:HD12	3:I:611:ILE:HD11	2.03	0.41
3:I:611:ILE:HG13	3:I:612:LEU:CD2	2.51	0.41
3:I:620:PHE:O	3:I:624:ILE:HG23	2.20	0.41
3:I:846:GLU:O	3:I:847:ASP:C	2.64	0.41
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.56	0.41
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	2.02	0.41
3:I:1247:LYS:HD3	3:I:1247:LYS:N	2.25	0.41
4:J:19:LEU:HD13	4:J:19:LEU:C	2.46	0.41
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.21	0.41
2:C:148:GLN:HB2	2:C:511:LEU:HD21	2.03	0.41
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.21	0.41
2:C:555:TYR:OH	2:C:637:ARG:NH2	2.54	0.41
2:C:697:LYS:HG3	2:C:698:PRO:HD2	2.03	0.41
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.51	0.41
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.51	0.41
3:D:1266:ILE:HG13	3:D:1274:PHE:O	2.20	0.41
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.38	0.41
5:X:119:ILE:CD1	5:X:122:ARG:HH21	2.34	0.41
5:X:312:SER:OG	5:X:314:THR:HG23	2.21	0.41
1:G:200:LYS:HG3	1:G:200:LYS:O	2.21	0.41
2:H:1010:GLN:HE21	2:H:1010:GLN:HB2	1.66	0.41
3:I:41:PRO:HG3	3:I:273:ILE:HG22	2.03	0.41
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.52	0.40
2:C:632:ASP:O	2:C:633:LEU:HD23	2.22	0.40
2:C:732:ILE:HD11	2:C:769:PRO:CB	2.50	0.40
2:C:1105:SER:HB2	3:D:731:ARG:HB2	2.03	0.40
2:C:1133:LYS:O	2:C:1134:GLN:HB2	2.22	0.40
2:C:1259:LEU:HD12	2:C:1259:LEU:C	2.45	0.40
2:C:1289:GLU:HB3	2:C:1315:MET:HE2	2.03	0.40
3:D:147:ILE:HD12	3:D:178:ALA:HB2	2.03	0.40
3:D:378:LYS:HD2	3:D:382:TYR:OH	2.20	0.40
3:D:555:TYR:HD1	3:D:589:TYR:HE2	1.70	0.40
3:D:558:ASP:OD1	3:D:559:ALA:N	2.53	0.40
5:X:541:ARG:O	5:X:545:HIS:HB2	2.22	0.40
1:F:45:ARG:NH2	1:G:37:HIS:HB3	2.37	0.40
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.03	0.40
2:H:54:ARG:HG2	2:H:55:SER:OG	2.21	0.40
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.02	0.40
3:I:438:GLU:HA	3:I:439:PRO:HD3	1.88	0.40
3:I:522:GLY:O	3:I:523:GLU:HG2	2.21	0.40
3:I:545:HIS:HA	3:I:546:ALA:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.42	0.40
5:Y:138:PRO:CG	5:Y:353:LEU:HD21	2.49	0.40
5:Y:418:LYS:O	5:Y:430:TYR:OH	2.33	0.40
2:C:542:ARG:HG2	2:C:543:ALA:N	2.35	0.40
2:C:994:ARG:HD3	2:C:994:ARG:N	2.36	0.40
3:D:292:VAL:O	3:D:296:LYS:HG3	2.22	0.40
3:D:374:LEU:HD22	3:D:381:ILE:CD1	2.51	0.40
3:D:1347:LEU:HD22	3:D:1357:ILE:HG23	2.03	0.40
5:X:112:THR:HG22	5:X:113:ARG:N	2.31	0.40
5:X:251:LYS:O	5:X:255:VAL:HG23	2.21	0.40
5:X:504:PRO:HB2	5:X:505:ILE:H	1.63	0.40
2:H:936:ARG:HH11	5:Y:495:ARG:HH11	1.68	0.40
2:H:1103:VAL:H	2:H:1104:PRO:HD2	1.84	0.40
3:I:109:SER:HA	3:I:110:PRO:HD3	1.98	0.40
3:I:205:LEU:HD13	3:I:217:LEU:CD2	2.50	0.40
3:I:227:PHE:O	3:I:230:SER:OG	2.23	0.40
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.52	0.40
3:I:387:LEU:HD23	3:I:387:LEU:C	2.45	0.40
3:I:704:GLU:HB3	3:I:705:THR:H	1.71	0.40
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.50	0.40
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.21	0.40
1:A:187:VAL:O	1:A:188:GLU:HB2	2.21	0.40
1:B:228:LEU:C	1:B:228:LEU:HD12	2.47	0.40
2:C:119:GLU:OE2	2:C:489:PRO:HB2	2.21	0.40
2:C:400:VAL:O	2:C:404:LYS:HE2	2.20	0.40
2:C:690:VAL:HG11	2:C:830:THR:HG21	2.04	0.40
2:C:818:VAL:HA	2:C:1096:ILE:HG22	2.03	0.40
2:C:1203:ASP:O	2:C:1204:LEU:HG	2.21	0.40
3:D:582:ILE:HG22	3:D:620:PHE:CE1	2.56	0.40
3:D:610:ARG:HG3	3:D:864:LEU:CD1	2.34	0.40
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	2.03	0.40
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.52	0.40
3:D:1329:THR:O	3:D:1333:THR:OG1	2.32	0.40
5:X:16:GLY:C	5:X:18:GLU:HA	2.47	0.40
5:X:145:LEU:HD13	5:X:145:LEU:C	2.46	0.40
5:X:240:ARG:HD3	5:X:244:THR:CB	2.45	0.40
1:F:28:LEU:HD13	1:G:231:PHE:HE2	1.86	0.40
1:G:188:GLU:O	1:G:200:LYS:HG2	2.22	0.40
2:H:685:MET:HE1	2:H:1073:LYS:HE2	2.03	0.40
2:H:1276:TRP:CE3	3:I:801:VAL:HG11	2.57	0.40
3:I:842:ARG:HB3	3:I:882:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:SER:OG	1:A:314:LEU:N	2.54	0.40
1:B:48:LEU:HD22	3:D:534:GLU:HG3	2.04	0.40
2:C:54:ARG:N	2:C:55:SER:CB	2.77	0.40
2:C:500:ALA:O	2:C:504:GLU:HB2	2.20	0.40
2:C:525:THR:O	2:C:529:ARG:NH1	2.54	0.40
2:C:820:GLU:HB2	2:C:1081:PRO:HA	2.04	0.40
2:C:1185:PRO:HB2	2:C:1186:VAL:H	1.67	0.40
3:D:97:VAL:HG13	3:D:101:ARG:CZ	2.51	0.40
3:D:370:LYS:HG3	3:D:371:LYS:H	1.85	0.40
3:D:479:GLU:O	3:D:483:LEU:HB2	2.22	0.40
3:D:545:HIS:HA	3:D:546:ALA:HA	1.79	0.40
3:D:901:ARG:CB	3:D:908:ILE:HA	2.52	0.40
3:D:1190:ILE:N	3:D:1190:ILE:HD12	2.37	0.40
5:X:11:LEU:HB3	5:X:15:ARG:NH1	2.36	0.40
5:X:28:ASN:HD22	5:X:28:ASN:C	2.29	0.40
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.55	0.40
1:G:90:VAL:HG13	1:G:121:VAL:HG13	2.02	0.40
2:H:131:THR:HG22	2:H:135:THR:H	1.86	0.40
2:H:479:LEU:HD22	2:H:492:MET:HE1	2.04	0.40
3:I:27:PRO:HD3	3:I:236:TRP:CE3	2.57	0.40
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.48	0.40
3:I:1297:LYS:NZ	3:I:1297:LYS:CA	2.81	0.40
5:Y:283:GLN:O	5:Y:287:ILE:HG13	2.22	0.40
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.56	0.40
1:B:178:SER:HA	1:B:179:PRO:HD3	1.91	0.40
2:C:161:LYS:HB3	2:C:161:LYS:NZ	2.36	0.40
2:C:539:THR:HB	2:C:540:ARG:H	1.65	0.40
2:C:643:SER:C	2:C:644:LEU:HD12	2.47	0.40
2:C:931:VAL:HG21	2:C:944:ARG:CZ	2.52	0.40
2:C:1054:LEU:HD12	2:C:1054:LEU:O	2.21	0.40
2:C:1164:PHE:HB3	2:C:1168:GLU:HG2	2.04	0.40
3:D:52:GLU:OE1	5:X:451:ARG:HD2	2.21	0.40
3:D:292:VAL:HG13	3:D:293:ARG:N	2.36	0.40
3:D:387:LEU:C	3:D:387:LEU:HD23	2.47	0.40
3:D:514:THR:HG23	3:D:576:ARG:HE	1.87	0.40
3:D:663:GLU:O	3:D:667:GLN:HG3	2.22	0.40
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.43	0.40
3:D:1167:LYS:HB3	3:D:1170:LYS:HB2	2.03	0.40
3:D:1170:LYS:O	3:D:1173:ARG:HD2	2.21	0.40
1:F:44:ARG:HA	1:F:183:ILE:HG21	2.03	0.40
1:F:181:GLU:OE1	1:F:181:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:468:LEU:HD12	2:H:468:LEU:HA	1.96	0.40
2:H:740:GLU:CD	2:H:740:GLU:H	2.28	0.40
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.36	0.40
3:I:1163:VAL:HG21	3:I:1198:VAL:HG11	2.03	0.40
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	2.03	0.40
3:I:1278:GLU:HG3	3:I:1279:GLN:H	1.86	0.40
3:I:1307:LEU:HD23	3:I:1307:LEU:H	1.86	0.40
5:Y:528:LEU:HD12	5:Y:528:LEU:C	2.46	0.40
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.20	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	321/329 (98%)	266 (83%)	40 (12%)	15 (5%)	2	17
1	B	217/329 (66%)	187 (86%)	22 (10%)	8 (4%)	2	21
1	F	227/329 (69%)	196 (86%)	25 (11%)	6 (3%)	4	26
1	G	213/329 (65%)	187 (88%)	22 (10%)	4 (2%)	6	32
2	C	1333/1342 (99%)	1069 (80%)	216 (16%)	48 (4%)	2	22
2	H	1333/1342 (99%)	1069 (80%)	215 (16%)	49 (4%)	2	21
3	D	1154/1407 (82%)	918 (80%)	194 (17%)	42 (4%)	2	22
3	I	1154/1407 (82%)	920 (80%)	192 (17%)	42 (4%)	2	22
4	E	88/91 (97%)	78 (89%)	5 (6%)	5 (6%)	1	15
4	J	74/91 (81%)	65 (88%)	4 (5%)	5 (7%)	1	12
5	X	511/613 (83%)	449 (88%)	49 (10%)	13 (2%)	4	27
5	Y	454/613 (74%)	410 (90%)	34 (8%)	10 (2%)	5	29
All	All	7079/8222 (86%)	5814 (82%)	1018 (14%)	247 (4%)	3	23

All (247) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	319	GLU
1	B	20	SER
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO
2	C	686	GLN
2	C	748	ILE
2	C	753	LEU
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	406	ALA
3	D	595	ALA
3	D	708	ASN
3	D	847	ASP
3	D	1268	ASN
3	D	1339	GLY
4	E	6	VAL
4	E	35	LYS
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
2	H	21	VAL
2	H	39	ILE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO

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Mol	Chain	Res	Type
2	H	1341	ASP
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	406	ALA
3	I	595	ALA
3	I	710	ASP
3	I	851	PRO
3	I	1339	GLY
4	J	6	VAL
4	J	35	LYS
5	Y	241	SER
1	A	193	GLU
1	B	19	VAL
1	B	188	GLU
2	C	53	PHE
2	C	79	VAL
2	C	437	ASN
2	C	699	LEU
2	C	1236	ASN
2	C	1239	VAL
2	C	1256	GLN
2	C	1341	ASP
3	D	89	GLY
3	D	155	GLU
3	D	255	LEU
3	D	316	ILE
3	D	404	GLU
3	D	417	ARG
3	D	542	ALA
3	D	590	SER
3	D	710	ASP
3	D	721	SER
3	D	851	PRO
3	D	901	ARG
3	D	913	GLU
3	D	914	ALA
5	X	23	THR
5	X	581	ASP
1	F	188	GLU
1	G	188	GLU
2	H	53	PHE

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Mol	Chain	Res	Type
2	H	78	PRO
2	H	170	VAL
2	H	535	PRO
2	H	669	PRO
2	H	753	LEU
2	H	1186	VAL
2	H	1236	ASN
2	H	1239	VAL
2	H	1256	GLN
3	I	53	ARG
3	I	89	GLY
3	I	155	GLU
3	I	345	LYS
3	I	417	ARG
3	I	542	ALA
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	847	ASP
3	I	914	ALA
3	I	1268	ASN
4	J	4	VAL
5	Y	490	PRO
1	A	14	VAL
1	A	160	HIS
1	A	166	ARG
2	C	44	GLU
2	C	56	VAL
2	C	78	PRO
2	C	143	ARG
2	C	298	ALA
2	C	740	GLU
2	C	1107	MET
2	C	1240	ASP
2	C	1270	PHE
3	D	53	ARG
3	D	108	ALA
3	D	132	LEU
3	D	559	ALA
3	D	707	ILE
3	D	731	ARG
3	D	1344	LEU

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Mol	Chain	Res	Type
3	D	1363	TYR
4	E	4	VAL
5	X	20	GLY
5	X	308	GLY
5	X	491	GLU
2	H	44	GLU
2	H	56	VAL
2	H	298	ALA
2	H	437	ASN
2	H	740	GLU
2	H	1270	PHE
3	I	108	ALA
3	I	132	LEU
3	I	210	SER
3	I	255	LEU
3	I	559	ALA
3	I	731	ARG
3	I	901	ARG
3	I	913	GLU
3	I	1195	GLN
3	I	1363	TYR
5	Y	108	VAL
5	Y	308	GLY
5	Y	491	GLU
1	A	93	GLN
1	A	194	GLN
1	B	235	ARG
2	C	543	ALA
2	C	1003	THR
2	C	1080	ASN
2	C	1139	ALA
3	D	62	PHE
3	D	210	SER
3	D	596	LEU
3	D	1195	GLN
4	E	5	THR
5	X	50	ASP
5	X	504	PRO
5	X	567	MET
1	F	153	VAL
1	F	160	HIS
1	F	166	ARG

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Mol	Chain	Res	Type
1	G	228	LEU
2	H	13	LYS
2	H	143	ARG
2	H	487	LEU
2	H	488	MET
2	H	699	LEU
2	H	895	LEU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1107	MET
2	H	1240	ASP
3	I	62	PHE
3	I	598	LYS
3	I	888	CYS
3	I	1344	LEU
5	Y	504	PRO
5	Y	567	MET
5	Y	581	ASP
1	A	187	VAL
1	A	188	GLU
1	A	195	ARG
1	A	322	PRO
1	B	177	TYR
2	C	13	LYS
2	C	69	GLN
2	C	746	ALA
2	C	812	PHE
2	C	895	LEU
3	D	598	LYS
3	D	848	VAL
3	D	888	CYS
5	X	600	HIS
1	F	33	ARG
2	H	736	VAL
2	H	746	ALA
2	H	1046	VAL
2	H	1139	ALA
3	I	590	SER
3	I	596	LEU
4	J	5	THR
5	Y	600	HIS

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Mol	Chain	Res	Type
1	A	163	GLU
1	B	49	SER
2	C	908	GLU
2	C	1093	PRO
2	C	1201	LEU
3	D	728	SER
3	D	855	ASP
3	D	1174	ARG
4	E	59	ILE
5	X	108	VAL
1	G	49	SER
2	H	516	ASP
2	H	812	PHE
2	H	908	GLU
3	I	848	VAL
3	I	850	LYS
3	I	855	ASP
3	I	1192	LYS
3	I	1194	ARG
2	H	43	PRO
4	J	59	ILE
1	A	232	VAL
2	C	104	ILE
2	C	373	GLY
2	C	736	VAL
2	C	1046	VAL
5	X	35	ILE
2	H	104	ILE
1	A	153	VAL
2	H	373	GLY
3	D	850	LYS
5	Y	564	GLY
1	B	154	PRO
3	I	706	VAL
2	H	489	PRO
2	H	1181	PRO
2	C	1181	PRO

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/286 (98%)	272 (97%)	9 (3%)	34	55
1	B	189/286 (66%)	186 (98%)	3 (2%)	55	67
1	F	197/286 (69%)	193 (98%)	4 (2%)	48	64
1	G	185/286 (65%)	179 (97%)	6 (3%)	34	55
2	C	1150/1157 (99%)	1074 (93%)	76 (7%)	15	42
2	H	1150/1157 (99%)	1073 (93%)	77 (7%)	15	42
3	D	971/1168 (83%)	908 (94%)	63 (6%)	15	42
3	I	971/1168 (83%)	908 (94%)	63 (6%)	15	42
4	E	74/75 (99%)	70 (95%)	4 (5%)	20	46
4	J	65/75 (87%)	61 (94%)	4 (6%)	16	43
5	X	460/540 (85%)	440 (96%)	20 (4%)	26	50
5	Y	407/540 (75%)	390 (96%)	17 (4%)	26	50
All	All	6100/7024 (87%)	5754 (94%)	346 (6%)	18	45

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	88	LEU
1	A	117	HIS
1	A	158	ARG
1	A	239	GLN
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	77	ASP
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN

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Mol	Chain	Res	Type
2	C	56	VAL
2	C	70	TYR
2	C	73	TYR
2	C	80	PHE
2	C	88	ARG
2	C	98	VAL
2	C	117	ILE
2	C	121	GLU
2	C	127	ILE
2	C	133	ASN
2	C	161	LYS
2	C	163	LYS
2	C	442	VAL
2	C	479	LEU
2	C	487	LEU
2	C	550	VAL
2	C	600	THR
2	C	603	ILE
2	C	645	PHE
2	C	650	VAL
2	C	661	VAL
2	C	690	VAL
2	C	693	LEU
2	C	700	VAL
2	C	704	MET
2	C	711	ASP
2	C	740	GLU
2	C	765	ILE
2	C	773	LEU
2	C	791	LEU
2	C	800	MET
2	C	817	LEU
2	C	844	LYS
2	C	845	LEU
2	C	890	LYS
2	C	908	GLU
2	C	909	LYS
2	C	920	VAL
2	C	941	LYS
2	C	944	ARG
2	C	953	LEU
2	C	964	LEU

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Mol	Chain	Res	Type
2	C	975	ILE
2	C	988	LYS
2	C	1002	LEU
2	C	1010	GLN
2	C	1017	GLN
2	C	1027	LYS
2	C	1032	LYS
2	C	1042	LEU
2	C	1060	ILE
2	C	1097	VAL
2	C	1119	MET
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1239	VAL
2	C	1248	THR
2	C	1259	LEU
2	C	1262	LYS
2	C	1264	GLN
2	C	1265	PHE
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
2	C	1341	ASP
3	D	9	LYS
3	D	13	LYS
3	D	20	ILE
3	D	50	LYS
3	D	66	LYS
3	D	74	LYS
3	D	92	VAL
3	D	114	ILE
3	D	117	LEU
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	155	GLU
3	D	169	LEU

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Mol	Chain	Res	Type
3	D	179	LYS
3	D	185	ILE
3	D	188	LEU
3	D	239	LEU
3	D	250	ARG
3	D	324	LEU
3	D	416	ILE
3	D	442	ILE
3	D	447	ILE
3	D	500	ILE
3	D	505	ASP
3	D	506	VAL
3	D	508	LEU
3	D	521	LYS
3	D	523	GLU
3	D	527	LEU
3	D	531	LYS
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	571	ASP
3	D	594	GLN
3	D	605	LEU
3	D	668	PHE
3	D	681	LYS
3	D	707	ILE
3	D	713	GLU
3	D	771	GLN
3	D	809	VAL
3	D	816	THR
3	D	826	ILE
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	882	VAL
3	D	909	ILE
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG

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Mol	Chain	Res	Type
3	D	1134	ILE
3	D	1148	ARG
3	D	1188	GLU
3	D	1247	LYS
3	D	1297	LYS
3	D	1306	LEU
3	D	1367	GLN
4	E	4	VAL
4	E	6	VAL
4	E	13	ILE
4	E	73	GLN
5	X	21	TYR
5	X	28	ASN
5	X	42	GLU
5	X	54	GLN
5	X	136	GLU
5	X	262	VAL
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	390	ILE
5	X	400	GLN
5	X	452	ILE
5	X	457	ILE
5	X	473	GLU
5	X	545	HIS
5	X	562	ARG
5	X	565	ILE
5	X	582	VAL
5	X	607	LEU
1	F	37	HIS
1	F	77	ASP
1	F	158	ARG
1	F	160	HIS
1	G	13	LEU
1	G	37	HIS
1	G	77	ASP
1	G	88	LEU
1	G	127	GLN
1	G	228	LEU
2	H	9	LYS

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Mol	Chain	Res	Type
2	H	15	PHE
2	H	18	ARG
2	H	32	LEU
2	H	37	LYS
2	H	41	GLN
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	98	VAL
2	H	99	LYS
2	H	117	ILE
2	H	127	ILE
2	H	161	LYS
2	H	311	CYS
2	H	442	VAL
2	H	479	LEU
2	H	481	LEU
2	H	488	MET
2	H	514	PHE
2	H	550	VAL
2	H	600	THR
2	H	603	ILE
2	H	645	PHE
2	H	661	VAL
2	H	690	VAL
2	H	700	VAL
2	H	704	MET
2	H	711	ASP
2	H	740	GLU
2	H	765	ILE
2	H	773	LEU
2	H	791	LEU
2	H	800	MET
2	H	817	LEU
2	H	844	LYS
2	H	845	LEU
2	H	865	LEU
2	H	890	LYS

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Mol	Chain	Res	Type
2	H	909	LYS
2	H	920	VAL
2	H	953	LEU
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	988	LYS
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1027	LYS
2	H	1032	LYS
2	H	1042	LEU
2	H	1060	ILE
2	H	1097	VAL
2	H	1119	MET
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1210	ILE
2	H	1211	ARG
2	H	1233	LEU
2	H	1239	VAL
2	H	1248	THR
2	H	1262	LYS
2	H	1264	GLN
2	H	1288	GLN
2	H	1291	LEU
2	H	1326	LEU
2	H	1335	ILE
2	H	1339	LEU
2	H	1341	ASP
3	I	9	LYS
3	I	31	ARG
3	I	50	LYS
3	I	66	LYS
3	I	74	LYS
3	I	92	VAL
3	I	114	ILE
3	I	117	LEU

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Mol	Chain	Res	Type
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	151	MET
3	I	155	GLU
3	I	169	LEU
3	I	179	LYS
3	I	185	ILE
3	I	188	LEU
3	I	239	LEU
3	I	316	ILE
3	I	324	LEU
3	I	325	LYS
3	I	416	ILE
3	I	430	HIS
3	I	442	ILE
3	I	447	ILE
3	I	475	GLU
3	I	500	ILE
3	I	505	ASP
3	I	506	VAL
3	I	521	LYS
3	I	523	GLU
3	I	527	LEU
3	I	531	LYS
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	605	LEU
3	I	681	LYS
3	I	707	ILE
3	I	771	GLN
3	I	809	VAL
3	I	816	THR
3	I	826	ILE
3	I	832	LYS
3	I	847	ASP
3	I	856	ILE
3	I	864	LEU
3	I	873	GLU

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Mol	Chain	Res	Type
3	I	882	VAL
3	I	909	ILE
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1226	VAL
3	I	1247	LYS
3	I	1297	LYS
3	I	1306	LEU
3	I	1369	ARG
4	J	4	VAL
4	J	6	VAL
4	J	13	ILE
4	J	73	GLN
5	Y	98	VAL
5	Y	136	GLU
5	Y	262	VAL
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	452	ILE
5	Y	457	ILE
5	Y	473	GLU
5	Y	545	HIS
5	Y	562	ARG
5	Y	565	ILE
5	Y	582	VAL
5	Y	589	GLN
5	Y	607	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	84	ASN
1	A	227	GLN
1	A	239	GLN

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Mol	Chain	Res	Type
1	B	66	HIS
1	B	84	ASN
2	C	69	GLN
2	C	133	ASN
2	C	139	ASN
2	C	219	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	450	ASN
2	C	462	ASN
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	573	ASN
2	C	673	HIS
2	C	684	ASN
2	C	799	ASN
2	C	834	GLN
2	C	932	GLN
2	C	952	GLN
2	C	955	GLN
2	C	1010	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1134	GLN
2	C	1175	ASN
2	C	1220	GLN
2	C	1264	GLN
3	D	94	GLN
3	D	209	ASN
3	D	300	GLN
3	D	364	HIS
3	D	680	ASN
3	D	690	ASN
3	D	739	GLN
3	D	875	ASN
3	D	921	GLN
3	D	1268	ASN
3	D	1326	GLN
4	E	31	GLN

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Mol	Chain	Res	Type
5	X	19	GLN
5	X	28	ASN
5	X	30	HIS
5	X	40	GLN
5	X	54	GLN
5	X	301	ASN
5	X	317	ASN
5	X	406	GLN
5	X	437	GLN
5	X	461	ASN
5	X	469	GLN
5	X	472	GLN
1	F	23	HIS
1	F	84	ASN
1	F	103	ASN
1	G	37	HIS
2	H	46	GLN
2	H	69	GLN
2	H	133	ASN
2	H	139	ASN
2	H	238	GLN
2	H	462	ASN
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	526	HIS
2	H	573	ASN
2	H	582	ASN
2	H	628	HIS
2	H	673	HIS
2	H	684	ASN
2	H	686	GLN
2	H	725	GLN
2	H	766	ASN
2	H	799	ASN
2	H	834	GLN
2	H	894	GLN
2	H	922	ASN
2	H	952	GLN
2	H	1010	GLN
2	H	1038	GLN
2	H	1134	GLN

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Mol	Chain	Res	Type
2	H	1175	ASN
2	H	1220	GLN
2	H	1264	GLN
2	H	1288	GLN
3	I	209	ASN
3	I	274	ASN
3	I	294	ASN
3	I	300	GLN
3	I	309	ASN
3	I	419	HIS
3	I	477	GLN
3	I	504	GLN
3	I	680	ASN
3	I	1268	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	242	HIS
5	Y	301	ASN
5	Y	342	GLN
5	Y	383	ASN
5	Y	437	GLN
5	Y	455	HIS
5	Y	469	GLN
5	Y	472	GLN
5	Y	589	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	1RM	H	1401	-	61,63,82	1.94	16 (26%)	83,96,120	1.93	21 (25%)
6	1RM	C	1401	-	80,82,82	1.74	16 (20%)	105,120,120	1.98	26 (24%)

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	1RM	H	1401	-	-	33/55/74/97	0/5/6/8
6	1RM	C	1401	-	-	39/68/97/97	0/7/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1401	1RM	O3-C6	8.17	1.52	1.37
6	C	1401	1RM	O3-C6	8.14	1.52	1.37
6	C	1401	1RM	O7-C25	-4.63	1.37	1.44
6	H	1401	1RM	O7-C25	-4.52	1.38	1.44
6	C	1401	1RM	C15-N1	4.28	1.45	1.37
6	H	1401	1RM	C15-N1	4.16	1.45	1.37
6	H	1401	1RM	C12-C11	-4.02	1.38	1.54
6	C	1401	1RM	C12-C11	-3.93	1.39	1.54
6	C	1401	1RM	C10-C4	3.65	1.51	1.46
6	H	1401	1RM	C10-C4	3.22	1.50	1.46
6	H	1401	1RM	O-C06	2.97	1.42	1.36
6	C	1401	1RM	C02-N3	2.73	1.43	1.38
6	C	1401	1RM	C32-C22	-2.60	1.48	1.53
6	H	1401	1RM	C32-C22	-2.58	1.48	1.53
6	H	1401	1RM	C02-N3	2.51	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	1RM	C-N03	2.48	1.38	1.32
6	H	1401	1RM	C18-C17	2.47	1.50	1.43
6	C	1401	1RM	O-C06	2.45	1.42	1.37
6	C	1401	1RM	C18-C17	2.36	1.50	1.43
6	C	1401	1RM	O6-C27	-2.25	1.38	1.43
6	H	1401	1RM	O6-C27	-2.23	1.38	1.43
6	H	1401	1RM	C14-C7	2.23	1.56	1.51
6	H	1401	1RM	C18-C19	2.19	1.41	1.33
6	H	1401	1RM	C5-C11	-2.17	1.40	1.45
6	C	1401	1RM	O9-C23	-2.16	1.37	1.43
6	C	1401	1RM	C18-C19	2.14	1.41	1.33
6	C	1401	1RM	C14-C7	2.13	1.55	1.51
6	C	1401	1RM	O10-C21	-2.11	1.37	1.43
6	H	1401	1RM	O9-C23	-2.11	1.37	1.43
6	H	1401	1RM	O10-C21	-2.09	1.37	1.43
6	H	1401	1RM	C6-C7	2.05	1.43	1.39
6	C	1401	1RM	C5-C11	-2.02	1.41	1.45

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	1RM	C6-C5-C11	-7.83	100.59	107.16
6	H	1401	1RM	C6-C5-C11	-7.16	101.15	107.16
6	C	1401	1RM	C9-C10-C5	-5.21	113.08	119.91
6	C	1401	1RM	C38-N02-C42	5.13	124.91	111.24
6	C	1401	1RM	C12-O3-C6	-4.95	99.42	107.69
6	H	1401	1RM	C9-C10-C5	-4.85	113.56	119.91
6	H	1401	1RM	C12-O3-C6	-4.61	99.99	107.69
6	H	1401	1RM	O7-C35-C36	4.61	119.31	111.09
6	C	1401	1RM	O7-C35-C36	4.41	118.96	111.09
6	H	1401	1RM	C37-O6-C27	4.35	122.97	112.99
6	C	1401	1RM	C39-N01-C44	3.84	121.47	111.24
6	C	1401	1RM	C37-O6-C27	3.81	121.71	112.99
6	C	1401	1RM	C44-N01-C41	3.56	116.51	108.84
6	C	1401	1RM	C18-C17-C16	-3.27	117.39	126.64
6	C	1401	1RM	C17-C18-C19	-3.18	117.07	124.43
6	C	1401	1RM	C5-C10-C4	3.16	128.72	122.13
6	H	1401	1RM	C31-C20-C21	3.05	117.97	111.45
6	H	1401	1RM	C18-C17-C16	-3.04	118.03	126.64
6	C	1401	1RM	C25-O7-C35	3.02	122.41	117.72
6	H	1401	1RM	C17-C18-C19	-2.89	117.73	124.43
6	C	1401	1RM	C8-C9-C1	-2.89	115.72	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	1RM	C10-C9-C8	2.87	123.77	119.65
6	C	1401	1RM	C31-C20-C21	2.86	117.58	111.45
6	H	1401	1RM	C5-C10-C4	2.85	128.08	122.13
6	H	1401	1RM	O4-C11-C5	-2.84	124.65	130.69
6	H	1401	1RM	C25-O7-C35	2.83	122.12	117.72
6	C	1401	1RM	O4-C11-C5	-2.82	124.68	130.69
6	C	1401	1RM	C43-C44-N01	2.82	116.34	110.65
6	C	1401	1RM	C16-C15-N1	2.81	120.30	115.01
6	C	1401	1RM	C3-C4-N3	-2.62	119.23	122.59
6	H	1401	1RM	C3-C4-N3	-2.54	119.34	122.59
6	H	1401	1RM	C8-C7-C6	-2.52	113.46	116.86
6	H	1401	1RM	C8-C9-C1	-2.51	116.39	120.85
6	H	1401	1RM	C10-C9-C8	2.49	123.23	119.65
6	H	1401	1RM	C16-C15-N1	2.42	119.57	115.01
6	C	1401	1RM	C8-C7-C6	-2.41	113.60	116.86
6	C	1401	1RM	C42-C41-N01	2.34	115.37	110.65
6	H	1401	1RM	C20-C19-C18	-2.25	121.46	126.11
6	C	1401	1RM	C12-O5-C29	2.18	123.21	117.84
6	H	1401	1RM	C1-C2-N1	2.16	119.93	115.21
6	C	1401	1RM	C38-N02-C43	2.15	116.98	111.24
6	C	1401	1RM	C20-C19-C18	-2.15	121.66	126.11
6	H	1401	1RM	C13-C12-C11	-2.15	108.60	113.90
6	H	1401	1RM	C12-O5-C29	2.15	123.12	117.84
6	H	1401	1RM	C30-C16-C17	-2.13	118.49	123.67
6	C	1401	1RM	C39-N01-C41	2.10	116.85	111.24
6	C	1401	1RM	C30-C16-C17	-2.03	118.73	123.67

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	1RM	C11-C12-O5-C29
6	C	1401	1RM	C13-C12-O5-C29
6	C	1401	1RM	O3-C12-O5-C29
6	C	1401	1RM	C30-C16-C17-C18
6	C	1401	1RM	C31-C20-C21-C22
6	C	1401	1RM	C21-C22-C23-C24
6	C	1401	1RM	C21-C22-C23-O9
6	C	1401	1RM	C32-C22-C23-C24
6	C	1401	1RM	C32-C22-C23-O9
6	C	1401	1RM	C23-C24-C25-C26
6	C	1401	1RM	C33-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	C	1401	1RM	C33-C24-C25-O7
6	C	1401	1RM	O7-C25-C26-C34
6	C	1401	1RM	C26-C27-C28-C29
6	H	1401	1RM	C11-C12-O5-C29
6	H	1401	1RM	C13-C12-O5-C29
6	H	1401	1RM	O3-C12-O5-C29
6	H	1401	1RM	C15-C16-C17-C18
6	H	1401	1RM	C30-C16-C17-C18
6	H	1401	1RM	C19-C20-C21-C22
6	H	1401	1RM	C19-C20-C21-O10
6	H	1401	1RM	C31-C20-C21-C22
6	H	1401	1RM	C21-C22-C23-C24
6	H	1401	1RM	C21-C22-C23-O9
6	H	1401	1RM	C32-C22-C23-C24
6	H	1401	1RM	C32-C22-C23-O9
6	H	1401	1RM	C23-C24-C25-C26
6	H	1401	1RM	C33-C24-C25-C26
6	H	1401	1RM	C33-C24-C25-O7
6	H	1401	1RM	O7-C25-C26-C34
6	H	1401	1RM	C26-C27-C28-C29
6	C	1401	1RM	C23-C24-C25-O7
6	H	1401	1RM	C23-C24-C25-O7
6	C	1401	1RM	C36-C35-O7-C25
6	C	1401	1RM	C17-C18-C19-C20
6	H	1401	1RM	C17-C18-C19-C20
6	C	1401	1RM	O7-C25-C26-C27
6	H	1401	1RM	O7-C25-C26-C27
6	C	1401	1RM	O8-C35-O7-C25
6	C	1401	1RM	C19-C20-C21-O10
6	H	1401	1RM	C31-C20-C21-O10
6	C	1401	1RM	C09-C38-N02-C42
6	C	1401	1RM	C19-C20-C21-C22
6	C	1401	1RM	C15-C16-C17-C18
6	H	1401	1RM	O8-C35-O7-C25
6	H	1401	1RM	C36-C35-O7-C25
6	H	1401	1RM	C16-C17-C18-C19
6	C	1401	1RM	C31-C20-C21-O10
6	C	1401	1RM	C16-C17-C18-C19
6	C	1401	1RM	C39-C40-N-C46
6	H	1401	1RM	C28-C29-O5-C12
6	C	1401	1RM	O6-C27-C28-C29
6	C	1401	1RM	O-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
6	C	1401	1RM	C24-C25-C26-C34
6	H	1401	1RM	C24-C25-C26-C34
6	C	1401	1RM	C39-C40-N-C
6	C	1401	1RM	N01-C39-C40-N
6	C	1401	1RM	N1-C15-C16-C17
6	C	1401	1RM	O11-C15-C16-C17
6	H	1401	1RM	C28-C27-O6-C37
6	C	1401	1RM	C40-C39-N01-C44
6	H	1401	1RM	N1-C15-C16-C17
6	H	1401	1RM	O11-C15-C16-C17
6	C	1401	1RM	C28-C29-O5-C12
6	H	1401	1RM	O6-C27-C28-C29
6	C	1401	1RM	C24-C25-C26-C27
6	H	1401	1RM	C24-C25-C26-C27
6	C	1401	1RM	N1-C15-C16-C30
6	C	1401	1RM	O11-C15-C16-C30
6	H	1401	1RM	O11-C15-C16-C30
6	C	1401	1RM	C02-C06-O-C07
6	H	1401	1RM	N1-C15-C16-C30

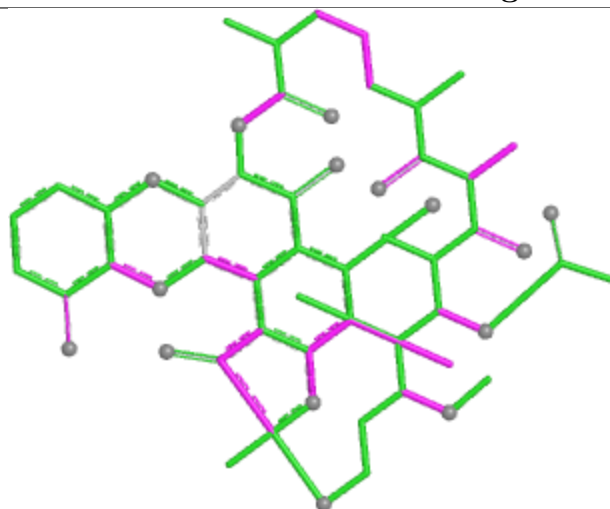
There are no ring outliers.

2 monomers are involved in 18 short contacts:

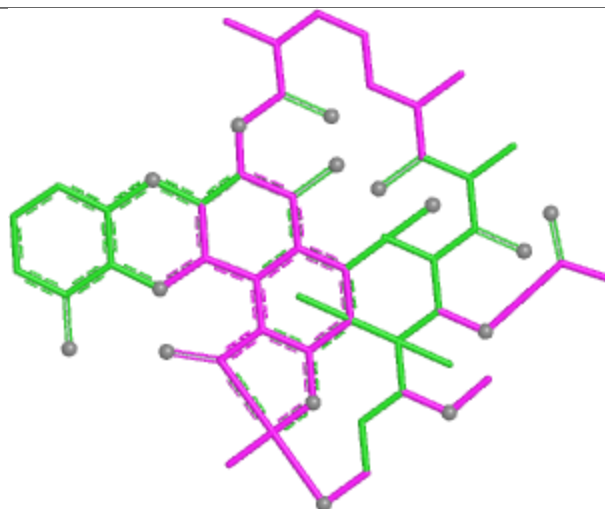
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1401	1RM	8	0
6	C	1401	1RM	10	0

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.

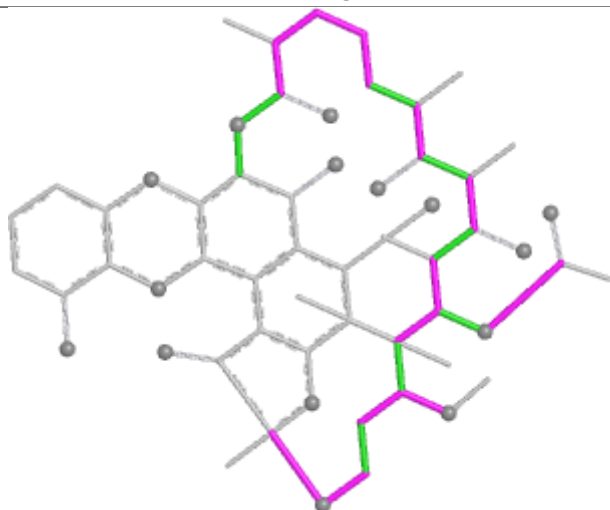
Ligand 1RM H 1401



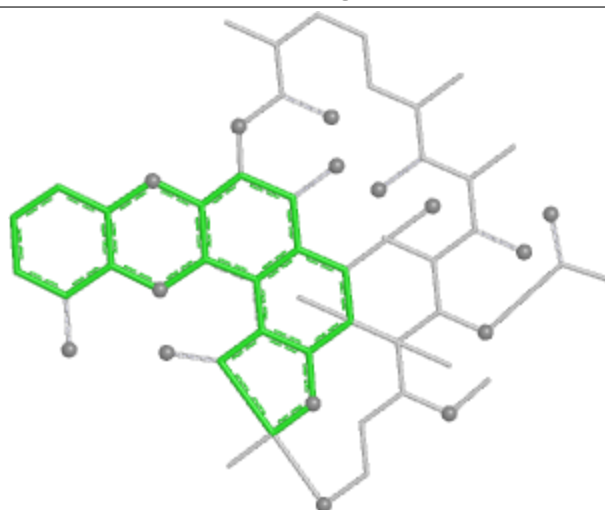
Bond lengths



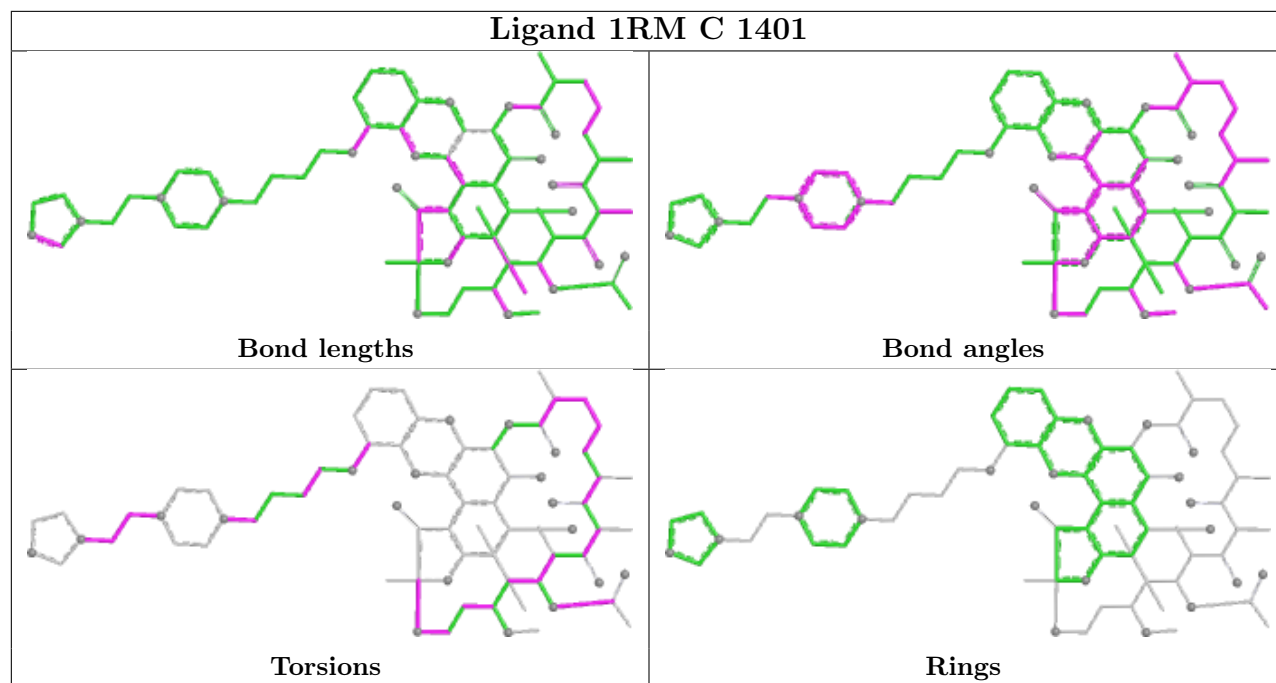
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	323/329 (98%)	-0.72	0	100 100	0, 59, 154, 247	0
1	B	221/329 (67%)	-0.54	0	100 100	5, 86, 172, 210	0
1	F	229/329 (69%)	-0.53	0	100 100	20, 107, 186, 257	0
1	G	217/329 (65%)	-0.59	1 (0%)	87 68	23, 106, 166, 211	0
2	C	1335/1342 (99%)	-0.70	1 (0%)	92 87	0, 35, 155, 279	0
2	H	1335/1342 (99%)	-0.61	0	100 100	1, 78, 192, 314	0
3	D	1160/1407 (82%)	-0.65	1 (0%)	92 87	0, 30, 149, 264	0
3	I	1160/1407 (82%)	-0.62	1 (0%)	92 87	1, 49, 170, 288	0
4	E	90/91 (98%)	-0.89	0	100 100	0, 32, 101, 141	0
4	J	76/91 (83%)	-0.65	0	100 100	7, 72, 156, 198	0
5	X	517/613 (84%)	-0.61	0	100 100	1, 95, 219, 329	0
5	Y	458/613 (74%)	-0.64	1 (0%)	91 80	2, 98, 217, 320	0
All	All	7121/8222 (86%)	-0.64	5 (0%)	92 87	0, 62, 183, 329	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	26	VAL	2.5
3	D	1142	ALA	2.5
2	C	116	ASP	2.4
5	Y	221	PHE	2.0
3	I	540	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

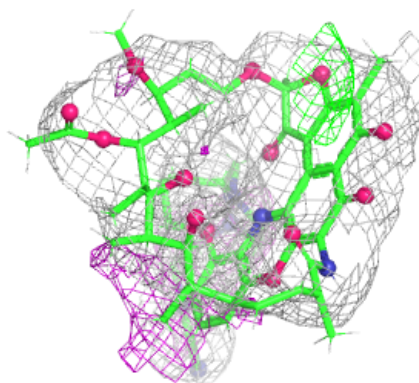
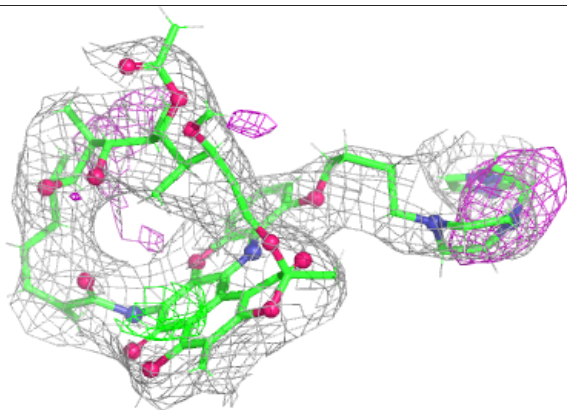
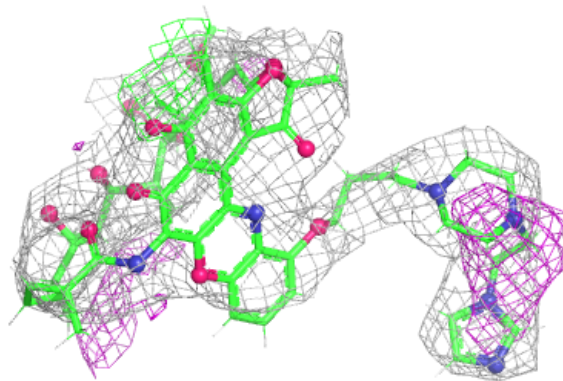
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1RM	C	1401	75/75	0.85	0.08	20,20,20,20	0
6	1RM	H	1401	58/75	0.85	0.08	20,20,20,20	0
8	MG	I	1503	1/1	0.93	0.24	20,20,20,20	0
8	MG	D	1503	1/1	0.98	0.14	24,24,24,24	0
7	ZN	I	1501	1/1	0.99	0.06	60,60,60,60	0
7	ZN	I	1502	1/1	0.99	0.06	49,49,49,49	0
7	ZN	D	1501	1/1	1.00	0.04	54,54,54,54	0
7	ZN	D	1502	1/1	1.00	0.06	8,8,8,8	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.

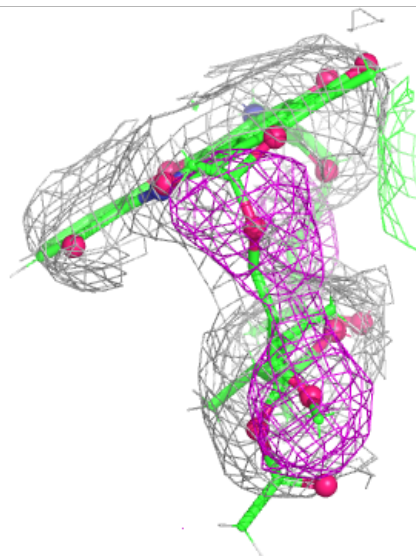
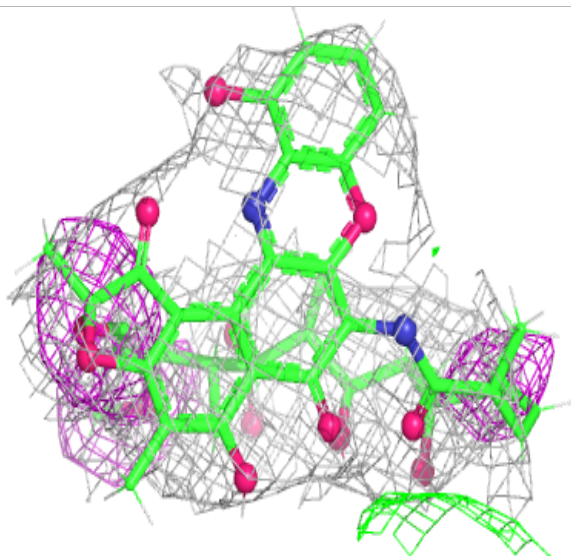
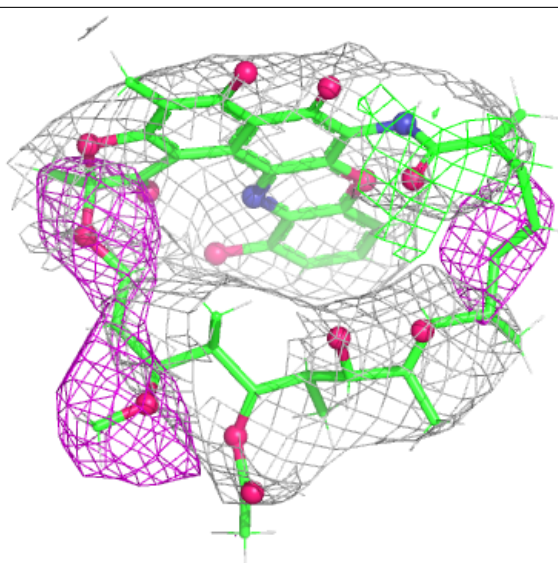
Electron density around 1RM C 1401:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 1RM H 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.