



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:22 AM GMT

PDB ID : 3OGL
Title : Structure of COI1-ASK1 in complex with JA-isoleucine and the JAZ1 degron
Authors : Sheard, L.B.; Tan, X.; Mao, H.; Withers, J.; Ben-Nissan, G.; Hinds, T.R.;
Hsu, F.; Sharon, M.; Browse, J.; He, S.Y.; Rizo, J.; Howe, G.A.; Zheng, N.
Deposited on : 2010-08-17
Resolution : 3.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

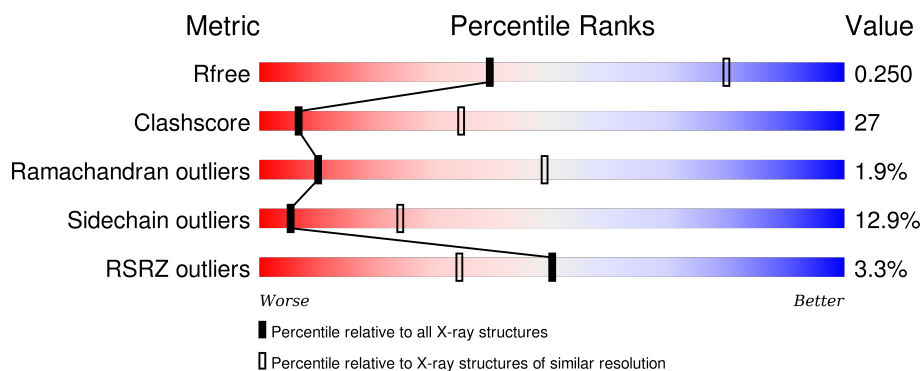
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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

Mol	Chain	Length	Quality of chain
1	A	160	<div> <div>3%</div> <div>49% 36% 5% 10%</div> </div>
1	C	160	<div> <div>5%</div> <div>49% 34% 6% 10%</div> </div>
1	E	160	<div> <div>%</div> <div>54% 29% 7% 10%</div> </div>
1	G	160	<div> <div></div> <div>53% 31% 7% 10%</div> </div>
1	I	160	<div> <div>5%</div> <div>48% 34% 8% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	160	
1	M	160	
1	O	160	
2	B	592	
2	D	592	
2	F	592	
2	H	592	
2	J	592	
2	L	592	
2	N	592	
2	P	592	
3	Q	21	
3	R	21	
3	S	21	
3	U	21	
3	V	21	
3	W	21	
3	X	21	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	7JA	B	1100	-	-	X	-
4	7JA	D	1100	-	-	X	-
4	7JA	F	1100	-	-	X	-
4	7JA	H	1100	-	-	X	X
4	7JA	J	1100	-	-	X	X
4	7JA	L	1100	-	-	X	-
4	7JA	N	1100	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	7JA	P	1100	-	-	X	-
5	PO4	B	1101	-	X	-	-
5	PO4	B	1102	-	X	-	X
5	PO4	B	1103	-	X	X	-
5	PO4	D	1101	-	X	-	-
5	PO4	D	1103	-	X	X	-
5	PO4	F	1101	-	X	-	X
5	PO4	F	1102	-	X	-	-
5	PO4	F	1103	-	-	X	-
5	PO4	H	1101	-	X	-	-
5	PO4	H	1103	-	-	X	-
5	PO4	H	1104	-	-	-	X
5	PO4	J	1102	-	-	-	X
5	PO4	J	1103	-	-	X	-
5	PO4	J	1104	-	-	-	X
5	PO4	L	1101	-	-	-	X
5	PO4	L	1102	-	-	-	X
5	PO4	L	1103	-	-	X	X
5	PO4	L	1104	-	-	-	X
5	PO4	N	1103	-	-	X	-
5	PO4	N	1104	-	-	-	X
5	PO4	P	1101	-	-	-	X
5	PO4	P	1103	-	-	X	-
5	PO4	P	1104	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	C	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	E	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	G	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	I	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	K	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	M	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	O	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			

- Molecule 2 is a protein called Coronatine-insensitive protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	D	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	F	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	H	562	Total	C	N	O	S	0	0	0
			4486	2840	779	831	36			
2	J	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	L	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

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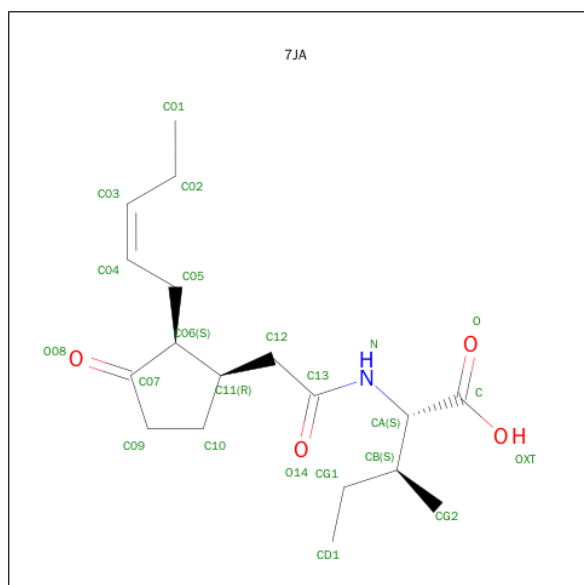
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	P	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

- Molecule 3 is a protein called JAZ1 incomplete degron peptide.

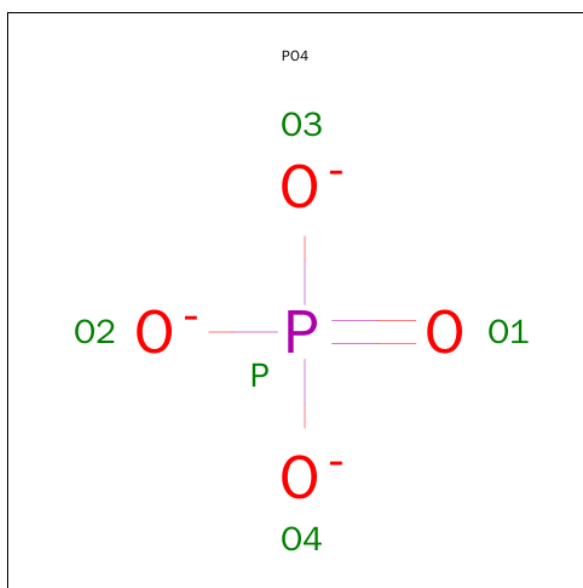
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	X	18	Total	C	N	O	0	0	0
			156	99	34	23			

- Molecule 4 is N-((1R,2S)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetyl)-L-isoLeucine (three-letter code: 7JA) (formula: C₁₈H₂₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			23	18	1	4		
4	D	1	Total	C	N	O	0	0
			23	18	1	4		
4	F	1	Total	C	N	O	0	0
			23	18	1	4		
4	H	1	Total	C	N	O	0	0
			23	18	1	4		
4	J	1	Total	C	N	O	0	0
			23	18	1	4		
4	L	1	Total	C	N	O	0	0
			23	18	1	4		
4	N	1	Total	C	N	O	0	0
			23	18	1	4		
4	P	1	Total	C	N	O	0	0
			23	18	1	4		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		

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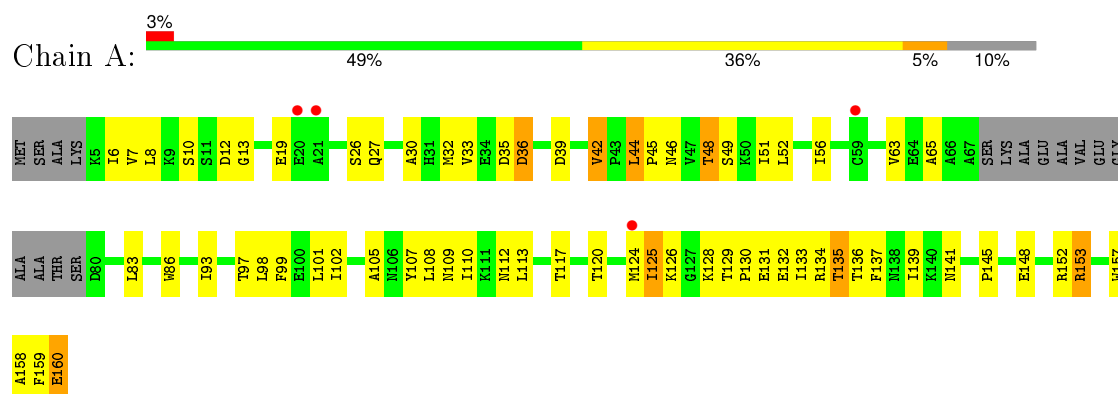
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		

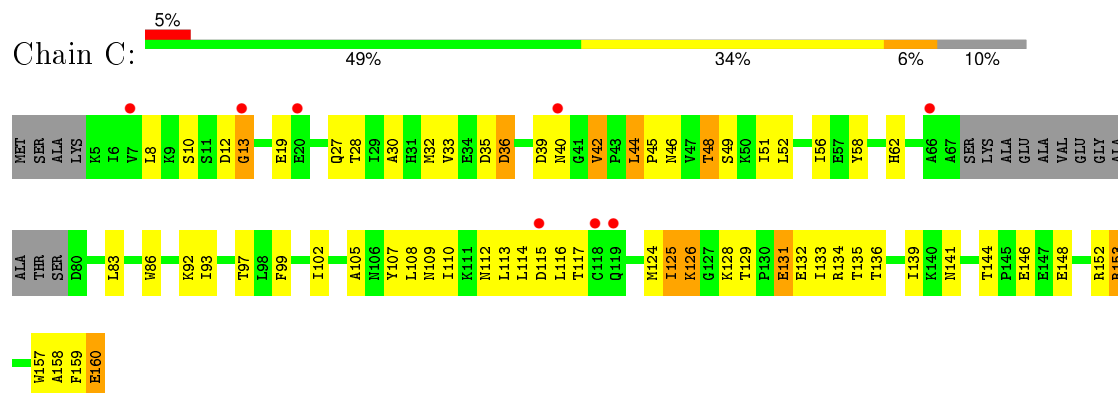
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

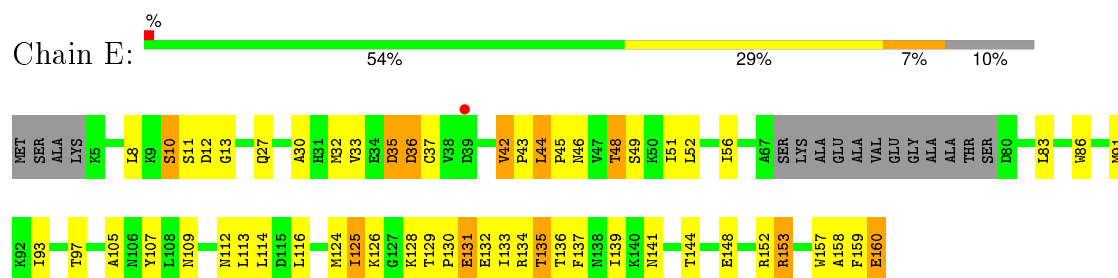
• Molecule 1: SKP1-like protein 1A



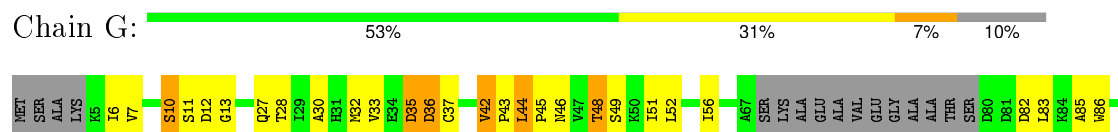
• Molecule 1: SKP1-like protein 1A



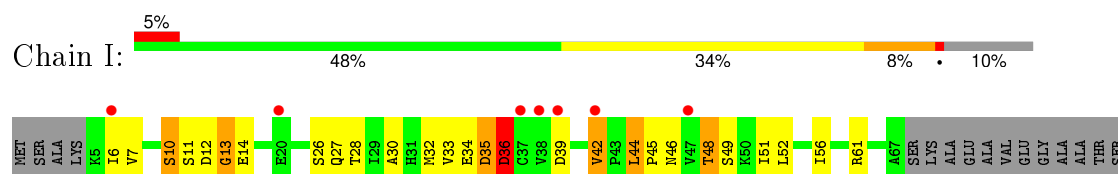
• Molecule 1: SKP1-like protein 1A



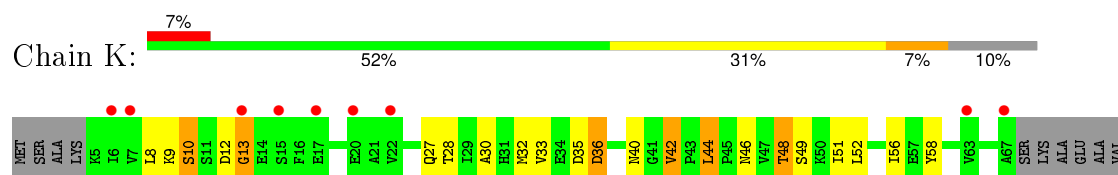
• Molecule 1: SKP1-like protein 1A



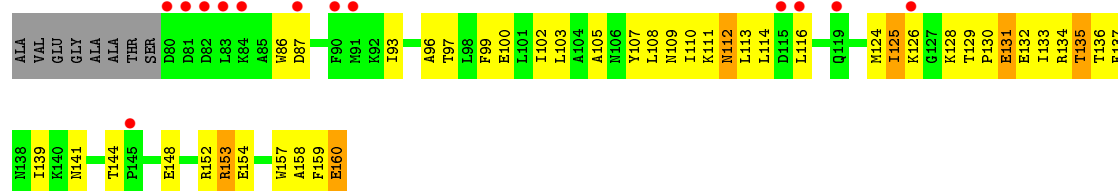
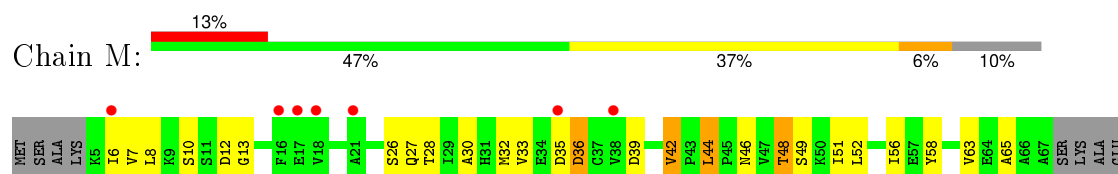
• Molecule 1: SKP1-like protein 1A



• Molecule 1: SKP1-like protein 1A

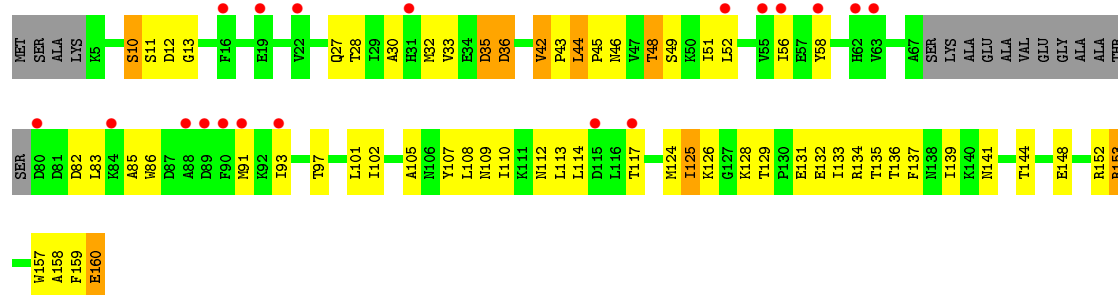


• Molecule 1: SKP1-like protein 1A

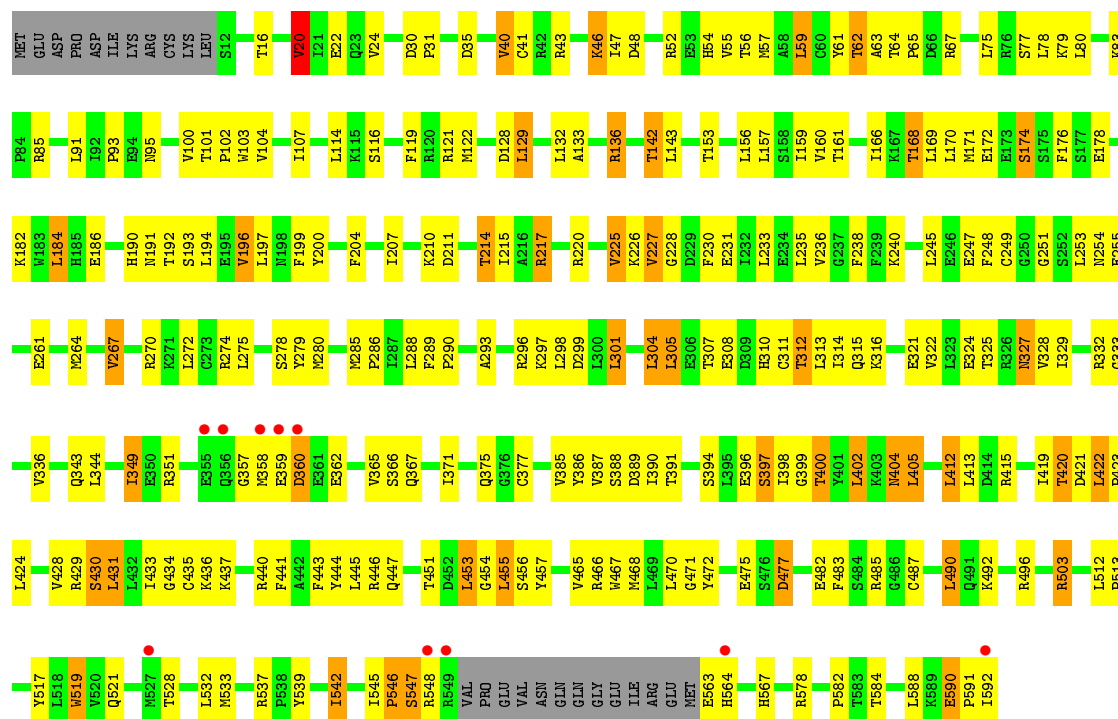


• Molecule 1: SKP1-like protein 1A

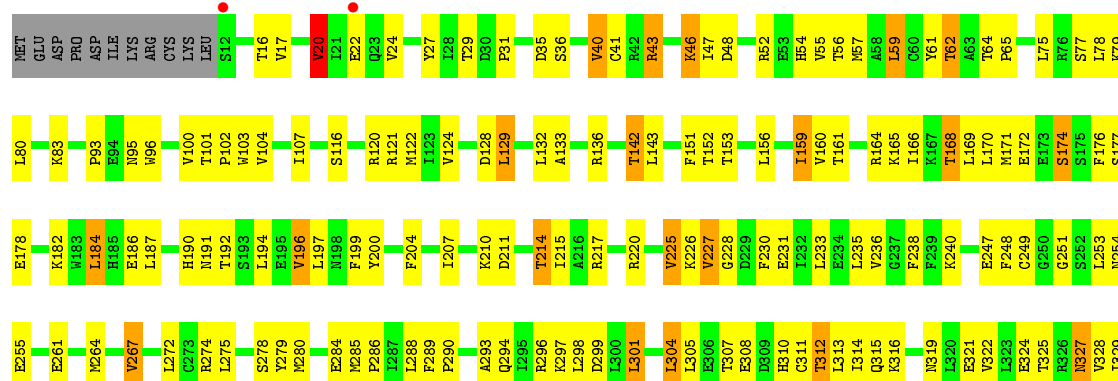


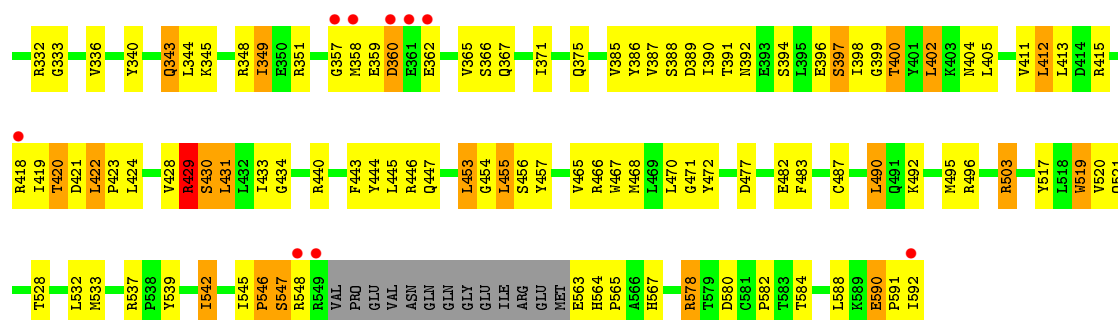


• Molecule 2: Coronatine-insensitive protein 1

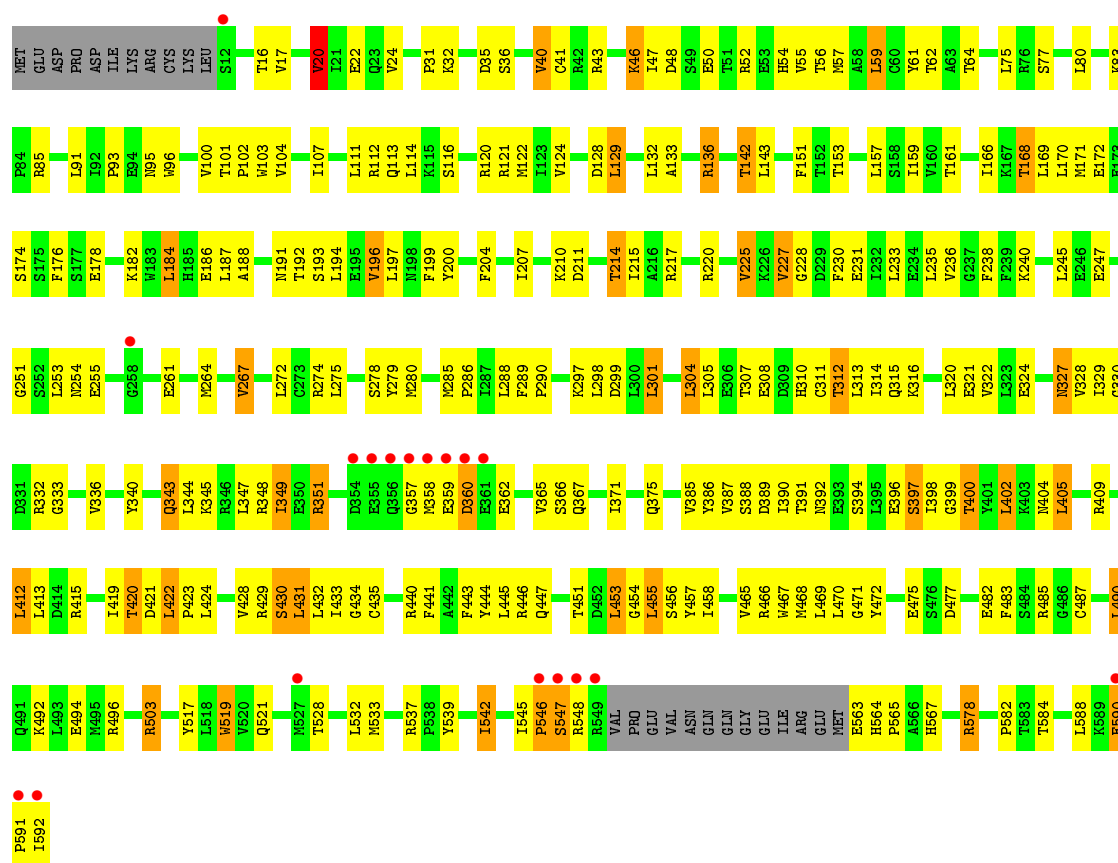


• Molecule 2: Coronatine-insensitive protein 1

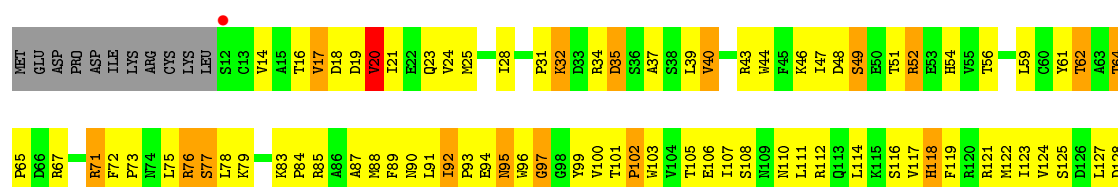




• Molecule 2: Coronatine-insensitive protein 1



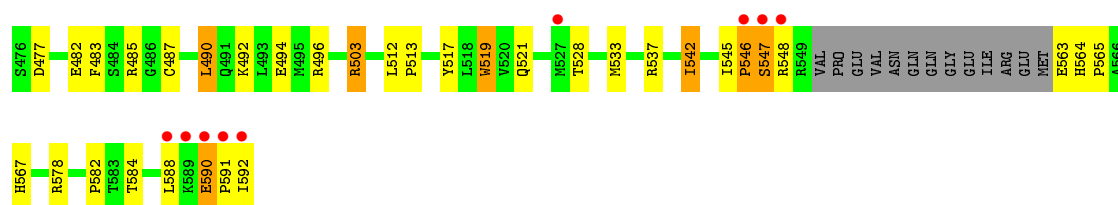
• Molecule 2: Coronatine-insensitive protein 1



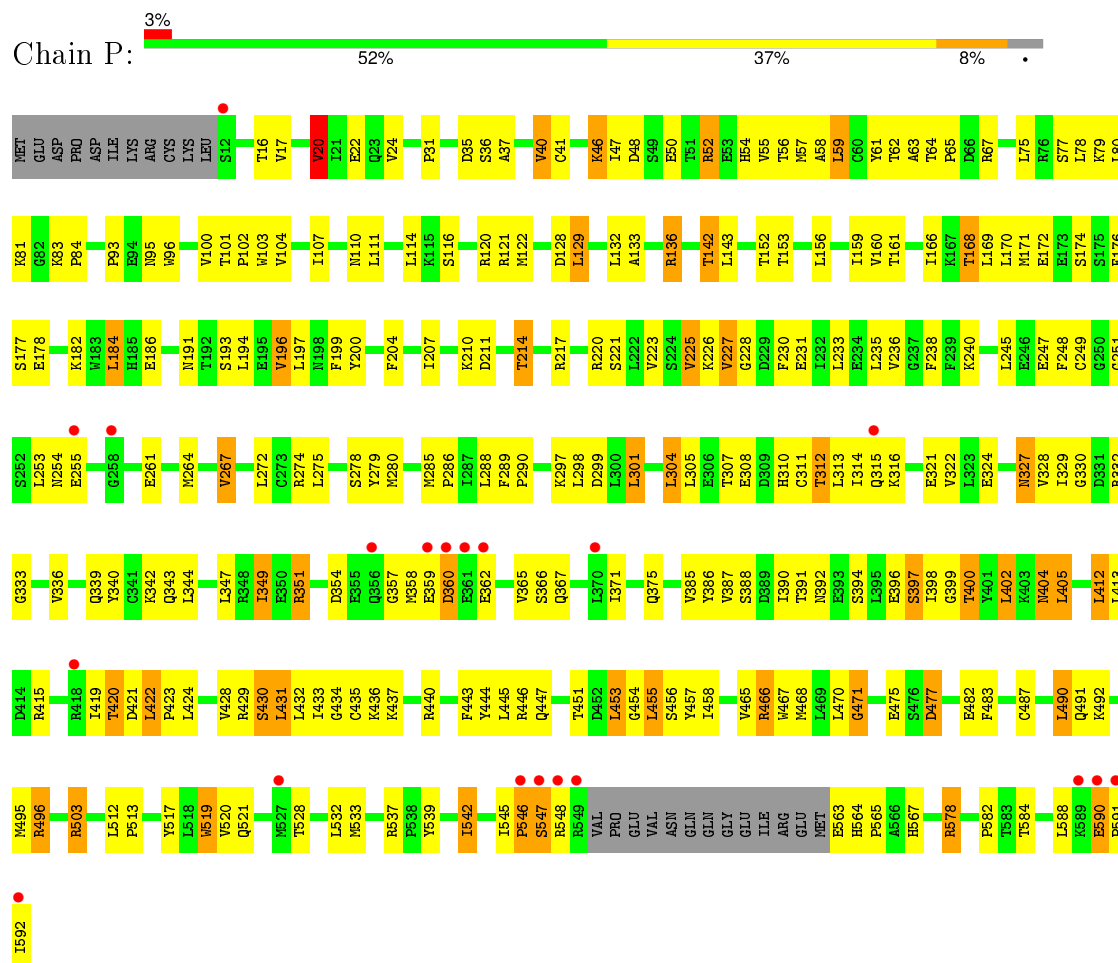


R503	R415	R332	E255	F176	P84
Y517	R418	R332	E255	F176	P84
L518	R419	E335	G258	E178	R85
M519	R420	E335	E261	K182	P93
W520	D421	V336	V336	L183	P94
Q521	L422	L337	L337	L184	N95
P423	L422	A338	M264	L185	M96
M527	L424	Q343	V267	E186	LYS
T528		L344			ARG
L532	V428	L347	L272	N191	CYS
M533	S430	R348	G273	T192	LYU
	L431	R349	R274	S193	S12
R537	L432	E350	L275	L194	T16
P538	L433	E351	S278	V196	V20
Y539	G434	R351	T279	L197	T21
		E355	M280	L198	E22
I542	R440	Q356		F199	Q23
I545	F441	G357	M285	Y200	V24
P546	L442	M358	P286		R120
S547	P443	E359	L287	F204	T29
	L444	D360	L288	T207	D30
R548	L445	E361	P289		P31
M549	R446	E362	P290		
VAL	Q447	V365	A293	K210	D128
PRO		S366	Q294	D211	L129
GLU	T451	Q367	T295	T214	L132
VAL	L452		R296	T215	A133
ASN	L453	I371	L297	R217	R136
GLN	G454		L298		A137
GLN	L455		D299		D138
GLY	S456	Q375	L300	R220	X46
GLU	Y457		L301		L47
ILE	L458	V385	L304	V225	T142
ARG		V386	L304	K226	L143
GLU	V465	V387	L305	V227	
MET	R466	S388	E306	G228	D146
E563	V467	D389	T307		T152
H564	V468	L390	E308	E231	T153
	L469	T391	S309	T232	
H567	L470	N392	H310	L233	L156
	G471	E393	C311	E234	A58
M578	Y472	S394	T312	L235	L159
		E396	L313	V236	V160
P582	E475	E397	T314	G237	C60
T583	S476	L398	Q315	F238	V61
T584	D477	G399	R316		T62
		Y400	K240		A63
L588	E482	T401	N319	L245	T64
K589	F483	L402	L320	E246	L166
E590		K403	E321	E247	K167
P591	C487	N404	V322	L169	T168
		L405	L323	F248	L170
I592	L490	V411	T325	G251	M171
	Q491	L412	R326	S252	E172
	R492	L413	T253	L263	E173
	R496	E414	V256	S474	S174
					S475
					Y82

MET	L75	L169	P238	E324	S397	L403	R403	L405	L412	L413	R415	L419	T420	L422	P423	L424	L428	V428	R429	S430	L431	L432	L433	G434	K437	R440	F441	R441	L442	F443	Y444	L445	R446	Q447	T451	D452	L453	G454	L455	S456	Y457	L458	V465	R466	W467	M468	L469	L470	G471	Y472	L475			
	L76	L170	P239	T325	R327	T400	L402	L405	L412	L413	R415	L419	T420	L422	P423	L424	L428	V428	R429	S430	L431	L432	L433	G434	K437	R440	F441	R441	L442	F443	Y444	L445	R446	Q447	T451	D452	L453	G454	L455	S456	Y457	L458	V465	R466	W467	M468	L469	L470	G471	Y472	L475			
	L77	M170	M171	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210	D211	T214	T215	A216	R217	R220	S221	L222	V223	E224	V225	F226	R227	G228	D229	F230	E231	I232	L233	E234	L235	V236	L237
	L78	L78	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210	D211	T214	T215	A216	R217	R220	S221	L222	V223	E224	V225	F226	R227	G228	D229	F230	E231	I232	L233	E234	L235	V236	L237	
	L79	L80	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210	D211	T214	T215	A216	R217	R220	S221	L222	V223	E224	V225	F226	R227	G228	D229	F230	E231	I232	L233	E234	L235	V236	L237	
	L81	L82	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210	D211	T214	T215	A216	R217	R220	S221	L222	V223	E224	V225	F226	R227	G228	D229	F230	E231	I232	L233	E234	L235	V236	L237	
	L83	P84	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210	D211	T214	T215	A216	R217	R220	S221	L222	V223	E224	V225	F226	R227	G228	D229	F230	E231	I232	L233	E234	L235	V236	L237	
	L84	P84	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210	D211	T214	T215	A216	R217	R220	S221	L222	V223	E224	V225	F226	R227	G228	D229	F230	E231	I232	L233	E234	L235	V236	L237	
	L85	P84	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210	D211	T214	T215	A216	R217	R220	S221	L222	V223	E224	V225	F226	R227	G228	D229	F230	E231	I232	L233	E234	L235	V236	L237	
	L86	P84	E172	E173	S174	S175	F176	S177	E178	K179	K182	W183	L184	H185	E186	M191	T192	S193	W194	F195	V196	L197	M198	F199	Y200	F204	A205	K206	T207	K210																								



• Molecule 2: Coronatine-insensitive protein 1



• Molecule 3: JAZ1 incomplete degron peptide



• Molecule 3: JAZ1 incomplete degron peptide



- Molecule 3: JAZ1 incomplete degron peptide

Chain S:  57% 29% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain U:  57% 29% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain V:  5% 57% 29% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain W:  5% 62% 24% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain X:  5% 52% 33% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.35Å 220.82Å 148.67Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	49.68 – 3.18 49.68 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (49.68-3.18) 91.1 (49.68-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.215 , 0.263 0.199 , 0.250	Depositor DCC
R_{free} test set	1886 reflections (1.62%)	DCC
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 123120 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	46877	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, 7JA

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	0.48	0/1162	0.60	0/1571
1	C	0.56	0/1162	0.63	0/1571
1	E	0.53	0/1162	0.63	0/1571
1	G	0.55	0/1162	0.69	0/1571
1	I	0.49	0/1162	0.61	0/1571
1	K	0.48	0/1162	0.61	0/1571
1	M	0.52	0/1162	0.61	0/1571
1	O	0.51	0/1162	0.60	0/1571
2	B	0.60	1/4623 (0.0%)	0.71	1/6238 (0.0%)
2	D	0.58	0/4623	0.71	2/6238 (0.0%)
2	F	0.53	0/4623	0.71	1/6238 (0.0%)
2	H	0.63	0/4566	0.87	3/6161 (0.0%)
2	J	0.54	0/4623	0.70	1/6238 (0.0%)
2	L	0.52	0/4623	0.70	1/6238 (0.0%)
2	N	0.61	0/4623	0.72	1/6238 (0.0%)
2	P	0.54	0/4623	0.70	1/6238 (0.0%)
3	Q	0.50	0/158	0.58	0/208
3	R	0.44	0/158	0.60	0/208
3	S	0.41	0/158	0.57	0/208
3	U	0.47	0/158	0.56	0/208
3	V	0.44	0/158	0.57	0/208
3	W	0.48	0/158	0.60	0/208
3	X	0.47	0/158	0.55	0/208
All	All	0.56	1/47329 (0.0%)	0.71	11/63851 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	377	CYS	CB-SG	-5.33	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	129	LEU	CA-CB-CG	7.85	133.35	115.30
2	D	129	LEU	CA-CB-CG	7.68	132.96	115.30
2	N	129	LEU	CA-CB-CG	7.36	132.23	115.30
2	B	129	LEU	CA-CB-CG	7.23	131.94	115.30
2	P	129	LEU	CA-CB-CG	7.20	131.85	115.30
2	J	129	LEU	CA-CB-CG	7.19	131.84	115.30
2	L	129	LEU	CA-CB-CG	6.66	130.61	115.30
2	H	170	LEU	CA-CB-CG	5.61	128.19	115.30
2	D	429	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	H	366	SER	N-CA-C	-5.26	96.79	111.00
2	H	156	LEU	CB-CG-CD1	-5.24	102.09	111.00

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	1146	0	1117	58	0
1	C	1146	0	1117	65	0
1	E	1146	0	1117	59	0
1	G	1146	0	1117	57	0
1	I	1146	0	1117	61	2
1	K	1146	0	1117	58	0
1	M	1146	0	1117	95	0
1	O	1146	0	1117	56	0
2	B	4541	0	4583	222	0
2	D	4541	0	4583	235	2
2	F	4541	0	4583	233	0
2	H	4486	0	4534	428	0
2	J	4541	0	4583	237	0
2	L	4541	0	4583	245	0
2	N	4541	0	4583	271	0
2	P	4541	0	4583	235	0
3	Q	156	0	171	5	0
3	R	156	0	171	5	0
3	S	156	0	171	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	156	0	171	5	0
3	V	156	0	171	5	0
3	W	156	0	171	4	0
3	X	156	0	171	5	0
4	B	23	0	29	16	0
4	D	23	0	28	15	0
4	F	23	0	28	19	0
4	H	23	0	29	21	0
4	J	23	0	28	17	0
4	L	23	0	28	16	0
4	N	23	0	28	17	0
4	P	23	0	28	15	0
5	B	20	0	0	2	0
5	D	20	0	0	3	0
5	F	20	0	0	4	0
5	H	20	0	0	3	0
5	J	20	0	0	2	0
5	L	20	0	0	3	0
5	N	20	0	0	2	0
5	P	20	0	0	3	0
All	All	46877	0	46974	2545	2

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 27.

All (2545) 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:B:168:THR:HB	2:B:196:VAL:HG13	1.28	1.14
2:L:168:THR:HB	2:L:196:VAL:HG13	1.22	1.14
4:J:1100:7JA:H04	4:J:1100:7JA:H12	1.29	1.13
2:F:168:THR:HB	2:F:196:VAL:HG13	1.27	1.13
1:G:151:VAL:HG11	2:H:39:LEU:HD21	1.28	1.13
4:F:1100:7JA:H04	4:F:1100:7JA:H12	1.27	1.13
4:D:1100:7JA:H12	4:D:1100:7JA:H04	1.29	1.12
2:D:168:THR:HB	2:D:196:VAL:HG13	1.25	1.11
2:J:168:THR:HB	2:J:196:VAL:HG13	1.26	1.11
2:H:390:ILE:HD11	2:H:412:LEU:HD21	1.28	1.11
4:P:1100:7JA:H04	4:P:1100:7JA:H12	1.30	1.11
4:L:1100:7JA:H04	4:L:1100:7JA:H12	1.29	1.10
2:H:519:TRP:HE1	4:H:1100:7JA:H01A	0.97	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:1100:7JA:H12	4:N:1100:7JA:H04	1.33	1.10
4:B:1100:7JA:H12	4:B:1100:7JA:H04	1.29	1.09
2:N:168:THR:HB	2:N:196:VAL:HG13	1.27	1.08
4:F:1100:7JA:C12	4:F:1100:7JA:H04	1.83	1.07
2:P:168:THR:HB	2:P:196:VAL:HG13	1.24	1.07
4:B:1100:7JA:H04	4:B:1100:7JA:C12	1.84	1.07
4:D:1100:7JA:H04	4:D:1100:7JA:C12	1.84	1.06
1:M:102:ILE:HD12	2:N:20:VAL:HG21	1.38	1.06
4:L:1100:7JA:H04	4:L:1100:7JA:C12	1.86	1.05
2:H:442:ALA:HB3	4:H:1100:7JA:HD1	1.36	1.04
4:J:1100:7JA:H04	4:J:1100:7JA:C12	1.87	1.03
2:H:398:ILE:HG23	2:H:402:LEU:HD11	1.39	1.03
4:P:1100:7JA:H04	4:P:1100:7JA:C12	1.87	1.02
2:H:366:SER:HB3	2:H:368:ARG:HG2	1.36	1.02
4:N:1100:7JA:C12	4:N:1100:7JA:H04	1.89	1.01
2:P:93:PRO:HA	2:P:548:ARG:HB2	1.42	1.01
1:G:151:VAL:CG1	2:H:39:LEU:HD21	1.91	1.01
2:H:274:ARG:HG2	2:H:297:LYS:HB3	1.43	1.00
2:L:93:PRO:HA	2:L:548:ARG:HB2	1.43	0.99
2:H:364:LEU:HB3	2:H:365:VAL:HG22	1.44	0.99
2:F:93:PRO:HA	2:F:548:ARG:HB2	1.45	0.99
2:D:386:TYR:CE1	4:D:1100:7JA:HG2	1.98	0.98
2:N:93:PRO:HA	2:N:548:ARG:HB2	1.42	0.98
2:H:519:TRP:NE1	4:H:1100:7JA:H01A	1.78	0.98
2:N:519:TRP:HE1	4:N:1100:7JA:H01A	1.28	0.98
2:D:80:LEU:HB2	2:D:122:MET:HE2	1.41	0.98
1:M:102:ILE:CD1	2:N:20:VAL:HG21	1.93	0.98
2:H:347:LEU:HD12	2:H:348:ARG:N	1.78	0.97
2:D:93:PRO:HA	2:D:548:ARG:HB2	1.46	0.97
2:N:386:TYR:CE1	4:N:1100:7JA:HG2	1.98	0.97
2:H:323:LEU:HD11	2:H:325:THR:HG22	1.46	0.97
2:N:444:TYR:HA	2:N:471:GLY:HA3	1.46	0.97
2:H:283:ASN:O	2:H:286:PRO:HD2	1.64	0.97
2:L:542:ILE:HD11	2:L:588:LEU:HD12	1.45	0.96
4:B:1100:7JA:C04	4:B:1100:7JA:C12	2.42	0.96
2:B:444:TYR:HA	2:B:471:GLY:HA3	1.47	0.96
2:L:386:TYR:CE1	4:L:1100:7JA:HG2	2.00	0.96
2:D:444:TYR:HA	2:D:471:GLY:HA3	1.47	0.95
2:F:386:TYR:CE1	4:F:1100:7JA:HG2	2.00	0.95
2:N:116:SER:HB2	2:N:142:THR:HG23	1.48	0.95
2:F:444:TYR:HA	2:F:471:GLY:HA3	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:ARG:HE	2:N:112:ARG:HG3	1.32	0.95
2:B:93:PRO:HA	2:B:548:ARG:HB2	1.46	0.95
2:P:519:TRP:HE1	4:P:1100:7JA:H01A	1.30	0.94
2:H:409:ARG:HB3	4:H:1100:7JA:H29	1.49	0.94
4:N:1100:7JA:C04	4:N:1100:7JA:C12	2.46	0.93
2:F:519:TRP:HE1	4:F:1100:7JA:H01A	1.32	0.93
2:N:546:PRO:HG2	2:N:584:THR:HB	1.50	0.93
2:J:386:TYR:CE1	4:J:1100:7JA:HG2	2.03	0.93
1:M:102:ILE:HG21	2:N:20:VAL:CG2	1.98	0.93
4:L:1100:7JA:C12	4:L:1100:7JA:C04	2.45	0.93
2:P:429:ARG:O	2:P:433:ILE:HG13	1.67	0.93
2:H:366:SER:CB	2:H:368:ARG:HG2	1.98	0.92
2:D:101:THR:HG22	2:D:128:ASP:OD1	1.69	0.92
2:J:93:PRO:HA	2:J:548:ARG:HB2	1.49	0.92
2:B:101:THR:HG22	2:B:128:ASP:OD1	1.69	0.91
2:F:101:THR:HG22	2:F:128:ASP:OD1	1.70	0.91
2:H:332:ARG:HH11	2:H:332:ARG:HG2	1.34	0.91
4:J:1100:7JA:C12	4:J:1100:7JA:C04	2.47	0.91
4:F:1100:7JA:C12	4:F:1100:7JA:C04	2.46	0.91
2:B:386:TYR:CE1	4:B:1100:7JA:HG2	2.04	0.91
2:B:542:ILE:HD11	2:B:588:LEU:HD12	1.51	0.91
2:P:101:THR:HG22	2:P:128:ASP:OD1	1.70	0.91
4:D:1100:7JA:C04	4:D:1100:7JA:C12	2.46	0.90
2:P:386:TYR:CE1	4:P:1100:7JA:HG2	2.06	0.90
2:J:519:TRP:NE1	4:J:1100:7JA:H01A	1.86	0.90
2:J:542:ILE:HD11	2:J:588:LEU:HD12	1.52	0.90
2:B:519:TRP:HE1	4:B:1100:7JA:H01A	1.34	0.90
2:F:546:PRO:HG2	2:F:584:THR:HB	1.53	0.90
2:F:542:ILE:HD11	2:F:588:LEU:HD12	1.52	0.90
4:P:1100:7JA:C04	4:P:1100:7JA:C12	2.47	0.90
2:H:97:GLY:HA3	2:H:123:ILE:HD11	1.52	0.90
4:B:1100:7JA:H12	4:B:1100:7JA:C04	2.01	0.89
2:N:142:THR:HB	2:N:168:THR:HG23	1.54	0.89
2:J:164:ARG:HE	2:N:112:ARG:CG	1.85	0.89
2:L:101:THR:HG22	2:L:128:ASP:OD1	1.72	0.89
2:P:444:TYR:HA	2:P:471:GLY:HA3	1.54	0.89
2:J:519:TRP:HE1	4:J:1100:7JA:H01A	1.35	0.89
2:L:519:TRP:HE1	4:L:1100:7JA:H01A	1.36	0.89
2:B:590:GLU:HB3	2:B:591:PRO:HD2	1.55	0.89
2:P:519:TRP:NE1	4:P:1100:7JA:H01A	1.88	0.89
2:H:305:LEU:HD23	2:H:305:LEU:H	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:590:GLU:HB3	2:N:591:PRO:HD2	1.55	0.88
2:P:590:GLU:HB3	2:P:591:PRO:HD2	1.55	0.88
2:N:519:TRP:NE1	4:N:1100:7JA:H01A	1.87	0.88
2:J:444:TYR:HA	2:J:471:GLY:HA3	1.53	0.88
2:N:429:ARG:O	2:N:433:ILE:HG13	1.72	0.88
1:M:96:ALA:HB1	2:N:14:VAL:HG12	1.55	0.88
2:L:444:TYR:HA	2:L:471:GLY:HA3	1.54	0.88
2:P:542:ILE:HD11	2:P:588:LEU:HD12	1.54	0.88
4:L:1100:7JA:H12	4:L:1100:7JA:C04	2.04	0.88
2:B:519:TRP:NE1	4:B:1100:7JA:H01A	1.88	0.88
2:N:542:ILE:HD11	2:N:588:LEU:HD12	1.56	0.88
1:C:48:THR:HG22	1:C:51:ILE:H	1.39	0.87
2:D:590:GLU:HB3	2:D:591:PRO:HD2	1.55	0.87
2:H:199:PHE:CZ	2:H:227:VAL:HG23	2.10	0.87
4:P:1100:7JA:C04	4:P:1100:7JA:H12	2.04	0.87
2:D:80:LEU:HB2	2:D:122:MET:CE	2.03	0.87
2:H:142:THR:HB	2:H:168:THR:OG1	1.74	0.86
2:F:519:TRP:NE1	4:F:1100:7JA:H01A	1.88	0.86
2:D:116:SER:HB2	2:D:142:THR:HG23	1.57	0.86
2:H:428:VAL:HG12	2:H:443:PHE:CZ	2.11	0.86
4:J:1100:7JA:C04	4:J:1100:7JA:H12	2.04	0.86
2:L:546:PRO:HG2	2:L:584:THR:HB	1.57	0.86
2:H:201:MET:HG3	2:H:302:TYR:CE1	2.09	0.86
2:H:311:CYS:HB3	2:H:336:VAL:HG21	1.55	0.86
2:P:286:PRO:HA	2:P:289:PHE:CE2	2.11	0.86
2:H:444:TYR:HA	2:H:471:GLY:HA3	1.58	0.86
2:H:371:ILE:HG22	2:H:375:GLN:HE21	1.40	0.86
2:D:519:TRP:NE1	4:D:1100:7JA:H01A	1.91	0.85
2:H:519:TRP:HH2	2:H:567:HIS:HD1	1.21	0.85
2:B:116:SER:HB2	2:B:142:THR:HG23	1.56	0.85
2:H:442:ALA:HB3	4:H:1100:7JA:CD1	2.04	0.85
2:J:590:GLU:HB3	2:J:591:PRO:HD2	1.56	0.85
2:L:590:GLU:HB3	2:L:591:PRO:HD2	1.55	0.85
2:P:142:THR:HB	2:P:168:THR:HG23	1.57	0.85
2:P:546:PRO:HG2	2:P:584:THR:HB	1.58	0.85
2:B:590:GLU:HB3	2:B:591:PRO:CD	2.07	0.85
1:K:102:ILE:HG12	1:K:117:THR:HB	1.58	0.85
2:J:80:LEU:HB2	2:J:122:MET:HE1	1.57	0.85
2:L:429:ARG:O	2:L:433:ILE:HG13	1.77	0.85
2:L:519:TRP:NE1	4:L:1100:7JA:H01A	1.91	0.85
2:D:542:ILE:HD11	2:D:588:LEU:HD12	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:SER:HB2	2:F:142:THR:HG23	1.59	0.84
2:D:590:GLU:HB3	2:D:591:PRO:CD	2.07	0.84
2:N:80:LEU:HB2	2:N:122:MET:HE2	1.57	0.84
2:P:590:GLU:HB3	2:P:591:PRO:CD	2.07	0.84
4:F:1100:7JA:C04	4:F:1100:7JA:H12	2.05	0.84
2:F:590:GLU:HB3	2:F:591:PRO:HD2	1.58	0.84
2:H:54:HIS:HE1	2:H:56:THR:OG1	1.61	0.84
2:D:519:TRP:HE1	4:D:1100:7JA:H01A	1.39	0.84
2:N:101:THR:HG22	2:N:128:ASP:OD1	1.77	0.84
2:H:409:ARG:HB3	4:H:1100:7JA:CG1	2.08	0.84
1:I:48:THR:HG22	1:I:51:ILE:H	1.42	0.84
2:J:101:THR:HG22	2:J:128:ASP:OD1	1.77	0.84
2:H:286:PRO:HA	2:H:289:PHE:CE2	2.12	0.83
2:P:116:SER:HB2	2:P:142:THR:HG23	1.59	0.83
2:N:590:GLU:HB3	2:N:591:PRO:CD	2.07	0.83
2:N:80:LEU:HB2	2:N:122:MET:CE	2.07	0.83
4:D:1100:7JA:H12	4:D:1100:7JA:C04	2.05	0.83
2:J:590:GLU:HB3	2:J:591:PRO:CD	2.08	0.83
1:E:48:THR:HG22	1:E:51:ILE:H	1.43	0.83
2:J:429:ARG:O	2:J:433:ILE:HG13	1.78	0.83
4:B:1100:7JA:C04	4:B:1100:7JA:H12A	2.08	0.83
2:B:429:ARG:O	2:B:433:ILE:HG13	1.78	0.83
2:J:546:PRO:HG2	2:J:584:THR:HB	1.60	0.83
2:L:590:GLU:HB3	2:L:591:PRO:CD	2.09	0.83
1:M:125:ILE:HG23	1:M:133:ILE:HD12	1.61	0.83
1:G:48:THR:HG22	1:G:51:ILE:H	1.43	0.82
1:C:125:ILE:HG23	1:C:133:ILE:HD12	1.59	0.82
2:N:519:TRP:HE1	4:N:1100:7JA:C01	1.92	0.82
2:H:390:ILE:HD12	2:H:410:LEU:HD21	1.62	0.82
2:J:80:LEU:HB2	2:J:122:MET:CE	2.08	0.82
1:M:102:ILE:CD1	2:N:20:VAL:CG2	2.58	0.82
2:F:429:ARG:O	2:F:433:ILE:HG13	1.79	0.82
2:H:542:ILE:HD12	2:H:542:ILE:C	1.99	0.82
2:H:492:LYS:NZ	2:H:516:ARG:HH11	1.77	0.81
1:K:125:ILE:HG23	1:K:133:ILE:HD12	1.63	0.81
2:F:142:THR:HB	2:F:168:THR:HG23	1.60	0.81
2:J:116:SER:HB2	2:J:142:THR:HG23	1.61	0.81
4:L:1100:7JA:C04	4:L:1100:7JA:H12A	2.11	0.81
2:F:590:GLU:HB3	2:F:591:PRO:CD	2.10	0.81
1:G:151:VAL:HG11	2:H:39:LEU:CD2	2.09	0.81
2:D:546:PRO:HG2	2:D:584:THR:HB	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:142:THR:HB	2:J:168:THR:HG23	1.62	0.81
1:K:93:ILE:HD12	1:K:97:THR:HG22	1.62	0.81
2:H:409:ARG:HB3	4:H:1100:7JA:CD1	2.11	0.81
2:J:519:TRP:HE1	4:J:1100:7JA:C01	1.94	0.80
2:H:328:VAL:HG13	2:H:359:GLU:HG2	1.62	0.80
1:M:96:ALA:HB1	2:N:14:VAL:CG1	2.10	0.80
2:H:201:MET:HG3	2:H:302:TYR:HE1	1.46	0.80
1:M:99:PHE:HD2	2:N:15:ALA:O	1.63	0.80
1:A:93:ILE:HD12	1:A:97:THR:HG22	1.61	0.80
1:C:93:ILE:HD12	1:C:97:THR:HG22	1.63	0.80
2:F:112:ARG:HG2	2:L:164:ARG:HD2	1.64	0.80
2:L:519:TRP:HE1	4:L:1100:7JA:C01	1.95	0.80
1:M:93:ILE:HD12	1:M:97:THR:HG22	1.63	0.80
2:L:116:SER:HB2	2:L:142:THR:HG23	1.62	0.80
4:N:1100:7JA:C04	4:N:1100:7JA:H12A	2.10	0.80
1:M:102:ILE:HG21	2:N:20:VAL:HG22	1.62	0.80
4:D:1100:7JA:C04	4:D:1100:7JA:H12A	2.12	0.80
2:B:142:THR:HB	2:B:168:THR:HG23	1.64	0.80
2:J:164:ARG:HD2	2:N:112:ARG:HG2	1.63	0.80
1:M:99:PHE:CD2	2:N:16:THR:C	2.56	0.80
1:A:48:THR:HG22	1:A:51:ILE:H	1.46	0.80
2:B:519:TRP:HE1	4:B:1100:7JA:C01	1.95	0.80
2:P:419:ILE:HD11	2:P:446:ARG:HH22	1.47	0.79
1:O:48:THR:HG22	1:O:51:ILE:H	1.46	0.79
2:L:286:PRO:HA	2:L:289:PHE:CE2	2.18	0.79
2:L:80:LEU:HB2	2:L:122:MET:CE	2.12	0.79
2:H:542:ILE:CG1	2:H:588:LEU:HB2	2.12	0.79
2:L:142:THR:HB	2:L:168:THR:HG23	1.64	0.79
2:H:266:LEU:HD13	2:H:267:VAL:H	1.48	0.78
4:F:1100:7JA:C04	4:F:1100:7JA:H12A	2.13	0.78
2:P:519:TRP:HE1	4:P:1100:7JA:C01	1.96	0.78
1:M:48:THR:HG22	1:M:51:ILE:H	1.48	0.78
1:E:93:ILE:HD12	1:E:97:THR:HG22	1.66	0.78
2:H:160:VAL:HG11	2:H:187:LEU:HG	1.65	0.78
2:N:286:PRO:HA	2:N:289:PHE:CE2	2.18	0.78
2:F:519:TRP:HE1	4:F:1100:7JA:C01	1.97	0.78
1:K:48:THR:HG22	1:K:51:ILE:H	1.47	0.78
2:F:80:LEU:HB2	2:F:122:MET:CE	2.14	0.78
2:H:230:PHE:HD1	2:H:235:LEU:HD21	1.49	0.78
2:H:125:SER:HB2	2:H:128:ASP:H	1.48	0.78
1:I:125:ILE:HG23	1:I:133:ILE:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:357:GLY:HA2	2:J:415:ARG:HH22	1.49	0.77
2:L:308:GLU:HG3	2:L:332:ARG:HH22	1.50	0.77
2:N:455:LEU:HD22	2:N:483:PHE:HB2	1.67	0.77
2:F:419:ILE:HD11	2:F:446:ARG:HH22	1.49	0.77
1:G:155:ASN:HB3	2:H:35:ASP:OD2	1.85	0.77
2:D:308:GLU:HG3	2:D:332:ARG:HH22	1.50	0.77
2:H:178:GLU:OE1	2:H:206:LYS:HB3	1.84	0.77
2:D:429:ARG:O	2:D:433:ILE:HG13	1.84	0.77
1:O:159:PHE:O	1:O:160:GLU:HB2	1.84	0.76
2:B:440:ARG:HB3	2:B:467:TRP:HE3	1.50	0.76
2:D:519:TRP:HE1	4:D:1100:7JA:C01	1.98	0.76
2:J:419:ILE:HD11	2:J:446:ARG:HH22	1.48	0.76
1:O:113:LEU:HG	1:O:113:LEU:O	1.83	0.76
2:H:92:ILE:HD13	2:H:93:PRO:HD2	1.67	0.76
2:P:80:LEU:HB2	2:P:122:MET:CE	2.15	0.76
2:F:455:LEU:HD22	2:F:483:PHE:HB2	1.67	0.76
2:L:349:ILE:HG13	2:L:385:VAL:HG22	1.67	0.76
2:J:398:ILE:HG23	2:J:402:LEU:HD11	1.68	0.76
2:B:546:PRO:HG2	2:B:584:THR:HB	1.65	0.76
2:D:419:ILE:HD11	2:D:446:ARG:HH22	1.49	0.76
2:B:80:LEU:HB2	2:B:122:MET:HE1	1.65	0.76
2:L:357:GLY:HA2	2:L:415:ARG:HH22	1.50	0.76
2:H:331:ASP:OD2	2:H:366:SER:HB2	1.84	0.76
1:O:125:ILE:HG23	1:O:133:ILE:HD12	1.67	0.76
2:H:285:MET:HE1	2:H:309:ASP:HB3	1.69	0.75
2:F:443:PHE:CE2	2:F:445:LEU:HD11	2.21	0.75
2:J:240:LYS:HG3	2:J:267:VAL:HG21	1.67	0.75
2:H:373:LEU:HD12	2:H:373:LEU:O	1.85	0.75
2:F:59:LEU:HD22	2:F:61:TYR:H	1.49	0.75
2:H:323:LEU:CD1	2:H:325:THR:HG22	2.16	0.75
1:M:159:PHE:O	1:M:160:GLU:HB2	1.84	0.75
2:F:286:PRO:HA	2:F:289:PHE:CE2	2.21	0.75
1:M:112:ASN:C	1:M:114:LEU:H	1.89	0.75
2:N:349:ILE:HG13	2:N:385:VAL:HG22	1.68	0.75
4:P:1100:7JA:C04	4:P:1100:7JA:H12A	2.16	0.75
2:H:519:TRP:HE1	4:H:1100:7JA:C01	1.90	0.75
2:H:519:TRP:CH2	2:H:567:HIS:ND1	2.53	0.75
2:L:455:LEU:HD22	2:L:483:PHE:HB2	1.68	0.75
2:P:310:HIS:O	2:P:314:ILE:HG12	1.87	0.75
2:H:400:THR:O	2:H:403:LYS:HE2	1.87	0.75
4:D:1100:7JA:H04	4:D:1100:7JA:H12A	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:OE2	1:A:160:GLU:HA	1.86	0.75
2:P:357:GLY:HA2	2:P:415:ARG:HH22	1.52	0.75
4:J:1100:7JA:H12A	4:J:1100:7JA:C04	2.14	0.75
2:P:55:VAL:HG23	2:P:75:LEU:HD21	1.68	0.75
4:F:1100:7JA:H12A	4:F:1100:7JA:H04	1.69	0.74
2:H:286:PRO:HA	2:H:289:PHE:CD2	2.22	0.74
1:K:159:PHE:O	1:K:160:GLU:HB2	1.85	0.74
2:N:299:ASP:OD2	2:N:301:LEU:HB2	1.86	0.74
2:H:396:GLU:O	2:H:400:THR:HG23	1.86	0.74
2:B:286:PRO:HA	2:B:289:PHE:CE2	2.22	0.74
1:C:159:PHE:O	1:C:160:GLU:HB2	1.87	0.74
1:I:93:ILE:HD12	1:I:97:THR:HG22	1.69	0.74
2:N:454:GLY:O	2:N:457:TYR:HB2	1.88	0.74
2:D:164:ARG:HD2	2:H:112:ARG:HD3	1.70	0.74
2:P:308:GLU:HG3	2:P:332:ARG:HH22	1.52	0.74
1:E:160:GLU:HA	1:E:160:GLU:OE2	1.86	0.74
2:P:440:ARG:HB3	2:P:467:TRP:HE3	1.53	0.74
2:N:419:ILE:HD11	2:N:446:ARG:HH22	1.51	0.74
2:B:308:GLU:HG3	2:B:332:ARG:HH22	1.53	0.74
2:B:419:ILE:HD11	2:B:446:ARG:HH22	1.51	0.74
1:G:160:GLU:OE1	1:G:160:GLU:HA	1.87	0.74
2:N:55:VAL:HG23	2:N:75:LEU:HD21	1.67	0.73
2:P:455:LEU:HD22	2:P:483:PHE:HB2	1.69	0.73
2:F:240:LYS:HG3	2:F:267:VAL:HG21	1.70	0.73
1:I:160:GLU:HA	1:I:160:GLU:OE2	1.86	0.73
2:B:80:LEU:HB2	2:B:122:MET:CE	2.17	0.73
2:J:440:ARG:HB3	2:J:467:TRP:HE3	1.53	0.73
2:N:357:GLY:HA2	2:N:415:ARG:HH22	1.53	0.73
2:N:240:LYS:HG3	2:N:267:VAL:HG21	1.71	0.73
2:F:308:GLU:HG3	2:F:332:ARG:HH22	1.51	0.73
2:B:191:ASN:HD21	2:B:194:LEU:H	1.34	0.73
2:H:428:VAL:CG1	2:H:443:PHE:CZ	2.71	0.73
2:L:443:PHE:CE2	2:L:445:LEU:HD11	2.24	0.73
2:J:311:CYS:HB3	2:J:336:VAL:HG21	1.69	0.73
1:O:93:ILE:HD12	1:O:97:THR:HG22	1.71	0.73
1:A:159:PHE:O	1:A:160:GLU:HB2	1.89	0.73
1:O:160:GLU:HA	1:O:160:GLU:OE2	1.89	0.72
1:G:93:ILE:HD12	1:G:97:THR:HG22	1.71	0.72
2:D:440:ARG:HB3	2:D:467:TRP:HE3	1.53	0.72
1:A:125:ILE:HG23	1:A:133:ILE:HD12	1.71	0.72
2:N:398:ILE:HG23	2:N:402:LEU:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:THR:HG22	1:M:51:ILE:HB	1.71	0.72
2:F:328:VAL:HG22	2:F:359:GLU:HB2	1.71	0.72
2:B:357:GLY:HA2	2:B:415:ARG:HH22	1.53	0.72
2:P:367:GLN:O	2:P:371:ILE:HG22	1.89	0.72
2:H:199:PHE:CE1	2:H:227:VAL:HG23	2.24	0.72
2:J:286:PRO:HA	2:J:289:PHE:CE2	2.24	0.72
2:D:357:GLY:HA2	2:D:415:ARG:HH22	1.55	0.72
2:J:308:GLU:HG3	2:J:332:ARG:HH22	1.53	0.72
2:L:398:ILE:HG23	2:L:402:LEU:HD11	1.71	0.72
2:D:142:THR:HB	2:D:168:THR:HG23	1.71	0.72
2:L:289:PHE:CD1	2:L:316:LYS:HD2	2.25	0.72
2:L:240:LYS:HG3	2:L:267:VAL:HG21	1.70	0.72
2:H:20:VAL:O	2:H:24:VAL:HG23	1.89	0.72
1:M:96:ALA:CB	2:N:14:VAL:HG12	2.19	0.72
2:H:213:GLU:CD	2:H:237:GLY:HA3	2.10	0.72
2:P:240:LYS:HG3	2:P:267:VAL:HG21	1.72	0.72
2:H:371:ILE:O	2:H:375:GLN:HG3	1.90	0.72
2:J:349:ILE:HG13	2:J:385:VAL:HG22	1.70	0.72
2:P:328:VAL:HG22	2:P:359:GLU:HB2	1.71	0.72
2:F:545:ILE:HB	2:F:567:HIS:HB2	1.72	0.72
1:E:159:PHE:O	1:E:160:GLU:HB2	1.90	0.72
2:P:184:LEU:HD12	2:P:207:ILE:HB	1.71	0.72
2:D:398:ILE:HG23	2:D:402:LEU:HD11	1.71	0.71
2:D:431:LEU:C	2:D:431:LEU:HD12	2.11	0.71
2:D:519:TRP:HH2	2:D:567:HIS:CE1	2.08	0.71
2:D:328:VAL:HG22	2:D:359:GLU:HB2	1.72	0.71
2:N:443:PHE:CE2	2:N:445:LEU:HD11	2.25	0.71
3:S:203:ILE:HD12	3:S:203:ILE:H	1.55	0.71
2:D:286:PRO:HA	2:D:289:PHE:CE2	2.26	0.71
2:D:191:ASN:HD21	2:D:194:LEU:H	1.39	0.71
2:J:419:ILE:HD13	2:J:446:ARG:HH12	1.54	0.71
2:H:277:LEU:O	2:H:278:SER:O	2.08	0.71
2:H:322:VAL:HG22	2:H:346:ARG:HB2	1.72	0.71
2:F:357:GLY:HA2	2:F:415:ARG:HH22	1.55	0.71
2:N:308:GLU:HG3	2:N:332:ARG:HH22	1.54	0.71
2:L:184:LEU:HD12	2:L:207:ILE:HB	1.73	0.71
2:D:240:LYS:HG3	2:D:267:VAL:HG21	1.71	0.71
2:B:349:ILE:HG13	2:B:385:VAL:HG22	1.71	0.71
2:H:364:LEU:HD22	2:H:387:VAL:HA	1.73	0.70
2:D:443:PHE:CE2	2:D:445:LEU:HD11	2.26	0.70
2:P:59:LEU:HD22	2:P:61:TYR:H	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:286:PRO:HA	2:P:289:PHE:CD2	2.26	0.70
1:E:48:THR:HG22	1:E:51:ILE:HB	1.73	0.70
2:L:419:ILE:HD11	2:L:446:ARG:HH22	1.54	0.70
2:L:59:LEU:HD22	2:L:61:TYR:H	1.55	0.70
4:P:1100:7JA:H04	4:P:1100:7JA:H12A	1.73	0.70
2:H:77:SER:HB3	2:H:116:SER:HB3	1.73	0.70
2:F:80:LEU:HB2	2:F:122:MET:HE1	1.73	0.70
2:J:55:VAL:HG23	2:J:75:LEU:HD21	1.74	0.70
2:F:310:HIS:O	2:F:314:ILE:HG12	1.91	0.70
2:H:468:MET:HG3	2:H:490:LEU:HD21	1.73	0.70
2:P:311:CYS:HB3	2:P:336:VAL:HG21	1.73	0.70
2:J:210:LYS:O	2:J:214:THR:HG22	1.92	0.70
2:B:59:LEU:HD22	2:B:61:TYR:H	1.57	0.70
2:H:160:VAL:CG1	2:H:187:LEU:HG	2.21	0.70
2:F:419:ILE:HD13	2:F:446:ARG:HH12	1.55	0.69
1:C:160:GLU:OE2	1:C:160:GLU:HA	1.91	0.69
2:N:328:VAL:HG22	2:N:359:GLU:HB2	1.73	0.69
2:F:454:GLY:O	2:F:457:TYR:HB2	1.92	0.69
2:F:398:ILE:HG23	2:F:402:LEU:HD11	1.73	0.69
2:L:328:VAL:HG22	2:L:359:GLU:HB2	1.73	0.69
2:J:328:VAL:HG22	2:J:359:GLU:HB2	1.74	0.69
2:P:545:ILE:HB	2:P:567:HIS:HB2	1.73	0.69
2:D:59:LEU:HD22	2:D:61:TYR:H	1.58	0.69
1:M:102:ILE:CG2	2:N:20:VAL:CG2	2.69	0.69
1:M:160:GLU:HA	1:M:160:GLU:OE2	1.91	0.69
2:B:455:LEU:HD22	2:B:483:PHE:HB2	1.74	0.69
4:N:1100:7JA:H12A	4:N:1100:7JA:H04	1.72	0.69
2:H:325:THR:OG1	2:H:326:ARG:O	2.11	0.69
1:M:129:THR:O	1:M:133:ILE:HG12	1.92	0.69
1:K:160:GLU:OE2	1:K:160:GLU:HA	1.90	0.69
2:P:398:ILE:HG23	2:P:402:LEU:HD11	1.74	0.69
2:L:431:LEU:HD12	2:L:431:LEU:C	2.13	0.69
2:J:164:ARG:NE	2:N:112:ARG:CG	2.55	0.69
2:J:59:LEU:HD22	2:J:61:TYR:H	1.57	0.69
2:B:143:LEU:HD23	2:B:159:ILE:HD13	1.74	0.69
2:D:251:GLY:O	2:D:278:SER:HB2	1.93	0.69
3:U:203:ILE:H	3:U:203:ILE:HD12	1.57	0.69
2:L:251:GLY:O	2:L:278:SER:HB2	1.93	0.69
3:V:203:ILE:HD12	3:V:203:ILE:H	1.57	0.69
2:F:191:ASN:HD21	2:F:194:LEU:H	1.39	0.69
2:D:563:GLU:O	2:D:563:GLU:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:299:ASP:OD2	2:J:301:LEU:HB2	1.94	0.68
2:H:492:LYS:HZ3	2:H:516:ARG:HH11	1.39	0.68
1:I:159:PHE:O	1:I:160:GLU:HB2	1.92	0.68
2:N:59:LEU:HD22	2:N:61:TYR:H	1.56	0.68
2:F:349:ILE:HG13	2:F:385:VAL:HG22	1.75	0.68
2:N:391:THR:HG23	2:N:394:SER:H	1.58	0.68
2:P:143:LEU:HD23	2:P:159:ILE:HD13	1.74	0.68
2:P:251:GLY:O	2:P:278:SER:HB2	1.93	0.68
2:N:440:ARG:HB3	2:N:467:TRP:HE3	1.58	0.68
2:J:563:GLU:O	2:J:563:GLU:HG3	1.93	0.68
2:D:419:ILE:HD13	2:D:446:ARG:HH12	1.59	0.68
2:B:210:LYS:O	2:B:214:THR:HG22	1.93	0.68
2:B:351:ARG:HD3	2:B:413:LEU:HD11	1.75	0.68
2:B:328:VAL:HG22	2:B:359:GLU:HB2	1.74	0.68
2:B:240:LYS:HG3	2:B:267:VAL:HG21	1.76	0.68
2:D:545:ILE:HB	2:D:567:HIS:HB2	1.73	0.68
1:M:102:ILE:HD13	2:N:20:VAL:HG22	1.75	0.68
2:J:164:ARG:CD	2:N:112:ARG:HG2	2.23	0.68
2:H:367:GLN:O	2:H:371:ILE:HG13	1.93	0.68
2:J:357:GLY:CA	2:J:415:ARG:HH22	2.07	0.68
2:H:428:VAL:HG23	2:H:429:ARG:N	2.08	0.68
4:N:1100:7JA:H12	4:N:1100:7JA:C04	2.05	0.68
1:O:48:THR:HG22	1:O:51:ILE:HB	1.76	0.68
2:H:278:SER:O	2:H:280:MET:N	2.26	0.68
2:F:55:VAL:HG23	2:F:75:LEU:HD21	1.75	0.68
2:L:80:LEU:HB2	2:L:122:MET:HE1	1.76	0.68
2:D:455:LEU:HD22	2:D:483:PHE:HB2	1.74	0.68
2:P:349:ILE:HG13	2:P:385:VAL:HG22	1.75	0.68
2:L:210:LYS:O	2:L:214:THR:HG22	1.92	0.68
2:P:443:PHE:CE2	2:P:445:LEU:HD11	2.29	0.68
2:P:191:ASN:HD21	2:P:194:LEU:H	1.40	0.68
2:F:251:GLY:O	2:F:278:SER:HB2	1.93	0.68
2:B:487:CYS:HB3	2:B:490:LEU:HB2	1.75	0.68
2:D:289:PHE:CD1	2:D:316:LYS:HD2	2.29	0.67
2:L:468:MET:HE3	2:L:470:LEU:HD21	1.75	0.67
2:N:307:THR:HG21	2:N:362:GLU:HB2	1.76	0.67
3:W:203:ILE:HD12	3:W:203:ILE:H	1.59	0.67
2:L:563:GLU:O	2:L:563:GLU:HG3	1.94	0.67
2:L:391:THR:HG23	2:L:394:SER:H	1.59	0.67
2:J:424:LEU:O	2:J:428:VAL:HG23	1.94	0.67
2:H:168:THR:HB	2:H:196:VAL:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:367:GLN:O	2:N:371:ILE:HG22	1.95	0.67
2:N:487:CYS:HB3	2:N:490:LEU:HB2	1.76	0.67
1:G:132:GLU:O	1:G:136:THR:HG23	1.93	0.67
2:N:545:ILE:HB	2:N:567:HIS:HB2	1.75	0.67
2:H:443:PHE:CE2	2:H:445:LEU:HD11	2.29	0.67
2:L:311:CYS:HB3	2:L:336:VAL:HG21	1.77	0.67
2:J:365:VAL:HG23	2:J:387:VAL:HA	1.77	0.67
2:P:357:GLY:CA	2:P:415:ARG:HH22	2.07	0.67
2:J:455:LEU:HD22	2:J:483:PHE:HB2	1.76	0.67
2:H:232:ILE:HG13	2:H:253:LEU:CD2	2.25	0.67
2:H:347:LEU:HD12	2:H:348:ARG:H	1.59	0.67
1:G:30:ALA:O	1:G:33:VAL:HG22	1.94	0.67
1:E:125:ILE:HG23	1:E:133:ILE:HD12	1.77	0.67
2:B:563:GLU:O	2:B:563:GLU:HG3	1.94	0.67
1:M:102:ILE:HD13	2:N:20:VAL:CG2	2.23	0.67
2:J:191:ASN:HD21	2:J:194:LEU:H	1.42	0.67
2:H:441:PHE:CZ	2:H:443:PHE:CD1	2.83	0.67
2:F:286:PRO:HA	2:F:289:PHE:CD2	2.30	0.67
2:B:365:VAL:HG23	2:B:387:VAL:HA	1.75	0.67
2:P:468:MET:HE3	2:P:470:LEU:HD21	1.77	0.67
1:E:45:PRO:HG3	2:L:293:ALA:HB3	1.75	0.67
2:J:545:ILE:HB	2:J:567:HIS:HB2	1.75	0.67
2:B:533:MET:HE3	2:B:588:LEU:HD13	1.76	0.67
2:P:289:PHE:CD1	2:P:316:LYS:HD2	2.29	0.67
1:A:48:THR:HG22	1:A:51:ILE:HB	1.77	0.67
2:L:431:LEU:HD12	2:L:431:LEU:O	1.95	0.67
2:J:184:LEU:HD12	2:J:207:ILE:HB	1.74	0.67
2:D:307:THR:HG21	2:D:362:GLU:HB2	1.77	0.67
1:I:158:ALA:HA	2:J:62:THR:HG21	1.77	0.67
1:G:48:THR:CG2	1:G:51:ILE:H	2.07	0.67
2:H:542:ILE:HD11	2:H:588:LEU:HB2	1.76	0.67
2:D:95:ASN:O	2:D:582:PRO:HG3	1.95	0.67
2:B:519:TRP:HH2	2:B:567:HIS:CE1	2.13	0.66
2:L:357:GLY:CA	2:L:415:ARG:HH22	2.07	0.66
2:P:93:PRO:HA	2:P:548:ARG:CB	2.22	0.66
2:F:311:CYS:HB3	2:F:336:VAL:HG21	1.77	0.66
2:D:349:ILE:HG13	2:D:385:VAL:HG22	1.77	0.66
2:F:289:PHE:CD1	2:F:316:LYS:HD2	2.31	0.66
2:B:357:GLY:CA	2:B:415:ARG:HH22	2.08	0.66
2:B:55:VAL:HG23	2:B:75:LEU:HD21	1.77	0.66
2:J:251:GLY:O	2:J:278:SER:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:545:ILE:HB	2:H:567:HIS:HB2	1.77	0.66
1:G:48:THR:HG22	1:G:51:ILE:HB	1.77	0.66
2:P:454:GLY:O	2:P:457:TYR:HB2	1.94	0.66
2:F:184:LEU:HD12	2:F:207:ILE:HB	1.78	0.66
2:F:211:ASP:HA	2:F:214:THR:HG23	1.78	0.66
2:P:519:TRP:HH2	2:P:567:HIS:CE1	2.13	0.66
2:D:54:HIS:HD2	2:D:77:SER:OG	1.78	0.66
2:J:454:GLY:O	2:J:457:TYR:HB2	1.96	0.66
2:H:332:ARG:CG	2:H:332:ARG:HH11	2.07	0.66
2:N:211:ASP:HA	2:N:214:THR:HG23	1.78	0.66
2:D:365:VAL:HG23	2:D:387:VAL:HA	1.77	0.66
1:I:153:ARG:HG2	1:I:157:TRP:CZ3	2.30	0.66
3:R:203:ILE:HD12	3:R:203:ILE:H	1.61	0.66
2:H:392:ASN:O	2:H:396:GLU:HG3	1.95	0.66
2:N:286:PRO:HA	2:N:289:PHE:CD2	2.31	0.66
1:G:128:LYS:HE3	1:G:136:THR:HG21	1.78	0.66
2:B:311:CYS:HB3	2:B:336:VAL:HG21	1.76	0.66
2:J:289:PHE:CD1	2:J:316:LYS:HD2	2.30	0.66
2:D:468:MET:HE3	2:D:470:LEU:HD21	1.78	0.66
2:L:55:VAL:HG23	2:L:75:LEU:HD21	1.76	0.66
1:A:102:ILE:CG1	1:A:117:THR:HB	2.25	0.66
1:G:144:THR:HG23	1:G:147:GLU:OE2	1.96	0.65
2:J:443:PHE:CE2	2:J:445:LEU:HD11	2.31	0.65
2:H:584:THR:HG22	2:H:584:THR:O	1.95	0.65
2:J:519:TRP:HH2	2:J:567:HIS:CE1	2.14	0.65
2:H:351:ARG:HD2	2:H:359:GLU:O	1.96	0.65
2:D:351:ARG:HD3	2:D:413:LEU:HD11	1.77	0.65
2:H:211:ASP:O	2:H:215:ILE:HG13	1.97	0.65
2:L:440:ARG:HB3	2:L:467:TRP:HE3	1.59	0.65
2:F:487:CYS:HB3	2:F:490:LEU:HB2	1.77	0.65
2:L:227:VAL:HG13	2:L:228:GLY:N	2.10	0.65
2:P:563:GLU:HG3	2:P:563:GLU:O	1.94	0.65
2:B:419:ILE:HD13	2:B:446:ARG:HH12	1.61	0.65
2:L:231:GLU:HG2	2:L:254:ASN:HD22	1.60	0.65
2:N:184:LEU:HD12	2:N:207:ILE:HB	1.78	0.65
3:X:203:ILE:HD12	3:X:203:ILE:H	1.60	0.65
2:D:386:TYR:HE1	4:D:1100:7JA:HG2	1.61	0.65
2:N:93:PRO:HA	2:N:548:ARG:CB	2.24	0.65
1:M:99:PHE:CD2	2:N:15:ALA:O	2.48	0.65
2:N:456:SER:HB3	2:N:482:GLU:HB3	1.79	0.65
2:H:54:HIS:CE1	2:H:56:THR:OG1	2.47	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:211:ASP:HA	2:J:214:THR:HG23	1.78	0.65
2:L:307:THR:HG21	2:L:362:GLU:HB2	1.79	0.65
2:P:211:ASP:HA	2:P:214:THR:HG23	1.78	0.65
2:H:441:PHE:O	2:H:468:MET:HA	1.95	0.65
2:L:419:ILE:HD13	2:L:446:ARG:HH12	1.61	0.65
2:F:563:GLU:HG3	2:F:563:GLU:O	1.95	0.65
2:N:419:ILE:HD13	2:N:446:ARG:HH12	1.62	0.65
2:N:251:GLY:O	2:N:278:SER:HB2	1.96	0.65
2:H:390:ILE:HD11	2:H:412:LEU:CD2	2.15	0.65
1:A:98:LEU:HD21	1:A:120:THR:HG22	1.78	0.65
4:L:1100:7JA:H04	4:L:1100:7JA:H12A	1.71	0.65
2:N:289:PHE:CD1	2:N:316:LYS:HD2	2.31	0.65
2:N:191:ASN:HD21	2:N:194:LEU:H	1.44	0.65
2:H:99:TYR:CD2	2:H:123:ILE:HD12	2.32	0.65
2:H:56:THR:HG23	2:H:79:LYS:HB3	1.77	0.65
2:H:56:THR:HG23	2:H:79:LYS:HD2	1.79	0.65
2:P:365:VAL:HG23	2:P:387:VAL:HA	1.79	0.65
2:L:454:GLY:O	2:L:457:TYR:HB2	1.96	0.65
2:F:365:VAL:HG23	2:F:387:VAL:HA	1.79	0.65
2:B:468:MET:HE3	2:B:470:LEU:HD21	1.77	0.65
2:H:305:LEU:HD23	2:H:305:LEU:N	2.10	0.64
1:E:30:ALA:O	1:E:33:VAL:HG22	1.97	0.64
2:F:231:GLU:HG2	2:F:254:ASN:HD22	1.61	0.64
2:H:34:ARG:NH1	2:H:48:ASP:OD1	2.27	0.64
2:P:419:ILE:HD13	2:P:446:ARG:HH12	1.61	0.64
2:P:80:LEU:HB2	2:P:122:MET:HE1	1.77	0.64
2:N:357:GLY:CA	2:N:415:ARG:HH22	2.09	0.64
2:D:319:ASN:ND2	1:G:43:PRO:HG3	2.12	0.64
2:B:307:THR:HG21	2:B:362:GLU:HB2	1.78	0.64
1:E:48:THR:CG2	1:E:51:ILE:H	2.09	0.64
2:D:299:ASP:OD2	2:D:301:LEU:HB2	1.98	0.64
2:B:443:PHE:CE2	2:B:445:LEU:HD11	2.31	0.64
2:P:431:LEU:C	2:P:431:LEU:HD12	2.18	0.64
1:O:30:ALA:O	1:O:33:VAL:HG22	1.98	0.64
2:D:487:CYS:HB3	2:D:490:LEU:HB2	1.80	0.64
2:D:210:LYS:O	2:D:214:THR:HG22	1.97	0.64
2:F:299:ASP:OD2	2:F:301:LEU:HB2	1.98	0.64
2:B:398:ILE:HG23	2:B:402:LEU:HD11	1.79	0.64
2:H:532:LEU:O	2:H:535:MET:HB3	1.98	0.64
2:J:54:HIS:HE1	2:J:56:THR:OG1	1.81	0.64
2:P:431:LEU:O	2:P:431:LEU:HD12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:431:LEU:HD12	2:F:431:LEU:C	2.18	0.64
2:N:563:GLU:HG3	2:N:563:GLU:O	1.97	0.64
2:H:143:LEU:HD12	2:H:144:LYS:H	1.62	0.64
2:F:424:LEU:O	2:F:428:VAL:HG23	1.97	0.64
1:I:30:ALA:O	1:I:33:VAL:HG22	1.97	0.64
2:N:431:LEU:HD12	2:N:431:LEU:C	2.17	0.64
2:D:412:LEU:HD12	2:D:412:LEU:O	1.98	0.64
2:N:519:TRP:HH2	2:N:567:HIS:CE1	2.16	0.64
1:M:102:ILE:HG21	2:N:20:VAL:HG23	1.78	0.64
2:F:468:MET:HE3	2:F:470:LEU:HD21	1.78	0.64
2:L:121:ARG:NH2	5:L:1103:PO4:O4	2.31	0.64
2:B:299:ASP:OD2	2:B:301:LEU:HB2	1.98	0.64
2:D:55:VAL:HG23	2:D:75:LEU:HD21	1.79	0.64
1:E:113:LEU:HG	1:E:113:LEU:O	1.98	0.64
2:L:487:CYS:HB3	2:L:490:LEU:HB2	1.80	0.64
2:B:54:HIS:HE1	2:B:56:THR:OG1	1.80	0.64
2:B:310:HIS:O	2:B:314:ILE:HG12	1.98	0.64
2:H:291:PHE:N	2:H:291:PHE:CD2	2.65	0.64
2:H:85:ARG:NH2	4:H:1100:7JA:O14	2.31	0.63
2:H:327:ASN:CG	2:H:351:ARG:HB2	2.18	0.63
2:L:286:PRO:HA	2:L:289:PHE:CD2	2.33	0.63
2:L:191:ASN:HD21	2:L:194:LEU:H	1.46	0.63
1:M:131:GLU:HA	1:M:131:GLU:OE2	1.97	0.63
2:L:80:LEU:HB2	2:L:122:MET:HE2	1.79	0.63
1:K:48:THR:HG22	1:K:51:ILE:HB	1.78	0.63
2:J:231:GLU:HG2	2:J:254:ASN:HD22	1.62	0.63
2:F:93:PRO:HA	2:F:548:ARG:CB	2.26	0.63
2:L:365:VAL:HG23	2:L:387:VAL:HA	1.78	0.63
2:B:286:PRO:HA	2:B:289:PHE:CD2	2.34	0.63
2:D:294:GLN:NE2	1:G:107:TYR:OH	2.31	0.63
2:J:487:CYS:HB3	2:J:490:LEU:HB2	1.80	0.63
2:P:227:VAL:HG13	2:P:228:GLY:N	2.13	0.63
2:D:159:ILE:HD12	2:D:166:ILE:HD11	1.81	0.63
2:F:519:TRP:HH2	2:F:567:HIS:CE1	2.17	0.63
1:M:102:ILE:CG2	2:N:20:VAL:HG23	2.28	0.63
1:K:102:ILE:CG1	1:K:117:THR:HB	2.27	0.63
2:B:412:LEU:HD12	2:B:412:LEU:O	1.99	0.63
2:H:307:THR:HB	2:H:328:VAL:O	1.99	0.63
2:H:143:LEU:HD12	2:H:144:LYS:N	2.14	0.63
2:L:519:TRP:HH2	2:L:567:HIS:CE1	2.16	0.63
2:H:542:ILE:CD1	2:H:588:LEU:HB2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:GLU:HG2	2:N:15:ALA:CB	2.29	0.63
1:O:48:THR:CG2	1:O:51:ILE:H	2.12	0.63
2:B:440:ARG:HB3	2:B:467:TRP:CE3	2.34	0.63
2:F:357:GLY:CA	2:F:415:ARG:HH22	2.10	0.63
2:F:391:THR:HG23	2:F:394:SER:H	1.64	0.63
2:D:424:LEU:O	2:D:428:VAL:HG23	1.99	0.63
2:N:365:VAL:HG23	2:N:387:VAL:HA	1.81	0.63
3:Q:203:ILE:HD12	3:Q:203:ILE:H	1.63	0.63
2:P:199:PHE:CE1	2:P:227:VAL:HG22	2.33	0.63
2:H:95:ASN:O	2:H:582:PRO:HG3	1.98	0.63
2:L:310:HIS:O	2:L:314:ILE:HG12	1.99	0.63
2:J:307:THR:HG21	2:J:362:GLU:HB2	1.79	0.63
2:N:301:LEU:HD23	2:N:324:GLU:HB3	1.81	0.62
2:N:310:HIS:O	2:N:314:ILE:HG12	1.98	0.62
2:F:307:THR:HG21	2:F:362:GLU:HB2	1.80	0.62
2:P:299:ASP:OD2	2:P:301:LEU:HB2	1.98	0.62
2:B:431:LEU:C	2:B:431:LEU:HD12	2.19	0.62
2:B:289:PHE:CD1	2:B:316:LYS:HD2	2.33	0.62
2:B:184:LEU:HD12	2:B:207:ILE:HB	1.79	0.62
2:N:396:GLU:O	2:N:400:THR:HB	1.98	0.62
2:D:231:GLU:HG2	2:D:254:ASN:HD22	1.64	0.62
2:B:454:GLY:O	2:B:457:TYR:HB2	1.97	0.62
2:B:545:ILE:HB	2:B:567:HIS:HB2	1.80	0.62
1:M:96:ALA:CB	2:N:14:VAL:CG1	2.76	0.62
2:J:286:PRO:HA	2:J:289:PHE:CD2	2.35	0.62
2:D:357:GLY:CA	2:D:415:ARG:HH22	2.11	0.62
2:H:442:ALA:CB	4:H:1100:7JA:CD1	2.75	0.62
2:L:542:ILE:CD1	2:L:588:LEU:HD12	2.27	0.62
2:B:251:GLY:O	2:B:278:SER:HB2	1.99	0.62
2:H:284:GLU:O	2:H:287:ILE:HD13	1.99	0.62
2:H:409:ARG:HB3	4:H:1100:7JA:HD1	1.80	0.62
2:H:365:VAL:HG21	2:H:387:VAL:HG13	1.81	0.62
1:M:100:GLU:HG2	2:N:15:ALA:HB2	1.81	0.62
2:H:125:SER:O	2:H:129:LEU:HB2	2.00	0.62
2:L:121:ARG:HH22	5:L:1103:PO4:P	2.23	0.62
2:L:424:LEU:O	2:L:428:VAL:HG23	1.99	0.62
1:K:48:THR:CG2	1:K:51:ILE:H	2.13	0.62
2:H:258:GLY:C	2:H:260:PRO:HD3	2.20	0.62
2:H:322:VAL:CG1	2:H:323:LEU:N	2.62	0.62
2:N:231:GLU:HG2	2:N:254:ASN:HD22	1.64	0.62
2:J:310:HIS:O	2:J:314:ILE:HG12	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:431:LEU:HD12	2:J:431:LEU:C	2.20	0.62
1:M:99:PHE:CE2	2:N:17:VAL:N	2.68	0.62
2:H:144:LYS:HG2	2:H:170:LEU:HD13	1.82	0.62
2:D:227:VAL:HG13	2:D:228:GLY:N	2.15	0.62
2:D:310:HIS:O	2:D:314:ILE:HG12	1.99	0.62
2:P:351:ARG:HD3	2:P:413:LEU:HD11	1.82	0.62
2:F:50:GLU:OE1	2:L:217:ARG:NH1	2.33	0.62
2:B:371:ILE:O	2:B:375:GLN:HG3	2.00	0.62
2:B:93:PRO:HA	2:B:548:ARG:CB	2.27	0.62
2:H:78:LEU:HD12	2:H:79:LYS:H	1.63	0.62
1:M:87:ASP:OD2	1:M:116:LEU:HD22	2.00	0.62
1:C:113:LEU:O	1:C:117:THR:HG23	1.99	0.62
2:F:297:LYS:HE2	2:F:322:VAL:HG21	1.82	0.62
2:J:412:LEU:O	2:J:412:LEU:HD12	1.99	0.62
2:B:533:MET:CE	2:B:588:LEU:HD13	2.29	0.61
2:H:443:PHE:HE2	2:H:445:LEU:HD11	1.65	0.61
1:A:48:THR:CG2	1:A:51:ILE:H	2.13	0.61
2:L:211:ASP:HA	2:L:214:THR:HG23	1.82	0.61
2:H:25:MET:HA	2:H:28:ILE:HD12	1.82	0.61
2:L:412:LEU:HD12	2:L:412:LEU:O	1.98	0.61
2:D:519:TRP:CH2	2:D:567:HIS:ND1	2.68	0.61
2:P:546:PRO:O	2:P:547:SER:HB2	2.01	0.61
2:L:93:PRO:HA	2:L:548:ARG:CB	2.25	0.61
2:H:431:LEU:C	2:H:431:LEU:HD23	2.20	0.61
2:B:391:THR:HG23	2:B:394:SER:H	1.65	0.61
2:H:225:VAL:O	2:H:248:PHE:HA	2.00	0.61
2:D:171:MET:O	2:D:174:SER:HB2	1.99	0.61
1:E:107:TYR:OH	2:L:294:GLN:NE2	2.33	0.61
2:J:419:ILE:HD13	2:J:446:ARG:NH1	2.15	0.61
2:D:367:GLN:O	2:D:371:ILE:HG22	1.99	0.61
2:D:211:ASP:HA	2:D:214:THR:HG23	1.81	0.61
2:F:440:ARG:HB3	2:F:467:TRP:HE3	1.65	0.61
2:N:444:TYR:HA	2:N:471:GLY:CA	2.28	0.61
2:J:233:LEU:O	2:J:236:VAL:HG23	2.00	0.61
1:K:158:ALA:HA	2:L:62:THR:HG21	1.81	0.61
1:M:99:PHE:HB2	2:N:15:ALA:CB	2.31	0.61
2:D:431:LEU:O	2:D:431:LEU:HD12	1.99	0.61
2:N:311:CYS:HB3	2:N:336:VAL:HG21	1.82	0.61
2:L:299:ASP:OD2	2:L:301:LEU:HB2	2.00	0.61
2:J:533:MET:HE3	2:J:588:LEU:HD13	1.82	0.61
1:M:48:THR:CG2	1:M:51:ILE:H	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:412:LEU:HD12	2:N:412:LEU:O	2.01	0.61
2:P:80:LEU:HB2	2:P:122:MET:HE2	1.82	0.61
1:O:158:ALA:HA	2:P:62:THR:HG21	1.82	0.61
2:B:397:SER:O	2:B:400:THR:HG22	2.00	0.61
2:H:395:LEU:H	2:H:395:LEU:CD2	2.13	0.60
1:C:48:THR:CG2	1:C:51:ILE:H	2.11	0.60
2:F:419:ILE:HD13	2:F:446:ARG:NH1	2.16	0.60
2:P:371:ILE:O	2:P:375:GLN:HG3	2.01	0.60
2:D:143:LEU:HD23	2:D:159:ILE:HD13	1.83	0.60
2:P:54:HIS:HE1	2:P:56:THR:OG1	1.83	0.60
2:L:472:TYR:OH	3:V:201:LEU:HB2	2.00	0.60
2:P:456:SER:CB	2:P:482:GLU:HB3	2.31	0.60
2:J:391:THR:HG23	2:J:394:SER:H	1.65	0.60
4:J:1100:7JA:H04	4:J:1100:7JA:H12A	1.73	0.60
2:H:386:TYR:CE1	4:H:1100:7JA:HG2B	2.36	0.60
2:N:386:TYR:CE1	4:N:1100:7JA:CG2	2.81	0.60
2:H:533:MET:C	2:H:535:MET:H	2.05	0.60
2:H:361:GLU:HA	2:H:364:LEU:HD12	1.81	0.60
2:L:351:ARG:HD3	2:L:413:LEU:HD11	1.83	0.60
2:B:227:VAL:HG13	2:B:228:GLY:N	2.16	0.60
2:J:93:PRO:HA	2:J:548:ARG:CB	2.30	0.60
2:N:143:LEU:HD23	2:N:159:ILE:HD13	1.82	0.60
2:H:477:ASP:OD2	2:H:504:ALA:HB2	2.01	0.60
2:J:95:ASN:O	2:J:582:PRO:HG3	2.01	0.60
2:D:293:ALA:HB3	1:G:45:PRO:HG3	1.84	0.60
1:I:131:GLU:OE2	1:I:131:GLU:HA	2.01	0.60
2:H:386:TYR:CZ	4:H:1100:7JA:HG2B	2.37	0.60
2:N:211:ASP:O	2:N:215:ILE:HG13	2.02	0.60
1:G:153:ARG:NH2	2:H:539:TYR:HE1	1.99	0.60
2:P:456:SER:HB3	2:P:482:GLU:HB3	1.83	0.60
1:A:30:ALA:O	1:A:33:VAL:HG22	2.01	0.60
2:N:521:GLN:HG3	2:N:567:HIS:HD2	1.66	0.60
2:P:159:ILE:HD12	2:P:166:ILE:HD11	1.83	0.60
2:N:133:ALA:HB2	2:N:159:ILE:HG22	1.84	0.60
1:M:30:ALA:O	1:M:33:VAL:HG22	2.01	0.60
1:C:30:ALA:O	1:C:33:VAL:HG22	2.00	0.60
2:H:285:MET:HG2	2:H:286:PRO:HD3	1.83	0.60
1:M:99:PHE:CZ	2:N:17:VAL:HG22	2.37	0.60
2:L:54:HIS:HD2	2:L:77:SER:OG	1.84	0.60
2:D:472:TYR:OH	3:R:201:LEU:HB2	2.02	0.60
2:H:407:ASP:OD1	2:H:440:ARG:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:397:SER:O	2:N:400:THR:HG22	2.02	0.60
2:J:367:GLN:O	2:J:371:ILE:HG22	2.01	0.60
2:D:184:LEU:HD12	2:D:207:ILE:HB	1.83	0.60
1:K:30:ALA:O	1:K:33:VAL:HG22	2.00	0.60
2:B:231:GLU:HG2	2:B:254:ASN:HD22	1.66	0.60
1:M:112:ASN:C	1:M:114:LEU:N	2.55	0.60
2:B:211:ASP:HA	2:B:214:THR:HG23	1.84	0.60
2:L:231:GLU:HG2	2:L:254:ASN:ND2	2.17	0.60
1:O:131:GLU:OE2	1:O:131:GLU:HA	2.02	0.60
2:H:92:ILE:HG22	2:H:93:PRO:O	2.02	0.59
2:D:419:ILE:HD13	2:D:446:ARG:NH1	2.17	0.59
2:H:259:MET:C	2:H:261:GLU:H	2.06	0.59
2:H:262:LYS:HD2	2:H:263:TYR:CE1	2.36	0.59
2:N:54:HIS:HE1	2:N:56:THR:OG1	1.85	0.59
2:N:121:ARG:NH2	5:N:1103:PO4:O4	2.35	0.59
2:H:343:GLN:CD	2:H:343:GLN:H	2.05	0.59
2:F:386:TYR:CE1	4:F:1100:7JA:CG2	2.83	0.59
2:P:391:THR:HG23	2:P:394:SER:H	1.65	0.59
2:P:231:GLU:HG2	2:P:254:ASN:HD22	1.67	0.59
2:P:412:LEU:HD12	2:P:412:LEU:O	2.01	0.59
2:H:347:LEU:HD11	2:H:349:ILE:HG13	1.83	0.59
2:D:440:ARG:HB3	2:D:467:TRP:CE3	2.35	0.59
1:M:27:GLN:HB2	1:M:109:ASN:HB3	1.83	0.59
2:B:279:TYR:HA	2:B:304:LEU:HD22	1.83	0.59
2:N:456:SER:CB	2:N:482:GLU:HB3	2.32	0.59
2:F:431:LEU:HD12	2:F:431:LEU:O	2.01	0.59
2:B:217:ARG:NH1	2:P:50:GLU:OE1	2.36	0.59
2:F:261:GLU:HG2	2:F:264:MET:HG3	1.84	0.59
2:B:121:ARG:NH2	5:B:1103:PO4:O4	2.36	0.59
1:C:131:GLU:HA	1:C:131:GLU:OE2	2.00	0.59
2:P:351:ARG:HG3	2:P:351:ARG:O	2.03	0.59
2:P:487:CYS:HB3	2:P:490:LEU:HB2	1.83	0.59
2:H:402:LEU:HD13	2:H:405:LEU:HG	1.85	0.59
2:F:112:ARG:HG3	2:L:164:ARG:HE	1.68	0.59
2:H:125:SER:HB3	2:H:127:LEU:H	1.66	0.59
2:L:367:GLN:O	2:L:371:ILE:HG22	2.01	0.59
2:L:297:LYS:HE2	2:L:322:VAL:HG21	1.83	0.59
2:F:472:TYR:OH	3:S:201:LEU:HB2	2.02	0.59
2:N:546:PRO:O	2:N:547:SER:HB2	2.03	0.59
2:J:468:MET:HE3	2:J:470:LEU:HD21	1.83	0.59
1:K:105:ALA:HB2	1:K:113:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:THR:CG2	1:I:51:ILE:H	2.15	0.59
2:N:170:LEU:HD23	2:N:170:LEU:C	2.23	0.59
2:H:375:GLN:HG2	2:H:401:TYR:CD1	2.38	0.59
1:C:158:ALA:HA	2:D:62:THR:HG21	1.84	0.59
2:N:468:MET:HE3	2:N:470:LEU:HD21	1.85	0.59
2:H:191:ASN:ND2	2:H:193:SER:H	2.01	0.59
2:F:227:VAL:HG13	2:F:228:GLY:N	2.17	0.59
2:L:533:MET:HE3	2:L:588:LEU:HD13	1.85	0.59
2:J:164:ARG:NE	2:N:112:ARG:HG2	2.18	0.59
1:M:153:ARG:HG2	1:M:157:TRP:CZ3	2.37	0.59
2:P:103:TRP:O	2:P:107:ILE:HG13	2.03	0.59
2:P:279:TYR:HA	2:P:304:LEU:HD22	1.84	0.59
1:M:158:ALA:HA	2:N:62:THR:HG21	1.83	0.59
2:N:275:LEU:HD11	2:N:288:LEU:HD21	1.84	0.59
2:F:456:SER:HB3	2:F:482:GLU:HB3	1.85	0.58
2:B:424:LEU:O	2:B:428:VAL:HG23	2.02	0.58
1:C:12:ASP:O	1:K:40:ASN:CB	2.50	0.58
2:D:311:CYS:HB3	2:D:336:VAL:HG21	1.83	0.58
2:J:546:PRO:O	2:J:547:SER:HB2	2.03	0.58
2:D:546:PRO:O	2:D:547:SER:HB2	2.02	0.58
2:F:533:MET:CE	2:F:588:LEU:HD13	2.33	0.58
2:L:54:HIS:HE1	2:L:56:THR:OG1	1.84	0.58
2:H:233:LEU:O	2:H:236:VAL:HG23	2.03	0.58
2:L:159:ILE:HD12	2:L:166:ILE:HD11	1.84	0.58
2:N:261:GLU:HG2	2:N:264:MET:HG3	1.85	0.58
2:J:143:LEU:HD23	2:J:159:ILE:HD13	1.85	0.58
2:H:392:ASN:HD21	2:H:422:LEU:HD13	1.68	0.58
2:H:371:ILE:CG2	2:H:375:GLN:HE21	2.14	0.58
2:J:440:ARG:HB3	2:J:467:TRP:CE3	2.36	0.58
1:A:102:ILE:HG13	1:A:117:THR:HB	1.84	0.58
2:P:301:LEU:HD23	2:P:324:GLU:HB3	1.85	0.58
2:B:367:GLN:O	2:B:371:ILE:HG22	2.04	0.58
2:J:422:LEU:HB3	2:J:423:PRO:HD3	1.85	0.58
2:F:80:LEU:HB2	2:F:122:MET:HE2	1.85	0.58
2:N:159:ILE:HD12	2:N:166:ILE:HD11	1.86	0.58
2:N:199:PHE:CE1	2:N:227:VAL:HG22	2.38	0.58
2:N:424:LEU:O	2:N:428:VAL:HG23	2.02	0.58
1:C:27:GLN:HB2	1:C:109:ASN:HB3	1.85	0.58
2:H:509:VAL:HG21	2:H:535:MET:SD	2.43	0.58
1:O:91:MET:SD	1:O:117:THR:HG22	2.44	0.58
1:M:148:GLU:HG2	1:M:152:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLU:O	1:C:136:THR:HG23	2.03	0.58
2:F:546:PRO:HG2	2:F:584:THR:CB	2.32	0.58
2:H:310:HIS:O	2:H:314:ILE:HG12	2.03	0.58
1:C:48:THR:HG22	1:C:51:ILE:N	2.14	0.58
1:C:102:ILE:HG21	2:D:20:VAL:CG2	2.34	0.58
2:B:161:THR:HG22	2:B:186:GLU:HG2	1.86	0.58
2:P:172:GLU:HG3	2:P:200:TYR:HB3	1.85	0.58
1:A:158:ALA:HA	2:B:62:THR:HG21	1.85	0.58
2:L:419:ILE:HD13	2:L:446:ARG:NH1	2.19	0.58
2:L:95:ASN:O	2:L:582:PRO:HG3	2.02	0.58
1:I:35:ASP:HB3	2:N:243:ALA:HB1	1.85	0.58
2:F:40:VAL:O	2:F:41:CYS:HB3	2.02	0.58
2:N:546:PRO:HG2	2:N:584:THR:CB	2.30	0.58
1:C:48:THR:HG22	1:C:51:ILE:HB	1.85	0.58
2:H:487:CYS:N	2:H:488:PRO:HD3	2.18	0.58
2:P:419:ILE:HD13	2:P:446:ARG:NH1	2.19	0.58
2:D:286:PRO:HA	2:D:289:PHE:CD2	2.38	0.58
2:F:159:ILE:HD12	2:F:166:ILE:HD11	1.85	0.58
1:E:153:ARG:HG2	1:E:157:TRP:CZ3	2.39	0.58
2:H:37:ALA:O	2:H:40:VAL:HG13	2.03	0.58
2:H:125:SER:HB3	2:H:127:LEU:N	2.18	0.58
2:N:440:ARG:HB3	2:N:467:TRP:CE3	2.39	0.58
2:F:275:LEU:HD11	2:F:288:LEU:HD21	1.86	0.58
2:H:382:TYR:C	2:H:382:TYR:CD1	2.77	0.58
2:H:99:TYR:CE2	2:H:123:ILE:HD12	2.39	0.58
1:M:128:LYS:HB2	1:M:133:ILE:CD1	2.34	0.58
2:P:440:ARG:HB3	2:P:467:TRP:CE3	2.36	0.58
2:B:159:ILE:HD11	2:B:169:LEU:HD13	1.86	0.58
2:L:307:THR:HG22	2:L:360:ASP:OD2	2.04	0.58
2:J:431:LEU:HD12	2:J:431:LEU:O	2.04	0.58
2:F:133:ALA:HB2	2:F:159:ILE:HG22	1.86	0.58
2:D:386:TYR:CE1	4:D:1100:7JA:CG2	2.83	0.57
2:L:545:ILE:HB	2:L:567:HIS:HB2	1.85	0.57
2:B:159:ILE:HD12	2:B:166:ILE:HD11	1.86	0.57
2:L:227:VAL:CG1	2:L:228:GLY:N	2.66	0.57
2:N:431:LEU:HD12	2:N:431:LEU:O	2.04	0.57
2:B:253:LEU:HD12	2:B:280:MET:HB2	1.86	0.57
2:P:133:ALA:HB2	2:P:159:ILE:HG22	1.85	0.57
2:D:454:GLY:O	2:D:457:TYR:HB2	2.04	0.57
2:P:397:SER:O	2:P:400:THR:HG22	2.04	0.57
2:J:227:VAL:HG13	2:J:228:GLY:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:521:GLN:HG3	2:N:567:HIS:CD2	2.39	0.57
1:O:159:PHE:O	1:O:160:GLU:CB	2.52	0.57
2:F:210:LYS:O	2:F:214:THR:HG22	2.04	0.57
2:H:96:TRP:HA	2:H:582:PRO:HG2	1.85	0.57
2:F:143:LEU:HD23	2:F:159:ILE:HD13	1.86	0.57
2:L:456:SER:HB3	2:L:482:GLU:HB3	1.86	0.57
2:N:297:LYS:HG3	2:N:322:VAL:HB	1.86	0.57
1:K:102:ILE:HG12	1:K:117:THR:CB	2.32	0.57
1:E:105:ALA:HB3	1:E:114:LEU:HD13	1.87	0.57
1:C:102:ILE:HG12	1:C:117:THR:HB	1.85	0.57
1:A:134:ARG:HH11	2:B:40:VAL:HA	1.70	0.57
2:B:419:ILE:HD13	2:B:446:ARG:NH1	2.20	0.57
2:J:307:THR:HG22	2:J:360:ASP:OD2	2.03	0.57
1:O:153:ARG:HG2	1:O:157:TRP:CZ3	2.39	0.57
2:N:351:ARG:O	2:N:351:ARG:HG3	2.04	0.57
2:N:396:GLU:HG2	2:N:430:SER:OG	2.05	0.57
2:L:456:SER:CB	2:L:482:GLU:HB3	2.35	0.57
1:M:132:GLU:O	1:M:136:THR:HG23	2.05	0.57
1:G:48:THR:HG22	1:G:51:ILE:N	2.18	0.57
2:N:297:LYS:HE2	2:N:322:VAL:HG21	1.86	0.57
1:E:43:PRO:HG3	2:L:319:ASN:ND2	2.20	0.57
2:H:180:ASP:OD1	2:H:182:LYS:HB2	2.04	0.57
2:D:547:SER:HB3	2:D:564:HIS:HB2	1.86	0.57
2:B:546:PRO:O	2:B:547:SER:HB2	2.03	0.57
2:J:533:MET:CE	2:J:588:LEU:HD13	2.35	0.57
2:F:231:GLU:HG2	2:F:254:ASN:ND2	2.18	0.57
2:J:121:ARG:HH22	5:J:1103:PO4:P	2.28	0.57
2:J:279:TYR:HA	2:J:304:LEU:HD22	1.86	0.57
2:L:397:SER:O	2:L:400:THR:HG22	2.04	0.57
2:H:147:LYS:HE2	2:H:173:GLU:OE1	2.04	0.57
2:D:233:LEU:O	2:D:236:VAL:HG23	2.05	0.57
2:D:580:ASP:HA	2:N:206:LYS:HE3	1.87	0.57
2:B:592:ILE:H	2:B:592:ILE:HD12	1.69	0.57
2:H:286:PRO:C	2:H:288:LEU:H	2.09	0.57
2:H:289:PHE:CE1	2:H:316:LYS:HD3	2.40	0.57
2:H:533:MET:HE3	2:H:588:LEU:HD13	1.86	0.57
2:J:275:LEU:HD11	2:J:288:LEU:HD21	1.87	0.57
2:D:307:THR:HG22	2:D:360:ASP:OD2	2.04	0.56
2:D:391:THR:HG23	2:D:394:SER:H	1.70	0.56
2:J:351:ARG:O	2:J:351:ARG:HG3	2.04	0.56
1:A:131:GLU:OE2	1:A:131:GLU:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:519:TRP:CH2	2:J:567:HIS:ND1	2.73	0.56
2:H:386:TYR:HD2	2:H:413:LEU:HD21	1.70	0.56
2:N:533:MET:HE3	2:N:588:LEU:HD13	1.86	0.56
1:C:40:ASN:HB3	1:K:13:GLY:O	2.04	0.56
2:L:592:ILE:HD12	2:L:592:ILE:H	1.70	0.56
2:L:386:TYR:CE1	4:L:1100:7JA:CG2	2.83	0.56
1:G:102:ILE:HG12	1:G:117:THR:OG1	2.06	0.56
2:J:54:HIS:HD2	2:J:77:SER:OG	1.88	0.56
2:N:210:LYS:O	2:N:214:THR:HG22	2.05	0.56
2:L:440:ARG:HB3	2:L:467:TRP:CE3	2.40	0.56
1:O:153:ARG:NH2	2:P:539:TYR:CE1	2.73	0.56
2:H:136:ARG:HA	2:H:136:ARG:NE	2.19	0.56
2:H:216:ALA:HB2	2:H:238:PHE:CD1	2.40	0.56
1:M:105:ALA:HB2	1:M:113:LEU:HD23	1.86	0.56
1:C:52:LEU:O	1:C:56:ILE:HG13	2.06	0.56
2:D:121:ARG:HH22	5:D:1103:PO4:P	2.28	0.56
2:N:95:ASN:O	2:N:582:PRO:HG3	2.05	0.56
2:J:547:SER:HB3	2:J:564:HIS:HB2	1.86	0.56
2:H:431:LEU:HD22	2:H:432:LEU:HD23	1.88	0.56
2:H:87:ALA:HB2	2:H:92:ILE:HB	1.87	0.56
2:J:231:GLU:HG2	2:J:254:ASN:ND2	2.20	0.56
2:F:199:PHE:CE1	2:F:227:VAL:HG22	2.40	0.56
2:J:159:ILE:HD12	2:J:166:ILE:HD11	1.86	0.56
2:P:275:LEU:HD11	2:P:288:LEU:HD21	1.87	0.56
2:D:519:TRP:CZ3	2:D:567:HIS:ND1	2.73	0.56
2:H:444:TYR:HA	2:H:471:GLY:CA	2.31	0.56
2:D:533:MET:CE	2:D:588:LEU:HD13	2.36	0.56
2:J:396:GLU:HG2	2:J:430:SER:OG	2.06	0.56
2:N:171:MET:O	2:N:174:SER:HB2	2.06	0.56
2:B:444:TYR:HA	2:B:471:GLY:CA	2.30	0.56
1:G:124:MET:O	1:G:128:LYS:HE2	2.05	0.56
2:N:57:MET:HE3	2:N:62:THR:HG22	1.87	0.56
2:J:351:ARG:HD3	2:J:413:LEU:HD11	1.86	0.56
1:K:131:GLU:OE2	1:K:131:GLU:HA	2.05	0.56
2:L:547:SER:HB3	2:L:564:HIS:HB2	1.88	0.56
2:B:547:SER:HB3	2:B:564:HIS:HB2	1.88	0.56
2:H:542:ILE:CD1	2:H:542:ILE:C	2.69	0.56
2:J:308:GLU:O	2:J:312:THR:HG23	2.06	0.56
2:L:199:PHE:CE1	2:L:227:VAL:HG22	2.41	0.56
2:J:456:SER:CB	2:J:482:GLU:HB3	2.36	0.56
2:F:521:GLN:HG3	2:F:567:HIS:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:351:ARG:HD3	2:N:413:LEU:HD11	1.87	0.56
2:H:170:LEU:HB2	2:H:198:ASN:HB3	1.88	0.56
2:D:371:ILE:O	2:D:375:GLN:HG3	2.06	0.56
2:L:143:LEU:HD23	2:L:159:ILE:HD13	1.88	0.56
1:A:132:GLU:O	1:A:136:THR:HG23	2.05	0.56
1:O:148:GLU:HG2	1:O:152:ARG:HH12	1.70	0.56
2:H:101:THR:HB	2:H:102:PRO:CD	2.36	0.56
2:J:261:GLU:HG2	2:J:264:MET:HG3	1.87	0.56
2:J:592:ILE:H	2:J:592:ILE:HD12	1.70	0.56
2:F:546:PRO:HD3	2:F:584:THR:O	2.06	0.56
2:L:386:TYR:HE1	4:L:1100:7JA:HG2	1.63	0.56
1:M:124:MET:O	1:M:128:LYS:HE2	2.04	0.56
2:H:542:ILE:HD12	2:H:543:GLU:N	2.21	0.56
1:M:99:PHE:HB2	2:N:15:ALA:HB3	1.88	0.56
2:H:156:LEU:O	2:H:160:VAL:HG22	2.05	0.56
2:P:307:THR:HG22	2:P:360:ASP:OD2	2.06	0.56
2:P:307:THR:HG21	2:P:362:GLU:HB2	1.86	0.56
1:O:27:GLN:HB2	1:O:109:ASN:HB3	1.86	0.56
2:H:533:MET:HE1	2:H:588:LEU:HB3	1.88	0.56
1:E:129:THR:O	1:E:133:ILE:HG12	2.06	0.56
2:D:412:LEU:HD12	2:D:412:LEU:C	2.25	0.56
2:H:259:MET:O	2:H:261:GLU:N	2.38	0.56
2:J:456:SER:HB3	2:J:482:GLU:HB3	1.88	0.56
2:D:456:SER:HB3	2:D:482:GLU:HB3	1.88	0.56
1:I:27:GLN:HB2	1:I:109:ASN:HB3	1.88	0.56
2:F:412:LEU:O	2:F:412:LEU:HD12	2.05	0.56
2:N:546:PRO:HD3	2:N:584:THR:O	2.05	0.55
2:H:428:VAL:CG2	2:H:429:ARG:N	2.68	0.55
2:H:304:LEU:HD13	2:H:304:LEU:O	2.05	0.55
2:P:121:ARG:NH2	5:P:1103:PO4:O4	2.38	0.55
2:H:47:ILE:O	2:H:51:THR:HG23	2.05	0.55
2:L:170:LEU:HD23	2:L:170:LEU:C	2.26	0.55
2:F:170:LEU:C	2:F:170:LEU:HD23	2.26	0.55
2:J:521:GLN:HG3	2:J:567:HIS:CD2	2.42	0.55
2:J:521:GLN:HG3	2:J:567:HIS:HD2	1.71	0.55
2:F:533:MET:HE3	2:F:588:LEU:HD13	1.87	0.55
1:O:129:THR:O	1:O:133:ILE:HG12	2.06	0.55
2:B:412:LEU:HD12	2:B:412:LEU:C	2.27	0.55
2:B:227:VAL:CG1	2:B:228:GLY:N	2.70	0.55
2:H:136:ARG:HG3	2:H:136:ARG:HH11	1.71	0.55
1:I:108:LEU:HD12	1:I:110:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:GLU:HG2	2:D:264:MET:HG3	1.87	0.55
2:D:296:ARG:HH22	1:G:35:ASP:HB2	1.71	0.55
2:N:472:TYR:OH	3:W:201:LEU:HB2	2.06	0.55
2:H:322:VAL:HG12	2:H:323:LEU:N	2.19	0.55
2:N:80:LEU:HB2	2:N:122:MET:HE1	1.87	0.55
2:N:327:ASN:HD22	2:N:328:VAL:N	2.04	0.55
2:D:301:LEU:HD23	2:D:324:GLU:HB3	1.88	0.55
2:J:121:ARG:NH2	5:J:1103:PO4:O4	2.39	0.55
2:L:546:PRO:O	2:L:547:SER:HB2	2.05	0.55
2:L:533:MET:CE	2:L:588:LEU:HD13	2.36	0.55
2:B:307:THR:HG22	2:B:360:ASP:OD2	2.05	0.55
1:E:105:ALA:HB2	1:E:113:LEU:HD23	1.88	0.55
2:P:170:LEU:HD23	2:P:170:LEU:C	2.27	0.55
2:B:519:TRP:CH2	2:B:567:HIS:ND1	2.75	0.55
1:M:159:PHE:O	1:M:160:GLU:CB	2.52	0.55
2:J:297:LYS:HE2	2:J:322:VAL:HG21	1.89	0.55
1:G:27:GLN:HB2	1:G:109:ASN:HB3	1.88	0.55
2:N:172:GLU:HG3	2:N:200:TYR:HB3	1.89	0.55
1:E:148:GLU:HG2	1:E:152:ARG:HH12	1.70	0.55
2:F:592:ILE:H	2:F:592:ILE:HD12	1.71	0.55
2:N:519:TRP:NE1	4:N:1100:7JA:C01	2.61	0.55
2:F:211:ASP:O	2:F:215:ILE:HG13	2.07	0.55
2:H:291:PHE:N	2:H:291:PHE:HD2	2.02	0.55
2:B:396:GLU:O	2:B:400:THR:HB	2.06	0.55
1:K:108:LEU:HD12	1:K:110:ILE:HD11	1.89	0.55
1:K:134:ARG:HH11	2:L:40:VAL:HA	1.72	0.55
1:A:153:ARG:HG2	1:A:157:TRP:CZ3	2.41	0.55
1:M:102:ILE:HD12	2:N:20:VAL:CG2	2.24	0.55
2:H:286:PRO:O	2:H:288:LEU:N	2.40	0.55
2:H:305:LEU:CD2	2:H:305:LEU:H	2.14	0.55
2:H:533:MET:CE	2:H:588:LEU:HD13	2.37	0.55
1:I:128:LYS:HB2	1:I:133:ILE:CD1	2.37	0.55
1:O:113:LEU:O	1:O:113:LEU:CG	2.54	0.55
2:J:57:MET:HE3	2:J:62:THR:HG22	1.89	0.55
2:H:84:PRO:HB3	2:H:517:TYR:OH	2.07	0.55
2:J:412:LEU:C	2:J:412:LEU:HD12	2.27	0.55
2:J:172:GLU:HG3	2:J:200:TYR:HB3	1.88	0.55
2:P:297:LYS:HE2	2:P:322:VAL:HG21	1.89	0.55
1:K:132:GLU:O	1:K:136:THR:HG23	2.06	0.55
2:H:419:ILE:HG13	2:H:419:ILE:O	2.06	0.55
2:N:347:LEU:HD21	2:N:349:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:LEU:O	2:B:431:LEU:HD12	2.07	0.55
1:A:135:THR:HG22	1:A:136:THR:N	2.22	0.55
2:H:456:SER:OG	2:H:482:GLU:HB3	2.06	0.55
2:F:521:GLN:HG3	2:F:567:HIS:CD2	2.42	0.55
2:B:101:THR:CG2	2:B:128:ASP:OD1	2.51	0.55
2:H:153:THR:HG23	2:H:178:GLU:HA	1.89	0.55
2:J:419:ILE:CD1	2:J:446:ARG:HH12	2.20	0.55
1:G:159:PHE:O	1:G:160:GLU:HB2	2.05	0.55
2:P:191:ASN:ND2	2:P:194:LEU:H	2.04	0.55
2:D:296:ARG:NH2	1:G:37:CYS:SG	2.80	0.55
2:H:502:GLU:OE1	2:H:526:SER:HB2	2.07	0.55
2:D:93:PRO:HA	2:D:548:ARG:CB	2.28	0.55
2:F:542:ILE:CD1	2:F:588:LEU:HD12	2.34	0.55
2:H:78:LEU:HD12	2:H:79:LYS:N	2.22	0.55
1:A:102:ILE:HG12	1:A:117:THR:HB	1.87	0.55
2:N:311:CYS:O	2:N:315:GLN:HB2	2.06	0.55
2:B:275:LEU:HD11	2:B:288:LEU:HD21	1.89	0.55
1:E:132:GLU:O	1:E:136:THR:HG23	2.07	0.55
2:P:592:ILE:H	2:P:592:ILE:HD12	1.72	0.55
2:H:176:PHE:CZ	2:H:204:PHE:CZ	2.95	0.55
2:F:546:PRO:O	2:F:547:SER:HB2	2.06	0.54
2:L:519:TRP:CH2	2:L:567:HIS:ND1	2.75	0.54
2:D:54:HIS:CD2	2:D:77:SER:OG	2.58	0.54
2:H:284:GLU:CD	2:H:284:GLU:H	2.10	0.54
2:H:138:ASP:OD2	2:H:164:ARG:HG3	2.07	0.54
1:I:148:GLU:HG2	1:I:152:ARG:HH12	1.72	0.54
2:J:235:LEU:O	2:J:238:PHE:HB3	2.07	0.54
2:F:396:GLU:O	2:F:400:THR:HB	2.07	0.54
2:B:521:GLN:HG3	2:B:567:HIS:HD2	1.72	0.54
1:M:125:ILE:HG23	1:M:133:ILE:CD1	2.36	0.54
1:I:129:THR:O	1:I:133:ILE:HG12	2.06	0.54
2:N:419:ILE:HD13	2:N:446:ARG:NH1	2.21	0.54
1:E:128:LYS:HB2	1:E:133:ILE:CD1	2.37	0.54
1:A:102:ILE:HG12	1:A:117:THR:CB	2.37	0.54
1:I:26:SER:HG	1:I:108:LEU:HB3	1.72	0.54
2:L:519:TRP:NE1	4:L:1100:7JA:C01	2.62	0.54
2:H:232:ILE:HG13	2:H:253:LEU:HD23	1.89	0.54
2:P:396:GLU:O	2:P:400:THR:HB	2.07	0.54
2:H:49:SER:HB2	2:H:71:ARG:O	2.07	0.54
1:C:134:ARG:HH11	2:D:40:VAL:HA	1.73	0.54
1:A:99:PHE:HZ	1:A:137:PHE:HE1	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:279:TYR:HA	2:F:304:LEU:HD22	1.89	0.54
2:H:274:ARG:CG	2:H:297:LYS:HB3	2.27	0.54
2:H:83:LYS:HA	2:H:96:TRP:CZ3	2.43	0.54
2:F:456:SER:CB	2:F:482:GLU:HB3	2.37	0.54
1:M:48:THR:HG22	1:M:51:ILE:CB	2.38	0.54
1:O:128:LYS:HB2	1:O:133:ILE:CD1	2.38	0.54
1:E:44:LEU:O	1:E:44:LEU:HD12	2.07	0.54
1:C:12:ASP:OD2	1:C:49:SER:HB2	2.08	0.54
2:H:106:GLU:HA	2:H:106:GLU:OE1	2.08	0.54
4:D:1100:7JA:OXT	4:D:1100:7JA:CG2	2.53	0.54
2:P:547:SER:HB3	2:P:564:HIS:HB2	1.90	0.54
2:P:519:TRP:CH2	2:P:567:HIS:ND1	2.76	0.54
2:F:367:GLN:O	2:F:371:ILE:HG22	2.07	0.54
1:E:135:THR:HG22	1:E:136:THR:N	2.21	0.54
2:F:253:LEU:HD12	2:F:280:MET:HB2	1.89	0.54
2:J:103:TRP:O	2:J:107:ILE:HG13	2.08	0.54
2:H:492:LYS:NZ	2:H:516:ARG:NH1	2.54	0.54
2:J:357:GLY:HA2	2:J:415:ARG:NH2	2.20	0.54
2:L:396:GLU:O	2:L:400:THR:HB	2.07	0.54
2:B:255:GLU:HG3	2:B:255:GLU:O	2.08	0.54
2:H:391:THR:O	2:H:395:LEU:HD23	2.07	0.54
2:P:533:MET:CE	2:P:588:LEU:HD13	2.38	0.54
2:J:397:SER:O	2:J:400:THR:HG22	2.08	0.54
2:B:297:LYS:HE2	2:B:322:VAL:HG21	1.90	0.54
2:J:519:TRP:NE1	4:J:1100:7JA:C01	2.60	0.54
2:H:328:VAL:HG13	2:H:359:GLU:CG	2.37	0.54
1:I:48:THR:HG22	1:I:51:ILE:HB	1.90	0.54
2:J:101:THR:OG1	2:J:102:PRO:HD3	2.08	0.54
2:P:308:GLU:O	2:P:312:THR:HG23	2.08	0.54
2:P:227:VAL:CG1	2:P:228:GLY:N	2.69	0.54
2:D:227:VAL:CG1	2:D:228:GLY:N	2.70	0.54
1:M:148:GLU:HG2	1:M:152:ARG:NH1	2.23	0.54
1:I:105:ALA:HB2	1:I:113:LEU:HD23	1.89	0.54
2:P:424:LEU:O	2:P:428:VAL:HG23	2.07	0.54
2:P:176:PHE:CZ	2:P:204:PHE:CZ	2.96	0.54
2:B:233:LEU:O	2:B:236:VAL:HG23	2.06	0.54
1:A:27:GLN:HB2	1:A:109:ASN:HB3	1.90	0.54
2:F:542:ILE:HG13	2:F:588:LEU:HB2	1.90	0.54
2:H:533:MET:CE	2:H:588:LEU:HB3	2.37	0.54
2:N:307:THR:HG22	2:N:360:ASP:OD2	2.07	0.54
2:D:54:HIS:HE1	2:D:56:THR:OG1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:ARG:NH2	5:D:1103:PO4:O4	2.41	0.54
2:D:456:SER:CB	2:D:482:GLU:HB3	2.38	0.54
1:E:37:CYS:SG	2:L:296:ARG:NH2	2.81	0.54
2:L:279:TYR:HA	2:L:304:LEU:HD22	1.90	0.54
2:D:492:LYS:HE3	2:D:517:TYR:CE2	2.43	0.54
2:H:118:HIS:HE1	2:H:146:ASP:OD2	1.90	0.53
2:B:357:GLY:HA2	2:B:415:ARG:NH2	2.23	0.53
2:D:159:ILE:HD11	2:D:169:LEU:HD13	1.90	0.53
2:D:422:LEU:HB3	2:D:423:PRO:HD3	1.89	0.53
1:E:107:TYR:HE1	2:L:294:GLN:HE22	1.56	0.53
2:P:54:HIS:HD2	2:P:77:SER:OG	1.90	0.53
2:F:227:VAL:CG1	2:F:228:GLY:N	2.72	0.53
2:P:422:LEU:HB3	2:P:423:PRO:HD3	1.90	0.53
1:I:132:GLU:O	1:I:136:THR:HG23	2.09	0.53
2:B:261:GLU:HG2	2:B:264:MET:HG3	1.90	0.53
2:B:171:MET:O	2:B:174:SER:HB2	2.08	0.53
2:J:386:TYR:CE1	4:J:1100:7JA:CG2	2.86	0.53
4:B:1100:7JA:O	4:B:1100:7JA:CG2	2.52	0.53
2:D:231:GLU:HG2	2:D:254:ASN:ND2	2.22	0.53
1:I:105:ALA:HB3	1:I:114:LEU:CD1	2.38	0.53
1:E:158:ALA:HA	2:F:62:THR:HG21	1.89	0.53
2:H:268:PHE:O	2:H:270:ARG:N	2.41	0.53
2:H:390:ILE:HB	2:H:395:LEU:HD21	1.90	0.53
2:N:547:SER:HB3	2:N:564:HIS:HB2	1.90	0.53
1:A:48:THR:HG22	1:A:51:ILE:N	2.20	0.53
2:L:227:VAL:HG13	2:L:228:GLY:H	1.73	0.53
2:L:412:LEU:HD12	2:L:412:LEU:C	2.29	0.53
2:B:121:ARG:HH22	5:B:1103:PO4:P	2.32	0.53
2:N:465:VAL:HG11	2:N:468:MET:HG3	1.90	0.53
2:J:289:PHE:N	2:J:290:PRO:HD2	2.23	0.53
2:F:422:LEU:HB3	2:F:423:PRO:HD3	1.91	0.53
2:J:371:ILE:O	2:J:375:GLN:HG3	2.08	0.53
2:F:351:ARG:HG3	2:F:351:ARG:O	2.09	0.53
2:N:545:ILE:HG22	2:N:546:PRO:N	2.24	0.53
2:L:542:ILE:CG1	2:L:588:LEU:HB2	2.38	0.53
1:C:159:PHE:O	1:C:160:GLU:CB	2.55	0.53
2:P:412:LEU:C	2:P:412:LEU:HD12	2.28	0.53
1:E:134:ARG:HH11	2:F:40:VAL:HA	1.74	0.53
2:H:18:ASP:OD2	2:H:43:ARG:NH1	2.34	0.53
1:C:153:ARG:HG2	1:C:157:TRP:CZ3	2.44	0.53
1:I:102:ILE:CG1	1:I:117:THR:HB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:GLN:HB2	1:E:109:ASN:HB3	1.90	0.53
1:C:114:LEU:C	1:C:116:LEU:H	2.12	0.53
2:P:521:GLN:HG3	2:P:567:HIS:HD2	1.73	0.53
2:P:533:MET:HE3	2:P:588:LEU:HD13	1.89	0.53
2:B:191:ASN:ND2	2:B:194:LEU:H	2.06	0.53
2:P:367:GLN:HB3	2:P:391:THR:HG22	1.91	0.53
2:L:465:VAL:HG11	2:L:468:MET:HG3	1.91	0.53
1:O:52:LEU:O	1:O:56:ILE:HG13	2.09	0.53
1:I:52:LEU:O	1:I:56:ILE:HG13	2.09	0.53
2:F:113:GLN:HE22	2:L:192:THR:CB	2.21	0.53
2:B:103:TRP:O	2:B:107:ILE:HG13	2.08	0.53
2:B:456:SER:CB	2:B:482:GLU:HB3	2.38	0.53
2:F:547:SER:HB3	2:F:564:HIS:HB2	1.90	0.53
2:L:547:SER:HB3	2:L:564:HIS:CB	2.39	0.53
2:H:366:SER:C	2:H:368:ARG:N	2.60	0.53
2:H:365:VAL:HG12	2:H:370:LEU:HG	1.89	0.53
2:L:289:PHE:N	2:L:290:PRO:HD2	2.24	0.53
1:E:159:PHE:O	1:E:160:GLU:CB	2.57	0.53
1:A:101:LEU:HB3	1:A:117:THR:HG21	1.91	0.53
2:F:307:THR:HG22	2:F:360:ASP:OD2	2.09	0.53
2:H:262:LYS:HD2	2:H:263:TYR:CZ	2.44	0.53
2:H:503:ARG:HE	2:H:503:ARG:H	1.57	0.53
2:D:396:GLU:HG2	2:D:430:SER:OG	2.08	0.53
2:D:235:LEU:O	2:D:238:PHE:HB3	2.09	0.53
2:L:255:GLU:HG3	2:L:255:GLU:O	2.08	0.53
2:D:101:THR:OG1	2:N:179:LYS:NZ	2.42	0.53
1:E:48:THR:HG22	1:E:51:ILE:N	2.19	0.53
1:G:48:THR:HG22	1:G:51:ILE:CB	2.38	0.53
1:A:159:PHE:O	1:A:160:GLU:CB	2.57	0.53
2:D:397:SER:O	2:D:400:THR:HG22	2.09	0.53
2:N:197:LEU:O	2:N:225:VAL:HA	2.09	0.53
2:P:78:LEU:HD12	2:P:79:LYS:H	1.73	0.53
2:J:78:LEU:HD12	2:J:79:LYS:H	1.74	0.53
2:H:327:ASN:HD22	2:H:364:LEU:HD21	1.73	0.53
2:B:231:GLU:HG2	2:B:254:ASN:ND2	2.24	0.53
2:F:397:SER:O	2:F:400:THR:HG22	2.09	0.53
2:D:161:THR:HG22	2:D:186:GLU:HG2	1.90	0.53
2:B:95:ASN:O	2:B:582:PRO:HG3	2.08	0.53
2:P:253:LEU:HD12	2:P:280:MET:HB2	1.91	0.53
2:L:542:ILE:HG13	2:L:588:LEU:HB2	1.91	0.53
2:F:542:ILE:CG1	2:F:588:LEU:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ARG:NH2	2:H:539:TYR:CE1	2.76	0.53
2:J:422:LEU:O	2:J:423:PRO:C	2.45	0.53
1:E:148:GLU:HG2	1:E:152:ARG:NH1	2.24	0.53
2:B:456:SER:HB3	2:B:482:GLU:HB3	1.90	0.53
1:K:27:GLN:HB2	1:K:109:ASN:HB3	1.89	0.53
2:H:418:ARG:HB3	2:H:421:ASP:HB2	1.91	0.53
2:B:422:LEU:HB3	2:B:423:PRO:HD3	1.91	0.53
2:B:472:TYR:OH	3:Q:201:LEU:HB2	2.08	0.53
2:J:547:SER:HB3	2:J:564:HIS:CB	2.38	0.52
2:P:519:TRP:CZ3	2:P:567:HIS:ND1	2.77	0.52
2:H:363:GLY:O	2:H:365:VAL:N	2.42	0.52
2:H:428:VAL:HG12	2:H:443:PHE:CE1	2.44	0.52
2:J:311:CYS:CB	2:J:336:VAL:HG21	2.38	0.52
2:L:371:ILE:O	2:L:375:GLN:HG3	2.08	0.52
2:N:121:ARG:HH22	5:N:1103:PO4:P	2.32	0.52
1:E:141:ASN:C	1:E:141:ASN:OD1	2.47	0.52
2:H:91:LEU:HD21	2:H:496:ARG:NH2	2.23	0.52
2:H:269:PRO:O	2:H:271:LYS:N	2.42	0.52
2:J:545:ILE:HG22	2:J:546:PRO:N	2.25	0.52
2:B:386:TYR:CE1	4:B:1100:7JA:CG2	2.87	0.52
1:K:46:ASN:HB2	1:K:107:TYR:CZ	2.44	0.52
1:A:12:ASP:OD2	1:A:49:SER:HB2	2.10	0.52
1:C:148:GLU:HG2	1:C:152:ARG:HH12	1.74	0.52
2:J:138:ASP:OD2	2:J:164:ARG:HG3	2.08	0.52
2:P:357:GLY:HA2	2:P:415:ARG:NH2	2.22	0.52
2:F:161:THR:HG22	2:F:186:GLU:HG2	1.90	0.52
2:H:447:GLN:HG3	2:H:447:GLN:O	2.09	0.52
2:P:386:TYR:CE1	4:P:1100:7JA:CG2	2.88	0.52
4:L:1100:7JA:CG2	4:L:1100:7JA:OXT	2.55	0.52
1:M:87:ASP:HB3	1:M:116:LEU:HD21	1.92	0.52
1:O:148:GLU:HG2	1:O:152:ARG:NH1	2.24	0.52
2:F:396:GLU:HG2	2:F:430:SER:OG	2.09	0.52
2:D:279:TYR:HA	2:D:304:LEU:HD22	1.89	0.52
2:F:54:HIS:HD2	2:F:77:SER:OG	1.93	0.52
2:J:171:MET:O	2:J:174:SER:HB2	2.09	0.52
2:J:170:LEU:C	2:J:170:LEU:HD23	2.30	0.52
2:F:519:TRP:CH2	2:F:567:HIS:ND1	2.77	0.52
2:B:545:ILE:HG22	2:B:546:PRO:N	2.23	0.52
2:F:357:GLY:HA2	2:F:415:ARG:NH2	2.24	0.52
2:N:371:ILE:O	2:N:375:GLN:HG3	2.09	0.52
1:E:105:ALA:HB3	1:E:114:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:ARG:HH22	5:P:1103:PO4:P	2.31	0.52
2:N:399:GLY:O	2:N:434:GLY:HA3	2.10	0.52
1:I:46:ASN:HB2	1:I:107:TYR:CZ	2.44	0.52
2:D:519:TRP:CH2	2:D:567:HIS:CE1	2.94	0.52
2:P:444:TYR:HA	2:P:471:GLY:CA	2.35	0.52
2:P:542:ILE:CG1	2:P:588:LEU:HB2	2.40	0.52
1:K:48:THR:HG22	1:K:51:ILE:N	2.21	0.52
1:K:159:PHE:O	1:K:160:GLU:CB	2.56	0.52
2:N:367:GLN:HB3	2:N:391:THR:HG22	1.92	0.52
1:A:98:LEU:CD2	1:A:120:THR:HG22	2.39	0.52
2:H:107:ILE:HG12	2:H:114:LEU:CD2	2.40	0.52
2:D:411:VAL:HG22	2:D:444:TYR:HB3	1.91	0.52
2:H:542:ILE:HD12	2:H:542:ILE:O	2.09	0.52
2:N:308:GLU:O	2:N:312:THR:HG23	2.10	0.52
2:J:159:ILE:HD11	2:J:169:LEU:HD13	1.91	0.52
2:L:197:LEU:O	2:L:225:VAL:HA	2.09	0.52
2:B:542:ILE:CD1	2:B:588:LEU:HD12	2.33	0.52
2:J:199:PHE:CE1	2:J:227:VAL:HG22	2.44	0.52
2:P:197:LEU:O	2:P:225:VAL:HA	2.09	0.52
2:L:253:LEU:HD12	2:L:280:MET:HB2	1.92	0.52
2:F:95:ASN:O	2:F:582:PRO:HG3	2.10	0.52
2:N:492:LYS:HE3	2:N:517:TYR:CE2	2.45	0.52
2:N:176:PHE:CZ	2:N:204:PHE:CZ	2.98	0.52
2:D:170:LEU:HD23	2:D:170:LEU:C	2.30	0.52
2:J:255:GLU:HG3	2:J:255:GLU:O	2.10	0.52
2:F:386:TYR:HE1	4:F:1100:7JA:HG2	1.66	0.52
2:D:519:TRP:NE1	4:D:1100:7JA:C01	2.64	0.52
2:H:395:LEU:N	2:H:395:LEU:CD2	2.73	0.52
2:N:519:TRP:CH2	2:N:567:HIS:ND1	2.77	0.52
2:H:362:GLU:O	2:H:363:GLY:C	2.48	0.52
1:K:129:THR:O	1:K:133:ILE:HG12	2.09	0.52
2:P:210:LYS:O	2:P:214:THR:HG22	2.10	0.52
2:F:371:ILE:O	2:F:375:GLN:HG3	2.09	0.52
1:C:105:ALA:HB2	1:C:113:LEU:HD23	1.91	0.52
2:L:351:ARG:O	2:L:351:ARG:HG3	2.10	0.52
2:B:40:VAL:O	2:B:41:CYS:HB3	2.10	0.52
2:N:386:TYR:HE1	4:N:1100:7JA:HG2	1.68	0.52
2:H:331:ASP:CG	2:H:366:SER:H	2.13	0.52
1:C:114:LEU:C	1:C:116:LEU:N	2.63	0.52
2:H:321:GLU:HA	2:H:344:LEU:HA	1.92	0.52
2:B:519:TRP:CZ3	2:B:567:HIS:ND1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:102:ILE:CB	2:N:20:VAL:CG2	2.87	0.51
2:P:542:ILE:HG13	2:P:588:LEU:HB2	1.92	0.51
1:C:125:ILE:HG23	1:C:133:ILE:CD1	2.34	0.51
1:I:124:MET:O	1:I:128:LYS:HE2	2.09	0.51
2:P:399:GLY:O	2:P:434:GLY:HA3	2.10	0.51
2:B:54:HIS:HD2	2:B:77:SER:OG	1.93	0.51
2:J:367:GLN:HB3	2:J:391:THR:HG22	1.92	0.51
1:O:134:ARG:HH11	2:P:40:VAL:HA	1.75	0.51
1:O:132:GLU:O	1:O:136:THR:HG23	2.09	0.51
1:M:44:LEU:O	1:M:44:LEU:HD12	2.11	0.51
2:J:542:ILE:HG13	2:J:588:LEU:HB2	1.92	0.51
2:N:289:PHE:N	2:N:290:PRO:HD2	2.25	0.51
2:J:301:LEU:HD23	2:J:324:GLU:HB3	1.91	0.51
2:D:365:VAL:CG2	2:D:387:VAL:HA	2.40	0.51
2:P:57:MET:HE3	2:P:62:THR:HG22	1.92	0.51
2:L:54:HIS:CD2	2:L:77:SER:OG	2.63	0.51
1:I:148:GLU:HG2	1:I:152:ARG:NH1	2.25	0.51
2:H:91:LEU:HD21	2:H:496:ARG:HH22	1.75	0.51
2:L:233:LEU:O	2:L:236:VAL:HG23	2.09	0.51
2:B:296:ARG:HH22	1:O:35:ASP:HB2	1.74	0.51
2:N:592:ILE:H	2:N:592:ILE:HD12	1.75	0.51
2:D:547:SER:HB3	2:D:564:HIS:CB	2.40	0.51
2:B:521:GLN:HG3	2:B:567:HIS:CD2	2.45	0.51
2:H:199:PHE:CE1	2:H:227:VAL:CG2	2.92	0.51
2:H:178:GLU:CD	2:H:206:LYS:HB3	2.30	0.51
2:P:311:CYS:CB	2:P:336:VAL:HG21	2.41	0.51
2:L:133:ALA:HB2	2:L:159:ILE:HG22	1.92	0.51
1:C:135:THR:HG22	1:C:136:THR:N	2.25	0.51
2:P:396:GLU:HG2	2:P:430:SER:OG	2.10	0.51
2:J:197:LEU:O	2:J:225:VAL:HA	2.11	0.51
2:P:547:SER:HB3	2:P:564:HIS:CB	2.41	0.51
2:F:419:ILE:CD1	2:F:446:ARG:HH12	2.23	0.51
2:J:389:ASP:OD2	2:J:419:ILE:HG23	2.10	0.51
1:G:160:GLU:HG2	2:H:52:ARG:HH21	1.76	0.51
2:F:301:LEU:HD23	2:F:324:GLU:HB3	1.93	0.51
2:N:231:GLU:HG2	2:N:254:ASN:ND2	2.25	0.51
2:L:57:MET:HE3	2:L:62:THR:HG22	1.92	0.51
2:H:256:ASP:OD2	2:H:259:MET:HG2	2.10	0.51
2:B:176:PHE:CZ	2:B:204:PHE:CZ	2.99	0.51
1:G:108:LEU:HD12	1:G:110:ILE:HD11	1.93	0.51
2:D:592:ILE:H	2:D:592:ILE:HD12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:248:PHE:CD2	2:P:248:PHE:C	2.83	0.51
2:P:519:TRP:NE1	4:P:1100:7JA:C01	2.65	0.51
2:H:405:LEU:HD13	2:H:408:PHE:HB2	1.91	0.51
2:B:289:PHE:N	2:B:290:PRO:CD	2.73	0.51
2:N:357:GLY:HA2	2:N:415:ARG:NH2	2.24	0.51
2:J:392:ASN:HD21	2:J:424:LEU:HA	1.75	0.51
1:E:124:MET:O	1:E:128:LYS:HE2	2.10	0.51
2:H:101:THR:HB	2:H:102:PRO:HD2	1.91	0.51
1:C:108:LEU:HD12	1:C:110:ILE:HD11	1.92	0.51
2:L:65:PRO:HG3	2:L:103:TRP:CE2	2.46	0.51
2:B:170:LEU:HD23	2:B:170:LEU:C	2.31	0.51
2:L:521:GLN:HG3	2:L:567:HIS:HD2	1.75	0.51
2:H:247:GLU:HA	2:H:274:ARG:O	2.10	0.51
2:L:357:GLY:HA2	2:L:415:ARG:NH2	2.21	0.51
2:B:157:LEU:O	2:B:161:THR:HG23	2.11	0.51
1:M:135:THR:HG22	1:M:136:THR:N	2.25	0.51
2:F:412:LEU:HD12	2:F:412:LEU:C	2.30	0.51
1:I:105:ALA:HB3	1:I:114:LEU:HD12	1.92	0.51
2:D:297:LYS:HE2	2:D:322:VAL:HG21	1.92	0.51
2:H:459:GLY:O	2:H:486:GLY:HA3	2.10	0.51
2:J:519:TRP:CZ3	2:J:567:HIS:ND1	2.78	0.51
1:C:129:THR:O	1:C:133:ILE:HG12	2.11	0.51
1:A:48:THR:HG22	1:A:51:ILE:CB	2.40	0.51
1:M:58:TYR:CD2	1:M:113:LEU:HD13	2.46	0.51
1:K:135:THR:HG22	1:K:136:THR:N	2.25	0.51
2:F:172:GLU:HG3	2:F:200:TYR:HB3	1.91	0.51
1:E:131:GLU:OE2	1:E:131:GLU:HA	2.11	0.51
2:D:542:ILE:HG13	2:D:588:LEU:HB2	1.93	0.51
2:L:289:PHE:N	2:L:290:PRO:CD	2.74	0.51
2:H:124:VAL:O	2:H:151:PHE:HB3	2.11	0.51
1:G:153:ARG:HB3	2:H:574:LEU:HD21	1.93	0.51
1:E:30:ALA:C	1:E:32:MET:H	2.15	0.51
2:D:422:LEU:O	2:D:423:PRO:C	2.48	0.51
2:J:227:VAL:CG1	2:J:228:GLY:N	2.73	0.51
2:F:171:MET:O	2:F:174:SER:HB2	2.10	0.51
2:P:521:GLN:HG3	2:P:567:HIS:CD2	2.45	0.51
2:B:547:SER:HB3	2:B:564:HIS:CB	2.40	0.51
1:E:48:THR:HG22	1:E:51:ILE:CB	2.39	0.51
1:C:128:LYS:HB2	1:C:133:ILE:CD1	2.41	0.51
1:M:99:PHE:CE2	2:N:16:THR:C	2.84	0.51
1:M:48:THR:HG22	1:M:51:ILE:N	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:327:ASN:HD22	2:J:328:VAL:N	2.09	0.51
2:F:440:ARG:HB3	2:F:467:TRP:CE3	2.46	0.51
2:H:107:ILE:HG12	2:H:114:LEU:HD22	1.92	0.51
2:N:279:TYR:HA	2:N:304:LEU:HD22	1.93	0.51
2:B:293:ALA:HB3	1:O:45:PRO:HG3	1.93	0.51
2:L:176:PHE:CZ	2:L:204:PHE:CZ	2.98	0.51
2:H:542:ILE:HD11	2:H:588:LEU:CB	2.41	0.51
2:F:328:VAL:CG2	2:F:359:GLU:HB2	2.41	0.51
2:P:327:ASN:HD22	2:P:328:VAL:N	2.08	0.51
1:G:28:THR:O	1:G:32:MET:HE2	2.11	0.51
2:P:365:VAL:CG2	2:P:387:VAL:HA	2.41	0.51
2:L:301:LEU:HD23	2:L:324:GLU:HB3	1.92	0.51
2:F:482:GLU:O	2:F:485:ARG:HG2	2.11	0.51
2:B:539:TYR:OH	1:C:146:GLU:HA	2.10	0.51
2:H:337:LEU:HD11	2:H:344:LEU:HD22	1.93	0.51
2:N:83:LYS:HA	2:N:96:TRP:CZ3	2.46	0.51
1:G:151:VAL:HG12	2:H:39:LEU:HD21	1.86	0.50
2:L:422:LEU:HB3	2:L:423:PRO:HD3	1.93	0.50
2:N:227:VAL:HG13	2:N:228:GLY:N	2.26	0.50
2:B:57:MET:HE3	2:B:62:THR:HG22	1.92	0.50
1:O:102:ILE:HD12	2:P:20:VAL:HG21	1.91	0.50
2:F:547:SER:HB3	2:F:564:HIS:CB	2.42	0.50
2:H:332:ARG:O	2:H:336:VAL:HG23	2.11	0.50
1:K:125:ILE:HG23	1:K:133:ILE:CD1	2.38	0.50
2:B:351:ARG:O	2:B:351:ARG:HG3	2.11	0.50
2:H:232:ILE:HG13	2:H:253:LEU:HD21	1.93	0.50
2:J:191:ASN:ND2	2:J:194:LEU:HB2	2.27	0.50
2:N:159:ILE:HD11	2:N:169:LEU:HD13	1.92	0.50
1:I:106:ASN:N	1:I:114:LEU:HD13	2.26	0.50
1:I:102:ILE:HG13	1:I:117:THR:HB	1.94	0.50
2:F:22:GLU:HG2	2:F:47:ILE:CD1	2.41	0.50
2:J:40:VAL:O	2:J:41:CYS:HB3	2.11	0.50
2:N:255:GLU:O	2:N:255:GLU:HG3	2.11	0.50
2:H:366:SER:HB3	2:H:368:ARG:CG	2.25	0.50
1:K:48:THR:HG22	1:K:51:ILE:CB	2.42	0.50
2:F:121:ARG:NH2	5:F:1103:PO4:O4	2.43	0.50
1:A:52:LEU:O	1:A:56:ILE:HG13	2.11	0.50
2:D:253:LEU:HD12	2:D:280:MET:HB2	1.93	0.50
2:L:519:TRP:CZ3	2:L:567:HIS:ND1	2.79	0.50
2:H:303:ALA:HB1	2:H:305:LEU:CD2	2.42	0.50
2:P:311:CYS:O	2:P:315:GLN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:ASN:ND2	2:F:194:LEU:H	2.08	0.50
2:D:396:GLU:O	2:D:400:THR:HB	2.12	0.50
2:N:253:LEU:HD12	2:N:280:MET:HB2	1.92	0.50
2:J:191:ASN:ND2	2:J:194:LEU:H	2.08	0.50
2:F:54:HIS:HE1	2:F:56:THR:OG1	1.95	0.50
1:M:12:ASP:OD2	1:M:49:SER:HB2	2.12	0.50
2:P:83:LYS:HA	2:P:96:TRP:CZ3	2.47	0.50
2:H:76:ARG:HG2	2:H:76:ARG:HH11	1.76	0.50
1:A:141:ASN:OD1	1:A:141:ASN:C	2.50	0.50
2:N:519:TRP:CZ3	2:N:567:HIS:ND1	2.80	0.50
1:I:48:THR:HG22	1:I:51:ILE:N	2.18	0.50
2:F:80:LEU:O	2:F:122:MET:HE2	2.12	0.50
2:N:412:LEU:HD12	2:N:412:LEU:C	2.32	0.50
2:N:54:HIS:HD2	2:N:77:SER:OG	1.94	0.50
2:H:587:VAL:O	2:H:587:VAL:HG12	2.10	0.50
2:B:270:ARG:HB3	1:O:107:TYR:CD1	2.47	0.50
2:B:78:LEU:HD12	2:B:79:LYS:H	1.77	0.50
2:N:321:GLU:HA	2:N:344:LEU:HA	1.92	0.50
2:N:101:THR:OG1	2:N:102:PRO:HD3	2.12	0.50
2:L:159:ILE:HD11	2:L:169:LEU:HD13	1.94	0.50
2:L:40:VAL:O	2:L:41:CYS:HB3	2.10	0.50
1:I:101:LEU:HB3	1:I:117:THR:HG21	1.93	0.50
2:B:399:GLY:O	2:B:434:GLY:HA3	2.12	0.50
2:J:220:ARG:HH21	2:N:22:GLU:HB3	1.76	0.50
2:N:35:ASP:O	2:N:38:SER:OG	2.29	0.50
1:G:52:LEU:O	1:G:56:ILE:HG13	2.11	0.50
2:J:546:PRO:HG2	2:J:584:THR:CB	2.38	0.50
2:H:462:SER:HB2	2:H:465:VAL:HB	1.92	0.50
1:M:99:PHE:CD2	2:N:16:THR:O	2.65	0.50
2:L:311:CYS:CB	2:L:336:VAL:HG21	2.42	0.50
2:L:261:GLU:HG2	2:L:264:MET:HG3	1.94	0.50
1:E:52:LEU:O	1:E:56:ILE:HG13	2.11	0.50
2:D:197:LEU:O	2:D:225:VAL:HA	2.11	0.50
1:M:108:LEU:HD12	1:M:110:ILE:HD11	1.93	0.50
1:K:52:LEU:O	1:K:56:ILE:HG13	2.12	0.50
2:P:261:GLU:HG2	2:P:264:MET:HG3	1.93	0.50
2:B:519:TRP:NE1	4:B:1100:7JA:C01	2.62	0.50
2:D:80:LEU:CB	2:D:122:MET:HE2	2.28	0.50
2:B:542:ILE:CG1	2:B:588:LEU:HB2	2.42	0.50
2:D:542:ILE:CG1	2:D:588:LEU:HB2	2.42	0.50
1:I:158:ALA:HA	2:J:62:THR:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:VAL:HG11	2:H:44:TRP:CE3	2.46	0.50
2:B:492:LYS:HE3	2:B:517:TYR:CE2	2.47	0.50
1:A:148:GLU:HG2	1:A:152:ARG:HH12	1.76	0.50
2:J:226:LYS:HA	2:J:249:CYS:O	2.12	0.50
2:P:156:LEU:O	2:P:160:VAL:HG22	2.12	0.50
2:L:503:ARG:NH1	2:L:503:ARG:HB3	2.27	0.50
2:P:546:PRO:HD3	2:P:584:THR:O	2.11	0.49
2:B:386:TYR:HE1	4:B:1100:7JA:HG2	1.70	0.49
2:H:331:ASP:OD1	2:H:366:SER:N	2.44	0.49
2:B:542:ILE:HG13	2:B:588:LEU:HB2	1.94	0.49
2:H:100:VAL:CG2	2:H:119:PHE:CE1	2.95	0.49
1:O:105:ALA:HB2	1:O:113:LEU:HD23	1.93	0.49
1:M:111:LYS:O	1:M:114:LEU:HB2	2.11	0.49
2:F:297:LYS:HG3	2:F:322:VAL:HB	1.92	0.49
1:I:26:SER:OG	1:I:108:LEU:HB3	2.12	0.49
2:F:22:GLU:HG2	2:F:47:ILE:HD13	1.94	0.49
2:L:85:ARG:NH2	4:L:1100:7JA:O14	2.40	0.49
2:L:545:ILE:HG22	2:L:546:PRO:N	2.27	0.49
2:H:85:ARG:HB3	2:H:85:ARG:CZ	2.41	0.49
2:N:547:SER:HB3	2:N:564:HIS:CB	2.42	0.49
1:O:48:THR:HG22	1:O:51:ILE:CB	2.40	0.49
2:J:365:VAL:CG2	2:J:387:VAL:HA	2.41	0.49
2:B:289:PHE:N	2:B:290:PRO:HD2	2.27	0.49
2:D:296:ARG:NE	1:G:37:CYS:SG	2.85	0.49
2:N:78:LEU:HD12	2:N:79:LYS:H	1.77	0.49
2:N:233:LEU:O	2:N:236:VAL:HG23	2.12	0.49
1:I:44:LEU:O	1:I:44:LEU:HD12	2.12	0.49
2:F:176:PHE:CZ	2:F:204:PHE:CZ	3.01	0.49
1:C:44:LEU:O	1:C:44:LEU:HD12	2.12	0.49
2:J:22:GLU:OE1	2:J:43:ARG:NH2	2.45	0.49
2:B:22:GLU:HG2	2:B:47:ILE:CD1	2.42	0.49
2:N:519:TRP:CH2	2:N:567:HIS:CG	3.00	0.49
2:H:385:VAL:HG13	2:H:387:VAL:HG23	1.94	0.49
2:D:357:GLY:HA2	2:D:415:ARG:NH2	2.25	0.49
2:H:277:LEU:O	2:H:278:SER:C	2.51	0.49
1:A:153:ARG:NH2	2:B:539:TYR:CE1	2.81	0.49
2:N:22:GLU:HG2	2:N:47:ILE:HD13	1.93	0.49
1:A:108:LEU:HD12	1:A:110:ILE:HD11	1.95	0.49
2:F:85:ARG:NH2	4:F:1100:7JA:O14	2.38	0.49
2:D:533:MET:HE3	2:D:588:LEU:HD13	1.93	0.49
2:H:543:GLU:C	2:H:544:LEU:HD23	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:VAL:HG11	2:H:124:VAL:HG22	1.94	0.49
2:F:365:VAL:CG2	2:F:387:VAL:HA	2.41	0.49
2:P:199:PHE:CZ	2:P:227:VAL:HG22	2.47	0.49
2:D:176:PHE:CZ	2:D:204:PHE:CZ	3.00	0.49
1:G:137:PHE:CD1	2:H:17:VAL:HG13	2.48	0.49
2:H:298:LEU:HD22	2:H:300:LEU:HG	1.94	0.49
1:K:12:ASP:OD2	1:K:49:SER:HB2	2.11	0.49
2:P:168:THR:HB	2:P:196:VAL:CG1	2.17	0.49
2:H:176:PHE:HZ	2:H:204:PHE:CZ	2.30	0.49
1:A:44:LEU:O	1:A:44:LEU:HD12	2.13	0.49
2:H:64:THR:O	2:H:65:PRO:C	2.47	0.49
2:H:390:ILE:HD11	2:H:410:LEU:HD11	1.94	0.49
2:N:533:MET:CE	2:N:588:LEU:HD13	2.42	0.49
2:H:428:VAL:O	2:H:432:LEU:HG	2.13	0.49
2:L:80:LEU:O	2:L:122:MET:HE2	2.12	0.49
2:H:153:THR:CG2	2:H:178:GLU:HA	2.41	0.49
2:B:327:ASN:HD22	2:B:328:VAL:N	2.11	0.49
2:L:311:CYS:O	2:L:315:GLN:HB2	2.13	0.49
2:B:301:LEU:HD23	2:B:324:GLU:HB3	1.94	0.49
2:N:275:LEU:HD11	2:N:288:LEU:CD2	2.43	0.49
2:J:133:ALA:HB2	2:J:159:ILE:HG22	1.94	0.49
2:N:22:GLU:HG2	2:N:47:ILE:CD1	2.43	0.49
2:L:161:THR:HG22	2:L:186:GLU:HG2	1.93	0.49
2:H:395:LEU:N	2:H:395:LEU:HD22	2.28	0.49
2:D:419:ILE:CD1	2:D:446:ARG:HH12	2.24	0.49
2:H:373:LEU:C	2:H:373:LEU:HD12	2.32	0.49
1:I:159:PHE:O	1:I:160:GLU:CB	2.59	0.49
2:B:422:LEU:O	2:B:423:PRO:C	2.51	0.49
2:F:121:ARG:HH22	5:F:1103:PO4:P	2.36	0.49
2:J:337:LEU:HD12	2:J:341:CYS:SG	2.53	0.49
2:J:253:LEU:HD12	2:J:280:MET:HB2	1.93	0.49
2:N:116:SER:CB	2:N:142:THR:HG23	2.32	0.49
2:L:542:ILE:HD11	2:L:588:LEU:CD1	2.31	0.49
2:H:478:GLU:O	2:H:482:GLU:HG2	2.13	0.49
2:N:124:VAL:O	2:N:151:PHE:HB3	2.12	0.49
2:D:275:LEU:HD11	2:D:288:LEU:HD21	1.94	0.49
1:M:52:LEU:O	1:M:56:ILE:HG13	2.12	0.49
2:H:386:TYR:CD2	2:H:413:LEU:HD21	2.48	0.49
2:D:444:TYR:HA	2:D:471:GLY:CA	2.31	0.49
1:G:102:ILE:HG21	2:H:20:VAL:HG22	1.95	0.49
2:D:199:PHE:CE1	2:D:227:VAL:HG22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:65:PRO:HA	2:H:103:TRP:CZ3	2.48	0.49
1:A:46:ASN:HB2	1:A:107:TYR:CZ	2.47	0.49
1:I:160:GLU:CG	2:J:31:PRO:HB3	2.43	0.49
2:H:170:LEU:HD23	2:H:170:LEU:C	2.33	0.49
2:F:367:GLN:HB3	2:F:391:THR:HG22	1.95	0.49
2:D:311:CYS:O	2:D:315:GLN:HB2	2.13	0.49
2:N:40:VAL:O	2:N:41:CYS:HB3	2.13	0.49
2:L:156:LEU:O	2:L:160:VAL:HG22	2.13	0.49
2:F:399:GLY:O	2:F:434:GLY:HA3	2.13	0.49
2:F:233:LEU:O	2:F:236:VAL:HG23	2.13	0.49
2:F:519:TRP:CZ3	2:F:567:HIS:ND1	2.81	0.48
2:H:331:ASP:OD2	2:H:366:SER:CB	2.59	0.48
2:J:542:ILE:CG1	2:J:588:LEU:HB2	2.43	0.48
2:H:465:VAL:HG11	2:H:468:MET:HG2	1.95	0.48
2:H:119:PHE:O	2:H:146:ASP:HB3	2.13	0.48
1:C:30:ALA:C	1:C:32:MET:H	2.16	0.48
2:B:275:LEU:HD11	2:B:288:LEU:CD2	2.42	0.48
1:O:137:PHE:CD1	2:P:17:VAL:HG21	2.47	0.48
2:P:22:GLU:HG2	2:P:47:ILE:HD13	1.94	0.48
2:P:171:MET:O	2:P:174:SER:HB2	2.12	0.48
2:P:152:THR:HG22	2:P:177:SER:HB2	1.95	0.48
2:N:65:PRO:HG3	2:N:103:TRP:CE2	2.48	0.48
2:F:519:TRP:NE1	4:F:1100:7JA:C01	2.65	0.48
2:H:542:ILE:HG12	2:H:588:LEU:HB2	1.92	0.48
2:P:80:LEU:O	2:P:122:MET:HE2	2.13	0.48
2:L:347:LEU:HD21	2:L:349:ILE:HD11	1.94	0.48
1:K:158:ALA:HA	2:L:62:THR:CG2	2.43	0.48
2:D:57:MET:HE3	2:D:62:THR:HG22	1.95	0.48
2:H:292:ALA:HA	2:H:295:ILE:HG12	1.95	0.48
2:D:542:ILE:CD1	2:D:588:LEU:HD12	2.38	0.48
2:F:327:ASN:HD22	2:F:328:VAL:N	2.11	0.48
2:N:392:ASN:HD21	2:N:424:LEU:HA	1.78	0.48
2:B:297:LYS:HG3	2:B:322:VAL:HB	1.95	0.48
2:N:103:TRP:O	2:N:107:ILE:HG13	2.13	0.48
2:N:432:LEU:CD1	2:N:458:ILE:HA	2.44	0.48
1:K:128:LYS:HB2	1:K:133:ILE:CD1	2.44	0.48
1:M:160:GLU:CG	2:N:31:PRO:HB3	2.43	0.48
2:B:365:VAL:CG2	2:B:387:VAL:HA	2.41	0.48
2:L:365:VAL:CG2	2:L:387:VAL:HA	2.43	0.48
2:D:211:ASP:O	2:D:215:ILE:HG13	2.13	0.48
2:J:465:VAL:HG11	2:J:468:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:422:LEU:HB3	2:N:423:PRO:HD3	1.94	0.48
1:C:134:ARG:HB2	1:C:139:ILE:O	2.14	0.48
1:E:35:ASP:HB2	2:L:296:ARG:HH22	1.79	0.48
2:D:280:MET:O	2:D:280:MET:HG2	2.13	0.48
2:D:247:GLU:HA	2:D:274:ARG:O	2.14	0.48
2:P:492:LYS:HE3	2:P:517:TYR:CE2	2.48	0.48
2:B:20:VAL:O	2:B:24:VAL:HG23	2.13	0.48
1:O:12:ASP:OD2	1:O:49:SER:HB2	2.13	0.48
2:D:519:TRP:CH2	2:D:567:HIS:CG	3.01	0.48
2:L:521:GLN:HG3	2:L:567:HIS:CD2	2.48	0.48
2:L:308:GLU:O	2:L:312:THR:HG23	2.13	0.48
1:G:30:ALA:C	1:G:32:MET:H	2.17	0.48
2:F:315:GLN:HG2	2:F:340:TYR:CE1	2.49	0.48
2:P:231:GLU:HG2	2:P:254:ASN:ND2	2.28	0.48
2:N:422:LEU:O	2:N:423:PRO:C	2.50	0.48
2:L:396:GLU:HG2	2:L:430:SER:OG	2.13	0.48
2:J:396:GLU:O	2:J:400:THR:HB	2.12	0.48
2:D:296:ARG:CZ	1:G:37:CYS:SG	3.01	0.48
1:K:141:ASN:C	1:K:141:ASN:OD1	2.52	0.48
1:I:134:ARG:HH11	2:J:40:VAL:HA	1.78	0.48
1:A:148:GLU:HG2	1:A:152:ARG:NH1	2.27	0.48
1:M:46:ASN:HB2	1:M:107:TYR:CZ	2.48	0.48
2:D:255:GLU:O	2:D:255:GLU:HG3	2.12	0.48
2:H:392:ASN:ND2	2:H:422:LEU:HD13	2.28	0.48
4:B:1100:7JA:H04	4:B:1100:7JA:H12A	1.69	0.48
2:H:343:GLN:N	2:H:343:GLN:CD	2.67	0.48
2:L:297:LYS:HE3	2:L:297:LYS:HB2	1.66	0.48
2:B:197:LEU:O	2:B:225:VAL:HA	2.14	0.48
2:N:503:ARG:HB3	2:N:503:ARG:NH1	2.29	0.48
2:H:412:LEU:HD13	2:H:446:ARG:NH2	2.28	0.48
2:H:442:ALA:CB	4:H:1100:7JA:HD1	2.25	0.48
2:N:542:ILE:CG1	2:N:588:LEU:HB2	2.44	0.48
1:G:129:THR:OG1	1:G:132:GLU:HG3	2.14	0.48
2:P:233:LEU:O	2:P:236:VAL:HG23	2.13	0.48
2:F:235:LEU:O	2:F:238:PHE:HB3	2.13	0.48
2:N:519:TRP:CZ3	2:N:567:HIS:CG	3.01	0.48
2:F:465:VAL:HG11	2:F:468:MET:HG3	1.96	0.48
1:O:124:MET:O	1:O:128:LYS:HE2	2.14	0.48
2:B:133:ALA:HB2	2:B:159:ILE:HG22	1.96	0.48
2:P:465:VAL:HG11	2:P:468:MET:HG3	1.96	0.48
2:F:311:CYS:O	2:F:315:GLN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:GLU:HG2	2:B:430:SER:OG	2.14	0.48
2:D:40:VAL:O	2:D:41:CYS:HB3	2.14	0.48
2:J:176:PHE:CZ	2:J:204:PHE:CZ	3.01	0.48
2:H:356:GLN:O	2:H:357:GLY:O	2.32	0.48
2:L:519:TRP:CH2	2:L:567:HIS:CG	3.02	0.48
2:J:80:LEU:HB2	2:J:122:MET:HE2	1.91	0.48
2:D:190:HIS:HB3	2:H:112:ARG:HD2	1.94	0.48
2:D:20:VAL:O	2:D:24:VAL:HG23	2.13	0.48
1:E:134:ARG:HB2	1:E:139:ILE:O	2.12	0.48
2:P:422:LEU:O	2:P:423:PRO:C	2.51	0.48
2:D:492:LYS:HG3	2:D:517:TYR:CD2	2.49	0.48
2:N:492:LYS:HG3	2:N:517:TYR:CD2	2.49	0.48
2:F:247:GLU:HA	2:F:274:ARG:O	2.14	0.48
2:P:321:GLU:HA	2:P:344:LEU:HA	1.94	0.48
2:P:46:LYS:HB2	2:P:46:LYS:HE3	1.49	0.48
2:D:248:PHE:CD2	2:D:248:PHE:C	2.86	0.48
2:P:546:PRO:HG2	2:P:584:THR:CB	2.37	0.48
2:P:328:VAL:CG2	2:P:359:GLU:HB2	2.43	0.48
1:K:114:LEU:C	1:K:116:LEU:H	2.16	0.48
2:B:156:LEU:O	2:B:160:VAL:HG22	2.14	0.48
2:H:395:LEU:HD23	2:H:395:LEU:H	1.79	0.47
2:B:519:TRP:CH2	2:B:567:HIS:CG	3.02	0.47
2:N:542:ILE:HG13	2:N:588:LEU:HB2	1.95	0.47
2:P:289:PHE:N	2:P:290:PRO:CD	2.77	0.47
2:J:285:MET:N	2:J:286:PRO:CD	2.77	0.47
2:L:419:ILE:CD1	2:L:446:ARG:HH12	2.27	0.47
1:A:30:ALA:C	1:A:32:MET:H	2.17	0.47
1:C:28:THR:O	1:C:32:MET:HE2	2.13	0.47
2:H:71:ARG:HG2	2:H:72:PHE:CD1	2.49	0.47
2:F:351:ARG:HD3	2:F:413:LEU:HD11	1.95	0.47
2:J:22:GLU:HG2	2:J:47:ILE:HD13	1.96	0.47
1:M:141:ASN:OD1	1:M:141:ASN:C	2.51	0.47
2:L:171:MET:O	2:L:174:SER:HB2	2.13	0.47
1:G:10:SER:OG	1:G:11:SER:N	2.47	0.47
2:P:503:ARG:HB3	2:P:503:ARG:NH1	2.28	0.47
2:J:248:PHE:CD2	2:J:248:PHE:C	2.87	0.47
4:J:1100:7JA:OXT	4:J:1100:7JA:CG2	2.56	0.47
4:F:1100:7JA:OXT	4:F:1100:7JA:CG2	2.54	0.47
2:H:391:THR:O	2:H:392:ASN:C	2.52	0.47
1:O:28:THR:O	1:O:32:MET:HE2	2.13	0.47
1:I:28:THR:O	1:I:32:MET:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:143:LEU:CD2	2:J:159:ILE:HD13	2.44	0.47
2:F:275:LEU:HD11	2:F:288:LEU:CD2	2.44	0.47
2:H:121:ARG:HA	2:H:147:LYS:O	2.13	0.47
2:H:101:THR:CB	2:H:102:PRO:CD	2.91	0.47
2:J:152:THR:HG22	2:J:177:SER:HB2	1.96	0.47
1:K:148:GLU:HG2	1:K:152:ARG:HH12	1.79	0.47
2:F:289:PHE:N	2:F:290:PRO:HD2	2.30	0.47
2:N:389:ASP:OD2	2:N:419:ILE:HG23	2.14	0.47
2:F:197:LEU:O	2:F:225:VAL:HA	2.14	0.47
2:H:386:TYR:HB3	2:H:413:LEU:HD21	1.97	0.47
2:F:157:LEU:O	2:F:161:THR:HG23	2.14	0.47
1:M:134:ARG:NE	1:M:141:ASN:HB2	2.30	0.47
2:N:153:THR:HG23	2:N:178:GLU:HA	1.95	0.47
2:D:124:VAL:O	2:D:151:PHE:HB3	2.15	0.47
3:Q:212:PHE:CD2	3:Q:213:LEU:HD23	2.48	0.47
1:G:82:ASP:O	1:G:85:ALA:HB3	2.14	0.47
2:H:201:MET:HG3	2:H:302:TYR:CD1	2.49	0.47
1:C:124:MET:O	1:C:128:LYS:HE2	2.14	0.47
2:H:153:THR:HG23	2:H:177:SER:O	2.14	0.47
2:J:289:PHE:N	2:J:290:PRO:CD	2.76	0.47
2:N:328:VAL:CG2	2:N:359:GLU:HB2	2.44	0.47
2:N:297:LYS:HB2	2:N:297:LYS:HE3	1.68	0.47
2:B:297:LYS:HB2	2:B:297:LYS:HE3	1.57	0.47
2:H:59:LEU:HD22	2:H:61:TYR:HB2	1.96	0.47
2:P:289:PHE:N	2:P:290:PRO:HD2	2.28	0.47
2:F:443:PHE:HE2	2:F:445:LEU:HD11	1.75	0.47
2:N:55:VAL:CG2	2:N:75:LEU:HD21	2.41	0.47
1:A:129:THR:O	1:A:133:ILE:HG12	2.14	0.47
2:P:366:SER:HB2	2:P:367:GLN:OE1	2.15	0.47
2:D:289:PHE:N	2:D:290:PRO:HD2	2.29	0.47
2:N:468:MET:CE	2:N:470:LEU:HD11	2.43	0.47
1:C:153:ARG:NH2	2:D:539:TYR:CE1	2.83	0.47
1:K:153:ARG:NH2	2:L:539:TYR:CE1	2.83	0.47
2:H:512:LEU:HA	2:H:513:PRO:HD3	1.64	0.47
2:J:221:SER:O	2:J:223:VAL:HG23	2.15	0.47
2:L:46:LYS:HE3	2:L:46:LYS:HB2	1.53	0.47
2:H:392:ASN:H	2:H:392:ASN:HD22	1.62	0.47
2:J:444:TYR:HA	2:J:471:GLY:CA	2.36	0.47
1:C:48:THR:HG22	1:C:51:ILE:CB	2.44	0.47
2:H:492:LYS:HZ1	2:H:516:ARG:HH11	1.59	0.47
2:F:112:ARG:CG	2:L:164:ARG:HD2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:308:GLU:O	2:F:312:THR:HG23	2.14	0.47
2:D:285:MET:N	2:D:286:PRO:CD	2.78	0.47
2:N:191:ASN:ND2	2:N:194:LEU:HB2	2.30	0.47
2:P:227:VAL:HG13	2:P:228:GLY:H	1.79	0.47
1:M:28:THR:O	1:M:32:MET:HE2	2.14	0.47
1:C:148:GLU:HG2	1:C:152:ARG:NH1	2.29	0.47
1:O:46:ASN:HB2	1:O:107:TYR:CZ	2.50	0.47
2:D:275:LEU:HD11	2:D:288:LEU:CD2	2.44	0.47
2:P:329:ILE:O	2:P:333:GLY:HA3	2.14	0.47
2:N:512:LEU:HA	2:N:513:PRO:HD2	1.77	0.47
2:J:83:LYS:HA	2:J:96:TRP:CZ3	2.49	0.47
2:P:161:THR:HG22	2:P:186:GLU:HG2	1.96	0.47
2:B:46:LYS:HB2	2:B:46:LYS:HE3	1.47	0.47
2:H:390:ILE:CD1	2:H:410:LEU:HD11	2.45	0.47
2:H:442:ALA:CB	4:H:1100:7JA:H28	2.44	0.47
2:H:85:ARG:O	2:H:88:MET:HG2	2.15	0.47
4:B:1100:7JA:O	4:B:1100:7JA:HG2A	2.10	0.47
2:P:101:THR:OG1	2:P:102:PRO:HD3	2.15	0.47
2:P:286:PRO:CA	2:P:289:PHE:CE2	2.92	0.47
2:L:78:LEU:HD21	2:L:80:LEU:HD21	1.96	0.47
1:M:153:ARG:CG	1:M:157:TRP:CZ3	2.98	0.47
2:D:96:TRP:O	2:D:578:ARG:NH2	2.39	0.47
2:F:57:MET:HE3	2:F:62:THR:HG22	1.96	0.47
1:I:141:ASN:OD1	1:I:141:ASN:C	2.52	0.47
2:P:22:GLU:HG2	2:P:47:ILE:CD1	2.45	0.47
2:H:286:PRO:C	2:H:288:LEU:N	2.69	0.47
2:J:270:ARG:O	1:M:46:ASN:OD1	2.33	0.47
2:H:423:PRO:HA	2:H:449:GLY:O	2.15	0.47
2:L:492:LYS:HE3	2:L:517:TYR:CE2	2.50	0.47
2:F:503:ARG:HB3	2:F:503:ARG:NH1	2.29	0.47
2:L:248:PHE:C	2:L:248:PHE:CD2	2.88	0.47
2:P:519:TRP:CH2	2:P:567:HIS:CE1	2.99	0.47
2:L:546:PRO:HG2	2:L:584:THR:CB	2.36	0.47
2:B:101:THR:OG1	2:B:102:PRO:HD3	2.15	0.47
2:P:419:ILE:CD1	2:P:446:ARG:HH12	2.26	0.47
2:B:465:VAL:HG11	2:B:468:MET:HG3	1.97	0.47
2:H:95:ASN:HD22	2:H:95:ASN:N	2.12	0.47
1:C:113:LEU:O	1:C:117:THR:CG2	2.63	0.47
2:B:199:PHE:CE1	2:B:227:VAL:HG22	2.49	0.47
1:G:134:ARG:HD3	2:H:40:VAL:O	2.15	0.47
2:H:136:ARG:HG3	2:H:136:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:LEU:C	1:K:116:LEU:N	2.66	0.47
2:N:337:LEU:HD12	2:N:341:CYS:SG	2.55	0.47
2:F:103:TRP:O	2:F:107:ILE:HG13	2.15	0.47
2:H:185:HIS:O	2:H:188:ALA:HB3	2.15	0.47
2:P:545:ILE:HG22	2:P:546:PRO:N	2.30	0.46
2:B:519:TRP:CH2	2:B:567:HIS:CE1	2.99	0.46
1:E:113:LEU:CG	1:E:113:LEU:O	2.63	0.46
2:L:422:LEU:O	2:L:423:PRO:C	2.53	0.46
1:C:58:TYR:CD2	1:C:113:LEU:HD13	2.50	0.46
2:B:492:LYS:HG3	2:B:517:TYR:CD2	2.50	0.46
2:F:101:THR:OG1	2:F:102:PRO:HD3	2.15	0.46
2:P:285:MET:N	2:P:286:PRO:CD	2.78	0.46
2:D:190:HIS:HE1	2:H:110:ASN:HA	1.81	0.46
2:D:289:PHE:N	2:D:290:PRO:CD	2.78	0.46
2:N:367:GLN:HG2	2:N:391:THR:HB	1.96	0.46
2:P:347:LEU:HD21	2:P:349:ILE:HD11	1.95	0.46
1:I:44:LEU:HA	1:I:45:PRO:HD3	1.71	0.46
1:G:12:ASP:OD2	1:G:49:SER:HB2	2.14	0.46
1:G:105:ALA:HB2	1:G:113:LEU:HD23	1.97	0.46
1:G:83:LEU:HA	1:G:83:LEU:HD23	1.77	0.46
2:N:248:PHE:C	2:N:248:PHE:CD2	2.88	0.46
2:L:546:PRO:HD3	2:L:584:THR:O	2.14	0.46
2:H:519:TRP:HH2	2:H:567:HIS:ND1	2.00	0.46
1:M:128:LYS:HB2	1:M:133:ILE:HD11	1.97	0.46
2:H:476:SER:C	2:H:478:GLU:N	2.67	0.46
1:M:134:ARG:HH11	2:N:40:VAL:HA	1.80	0.46
2:P:492:LYS:HG3	2:P:517:TYR:CD2	2.50	0.46
2:H:59:LEU:CD2	2:H:61:TYR:HB2	2.45	0.46
2:P:477:ASP:OD1	2:P:477:ASP:N	2.48	0.46
1:M:102:ILE:HB	2:N:20:VAL:CG2	2.46	0.46
1:A:128:LYS:HB2	1:A:133:ILE:CD1	2.46	0.46
1:I:12:ASP:OD2	1:I:49:SER:HB2	2.16	0.46
2:H:266:LEU:CD1	2:H:267:VAL:H	2.26	0.46
1:A:160:GLU:CG	2:B:31:PRO:HB3	2.45	0.46
2:J:54:HIS:CE1	2:J:56:THR:OG1	2.66	0.46
1:M:158:ALA:HA	2:N:62:THR:CG2	2.46	0.46
1:I:135:THR:HG22	1:I:136:THR:N	2.31	0.46
2:L:321:GLU:HA	2:L:344:LEU:HA	1.97	0.46
2:B:321:GLU:HA	2:B:344:LEU:HA	1.96	0.46
2:J:321:GLU:HA	2:J:344:LEU:HA	1.97	0.46
2:D:156:LEU:O	2:D:160:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:LEU:HA	2:H:39:LEU:HD23	1.56	0.46
4:P:1100:7JA:CG2	4:P:1100:7JA:OXT	2.58	0.46
4:N:1100:7JA:H05	4:N:1100:7JA:H27	1.74	0.46
2:H:347:LEU:HD12	2:H:347:LEU:C	2.33	0.46
2:F:444:TYR:HA	2:F:471:GLY:CA	2.33	0.46
1:C:93:ILE:CD1	1:C:97:THR:HG22	2.42	0.46
2:N:419:ILE:CD1	2:N:446:ARG:HH12	2.29	0.46
2:B:308:GLU:O	2:B:312:THR:HG23	2.16	0.46
2:L:387:VAL:HG22	2:L:389:ASP:H	1.79	0.46
2:F:55:VAL:CG2	2:F:75:LEU:HD21	2.45	0.46
2:D:367:GLN:HB3	2:D:391:THR:HG22	1.98	0.46
1:C:158:ALA:HA	2:D:62:THR:CG2	2.45	0.46
2:F:124:VAL:O	2:F:151:PHE:HB3	2.16	0.46
2:H:278:SER:C	2:H:280:MET:H	2.19	0.46
1:A:158:ALA:HA	2:B:62:THR:CG2	2.46	0.46
2:J:472:TYR:OH	3:U:201:LEU:HB2	2.16	0.46
2:B:235:LEU:O	2:B:238:PHE:HB3	2.16	0.46
2:L:399:GLY:O	2:L:434:GLY:HA3	2.16	0.46
2:F:519:TRP:CH2	2:F:567:HIS:CE1	3.03	0.46
2:H:494:GLU:HA	2:H:519:TRP:O	2.15	0.46
2:H:168:THR:HB	2:H:196:VAL:CG1	2.45	0.46
2:H:533:MET:O	2:H:535:MET:N	2.46	0.46
2:D:465:VAL:HG11	2:D:468:MET:HG3	1.98	0.46
3:V:201:LEU:HD23	3:V:201:LEU:HA	1.72	0.46
1:K:30:ALA:C	1:K:32:MET:H	2.19	0.46
2:D:296:ARG:NH1	1:G:35:ASP:OD1	2.41	0.46
1:I:134:ARG:NE	1:I:141:ASN:HB2	2.31	0.46
1:K:148:GLU:HG2	1:K:152:ARG:NH1	2.31	0.46
2:D:103:TRP:O	2:D:107:ILE:HG13	2.14	0.46
2:L:22:GLU:HG2	2:L:47:ILE:CD1	2.45	0.46
2:P:226:LYS:HA	2:P:249:CYS:O	2.15	0.46
2:P:153:THR:HG23	2:P:178:GLU:HA	1.97	0.46
2:F:83:LYS:HA	2:F:96:TRP:CZ3	2.51	0.46
2:H:366:SER:OG	2:H:368:ARG:HG2	2.16	0.46
2:P:542:ILE:CD1	2:P:588:LEU:HD12	2.36	0.46
2:P:332:ARG:O	2:P:336:VAL:HG23	2.15	0.46
2:D:191:ASN:ND2	2:D:194:LEU:HB2	2.30	0.46
2:P:194:LEU:HD12	2:P:194:LEU:HA	1.81	0.46
3:S:201:LEU:HD23	3:S:201:LEU:HA	1.61	0.46
2:P:297:LYS:HB2	2:P:297:LYS:HE3	1.68	0.46
2:P:40:VAL:O	2:P:41:CYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:134:ARG:HB2	1:M:139:ILE:O	2.15	0.46
2:H:59:LEU:CD2	2:H:61:TYR:H	2.29	0.46
2:H:108:SER:OG	2:H:135:ALA:HB2	2.16	0.46
2:F:564:HIS:HA	2:F:565:PRO:HD2	1.76	0.46
2:N:519:TRP:CH2	2:N:567:HIS:CE1	3.02	0.46
2:N:519:TRP:CZ3	2:N:567:HIS:HB3	2.51	0.46
2:J:542:ILE:CD1	2:J:588:LEU:HD12	2.36	0.46
1:K:160:GLU:CG	2:L:31:PRO:HB3	2.46	0.46
1:E:160:GLU:CG	2:F:31:PRO:HB3	2.45	0.46
2:N:443:PHE:HE2	2:N:445:LEU:HD11	1.80	0.46
2:H:94:GLU:CG	2:H:95:ASN:H	2.29	0.46
1:K:134:ARG:HB2	1:K:139:ILE:O	2.16	0.46
1:O:42:VAL:HA	1:O:43:PRO:HD3	1.82	0.46
2:J:329:ILE:O	2:J:333:GLY:HA3	2.16	0.46
2:P:432:LEU:CD1	2:P:458:ILE:HA	2.46	0.46
2:H:327:ASN:HA	2:H:349:ILE:CG2	2.46	0.45
2:L:285:MET:N	2:L:286:PRO:CD	2.79	0.45
2:B:419:ILE:HD11	2:B:446:ARG:NH2	2.27	0.45
2:P:211:ASP:HA	2:P:214:THR:CG2	2.43	0.45
1:O:30:ALA:C	1:O:32:MET:H	2.20	0.45
2:P:275:LEU:HD11	2:P:288:LEU:CD2	2.46	0.45
2:J:20:VAL:O	2:J:24:VAL:HG23	2.16	0.45
2:H:317:CYS:O	2:H:320:LEU:HB2	2.16	0.45
2:N:338:ALA:O	2:N:376:GLY:HA3	2.16	0.45
2:L:172:GLU:HG3	2:L:200:TYR:HB3	1.96	0.45
2:N:20:VAL:O	2:N:24:VAL:HG23	2.17	0.45
2:H:351:ARG:HG3	2:H:359:GLU:HB3	1.97	0.45
2:J:164:ARG:HE	2:N:112:ARG:HG2	1.69	0.45
2:H:375:GLN:HG2	2:H:401:TYR:CE1	2.51	0.45
2:P:159:ILE:HD11	2:P:169:LEU:HD13	1.99	0.45
1:A:102:ILE:HG12	1:A:117:THR:OG1	2.16	0.45
2:B:310:HIS:HE1	2:B:325:THR:OG1	1.98	0.45
2:L:194:LEU:HD12	2:L:194:LEU:HA	1.74	0.45
2:D:133:ALA:HB2	2:D:159:ILE:HG22	1.98	0.45
2:B:431:LEU:CD1	2:B:435:CYS:SG	3.04	0.45
1:E:130:PRO:O	1:E:134:ARG:HG2	2.16	0.45
3:X:201:LEU:HD23	3:X:201:LEU:HA	1.69	0.45
1:M:103:LEU:HD11	2:N:19:ASP:HB3	1.98	0.45
2:J:495:MET:O	2:J:520:VAL:HA	2.16	0.45
2:F:255:GLU:HG3	2:F:255:GLU:O	2.16	0.45
2:F:168:THR:HB	2:F:196:VAL:CG1	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:314:ILE:HG22	2:H:341:CYS:SG	2.56	0.45
2:H:327:ASN:HD22	2:H:364:LEU:CD2	2.30	0.45
2:J:311:CYS:O	2:J:315:GLN:HB2	2.16	0.45
2:D:191:ASN:ND2	2:D:194:LEU:H	2.10	0.45
2:L:367:GLN:HG2	2:L:391:THR:HB	1.98	0.45
2:N:310:HIS:HE1	2:N:325:THR:OG1	2.00	0.45
1:K:158:ALA:CB	2:L:62:THR:HG23	2.47	0.45
3:R:201:LEU:HD23	3:R:201:LEU:HA	1.74	0.45
1:K:134:ARG:NE	1:K:141:ASN:HB2	2.31	0.45
2:H:16:THR:O	2:H:17:VAL:C	2.54	0.45
1:G:137:PHE:CD1	2:H:17:VAL:CG1	3.00	0.45
2:L:22:GLU:OE1	2:L:43:ARG:NH2	2.49	0.45
2:J:298:LEU:HA	2:J:298:LEU:HD12	1.67	0.45
2:L:275:LEU:HD11	2:L:288:LEU:HD21	1.97	0.45
2:F:321:GLU:HA	2:F:344:LEU:HA	1.99	0.45
2:N:451:THR:HA	2:N:475:GLU:HG3	1.98	0.45
2:D:321:GLU:HA	2:D:344:LEU:HA	1.98	0.45
2:D:101:THR:OG1	2:D:102:PRO:HD3	2.17	0.45
2:H:230:PHE:CD1	2:H:235:LEU:HD21	2.39	0.45
2:D:194:LEU:HA	2:D:194:LEU:HD12	1.80	0.45
2:D:351:ARG:HG3	2:D:351:ARG:O	2.16	0.45
2:P:54:HIS:CE1	2:P:56:THR:OG1	2.66	0.45
2:D:297:LYS:HG3	2:D:322:VAL:HB	1.98	0.45
2:F:20:VAL:O	2:F:24:VAL:HG23	2.17	0.45
2:F:329:ILE:O	2:F:333:GLY:HA3	2.17	0.45
2:B:503:ARG:HB3	2:B:503:ARG:NH1	2.31	0.45
2:J:519:TRP:CH2	2:J:567:HIS:CG	3.04	0.45
2:B:545:ILE:HA	2:B:546:PRO:HD3	1.76	0.45
2:B:546:PRO:HG2	2:B:584:THR:CB	2.42	0.45
1:O:105:ALA:HB3	1:O:114:LEU:HD13	1.98	0.45
2:F:240:LYS:CG	2:F:267:VAL:HG21	2.44	0.45
2:J:54:HIS:CD2	2:J:77:SER:OG	2.69	0.45
2:F:387:VAL:HG22	2:F:389:ASP:H	1.80	0.45
2:L:54:HIS:CE1	2:L:56:THR:OG1	2.69	0.45
2:N:65:PRO:HA	2:N:103:TRP:CZ3	2.52	0.45
2:B:114:LEU:O	2:B:136:ARG:NH1	2.48	0.45
2:D:22:GLU:OE1	2:D:43:ARG:NH2	2.49	0.45
2:N:404:ASN:HA	2:N:437:LYS:HD2	1.99	0.45
2:P:63:ALA:HB1	2:P:67:ARG:HD2	1.99	0.45
2:J:399:GLY:O	2:J:434:GLY:HA3	2.17	0.45
2:P:95:ASN:O	2:P:582:PRO:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:ILE:O	2:D:333:GLY:HA3	2.17	0.45
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.84	0.45
1:K:44:LEU:O	1:K:44:LEU:HD12	2.17	0.45
2:H:32:LYS:HD3	2:H:32:LYS:HA	1.49	0.45
4:F:1100:7JA:OXT	4:F:1100:7JA:HG2A	2.13	0.45
2:D:546:PRO:HG2	2:D:584:THR:CB	2.40	0.45
2:J:419:ILE:O	2:J:420:THR:C	2.55	0.45
1:M:112:ASN:O	1:M:114:LEU:N	2.46	0.45
1:I:153:ARG:NH2	2:J:539:TYR:CE1	2.85	0.45
2:J:199:PHE:CZ	2:J:227:VAL:HG22	2.52	0.45
2:N:343:GLN:O	2:N:345:LYS:HG2	2.17	0.45
2:P:512:LEU:HA	2:P:513:PRO:HD2	1.76	0.45
3:R:212:PHE:CD2	3:R:213:LEU:HD23	2.52	0.45
2:L:305:LEU:H	2:L:305:LEU:HD22	1.80	0.45
2:P:255:GLU:O	2:P:255:GLU:HG3	2.16	0.45
4:J:1100:7JA:HG2A	4:J:1100:7JA:OXT	2.12	0.45
4:F:1100:7JA:H05	4:F:1100:7JA:H27	1.65	0.45
1:K:124:MET:O	1:K:128:LYS:HE2	2.16	0.45
2:L:80:LEU:HD12	2:L:122:MET:HE1	1.97	0.45
2:H:100:VAL:HG21	2:H:119:PHE:CZ	2.51	0.45
2:N:398:ILE:CG2	2:N:402:LEU:HD11	2.45	0.45
1:E:128:LYS:HB2	1:E:133:ILE:HD11	1.99	0.45
2:N:199:PHE:CZ	2:N:227:VAL:HG22	2.52	0.45
1:E:137:PHE:CD1	2:F:17:VAL:HG21	2.52	0.45
2:N:247:GLU:HA	2:N:274:ARG:O	2.16	0.45
2:H:455:LEU:HA	2:H:455:LEU:HD23	1.66	0.45
2:F:545:ILE:HG22	2:F:546:PRO:N	2.32	0.45
2:N:91:LEU:O	2:N:567:HIS:HE1	2.00	0.45
2:H:371:ILE:HG22	2:H:375:GLN:NE2	2.20	0.45
2:J:80:LEU:O	2:J:122:MET:HE2	2.16	0.45
2:H:100:VAL:HG23	2:H:122:MET:HE2	1.98	0.45
1:I:128:LYS:HB2	1:I:133:ILE:HD11	1.99	0.45
2:D:419:ILE:HD11	2:D:446:ARG:NH2	2.25	0.45
2:N:301:LEU:CD2	2:N:324:GLU:HB3	2.46	0.45
2:F:392:ASN:HD21	2:F:424:LEU:HA	1.82	0.45
1:A:134:ARG:NH1	2:B:40:VAL:HA	2.31	0.45
1:K:153:ARG:HG2	1:K:157:TRP:CZ3	2.52	0.45
2:F:153:THR:HG23	2:F:178:GLU:HA	1.99	0.45
1:E:91:MET:HG3	1:E:116:LEU:HD11	1.98	0.45
2:B:245:LEU:HA	2:B:245:LEU:HD12	1.80	0.45
1:O:160:GLU:CG	2:P:31:PRO:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:431:LEU:CD1	2:P:435:CYS:SG	3.05	0.45
2:H:477:ASP:HB3	2:H:504:ALA:CB	2.47	0.45
1:M:30:ALA:C	1:M:32:MET:H	2.21	0.45
2:J:275:LEU:HD11	2:J:288:LEU:CD2	2.46	0.45
1:O:134:ARG:HB2	1:O:139:ILE:O	2.17	0.45
2:J:37:ALA:O	2:J:40:VAL:HG13	2.17	0.45
1:A:8:LEU:HD23	1:A:42:VAL:HG13	1.98	0.45
2:F:46:LYS:HE3	2:F:46:LYS:HB2	1.56	0.45
2:H:410:LEU:HD13	2:H:411:VAL:N	2.32	0.44
2:H:310:HIS:NE2	2:H:328:VAL:HG23	2.31	0.44
2:H:314:ILE:C	2:H:316:LYS:H	2.18	0.44
1:M:99:PHE:HZ	2:N:17:VAL:HG22	1.82	0.44
2:D:429:ARG:HG2	2:D:433:ILE:HD11	1.99	0.44
1:I:158:ALA:CB	2:J:62:THR:HG23	2.47	0.44
2:P:301:LEU:CD2	2:P:324:GLU:HB3	2.47	0.44
1:O:141:ASN:OD1	1:O:141:ASN:C	2.55	0.44
1:I:134:ARG:HB2	1:I:139:ILE:O	2.17	0.44
2:D:172:GLU:HG3	2:D:200:TYR:HB3	1.99	0.44
2:P:405:LEU:HD23	2:P:405:LEU:HA	1.80	0.44
2:P:101:THR:CG2	2:P:128:ASP:OD1	2.55	0.44
2:H:142:THR:HA	2:H:168:THR:O	2.17	0.44
2:H:156:LEU:HD11	2:H:171:MET:HE3	2.00	0.44
1:M:111:LYS:O	1:M:114:LEU:CB	2.65	0.44
2:B:419:ILE:CD1	2:B:446:ARG:HH12	2.27	0.44
2:H:161:THR:HG22	2:H:186:GLU:HG2	1.99	0.44
2:N:469:LEU:HA	2:N:494:GLU:O	2.17	0.44
2:J:519:TRP:CH2	2:J:567:HIS:CE1	3.00	0.44
2:P:519:TRP:CH2	2:P:567:HIS:CG	3.05	0.44
2:H:366:SER:O	2:H:369:GLY:N	2.49	0.44
2:J:164:ARG:NE	2:N:112:ARG:HG3	2.14	0.44
2:L:101:THR:OG1	2:L:102:PRO:HD3	2.17	0.44
1:O:48:THR:HG22	1:O:51:ILE:N	2.22	0.44
2:B:389:ASP:OD2	2:B:419:ILE:HG23	2.17	0.44
2:F:301:LEU:CD2	2:F:324:GLU:HB3	2.48	0.44
1:K:28:THR:O	1:K:32:MET:HE2	2.18	0.44
2:N:227:VAL:CG1	2:N:228:GLY:N	2.81	0.44
2:J:22:GLU:HG2	2:J:47:ILE:CD1	2.46	0.44
2:J:432:LEU:CD1	2:J:458:ILE:HA	2.48	0.44
2:L:532:LEU:HA	2:L:532:LEU:HD23	1.75	0.44
2:P:245:LEU:HD12	2:P:245:LEU:HA	1.85	0.44
2:P:532:LEU:HD23	2:P:532:LEU:HA	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:521:GLN:HG3	2:D:567:HIS:HD2	1.82	0.44
2:H:56:THR:CG2	2:H:79:LYS:HD2	2.46	0.44
2:H:117:VAL:HG11	2:H:119:PHE:CZ	2.52	0.44
2:B:328:VAL:CG2	2:B:359:GLU:HB2	2.45	0.44
1:E:44:LEU:HA	1:E:45:PRO:HD3	1.71	0.44
2:L:199:PHE:CZ	2:L:227:VAL:HG22	2.52	0.44
2:H:64:THR:O	2:H:67:ARG:N	2.47	0.44
1:M:154:GLU:OE1	2:N:67:ARG:NH1	2.51	0.44
2:N:34:ARG:NH1	2:N:48:ASP:OD1	2.50	0.44
2:D:46:LYS:HE3	2:D:46:LYS:HB2	1.51	0.44
2:H:409:ARG:CB	4:H:1100:7JA:HD1	2.48	0.44
2:N:351:ARG:HB3	2:N:386:TYR:CG	2.52	0.44
2:N:101:THR:N	2:N:102:PRO:CD	2.81	0.44
2:H:506:ALA:HB1	2:H:535:MET:HB2	1.99	0.44
2:P:443:PHE:HE2	2:P:445:LEU:HD11	1.82	0.44
2:L:441:PHE:O	2:L:468:MET:HA	2.18	0.44
2:F:366:SER:HB2	2:F:367:GLN:OE1	2.17	0.44
2:J:431:LEU:CD1	2:J:435:CYS:SG	3.05	0.44
1:E:153:ARG:NH2	2:F:539:TYR:CE1	2.85	0.44
2:H:121:ARG:NH2	5:H:1103:PO4:O4	2.49	0.44
2:H:71:ARG:HG2	2:H:72:PHE:CE1	2.52	0.44
1:M:130:PRO:O	1:M:134:ARG:HG2	2.17	0.44
2:H:320:LEU:HD12	2:H:320:LEU:HA	1.71	0.44
2:H:495:MET:HB2	2:H:520:VAL:HG22	1.99	0.44
2:H:390:ILE:HD13	2:H:390:ILE:N	2.32	0.44
2:H:392:ASN:H	2:H:392:ASN:ND2	2.15	0.44
4:P:1100:7JA:H05	4:P:1100:7JA:H27	1.67	0.44
2:P:519:TRP:CZ3	2:P:567:HIS:CG	3.05	0.44
2:L:519:TRP:CZ3	2:L:567:HIS:CG	3.06	0.44
2:B:519:TRP:CZ3	2:B:567:HIS:CG	3.06	0.44
2:L:444:TYR:HA	2:L:471:GLY:CA	2.37	0.44
2:D:308:GLU:O	2:D:312:THR:HG23	2.18	0.44
1:O:125:ILE:HG23	1:O:133:ILE:CD1	2.42	0.44
2:H:211:ASP:HA	2:H:214:THR:HG23	1.99	0.44
2:N:315:GLN:HG2	2:N:340:TYR:CE1	2.53	0.44
2:P:83:LYS:HA	2:P:84:PRO:HD3	1.88	0.44
2:H:424:LEU:O	2:H:427:GLY:N	2.50	0.44
2:J:117:VAL:HG11	2:J:119:PHE:CZ	2.52	0.44
2:P:495:MET:O	2:P:520:VAL:HA	2.16	0.44
2:L:578:ARG:HG3	2:L:578:ARG:H	1.46	0.44
1:G:125:ILE:HG23	1:G:133:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:GLU:HG3	2:B:200:TYR:HB3	1.98	0.44
2:B:247:GLU:HA	2:B:274:ARG:O	2.17	0.44
1:C:46:ASN:HB2	1:C:107:TYR:CZ	2.53	0.44
1:A:105:ALA:HB2	1:A:113:LEU:HD23	1.99	0.44
2:H:75:LEU:HA	2:H:75:LEU:HD23	1.60	0.44
2:J:546:PRO:HD3	2:J:584:THR:O	2.18	0.44
2:P:533:MET:HE3	2:P:588:LEU:HB3	2.00	0.44
2:P:191:ASN:HD21	2:P:194:LEU:N	2.09	0.44
2:H:96:TRP:O	2:H:578:ARG:NH2	2.51	0.44
2:P:456:SER:HB2	2:P:482:GLU:HB3	1.97	0.44
3:R:201:LEU:HA	3:R:202:PRO:HD3	1.83	0.44
2:H:121:ARG:NH2	5:H:1103:PO4:P	2.91	0.44
3:W:201:LEU:HD23	3:W:201:LEU:HA	1.68	0.44
1:E:158:ALA:HA	2:F:62:THR:CG2	2.48	0.44
2:H:424:LEU:N	2:H:449:GLY:O	2.47	0.44
2:D:165:LYS:NZ	2:H:139:ASP:OD1	2.46	0.44
2:F:492:LYS:HG3	2:F:517:TYR:CD2	2.53	0.44
2:L:545:ILE:HA	2:L:546:PRO:HD3	1.74	0.44
2:F:429:ARG:HG2	2:F:433:ILE:HD11	2.00	0.44
1:M:99:PHE:CD2	2:N:16:THR:CA	3.00	0.44
2:F:311:CYS:CB	2:F:336:VAL:HG21	2.45	0.44
1:G:147:GLU:O	1:G:148:GLU:C	2.54	0.44
2:N:441:PHE:O	2:N:468:MET:HA	2.17	0.44
1:C:134:ARG:NE	1:C:141:ASN:HB2	2.33	0.44
2:B:22:GLU:OE1	2:B:43:ARG:NH2	2.51	0.44
2:J:46:LYS:HE3	2:J:46:LYS:HB2	1.50	0.44
1:G:152:ARG:O	1:G:153:ARG:C	2.56	0.44
2:H:255:GLU:HB3	2:H:263:TYR:HE1	1.83	0.44
2:F:343:GLN:O	2:F:345:LYS:HG2	2.18	0.44
2:L:320:LEU:HD21	2:L:323:LEU:HB2	1.99	0.44
1:E:12:ASP:OD2	1:E:49:SER:HB2	2.17	0.44
2:F:405:LEU:HA	2:F:405:LEU:HD23	1.77	0.44
2:L:519:TRP:CH2	2:L:567:HIS:CE1	3.02	0.43
2:H:314:ILE:O	2:H:316:LYS:N	2.51	0.43
2:B:542:ILE:HD11	2:B:588:LEU:CD1	2.37	0.43
2:J:80:LEU:HD12	2:J:122:MET:HE1	2.00	0.43
2:L:138:ASP:OD2	2:L:164:ARG:HG3	2.18	0.43
2:H:124:VAL:CG1	2:H:129:LEU:HD13	2.48	0.43
2:H:206:LYS:HE3	2:H:206:LYS:HB2	1.81	0.43
2:B:285:MET:N	2:B:286:PRO:CD	2.81	0.43
1:A:125:ILE:HG23	1:A:133:ILE:CD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:328:VAL:CG2	2:L:359:GLU:HB2	2.43	0.43
2:L:310:HIS:HE1	2:L:325:THR:OG1	2.00	0.43
2:L:103:TRP:O	2:L:107:ILE:HG13	2.18	0.43
2:N:37:ALA:O	2:N:40:VAL:HG13	2.18	0.43
2:P:451:THR:HB	2:P:475:GLU:OE2	2.18	0.43
2:H:140:LEU:HD23	2:H:163:CYS:SG	2.58	0.43
1:C:8:LEU:HD23	1:C:42:VAL:HG13	1.99	0.43
2:F:519:TRP:CH2	2:F:567:HIS:CG	3.06	0.43
2:D:348:ARG:HH22	4:D:1100:7JA:C	2.32	0.43
2:B:546:PRO:HD3	2:B:584:THR:O	2.18	0.43
2:H:328:VAL:CG1	2:H:359:GLU:HG2	2.40	0.43
2:B:101:THR:HG22	2:B:128:ASP:CG	2.37	0.43
1:M:137:PHE:CD1	2:N:17:VAL:HG21	2.52	0.43
1:O:128:LYS:HB2	1:O:133:ILE:HD11	1.99	0.43
2:H:225:VAL:HG23	2:H:225:VAL:O	2.17	0.43
2:B:83:LYS:O	2:B:121:ARG:HD2	2.19	0.43
2:F:199:PHE:CZ	2:F:227:VAL:HG22	2.53	0.43
2:D:297:LYS:HE3	2:D:297:LYS:HB2	1.67	0.43
2:D:22:GLU:HG2	2:D:47:ILE:HD13	2.01	0.43
1:I:6:ILE:HG22	1:I:7:VAL:N	2.33	0.43
2:F:432:LEU:CD1	2:F:458:ILE:HA	2.48	0.43
2:P:235:LEU:O	2:P:238:PHE:HB3	2.17	0.43
2:D:519:TRP:CZ3	2:D:567:HIS:CG	3.06	0.43
2:D:546:PRO:HD3	2:D:584:THR:O	2.17	0.43
2:N:545:ILE:HG23	2:N:546:PRO:HD2	2.01	0.43
2:H:351:ARG:HH11	2:H:360:ASP:HA	1.83	0.43
2:H:542:ILE:HD13	2:H:544:LEU:HD21	2.00	0.43
2:L:211:ASP:HA	2:L:214:THR:CG2	2.47	0.43
2:N:482:GLU:O	2:N:485:ARG:HG2	2.18	0.43
2:J:490:LEU:HD23	2:J:490:LEU:HA	1.86	0.43
1:C:13:GLY:HA3	1:K:9:LYS:NZ	2.32	0.43
1:M:6:ILE:HG22	1:M:7:VAL:N	2.33	0.43
2:B:477:ASP:N	2:B:477:ASP:OD1	2.50	0.43
2:B:546:PRO:HB2	2:B:547:SER:H	1.60	0.43
2:P:285:MET:HB3	2:P:286:PRO:HD3	2.00	0.43
2:N:419:ILE:O	2:N:420:THR:C	2.57	0.43
2:D:398:ILE:CG2	2:D:402:LEU:HD11	2.43	0.43
2:F:422:LEU:O	2:F:424:LEU:HG	2.18	0.43
1:I:30:ALA:C	1:I:32:MET:H	2.22	0.43
2:F:297:LYS:HE2	2:F:322:VAL:CG2	2.48	0.43
2:L:297:LYS:HE2	2:L:322:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:491:GLN:HA	2:H:515:LEU:HA	1.99	0.43
1:O:108:LEU:HD12	1:O:110:ILE:HD11	2.00	0.43
3:U:212:PHE:CD2	3:U:213:LEU:HD23	2.53	0.43
2:P:114:LEU:O	2:P:136:ARG:NH1	2.49	0.43
2:L:114:LEU:HD12	2:L:114:LEU:HA	1.80	0.43
1:M:8:LEU:HD23	1:M:42:VAL:HG13	2.00	0.43
1:G:142:ASP:N	1:G:142:ASP:OD2	2.51	0.43
4:H:1100:7JA:H12	4:H:1100:7JA:H05A	1.84	0.43
2:H:328:VAL:CG1	2:H:359:GLU:CG	2.96	0.43
2:H:364:LEU:HD13	2:H:388:SER:CB	2.49	0.43
2:F:101:THR:N	2:F:102:PRO:CD	2.82	0.43
2:N:194:LEU:HA	2:N:194:LEU:HD12	1.73	0.43
2:L:247:GLU:HA	2:L:274:ARG:O	2.18	0.43
2:D:78:LEU:HD12	2:D:79:LYS:H	1.83	0.43
1:I:42:VAL:HG22	1:I:42:VAL:O	2.18	0.43
2:J:503:ARG:HB3	2:J:503:ARG:NH1	2.34	0.43
2:D:503:ARG:NH1	2:D:503:ARG:HB3	2.34	0.43
2:N:298:LEU:HD12	2:N:298:LEU:HA	1.70	0.43
2:D:521:GLN:HG3	2:D:567:HIS:CD2	2.53	0.43
2:L:85:ARG:NH1	5:L:1101:PO4:O3	2.51	0.43
2:J:398:ILE:CG2	2:J:402:LEU:HD11	2.43	0.43
2:P:315:GLN:HG2	2:P:340:TYR:CE1	2.54	0.43
2:P:453:LEU:HD11	2:P:457:TYR:OH	2.18	0.43
1:G:148:GLU:HG2	1:G:152:ARG:NH1	2.33	0.43
1:G:46:ASN:HB2	1:G:107:TYR:CZ	2.53	0.43
1:E:46:ASN:HB2	1:E:107:TYR:CZ	2.54	0.43
1:O:158:ALA:HA	2:P:62:THR:CG2	2.46	0.43
1:O:10:SER:OG	1:O:11:SER:N	2.51	0.43
2:J:512:LEU:HA	2:J:513:PRO:HD2	1.73	0.43
2:L:405:LEU:HA	2:L:405:LEU:HD23	1.84	0.43
2:J:547:SER:CB	2:J:564:HIS:CB	2.96	0.43
2:F:409:ARG:HB3	4:F:1100:7JA:HG1	2.01	0.43
2:H:385:VAL:HG13	2:H:387:VAL:CG2	2.48	0.43
2:J:411:VAL:HG22	2:J:444:TYR:HB3	1.99	0.43
2:L:429:ARG:HG2	2:L:433:ILE:HD11	2.01	0.43
2:H:207:ILE:HD12	2:H:230:PHE:HZ	1.84	0.43
2:J:315:GLN:HG2	2:J:340:TYR:CE1	2.54	0.43
2:H:213:GLU:OE2	2:H:237:GLY:HA3	2.18	0.43
2:P:563:GLU:O	2:P:563:GLU:CG	2.66	0.43
2:H:96:TRP:HA	2:H:582:PRO:CG	2.47	0.43
2:H:233:LEU:HD11	2:H:262:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:297:LYS:HG3	2:L:322:VAL:HB	2.01	0.43
2:D:578:ARG:H	2:D:578:ARG:HG3	1.48	0.43
2:N:83:LYS:HA	2:N:84:PRO:HD3	1.88	0.43
1:E:91:MET:HG2	1:E:116:LEU:HD21	2.00	0.43
2:L:114:LEU:O	2:L:136:ARG:NH1	2.50	0.43
1:I:126:LYS:HZ1	2:J:29:THR:H	1.67	0.43
2:J:120:ARG:HD2	2:J:146:ASP:OD2	2.18	0.43
2:B:404:ASN:HA	2:B:437:LYS:HD2	2.01	0.43
2:B:451:THR:HA	2:B:475:GLU:HG3	2.00	0.43
2:D:187:LEU:HD23	2:D:187:LEU:HA	1.85	0.43
2:D:547:SER:CB	2:D:564:HIS:CB	2.97	0.43
2:B:85:ARG:NH2	4:B:1100:7JA:O14	2.45	0.43
2:H:227:VAL:O	2:H:250:GLY:HA3	2.19	0.43
2:F:112:ARG:HG2	2:L:164:ARG:CD	2.43	0.43
2:L:78:LEU:HD12	2:L:79:LYS:H	1.84	0.43
1:A:124:MET:O	1:A:128:LYS:HE2	2.18	0.43
2:D:431:LEU:C	2:D:431:LEU:CD1	2.82	0.43
2:L:419:ILE:HD11	2:L:446:ARG:NH2	2.29	0.43
2:L:389:ASP:OD2	2:L:419:ILE:HG23	2.18	0.43
2:J:191:ASN:HD21	2:J:194:LEU:N	2.12	0.43
2:N:311:CYS:CB	2:N:336:VAL:HG21	2.48	0.43
1:O:153:ARG:CG	1:O:157:TRP:CZ3	3.02	0.43
2:F:107:ILE:HG12	2:F:111:LEU:HD12	2.00	0.43
2:J:344:LEU:HD23	2:J:380:LEU:HD21	2.00	0.43
2:L:20:VAL:O	2:L:24:VAL:HG23	2.19	0.43
2:P:339:GLN:HA	2:P:342:LYS:HE2	2.00	0.43
2:P:52:ARG:HH11	2:P:52:ARG:HD3	1.70	0.43
2:P:419:ILE:O	2:P:420:THR:C	2.57	0.43
2:H:100:VAL:HG21	2:H:119:PHE:CE1	2.53	0.43
2:F:211:ASP:HA	2:F:214:THR:CG2	2.48	0.43
2:N:365:VAL:CG2	2:N:387:VAL:HA	2.46	0.43
2:P:304:LEU:HD11	3:X:216:ARG:HG3	2.00	0.43
2:H:121:ARG:HH22	5:H:1103:PO4:P	2.41	0.43
2:J:297:LYS:HG3	2:J:322:VAL:HB	2.00	0.43
2:B:65:PRO:HG3	2:B:103:TRP:CE2	2.54	0.43
1:O:135:THR:HG22	1:O:136:THR:N	2.33	0.43
2:H:495:MET:HE2	2:H:520:VAL:HG22	2.00	0.43
2:F:114:LEU:HD12	2:F:114:LEU:HA	1.79	0.43
2:J:492:LYS:HG3	2:J:517:TYR:CD2	2.54	0.43
2:H:467:TRP:CZ3	2:H:494:GLU:OE1	2.72	0.43
2:N:542:ILE:CD1	2:N:588:LEU:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:542:ILE:HG13	2:H:588:LEU:HB2	1.97	0.43
1:C:160:GLU:CG	2:D:31:PRO:HB3	2.49	0.43
2:D:328:VAL:CG2	2:D:359:GLU:HB2	2.44	0.43
2:B:143:LEU:CD2	2:B:159:ILE:HD13	2.47	0.43
2:B:367:GLN:HG2	2:B:391:THR:HB	2.01	0.43
1:I:102:ILE:HG12	1:I:117:THR:HB	2.01	0.43
1:M:26:SER:OG	1:M:108:LEU:HB3	2.19	0.43
2:L:451:THR:HA	2:L:475:GLU:HG3	2.00	0.43
1:K:126:LYS:HZ1	2:L:29:THR:H	1.67	0.43
2:P:545:ILE:HA	2:P:546:PRO:HD3	1.76	0.42
2:H:487:CYS:N	2:H:488:PRO:CD	2.82	0.42
2:L:443:PHE:HE2	2:L:445:LEU:HD11	1.80	0.42
2:L:468:MET:CE	2:L:470:LEU:HD11	2.49	0.42
1:G:149:GLU:OE1	1:G:153:ARG:NE	2.52	0.42
2:B:441:PHE:O	2:B:468:MET:HA	2.19	0.42
2:H:43:ARG:NH2	2:H:47:ILE:HD11	2.34	0.42
2:P:17:VAL:O	2:P:20:VAL:HG12	2.19	0.42
2:L:432:LEU:CD1	2:L:458:ILE:HA	2.49	0.42
2:D:495:MET:O	2:D:520:VAL:HA	2.19	0.42
2:N:161:THR:HG22	2:N:186:GLU:HG2	2.00	0.42
2:F:245:LEU:HD12	2:F:245:LEU:HA	1.79	0.42
1:C:19:GLU:OE1	1:C:19:GLU:N	2.49	0.42
2:L:168:THR:HB	2:L:196:VAL:CG1	2.16	0.42
2:H:440:ARG:HB3	2:H:467:TRP:CD1	2.54	0.42
2:N:564:HIS:HA	2:N:565:PRO:HD2	1.76	0.42
2:H:289:PHE:N	2:H:290:PRO:HD2	2.34	0.42
2:F:289:PHE:N	2:F:290:PRO:CD	2.81	0.42
2:N:453:LEU:HD11	2:N:457:TYR:OH	2.19	0.42
2:F:563:GLU:O	2:F:563:GLU:CG	2.67	0.42
2:H:198:ASN:OD1	2:H:198:ASN:O	2.38	0.42
2:H:94:GLU:CG	2:H:95:ASN:N	2.82	0.42
1:C:12:ASP:O	1:K:40:ASN:HB2	2.19	0.42
1:A:134:ARG:HB2	1:A:139:ILE:O	2.19	0.42
2:P:297:LYS:HG3	2:P:322:VAL:HB	1.99	0.42
3:Q:201:LEU:HA	3:Q:202:PRO:HD3	1.81	0.42
2:L:233:LEU:HA	2:L:233:LEU:HD23	1.88	0.42
2:J:58:ALA:O	2:J:81:LYS:HB2	2.19	0.42
2:H:542:ILE:HD12	2:H:543:GLU:CA	2.49	0.42
2:H:92:ILE:CG2	2:H:93:PRO:O	2.68	0.42
2:L:191:ASN:ND2	2:L:194:LEU:HB2	2.35	0.42
1:E:134:ARG:NH1	2:F:40:VAL:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:453:LEU:HD11	2:D:457:TYR:OH	2.19	0.42
2:P:37:ALA:O	2:P:40:VAL:HG13	2.20	0.42
2:J:96:TRP:O	2:J:578:ARG:NH2	2.45	0.42
2:F:298:LEU:HB2	2:F:320:LEU:HD11	2.02	0.42
2:H:537:ARG:HB3	2:H:538:PRO:CD	2.49	0.42
2:J:247:GLU:HA	2:J:274:ARG:O	2.20	0.42
2:F:32:LYS:HD2	2:F:32:LYS:HA	1.91	0.42
2:P:386:TYR:HE1	4:P:1100:7JA:HG2	1.72	0.42
2:D:101:THR:CG2	2:D:128:ASP:OD1	2.55	0.42
2:F:191:ASN:ND2	2:F:194:LEU:HB2	2.34	0.42
2:J:194:LEU:HD12	2:J:194:LEU:HA	1.74	0.42
2:F:422:LEU:O	2:F:423:PRO:C	2.57	0.42
1:C:12:ASP:O	1:K:40:ASN:HB3	2.19	0.42
2:H:21:ILE:HG23	2:H:47:ILE:HD13	2.02	0.42
2:H:502:GLU:CD	2:H:526:SER:HB2	2.40	0.42
2:F:578:ARG:HG3	2:F:578:ARG:H	1.48	0.42
2:N:335:GLU:O	2:N:338:ALA:HB3	2.20	0.42
2:P:451:THR:HA	2:P:475:GLU:HG3	2.02	0.42
1:K:8:LEU:HD23	1:K:42:VAL:HG13	2.00	0.42
1:O:82:ASP:O	1:O:85:ALA:HB3	2.19	0.42
1:C:99:PHE:CZ	2:D:17:VAL:HG22	2.55	0.42
2:H:200:TYR:C	2:H:200:TYR:CD1	2.90	0.42
2:B:248:PHE:C	2:B:248:PHE:CD2	2.92	0.42
2:B:298:LEU:HA	2:B:298:LEU:HD12	1.77	0.42
2:H:409:ARG:CB	4:H:1100:7JA:H29	2.35	0.42
2:J:101:THR:CG2	2:J:128:ASP:OD1	2.59	0.42
1:M:100:GLU:CG	2:N:15:ALA:HB2	2.48	0.42
2:J:387:VAL:HG22	2:J:389:ASP:H	1.84	0.42
2:J:419:ILE:HD11	2:J:446:ARG:NH2	2.25	0.42
1:M:114:LEU:C	1:M:116:LEU:N	2.72	0.42
1:A:160:GLU:HG3	2:B:31:PRO:HB3	2.01	0.42
2:B:419:ILE:O	2:B:420:THR:C	2.57	0.42
2:F:188:ALA:HA	2:F:215:ILE:HG12	2.02	0.42
2:F:490:LEU:HD23	2:F:490:LEU:HA	1.89	0.42
2:F:431:LEU:CD1	2:F:435:CYS:SG	3.08	0.42
2:N:297:LYS:HE2	2:N:322:VAL:CG2	2.49	0.42
2:F:96:TRP:O	2:F:578:ARG:NH2	2.45	0.42
3:X:201:LEU:HA	3:X:202:PRO:HD3	1.83	0.42
2:F:187:LEU:HD23	2:F:187:LEU:HA	1.83	0.42
1:E:10:SER:OG	1:E:11:SER:N	2.50	0.42
2:N:289:PHE:HB2	2:N:290:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:ALA:C	2:H:89:PHE:H	2.23	0.42
2:J:366:SER:HB2	2:J:367:GLN:OE1	2.19	0.42
1:O:44:LEU:HA	1:O:45:PRO:HD3	1.77	0.42
2:P:466:ARG:HG2	2:P:491:GLN:OE1	2.19	0.42
2:D:343:GLN:O	2:D:345:LYS:HG2	2.20	0.42
1:A:63:VAL:C	1:A:65:ALA:H	2.22	0.42
2:H:345:LYS:NZ	2:H:345:LYS:HB3	2.35	0.42
4:N:1100:7JA:HN	4:N:1100:7JA:H10	1.85	0.42
2:H:302:TYR:N	2:H:302:TYR:CD2	2.83	0.42
2:J:101:THR:N	2:J:102:PRO:CD	2.82	0.42
2:N:285:MET:N	2:N:286:PRO:CD	2.82	0.42
1:G:160:GLU:HB3	2:H:31:PRO:HB3	2.02	0.42
2:H:343:GLN:NE2	2:H:343:GLN:N	2.67	0.42
2:H:107:ILE:HA	2:H:111:LEU:HB2	2.02	0.42
1:C:141:ASN:OD1	1:C:141:ASN:C	2.58	0.42
2:B:22:GLU:HG2	2:B:47:ILE:HD13	2.00	0.42
2:L:22:GLU:HG2	2:L:47:ILE:HD13	2.01	0.42
2:B:226:LYS:HA	2:B:249:CYS:O	2.20	0.42
2:N:235:LEU:O	2:N:238:PHE:HB3	2.19	0.42
2:L:235:LEU:O	2:L:238:PHE:HB3	2.19	0.42
2:J:335:GLU:O	2:J:338:ALA:HB3	2.20	0.42
2:P:298:LEU:HA	2:P:298:LEU:HD12	1.87	0.42
2:F:532:LEU:HA	2:F:532:LEU:HD23	1.70	0.42
1:M:102:ILE:CB	2:N:20:VAL:HG21	2.50	0.42
2:H:364:LEU:O	2:H:365:VAL:HG13	2.20	0.42
2:D:411:VAL:HG22	2:D:444:TYR:CB	2.49	0.42
2:F:285:MET:N	2:F:286:PRO:CD	2.81	0.42
2:B:419:ILE:HD12	2:B:419:ILE:N	2.35	0.42
2:J:328:VAL:CG2	2:J:359:GLU:HB2	2.44	0.42
2:N:54:HIS:CD2	2:N:77:SER:OG	2.71	0.42
2:F:114:LEU:O	2:F:136:ARG:NH1	2.52	0.42
2:B:329:ILE:O	2:B:333:GLY:HA3	2.19	0.42
2:H:510:THR:HG22	2:H:511:LYS:N	2.35	0.42
3:X:212:PHE:CD2	3:X:213:LEU:HD23	2.55	0.42
2:D:152:THR:HG22	2:D:177:SER:HB2	2.02	0.42
1:G:42:VAL:O	1:G:42:VAL:HG22	2.20	0.42
2:H:172:GLU:O	2:H:202:THR:CG2	2.68	0.42
2:B:545:ILE:HG23	2:B:546:PRO:HD2	2.01	0.42
2:F:542:ILE:HD11	2:F:588:LEU:CD1	2.36	0.42
2:L:367:GLN:HB3	2:L:391:THR:HG22	2.01	0.42
2:L:419:ILE:O	2:L:420:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:LEU:O	2:D:424:LEU:HG	2.20	0.42
2:B:366:SER:HB2	2:B:367:GLN:OE1	2.19	0.42
2:L:492:LYS:HG3	2:L:517:TYR:CD2	2.55	0.42
1:I:111:LYS:O	1:I:115:ASP:HB2	2.19	0.42
1:I:10:SER:OG	1:I:11:SER:N	2.52	0.42
1:A:6:ILE:HG22	1:A:7:VAL:N	2.35	0.42
2:J:161:THR:HG22	2:J:186:GLU:HG2	2.02	0.42
2:B:305:LEU:HD22	2:B:305:LEU:H	1.85	0.42
1:K:83:LEU:HD23	1:K:83:LEU:HA	1.81	0.42
2:B:547:SER:CB	2:B:564:HIS:CB	2.97	0.42
1:M:102:ILE:HB	2:N:20:VAL:HG21	2.02	0.42
1:I:48:THR:HG22	1:I:51:ILE:CB	2.50	0.42
1:A:93:ILE:CD1	1:A:97:THR:HG22	2.42	0.42
2:F:419:ILE:HD11	2:F:446:ARG:NH2	2.27	0.42
2:B:30:ASP:HA	2:B:31:PRO:HD3	1.90	0.42
2:B:387:VAL:HG22	2:B:389:ASP:H	1.84	0.42
1:I:153:ARG:CG	1:I:157:TRP:CZ3	3.01	0.42
2:F:159:ILE:HD11	2:F:169:LEU:HD13	2.02	0.42
2:N:63:ALA:HB1	2:N:67:ARG:HD2	2.02	0.42
3:W:212:PHE:CD2	3:W:213:LEU:HD23	2.55	0.42
2:D:226:LYS:HA	2:D:249:CYS:O	2.19	0.42
3:S:212:PHE:CD2	3:S:213:LEU:HD23	2.55	0.42
2:J:405:LEU:HA	2:J:405:LEU:HD23	1.74	0.42
2:J:91:LEU:O	2:J:567:HIS:HE1	2.03	0.41
4:L:1100:7JA:OXT	4:L:1100:7JA:HG2A	2.11	0.41
2:H:123:ILE:HD13	2:H:123:ILE:HG21	1.88	0.41
2:H:227:VAL:HG22	2:H:228:GLY:H	1.85	0.41
1:K:160:GLU:HG3	2:L:31:PRO:HB3	2.02	0.41
2:L:30:ASP:HA	2:L:31:PRO:HD3	1.93	0.41
2:B:490:LEU:HA	2:B:490:LEU:HD23	1.85	0.41
3:V:201:LEU:HA	3:V:202:PRO:HD3	1.83	0.41
2:D:315:GLN:HG2	2:D:340:TYR:CE1	2.55	0.41
1:E:8:LEU:HD23	1:E:42:VAL:HG13	2.02	0.41
2:H:114:LEU:O	2:H:136:ARG:NH1	2.53	0.41
2:D:83:LYS:HA	2:D:96:TRP:CZ3	2.55	0.41
2:P:392:ASN:HD21	2:P:424:LEU:HA	1.85	0.41
2:B:482:GLU:O	2:B:485:ARG:HG2	2.20	0.41
2:P:20:VAL:O	2:P:24:VAL:HG23	2.20	0.41
2:N:221:SER:O	2:N:223:VAL:HG23	2.19	0.41
1:C:126:LYS:HZ3	2:D:29:THR:H	1.67	0.41
2:N:405:LEU:HA	2:N:405:LEU:HD23	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:532:LEU:HA	2:J:532:LEU:HD23	1.75	0.41
2:F:348:ARG:HH22	4:F:1100:7JA:C	2.33	0.41
2:D:545:ILE:HG22	2:D:546:PRO:N	2.35	0.41
2:H:429:ARG:HB2	2:H:457:TYR:CD1	2.55	0.41
2:F:453:LEU:HD11	2:F:457:TYR:OH	2.20	0.41
2:F:194:LEU:HD12	2:F:194:LEU:HA	1.79	0.41
2:J:392:ASN:ND2	2:J:424:LEU:HA	2.34	0.41
2:L:75:LEU:HD23	2:L:75:LEU:HA	1.83	0.41
2:D:392:ASN:HD21	2:D:424:LEU:HA	1.85	0.41
2:H:216:ALA:HB2	2:H:238:PHE:HD1	1.83	0.41
1:K:82:ASP:O	1:K:85:ALA:HB3	2.20	0.41
1:M:63:VAL:C	1:M:65:ALA:H	2.24	0.41
2:H:350:GLU:HG3	2:H:350:GLU:O	2.20	0.41
2:P:496:ARG:HA	2:P:521:GLN:O	2.21	0.41
1:C:128:LYS:HB2	1:C:133:ILE:HD11	2.03	0.41
2:L:392:ASN:HD21	2:L:424:LEU:HA	1.85	0.41
2:J:367:GLN:CG	2:J:391:THR:HG22	2.50	0.41
2:J:297:LYS:HE3	2:J:297:LYS:HB2	1.69	0.41
1:A:145:PRO:HB2	2:D:539:TYR:CE2	2.54	0.41
2:N:304:LEU:HA	2:N:304:LEU:HD12	1.93	0.41
1:K:10:SER:HB2	1:K:52:LEU:HD23	2.02	0.41
2:L:83:LYS:HA	2:L:96:TRP:CZ3	2.55	0.41
2:J:451:THR:HA	2:J:475:GLU:HG3	2.02	0.41
2:B:153:THR:HG23	2:B:178:GLU:HA	2.02	0.41
2:P:221:SER:O	2:P:223:VAL:HG23	2.20	0.41
2:H:543:GLU:O	2:H:544:LEU:HD23	2.20	0.41
1:O:58:TYR:CD2	1:O:113:LEU:HD13	2.55	0.41
1:M:114:LEU:C	1:M:116:LEU:H	2.24	0.41
2:B:191:ASN:ND2	2:B:194:LEU:HB2	2.36	0.41
2:P:398:ILE:CG2	2:P:402:LEU:HD11	2.48	0.41
2:L:453:LEU:HD11	2:L:457:TYR:OH	2.20	0.41
2:P:431:LEU:C	2:P:431:LEU:CD1	2.88	0.41
2:P:399:GLY:HA3	2:P:431:LEU:HA	2.03	0.41
2:B:54:HIS:CE1	2:B:56:THR:OG1	2.65	0.41
2:L:422:LEU:O	2:L:424:LEU:HG	2.21	0.41
2:D:310:HIS:HE1	2:D:325:THR:OG1	2.03	0.41
3:S:201:LEU:HA	3:S:202:PRO:HD3	1.82	0.41
1:C:134:ARG:NH1	2:D:40:VAL:HA	2.35	0.41
2:D:22:GLU:HG2	2:D:47:ILE:CD1	2.50	0.41
2:H:301:LEU:HD13	2:H:301:LEU:HA	1.68	0.41
2:N:32:LYS:HD2	2:N:32:LYS:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:409:ARG:HD2	4:H:1100:7JA:H29	2.02	0.41
2:H:314:ILE:HG12	2:H:314:ILE:H	1.51	0.41
2:L:411:VAL:HG22	2:L:444:TYR:HB3	2.02	0.41
2:H:152:THR:HB	2:H:177:SER:HB2	2.02	0.41
2:H:255:GLU:HB3	2:H:263:TYR:CE1	2.55	0.41
1:A:130:PRO:O	1:A:134:ARG:HG2	2.21	0.41
2:J:456:SER:HB2	2:J:482:GLU:HB3	2.01	0.41
2:L:305:LEU:H	2:L:305:LEU:CD2	2.33	0.41
1:I:154:GLU:OE1	2:J:67:ARG:NH1	2.53	0.41
2:N:222:LEU:HA	2:N:222:LEU:HD12	1.85	0.41
2:B:63:ALA:HB1	2:B:67:ARG:HD2	2.02	0.41
2:P:546:PRO:HB2	2:P:547:SER:H	1.63	0.41
2:H:347:LEU:HD11	2:H:349:ILE:CG1	2.48	0.41
2:H:492:LYS:HZ1	2:H:516:ARG:NH1	2.18	0.41
2:F:419:ILE:O	2:F:420:THR:C	2.58	0.41
2:H:83:LYS:HA	2:H:84:PRO:HD3	1.88	0.41
1:K:58:TYR:CD2	1:K:113:LEU:HD13	2.55	0.41
2:P:107:ILE:HG12	2:P:111:LEU:HD12	2.02	0.41
1:E:42:VAL:HA	1:E:43:PRO:HD3	1.84	0.41
1:O:44:LEU:O	1:O:44:LEU:HD12	2.20	0.41
1:M:134:ARG:NH2	1:M:141:ASN:HD22	2.18	0.41
2:P:436:LYS:HB3	2:P:436:LYS:HE2	1.89	0.41
4:J:1100:7JA:H27	4:J:1100:7JA:H05	1.65	0.41
2:J:386:TYR:HE1	4:J:1100:7JA:HG2	1.73	0.41
2:F:91:LEU:O	2:F:567:HIS:HE1	2.03	0.41
2:H:442:ALA:HB1	4:H:1100:7JA:H28	2.02	0.41
1:E:51:ILE:HA	1:E:51:ILE:HD13	1.91	0.41
2:N:289:PHE:N	2:N:290:PRO:CD	2.82	0.41
2:B:80:LEU:HB2	2:B:122:MET:HE2	1.97	0.41
2:D:443:PHE:HE2	2:D:445:LEU:HD11	1.80	0.41
1:C:58:TYR:CE1	1:C:62:HIS:CE1	3.09	0.41
1:E:134:ARG:NE	1:E:141:ASN:HB2	2.34	0.41
2:H:481:MET:O	2:H:482:GLU:C	2.57	0.41
1:E:158:ALA:CB	2:F:62:THR:HG23	2.51	0.41
2:D:304:LEU:HA	2:D:304:LEU:HD12	1.91	0.41
2:F:120:ARG:NH2	5:F:1103:PO4:O4	2.53	0.41
2:H:587:VAL:HG12	2:H:589:LYS:HD3	2.02	0.41
1:C:115:ASP:HA	2:D:27:TYR:HE2	1.85	0.41
2:J:209:PRO:HD3	2:J:230:PHE:CE2	2.56	0.41
2:J:564:HIS:HA	2:J:565:PRO:HD2	1.80	0.41
2:B:91:LEU:O	2:B:567:HIS:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:327:ASN:HD22	2:D:328:VAL:N	2.19	0.41
2:D:314:ILE:H	2:D:314:ILE:HG12	1.65	0.41
2:L:456:SER:HB2	2:L:482:GLU:HB3	2.01	0.41
2:D:120:ARG:NH2	5:D:1103:PO4:O4	2.54	0.41
1:O:134:ARG:NE	1:O:141:ASN:HB2	2.36	0.41
2:N:120:ARG:HD2	2:N:146:ASP:OD2	2.20	0.41
3:V:212:PHE:CD2	3:V:213:LEU:HD23	2.56	0.41
2:L:466:ARG:HG2	2:L:491:GLN:OE1	2.21	0.41
1:I:13:GLY:O	1:I:14:GLU:HG2	2.20	0.41
2:L:120:ARG:HD2	2:L:146:ASP:OD2	2.20	0.41
2:J:527:MET:O	2:J:528:THR:C	2.59	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.80	0.41
2:N:386:TYR:OH	4:N:1100:7JA:HG2B	2.21	0.41
2:H:289:PHE:O	2:H:290:PRO:C	2.58	0.41
2:D:80:LEU:HB2	2:D:122:MET:HE1	1.95	0.41
2:H:431:LEU:CD2	2:H:432:LEU:HD23	2.48	0.41
1:M:128:LYS:HB2	1:M:133:ILE:HD13	2.02	0.41
2:D:419:ILE:O	2:D:420:THR:C	2.59	0.41
2:B:80:LEU:HD12	2:B:122:MET:HE1	2.03	0.41
2:D:389:ASP:OD2	2:D:419:ILE:HG23	2.21	0.41
2:P:367:GLN:HG2	2:P:391:THR:HB	2.03	0.41
2:L:419:ILE:HD12	2:L:419:ILE:N	2.36	0.41
2:J:55:VAL:HG12	2:J:56:THR:N	2.36	0.41
2:J:211:ASP:HA	2:J:214:THR:CG2	2.47	0.41
2:F:347:LEU:HD21	2:F:349:ILE:HD11	2.02	0.41
2:J:57:MET:CE	2:J:62:THR:HG22	2.50	0.41
2:B:55:VAL:CG2	2:B:75:LEU:HD21	2.46	0.41
1:A:98:LEU:HD21	1:A:120:THR:CG2	2.48	0.41
2:B:453:LEU:HD11	2:B:457:TYR:OH	2.21	0.41
2:J:367:GLN:HG2	2:J:391:THR:HB	2.03	0.41
2:D:83:LYS:O	2:D:121:ARG:HD2	2.21	0.41
2:H:71:ARG:C	2:H:73:PRO:HD3	2.41	0.41
3:Q:201:LEU:HA	3:Q:201:LEU:HD23	1.74	0.41
1:C:44:LEU:HA	1:C:45:PRO:HD3	1.76	0.41
2:H:300:LEU:HD23	2:H:300:LEU:HA	1.89	0.41
2:J:298:LEU:HB2	2:J:320:LEU:HD11	2.01	0.41
2:F:298:LEU:HD12	2:F:298:LEU:HA	1.73	0.41
2:J:157:LEU:O	2:J:161:THR:HG23	2.20	0.41
2:F:451:THR:HA	2:F:475:GLU:HG3	2.03	0.41
1:I:137:PHE:CD1	2:J:17:VAL:HG21	2.55	0.41
2:L:335:GLU:O	2:L:338:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:527:MET:O	2:L:528:THR:C	2.58	0.41
1:O:101:LEU:HA	1:O:101:LEU:HD23	1.92	0.41
1:A:19:GLU:OE1	1:A:19:GLU:N	2.52	0.41
2:D:532:LEU:HA	2:D:532:LEU:HD23	1.74	0.41
2:F:545:ILE:HA	2:F:546:PRO:HD3	1.79	0.41
2:F:519:TRP:CZ3	2:F:567:HIS:CG	3.09	0.41
4:N:1100:7JA:OXT	4:N:1100:7JA:CG2	2.66	0.41
2:H:425:ASP:OD1	2:H:454:GLY:HA3	2.21	0.41
1:M:99:PHE:CB	2:N:15:ALA:HB1	2.51	0.41
2:H:266:LEU:HA	2:H:266:LEU:HD22	1.89	0.41
2:P:55:VAL:CG2	2:P:75:LEU:HD21	2.42	0.41
2:L:211:ASP:O	2:L:215:ILE:HG13	2.21	0.41
1:E:105:ALA:CB	1:E:114:LEU:HD13	2.50	0.41
2:F:297:LYS:HE3	2:F:297:LYS:HB2	1.67	0.41
2:D:366:SER:HB2	2:D:367:GLN:OE1	2.21	0.41
2:N:465:VAL:CG1	2:N:468:MET:HG3	2.50	0.41
2:N:422:LEU:O	2:N:424:LEU:HG	2.21	0.41
1:A:26:SER:OG	1:A:108:LEU:HB3	2.20	0.41
2:H:511:LYS:HB2	2:H:511:LYS:HE2	1.91	0.41
2:L:152:THR:HG22	2:L:177:SER:HB2	2.04	0.41
1:I:34:GLU:C	1:I:36:ASP:H	2.24	0.41
1:G:44:LEU:HD12	1:G:44:LEU:O	2.20	0.41
2:D:564:HIS:HA	2:D:565:PRO:HD2	1.77	0.40
2:N:545:ILE:HA	2:N:546:PRO:HD3	1.78	0.40
2:B:546:PRO:O	2:B:547:SER:CB	2.70	0.40
2:H:490:LEU:HD23	2:H:490:LEU:HA	1.85	0.40
2:H:544:LEU:HD23	2:H:544:LEU:N	2.36	0.40
2:F:289:PHE:HB2	2:F:290:PRO:HD3	2.03	0.40
2:B:191:ASN:HD21	2:B:194:LEU:N	2.11	0.40
2:L:55:VAL:CG2	2:L:75:LEU:HD21	2.49	0.40
2:D:367:GLN:HG2	2:D:391:THR:HB	2.03	0.40
2:D:311:CYS:CB	2:D:336:VAL:HG21	2.47	0.40
3:U:201:LEU:HA	3:U:201:LEU:HD23	1.69	0.40
2:L:153:THR:HG23	2:L:178:GLU:HA	2.02	0.40
2:B:190:HIS:HE1	2:P:110:ASN:HA	1.86	0.40
2:P:247:GLU:HA	2:P:274:ARG:O	2.20	0.40
1:K:144:THR:OG1	1:K:147:GLU:HG3	2.22	0.40
2:H:220:ARG:NE	2:H:220:ARG:HA	2.36	0.40
1:O:83:LEU:HD23	1:O:83:LEU:HA	1.80	0.40
2:J:348:ARG:HH22	4:J:1100:7JA:C	2.35	0.40
2:L:533:MET:HE3	2:L:588:LEU:HB3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:432:LEU:HD11	2:H:458:ILE:CD1	2.52	0.40
1:M:99:PHE:HD2	2:N:15:ALA:C	2.20	0.40
2:J:75:LEU:HD23	2:J:75:LEU:HA	1.87	0.40
2:L:191:ASN:ND2	2:L:194:LEU:H	2.16	0.40
2:L:301:LEU:CD2	2:L:324:GLU:HB3	2.52	0.40
2:P:65:PRO:HG3	2:P:103:TRP:CE2	2.56	0.40
2:H:279:TYR:O	2:H:304:LEU:HB2	2.22	0.40
2:N:107:ILE:HA	2:N:111:LEU:HB2	2.03	0.40
2:D:153:THR:HG23	2:D:178:GLU:HA	2.03	0.40
2:P:58:ALA:O	2:P:81:LYS:HB2	2.22	0.40
2:B:532:LEU:HA	2:B:532:LEU:HD23	1.76	0.40
2:P:564:HIS:HA	2:P:565:PRO:HD2	1.78	0.40
2:H:348:ARG:HG3	2:H:384:ALA:HB3	2.03	0.40
2:P:429:ARG:HG2	2:P:433:ILE:HD11	2.04	0.40
2:H:454:GLY:O	2:H:457:TYR:HB2	2.20	0.40
2:H:487:CYS:HB3	2:H:490:LEU:HB2	2.03	0.40
1:I:125:ILE:HG23	1:I:133:ILE:CD1	2.42	0.40
2:D:267:VAL:HG23	2:D:267:VAL:O	2.22	0.40
2:D:563:GLU:CG	2:D:563:GLU:O	2.65	0.40
1:A:101:LEU:HA	1:A:101:LEU:HD23	1.92	0.40
2:D:75:LEU:HA	2:D:75:LEU:HD23	1.85	0.40
2:D:227:VAL:HG13	2:D:228:GLY:H	1.83	0.40
2:J:233:LEU:HA	2:J:233:LEU:HD23	1.82	0.40
1:C:158:ALA:CB	2:D:62:THR:HG23	2.51	0.40
2:H:59:LEU:O	2:H:62:THR:HB	2.21	0.40
2:B:512:LEU:HA	2:B:513:PRO:HD2	1.78	0.40
2:H:461:TYR:C	2:H:463:PRO:HD3	2.41	0.40
2:D:298:LEU:HD12	2:D:298:LEU:HA	1.72	0.40
1:E:83:LEU:HD23	1:E:83:LEU:HA	1.82	0.40
2:L:547:SER:CB	2:L:564:HIS:CB	2.99	0.40
2:H:492:LYS:NZ	2:H:516:ARG:HD2	2.35	0.40
2:F:468:MET:HE1	2:F:483:PHE:CE1	2.55	0.40
2:F:285:MET:HB3	2:F:286:PRO:HD3	2.03	0.40
2:B:311:CYS:O	2:B:315:GLN:HB2	2.21	0.40
2:F:431:LEU:CD1	2:F:431:LEU:C	2.89	0.40
2:H:517:TYR:CE1	2:H:569:LEU:HD11	2.57	0.40
1:C:102:ILE:HG21	2:D:20:VAL:HG22	2.02	0.40
2:H:259:MET:C	2:H:261:GLU:N	2.72	0.40
2:H:482:GLU:HG2	2:H:482:GLU:H	1.60	0.40
1:C:134:ARG:NH2	1:C:141:ASN:HD22	2.19	0.40
2:H:501:SER:HB2	2:H:503:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:201:LEU:HA	3:U:202:PRO:HD3	1.80	0.40
2:D:65:PRO:HA	2:D:103:TRP:CZ3	2.57	0.40
2:L:275:LEU:HD11	2:L:288:LEU:CD2	2.51	0.40
2:D:399:GLY:O	2:D:434:GLY:HA3	2.22	0.40
2:F:85:ARG:NH1	5:F:1101:PO4:O3	2.54	0.40
4:H:1100:7JA:C04	4:H:1100:7JA:H12A	2.50	0.40
2:H:306:GLU:OE2	2:H:307:THR:HG22	2.21	0.40
2:H:363:GLY:O	2:H:364:LEU:C	2.60	0.40
2:L:588:LEU:HA	2:L:588:LEU:HD23	1.97	0.40
2:F:441:PHE:O	2:F:468:MET:HA	2.22	0.40
2:B:119:PHE:CD1	2:B:122:MET:HE3	2.57	0.40
2:L:367:GLN:NE2	2:L:389:ASP:OD1	2.53	0.40
2:N:366:SER:HB2	2:N:367:GLN:OE1	2.21	0.40
2:B:211:ASP:O	2:B:215:ILE:HG13	2.21	0.40
2:P:120:ARG:NH2	5:P:1103:PO4:O4	2.52	0.40
2:H:21:ILE:C	2:H:23:GLN:N	2.75	0.40
1:K:134:ARG:NH1	2:L:40:VAL:HA	2.35	0.40
2:P:422:LEU:O	2:P:424:LEU:HG	2.21	0.40
2:B:456:SER:HB2	2:B:482:GLU:HB3	2.03	0.40
2:P:329:ILE:HG23	2:P:330:GLY:N	2.35	0.40
2:F:329:ILE:HG23	2:F:330:GLY:N	2.36	0.40
2:L:96:TRP:O	2:L:578:ARG:NH2	2.44	0.40
2:F:469:LEU:HA	2:F:494:GLU:O	2.22	0.40
1:G:6:ILE:HG22	1:G:7:VAL:N	2.36	0.40
2:P:404:ASN:HA	2:P:437:LYS:HD2	2.02	0.40
2:L:245:LEU:HD12	2:L:245:LEU:HA	1.80	0.40
2:P:578:ARG:HG3	2:P:578:ARG:H	1.41	0.40
2:J:114:LEU:HA	2:J:114:LEU:HD12	1.72	0.40
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.84	0.40
2:B:436:LYS:HE2	2:B:436:LYS:HB3	1.96	0.40
2:L:298:LEU:HA	2:L:298:LEU:HD12	1.82	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:ARG:NH2	1:I:61:ARG:NH1[2_555]	2.06	0.14
2:D:429:ARG:NH1	1:I:86:TRP:CE3[2_555]	2.14	0.06

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	140/160 (88%)	115 (82%)	22 (16%)	3 (2%)	9	45
1	C	140/160 (88%)	113 (81%)	23 (16%)	4 (3%)	6	35
1	E	140/160 (88%)	114 (81%)	23 (16%)	3 (2%)	9	45
1	G	140/160 (88%)	114 (81%)	22 (16%)	4 (3%)	6	35
1	I	140/160 (88%)	117 (84%)	20 (14%)	3 (2%)	9	45
1	K	140/160 (88%)	117 (84%)	19 (14%)	4 (3%)	6	35
1	M	140/160 (88%)	110 (79%)	27 (19%)	3 (2%)	9	45
1	O	140/160 (88%)	112 (80%)	25 (18%)	3 (2%)	9	45
2	B	564/592 (95%)	500 (89%)	57 (10%)	7 (1%)	16	60
2	D	564/592 (95%)	504 (89%)	53 (9%)	7 (1%)	16	60
2	F	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	16	60
2	H	558/592 (94%)	430 (77%)	98 (18%)	30 (5%)	2	18
2	J	564/592 (95%)	504 (89%)	52 (9%)	8 (1%)	14	56
2	L	564/592 (95%)	503 (89%)	54 (10%)	7 (1%)	16	60
2	N	564/592 (95%)	504 (89%)	51 (9%)	9 (2%)	12	53
2	P	564/592 (95%)	500 (89%)	56 (10%)	8 (1%)	14	56
3	Q	16/21 (76%)	16 (100%)	0	0	100	100
3	R	16/21 (76%)	16 (100%)	0	0	100	100
3	S	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	U	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	V	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	W	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	X	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
All	All	5738/6163 (93%)	4969 (87%)	659 (12%)	110 (2%)	10	49

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
2	B	420	THR
2	B	546	PRO
1	C	36	ASP
2	D	420	THR
2	D	546	PRO
1	E	36	ASP
2	F	420	THR
2	F	546	PRO
1	G	36	ASP
2	H	97	GLY
2	H	200	TYR
2	H	269	PRO
2	H	270	ARG
2	H	278	SER
2	H	364	LEU
2	H	365	VAL
1	I	36	ASP
2	J	420	THR
2	J	546	PRO
1	K	36	ASP
2	L	420	THR
2	L	546	PRO
1	M	36	ASP
2	N	420	THR
2	N	546	PRO
1	O	36	ASP
2	P	420	THR
2	P	546	PRO
1	A	13	GLY
2	B	590	GLU
1	C	13	GLY
2	D	590	GLU
1	E	13	GLY
2	F	20	VAL
2	F	590	GLU
1	G	13	GLY
1	G	128	LYS
2	H	20	VAL
2	H	228	GLY
2	H	254	ASN
2	H	279	TYR

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Mol	Chain	Res	Type
2	H	287	ILE
2	H	357	GLY
1	I	13	GLY
2	J	358	MET
2	J	590	GLU
1	K	13	GLY
2	L	20	VAL
2	L	590	GLU
1	M	13	GLY
1	M	126	LYS
2	N	590	GLU
1	O	13	GLY
2	P	20	VAL
2	P	590	GLU
2	B	20	VAL
2	B	358	MET
1	C	92	LYS
1	C	126	LYS
2	D	358	MET
2	D	547	SER
2	F	358	MET
2	H	102	PRO
2	H	524	ARG
2	H	525	ALA
2	H	534	GLN
2	H	538	PRO
1	I	126	LYS
2	J	20	VAL
2	J	547	SER
1	K	126	LYS
2	L	358	MET
2	L	547	SER
2	N	20	VAL
2	N	358	MET
2	P	358	MET
2	P	547	SER
1	A	126	LYS
2	B	547	SER
2	D	20	VAL
1	E	126	LYS
2	F	547	SER
2	H	206	LYS

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Mol	Chain	Res	Type
2	H	273	CYS
2	H	315	GLN
2	H	330	GLY
2	H	359	GLU
2	H	575	ALA
2	J	422	LEU
1	K	92	LYS
2	N	547	SER
1	O	126	LYS
2	B	422	LEU
2	D	422	LEU
2	F	422	LEU
1	G	138	ASN
2	H	188	ALA
2	H	260	PRO
2	H	482	GLU
2	H	546	PRO
2	L	422	LEU
2	N	422	LEU
2	P	422	LEU
2	H	290	PRO
2	N	290	PRO
2	J	471	GLY
2	N	471	GLY
2	P	471	GLY
2	H	314	ILE

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	127/137 (93%)	113 (89%)	14 (11%)	8	32
1	C	127/137 (93%)	113 (89%)	14 (11%)	8	32
1	E	127/137 (93%)	113 (89%)	14 (11%)	8	32
1	G	127/137 (93%)	115 (91%)	12 (9%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	127/137 (93%)	113 (89%)	14 (11%)	8	32
1	K	127/137 (93%)	116 (91%)	11 (9%)	13	44
1	M	127/137 (93%)	112 (88%)	15 (12%)	6	28
1	O	127/137 (93%)	115 (91%)	12 (9%)	11	39
2	B	500/523 (96%)	436 (87%)	64 (13%)	5	24
2	D	500/523 (96%)	431 (86%)	69 (14%)	4	20
2	F	500/523 (96%)	435 (87%)	65 (13%)	5	24
2	H	494/523 (94%)	395 (80%)	99 (20%)	1	8
2	J	500/523 (96%)	436 (87%)	64 (13%)	5	24
2	L	500/523 (96%)	439 (88%)	61 (12%)	6	27
2	N	500/523 (96%)	437 (87%)	63 (13%)	5	25
2	P	500/523 (96%)	436 (87%)	64 (13%)	5	24
3	Q	16/19 (84%)	15 (94%)	1 (6%)	22	62
3	R	16/19 (84%)	15 (94%)	1 (6%)	22	62
3	S	16/19 (84%)	15 (94%)	1 (6%)	22	62
3	U	16/19 (84%)	15 (94%)	1 (6%)	22	62
3	V	16/19 (84%)	15 (94%)	1 (6%)	22	62
3	W	16/19 (84%)	15 (94%)	1 (6%)	22	62
3	X	16/19 (84%)	15 (94%)	1 (6%)	22	62
All	All	5122/5413 (95%)	4460 (87%)	662 (13%)	5	24

All (662) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	35	ASP
1	A	36	ASP
1	A	39	ASP
1	A	42	VAL
1	A	44	LEU
1	A	45	PRO
1	A	48	THR
1	A	86	TRP
1	A	112	ASN
1	A	125	ILE

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Mol	Chain	Res	Type
1	A	135	THR
1	A	153	ARG
1	A	160	GLU
2	B	16	THR
2	B	20	VAL
2	B	35	ASP
2	B	40	VAL
2	B	46	LYS
2	B	48	ASP
2	B	52	ARG
2	B	59	LEU
2	B	62	THR
2	B	64	THR
2	B	100	VAL
2	B	104	VAL
2	B	129	LEU
2	B	132	LEU
2	B	136	ARG
2	B	142	THR
2	B	168	THR
2	B	174	SER
2	B	182	LYS
2	B	184	LEU
2	B	192	THR
2	B	193	SER
2	B	196	VAL
2	B	214	THR
2	B	217	ARG
2	B	220	ARG
2	B	225	VAL
2	B	227	VAL
2	B	230	PHE
2	B	267	VAL
2	B	272	LEU
2	B	301	LEU
2	B	304	LEU
2	B	305	LEU
2	B	312	THR
2	B	313	LEU
2	B	327	ASN
2	B	343	GLN
2	B	349	ILE

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Mol	Chain	Res	Type
2	B	360	ASP
2	B	388	SER
2	B	390	ILE
2	B	397	SER
2	B	400	THR
2	B	402	LEU
2	B	404	ASN
2	B	405	LEU
2	B	412	LEU
2	B	421	ASP
2	B	430	SER
2	B	431	LEU
2	B	447	GLN
2	B	453	LEU
2	B	455	LEU
2	B	466	ARG
2	B	477	ASP
2	B	490	LEU
2	B	496	ARG
2	B	503	ARG
2	B	519	TRP
2	B	528	THR
2	B	537	ARG
2	B	542	ILE
2	B	578	ARG
3	Q	200	GLU
1	C	10	SER
1	C	35	ASP
1	C	36	ASP
1	C	39	ASP
1	C	42	VAL
1	C	44	LEU
1	C	48	THR
1	C	86	TRP
1	C	112	ASN
1	C	125	ILE
1	C	131	GLU
1	C	144	THR
1	C	153	ARG
1	C	160	GLU
2	D	16	THR
2	D	20	VAL

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Mol	Chain	Res	Type
2	D	35	ASP
2	D	36	SER
2	D	40	VAL
2	D	43	ARG
2	D	46	LYS
2	D	48	ASP
2	D	52	ARG
2	D	59	LEU
2	D	62	THR
2	D	64	THR
2	D	100	VAL
2	D	104	VAL
2	D	129	LEU
2	D	132	LEU
2	D	136	ARG
2	D	142	THR
2	D	159	ILE
2	D	168	THR
2	D	174	SER
2	D	182	LYS
2	D	184	LEU
2	D	192	THR
2	D	196	VAL
2	D	214	THR
2	D	217	ARG
2	D	220	ARG
2	D	225	VAL
2	D	227	VAL
2	D	230	PHE
2	D	267	VAL
2	D	272	LEU
2	D	284	GLU
2	D	301	LEU
2	D	304	LEU
2	D	305	LEU
2	D	312	THR
2	D	313	LEU
2	D	327	ASN
2	D	343	GLN
2	D	349	ILE
2	D	360	ASP
2	D	388	SER

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Mol	Chain	Res	Type
2	D	390	ILE
2	D	397	SER
2	D	400	THR
2	D	402	LEU
2	D	404	ASN
2	D	405	LEU
2	D	412	LEU
2	D	418	ARG
2	D	421	ASP
2	D	429	ARG
2	D	430	SER
2	D	431	LEU
2	D	447	GLN
2	D	453	LEU
2	D	455	LEU
2	D	466	ARG
2	D	477	ASP
2	D	490	LEU
2	D	496	ARG
2	D	503	ARG
2	D	519	TRP
2	D	528	THR
2	D	537	ARG
2	D	542	ILE
2	D	578	ARG
3	R	200	GLU
1	E	10	SER
1	E	35	ASP
1	E	36	ASP
1	E	42	VAL
1	E	44	LEU
1	E	48	THR
1	E	86	TRP
1	E	112	ASN
1	E	125	ILE
1	E	131	GLU
1	E	135	THR
1	E	144	THR
1	E	153	ARG
1	E	160	GLU
2	F	16	THR
2	F	20	VAL

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Mol	Chain	Res	Type
2	F	35	ASP
2	F	36	SER
2	F	40	VAL
2	F	43	ARG
2	F	46	LYS
2	F	48	ASP
2	F	52	ARG
2	F	59	LEU
2	F	64	THR
2	F	100	VAL
2	F	104	VAL
2	F	129	LEU
2	F	132	LEU
2	F	136	ARG
2	F	142	THR
2	F	168	THR
2	F	182	LYS
2	F	184	LEU
2	F	192	THR
2	F	193	SER
2	F	196	VAL
2	F	214	THR
2	F	217	ARG
2	F	220	ARG
2	F	225	VAL
2	F	227	VAL
2	F	230	PHE
2	F	267	VAL
2	F	272	LEU
2	F	301	LEU
2	F	304	LEU
2	F	305	LEU
2	F	312	THR
2	F	313	LEU
2	F	327	ASN
2	F	343	GLN
2	F	349	ILE
2	F	351	ARG
2	F	360	ASP
2	F	388	SER
2	F	390	ILE
2	F	397	SER

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Mol	Chain	Res	Type
2	F	400	THR
2	F	402	LEU
2	F	404	ASN
2	F	405	LEU
2	F	412	LEU
2	F	421	ASP
2	F	430	SER
2	F	431	LEU
2	F	447	GLN
2	F	453	LEU
2	F	455	LEU
2	F	466	ARG
2	F	477	ASP
2	F	490	LEU
2	F	496	ARG
2	F	503	ARG
2	F	519	TRP
2	F	528	THR
2	F	537	ARG
2	F	542	ILE
2	F	578	ARG
3	S	200	GLU
1	G	10	SER
1	G	35	ASP
1	G	36	ASP
1	G	42	VAL
1	G	44	LEU
1	G	48	THR
1	G	86	TRP
1	G	112	ASN
1	G	133	ILE
1	G	142	ASP
1	G	144	THR
1	G	153	ARG
2	H	14	VAL
2	H	17	VAL
2	H	19	ASP
2	H	20	VAL
2	H	32	LYS
2	H	35	ASP
2	H	40	VAL
2	H	46	LYS

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Mol	Chain	Res	Type
2	H	49	SER
2	H	52	ARG
2	H	62	THR
2	H	64	THR
2	H	71	ARG
2	H	76	ARG
2	H	77	SER
2	H	90	ASN
2	H	92	ILE
2	H	95	ASN
2	H	105	THR
2	H	118	HIS
2	H	130	ASP
2	H	132	LEU
2	H	136	ARG
2	H	139	ASP
2	H	140	LEU
2	H	156	LEU
2	H	159	ILE
2	H	160	VAL
2	H	166	ILE
2	H	168	THR
2	H	170	LEU
2	H	175	SER
2	H	177	SER
2	H	184	LEU
2	H	191	ASN
2	H	193	SER
2	H	203	GLU
2	H	214	THR
2	H	220	ARG
2	H	223	VAL
2	H	224	SER
2	H	231	GLU
2	H	236	VAL
2	H	257	ILE
2	H	263	TYR
2	H	266	LEU
2	H	267	VAL
2	H	273	CYS
2	H	285	MET
2	H	287	ILE

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Mol	Chain	Res	Type
2	H	288	LEU
2	H	291	PHE
2	H	298	LEU
2	H	301	LEU
2	H	304	LEU
2	H	305	LEU
2	H	307	THR
2	H	311	CYS
2	H	312	THR
2	H	313	LEU
2	H	314	ILE
2	H	317	CYS
2	H	325	THR
2	H	329	ILE
2	H	332	ARG
2	H	339	GLN
2	H	343	GLN
2	H	345	LYS
2	H	347	LEU
2	H	359	GLU
2	H	365	VAL
2	H	382	TYR
2	H	389	ASP
2	H	390	ILE
2	H	391	THR
2	H	395	LEU
2	H	402	LEU
2	H	410	LEU
2	H	421	ASP
2	H	422	LEU
2	H	453	LEU
2	H	455	LEU
2	H	462	SER
2	H	466	ARG
2	H	467	TRP
2	H	475	GLU
2	H	490	LEU
2	H	491	GLN
2	H	496	ARG
2	H	499	CYS
2	H	503	ARG
2	H	511	LYS

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Mol	Chain	Res	Type
2	H	514	SER
2	H	515	LEU
2	H	516	ARG
2	H	534	GLN
2	H	542	ILE
2	H	583	THR
2	H	589	LYS
1	I	10	SER
1	I	35	ASP
1	I	36	ASP
1	I	39	ASP
1	I	42	VAL
1	I	44	LEU
1	I	48	THR
1	I	86	TRP
1	I	112	ASN
1	I	125	ILE
1	I	131	GLU
1	I	144	THR
1	I	153	ARG
1	I	160	GLU
2	J	16	THR
2	J	20	VAL
2	J	35	ASP
2	J	36	SER
2	J	40	VAL
2	J	46	LYS
2	J	48	ASP
2	J	52	ARG
2	J	59	LEU
2	J	62	THR
2	J	64	THR
2	J	100	VAL
2	J	104	VAL
2	J	129	LEU
2	J	132	LEU
2	J	136	ARG
2	J	142	THR
2	J	168	THR
2	J	174	SER
2	J	182	LYS
2	J	184	LEU

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Mol	Chain	Res	Type
2	J	193	SER
2	J	196	VAL
2	J	214	THR
2	J	217	ARG
2	J	220	ARG
2	J	225	VAL
2	J	267	VAL
2	J	272	LEU
2	J	301	LEU
2	J	304	LEU
2	J	305	LEU
2	J	312	THR
2	J	313	LEU
2	J	327	ASN
2	J	343	GLN
2	J	349	ILE
2	J	351	ARG
2	J	360	ASP
2	J	388	SER
2	J	390	ILE
2	J	397	SER
2	J	400	THR
2	J	402	LEU
2	J	404	ASN
2	J	405	LEU
2	J	412	LEU
2	J	421	ASP
2	J	430	SER
2	J	431	LEU
2	J	447	GLN
2	J	453	LEU
2	J	455	LEU
2	J	466	ARG
2	J	477	ASP
2	J	490	LEU
2	J	495	MET
2	J	496	ARG
2	J	503	ARG
2	J	519	TRP
2	J	528	THR
2	J	537	ARG
2	J	542	ILE

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Mol	Chain	Res	Type
2	J	578	ARG
3	U	200	GLU
1	K	10	SER
1	K	35	ASP
1	K	36	ASP
1	K	42	VAL
1	K	44	LEU
1	K	48	THR
1	K	112	ASN
1	K	125	ILE
1	K	131	GLU
1	K	153	ARG
1	K	160	GLU
2	L	16	THR
2	L	20	VAL
2	L	35	ASP
2	L	36	SER
2	L	40	VAL
2	L	46	LYS
2	L	48	ASP
2	L	52	ARG
2	L	59	LEU
2	L	64	THR
2	L	100	VAL
2	L	104	VAL
2	L	132	LEU
2	L	136	ARG
2	L	142	THR
2	L	168	THR
2	L	182	LYS
2	L	184	LEU
2	L	192	THR
2	L	193	SER
2	L	196	VAL
2	L	214	THR
2	L	220	ARG
2	L	225	VAL
2	L	227	VAL
2	L	267	VAL
2	L	272	LEU
2	L	301	LEU
2	L	304	LEU

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Mol	Chain	Res	Type
2	L	305	LEU
2	L	312	THR
2	L	313	LEU
2	L	327	ASN
2	L	343	GLN
2	L	349	ILE
2	L	360	ASP
2	L	388	SER
2	L	390	ILE
2	L	397	SER
2	L	400	THR
2	L	402	LEU
2	L	404	ASN
2	L	405	LEU
2	L	412	LEU
2	L	418	ARG
2	L	421	ASP
2	L	430	SER
2	L	431	LEU
2	L	447	GLN
2	L	453	LEU
2	L	455	LEU
2	L	466	ARG
2	L	477	ASP
2	L	490	LEU
2	L	496	ARG
2	L	503	ARG
2	L	519	TRP
2	L	528	THR
2	L	537	ARG
2	L	542	ILE
2	L	578	ARG
3	V	200	GLU
1	M	10	SER
1	M	35	ASP
1	M	36	ASP
1	M	39	ASP
1	M	42	VAL
1	M	44	LEU
1	M	48	THR
1	M	86	TRP
1	M	112	ASN

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Mol	Chain	Res	Type
1	M	125	ILE
1	M	131	GLU
1	M	135	THR
1	M	144	THR
1	M	153	ARG
1	M	160	GLU
2	N	16	THR
2	N	20	VAL
2	N	35	ASP
2	N	36	SER
2	N	40	VAL
2	N	43	ARG
2	N	46	LYS
2	N	48	ASP
2	N	52	ARG
2	N	59	LEU
2	N	64	THR
2	N	100	VAL
2	N	104	VAL
2	N	129	LEU
2	N	132	LEU
2	N	136	ARG
2	N	142	THR
2	N	168	THR
2	N	182	LYS
2	N	184	LEU
2	N	192	THR
2	N	196	VAL
2	N	214	THR
2	N	217	ARG
2	N	220	ARG
2	N	225	VAL
2	N	230	PHE
2	N	267	VAL
2	N	272	LEU
2	N	301	LEU
2	N	304	LEU
2	N	305	LEU
2	N	312	THR
2	N	313	LEU
2	N	327	ASN
2	N	343	GLN

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Mol	Chain	Res	Type
2	N	349	ILE
2	N	351	ARG
2	N	360	ASP
2	N	388	SER
2	N	390	ILE
2	N	397	SER
2	N	400	THR
2	N	402	LEU
2	N	404	ASN
2	N	405	LEU
2	N	412	LEU
2	N	421	ASP
2	N	430	SER
2	N	431	LEU
2	N	447	GLN
2	N	453	LEU
2	N	455	LEU
2	N	466	ARG
2	N	477	ASP
2	N	490	LEU
2	N	496	ARG
2	N	503	ARG
2	N	519	TRP
2	N	528	THR
2	N	537	ARG
2	N	542	ILE
2	N	578	ARG
3	W	200	GLU
1	O	10	SER
1	O	35	ASP
1	O	36	ASP
1	O	42	VAL
1	O	44	LEU
1	O	48	THR
1	O	86	TRP
1	O	112	ASN
1	O	125	ILE
1	O	144	THR
1	O	153	ARG
1	O	160	GLU
2	P	16	THR
2	P	20	VAL

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Mol	Chain	Res	Type
2	P	35	ASP
2	P	36	SER
2	P	40	VAL
2	P	46	LYS
2	P	48	ASP
2	P	52	ARG
2	P	59	LEU
2	P	64	THR
2	P	100	VAL
2	P	104	VAL
2	P	129	LEU
2	P	132	LEU
2	P	136	ARG
2	P	142	THR
2	P	168	THR
2	P	182	LYS
2	P	184	LEU
2	P	193	SER
2	P	196	VAL
2	P	214	THR
2	P	217	ARG
2	P	220	ARG
2	P	225	VAL
2	P	227	VAL
2	P	230	PHE
2	P	267	VAL
2	P	272	LEU
2	P	301	LEU
2	P	304	LEU
2	P	305	LEU
2	P	312	THR
2	P	313	LEU
2	P	327	ASN
2	P	343	GLN
2	P	349	ILE
2	P	351	ARG
2	P	354	ASP
2	P	360	ASP
2	P	388	SER
2	P	390	ILE
2	P	397	SER
2	P	400	THR

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Mol	Chain	Res	Type
2	P	402	LEU
2	P	404	ASN
2	P	405	LEU
2	P	412	LEU
2	P	421	ASP
2	P	430	SER
2	P	431	LEU
2	P	447	GLN
2	P	453	LEU
2	P	455	LEU
2	P	466	ARG
2	P	477	ASP
2	P	490	LEU
2	P	496	ARG
2	P	503	ARG
2	P	519	TRP
2	P	528	THR
2	P	537	ARG
2	P	542	ILE
2	P	578	ARG
3	X	200	GLU

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

Mol	Chain	Res	Type
1	A	31	HIS
1	A	46	ASN
1	A	62	HIS
1	A	95	GLN
2	B	54	HIS
2	B	109	ASN
2	B	190	HIS
2	B	191	ASN
2	B	254	ASN
2	B	294	GLN
2	B	310	HIS
2	B	319	ASN
2	B	327	ASN
2	B	343	GLN
2	B	460	GLN
2	B	489	ASN
1	C	31	HIS

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Mol	Chain	Res	Type
1	C	46	ASN
1	C	62	HIS
2	D	54	HIS
2	D	109	ASN
2	D	190	HIS
2	D	191	ASN
2	D	254	ASN
2	D	294	GLN
2	D	310	HIS
2	D	319	ASN
2	D	327	ASN
2	D	343	GLN
2	D	460	GLN
2	D	489	ASN
1	E	31	HIS
1	E	46	ASN
1	E	62	HIS
2	F	54	HIS
2	F	109	ASN
2	F	113	GLN
2	F	191	ASN
2	F	254	ASN
2	F	310	HIS
2	F	327	ASN
2	F	343	GLN
2	F	460	GLN
2	F	489	ASN
1	G	31	HIS
1	G	46	ASN
1	G	62	HIS
2	H	23	GLN
2	H	54	HIS
2	H	74	ASN
2	H	95	ASN
2	H	110	ASN
2	H	118	HIS
2	H	191	ASN
2	H	198	ASN
2	H	319	ASN
2	H	343	GLN
2	H	375	GLN
2	H	392	ASN

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Mol	Chain	Res	Type
2	H	460	GLN
2	H	489	ASN
2	H	577	GLN
1	I	31	HIS
1	I	46	ASN
1	I	62	HIS
2	J	54	HIS
2	J	109	ASN
2	J	191	ASN
2	J	254	ASN
2	J	294	GLN
2	J	310	HIS
2	J	327	ASN
2	J	343	GLN
2	J	460	GLN
2	J	489	ASN
1	K	31	HIS
1	K	46	ASN
1	K	62	HIS
2	L	54	HIS
2	L	109	ASN
2	L	190	HIS
2	L	191	ASN
2	L	254	ASN
2	L	294	GLN
2	L	310	HIS
2	L	319	ASN
2	L	327	ASN
2	L	343	GLN
2	L	460	GLN
2	L	489	ASN
1	M	31	HIS
1	M	62	HIS
2	N	54	HIS
2	N	109	ASN
2	N	191	ASN
2	N	254	ASN
2	N	310	HIS
2	N	327	ASN
2	N	343	GLN
2	N	460	GLN
2	N	489	ASN

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Mol	Chain	Res	Type
1	O	31	HIS
1	O	46	ASN
1	O	62	HIS
2	P	54	HIS
2	P	109	ASN
2	P	191	ASN
2	P	254	ASN
2	P	310	HIS
2	P	327	ASN
2	P	343	GLN
2	P	460	GLN
2	P	489	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

40 ligands are modelled in this entry.

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	$\# Z > 2$
4	7JA	B	1100	-	20,23,23	1.61	3 (15%)	20,30,30	1.92	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	B	1101	-	4,4,4	2.98	4 (100%)	6,6,6	0.29	0
5	PO4	B	1102	-	4,4,4	2.89	4 (100%)	6,6,6	0.27	0
5	PO4	B	1103	-	4,4,4	2.78	4 (100%)	6,6,6	0.28	0
5	PO4	B	1104	-	4,4,4	3.01	3 (75%)	6,6,6	0.30	0
4	7JA	D	1100	-	20,23,23	1.50	3 (15%)	20,30,30	1.73	4 (20%)
5	PO4	D	1101	-	4,4,4	2.91	4 (100%)	6,6,6	0.30	0
5	PO4	D	1102	-	4,4,4	2.89	3 (75%)	6,6,6	0.26	0
5	PO4	D	1103	-	4,4,4	2.84	4 (100%)	6,6,6	0.30	0
5	PO4	D	1104	-	4,4,4	2.90	3 (75%)	6,6,6	0.31	0
4	7JA	F	1100	-	20,23,23	1.56	3 (15%)	20,30,30	1.82	4 (20%)
5	PO4	F	1101	-	4,4,4	2.97	4 (100%)	6,6,6	0.35	0
5	PO4	F	1102	-	4,4,4	3.00	4 (100%)	6,6,6	0.26	0
5	PO4	F	1103	-	4,4,4	2.79	3 (75%)	6,6,6	0.28	0
5	PO4	F	1104	-	4,4,4	2.92	3 (75%)	6,6,6	0.32	0
4	7JA	H	1100	-	20,23,23	1.47	3 (15%)	20,30,30	1.78	5 (25%)
5	PO4	H	1101	-	4,4,4	3.17	4 (100%)	6,6,6	0.30	0
5	PO4	H	1102	-	4,4,4	3.05	3 (75%)	6,6,6	0.28	0
5	PO4	H	1103	-	4,4,4	2.99	3 (75%)	6,6,6	0.28	0
5	PO4	H	1104	-	4,4,4	3.05	3 (75%)	6,6,6	0.36	0
4	7JA	J	1100	-	20,23,23	1.51	3 (15%)	20,30,30	1.75	4 (20%)
5	PO4	J	1101	-	4,4,4	2.93	3 (75%)	6,6,6	0.31	0
5	PO4	J	1102	-	4,4,4	3.06	3 (75%)	6,6,6	0.27	0
5	PO4	J	1103	-	4,4,4	2.91	3 (75%)	6,6,6	0.28	0
5	PO4	J	1104	-	4,4,4	2.79	3 (75%)	6,6,6	0.28	0
4	7JA	L	1100	-	20,23,23	1.46	2 (10%)	20,30,30	1.51	1 (5%)
5	PO4	L	1101	-	4,4,4	2.83	3 (75%)	6,6,6	0.29	0
5	PO4	L	1102	-	4,4,4	3.03	3 (75%)	6,6,6	0.26	0
5	PO4	L	1103	-	4,4,4	2.96	3 (75%)	6,6,6	0.28	0
5	PO4	L	1104	-	4,4,4	2.94	3 (75%)	6,6,6	0.29	0
4	7JA	N	1100	-	20,23,23	1.47	3 (15%)	20,30,30	1.78	2 (10%)
5	PO4	N	1101	-	4,4,4	2.97	3 (75%)	6,6,6	0.32	0
5	PO4	N	1102	-	4,4,4	3.07	3 (75%)	6,6,6	0.28	0
5	PO4	N	1103	-	4,4,4	2.89	3 (75%)	6,6,6	0.31	0
5	PO4	N	1104	-	4,4,4	3.08	3 (75%)	6,6,6	0.31	0
4	7JA	P	1100	-	20,23,23	1.52	3 (15%)	20,30,30	1.65	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	P	1101	-	4,4,4	3.00	3 (75%)	6,6,6	0.29	0
5	PO4	P	1102	-	4,4,4	3.06	3 (75%)	6,6,6	0.27	0
5	PO4	P	1103	-	4,4,4	2.90	3 (75%)	6,6,6	0.29	0
5	PO4	P	1104	-	4,4,4	2.88	3 (75%)	6,6,6	0.30	0

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
4	7JA	B	1100	-	-	0/19/36/36	0/1/1/1
5	PO4	B	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1104	-	-	0/0/0/0	0/0/0/0
4	7JA	D	1100	-	-	0/19/36/36	0/1/1/1
5	PO4	D	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1104	-	-	0/0/0/0	0/0/0/0
4	7JA	F	1100	-	-	0/19/36/36	0/1/1/1
5	PO4	F	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1104	-	-	0/0/0/0	0/0/0/0
4	7JA	H	1100	-	-	0/19/36/36	0/1/1/1
5	PO4	H	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1104	-	-	0/0/0/0	0/0/0/0
4	7JA	J	1100	-	-	0/19/36/36	0/1/1/1
5	PO4	J	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1104	-	-	0/0/0/0	0/0/0/0
4	7JA	L	1100	-	-	0/19/36/36	0/1/1/1
5	PO4	L	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1104	-	-	0/0/0/0	0/0/0/0
4	7JA	N	1100	-	-	0/19/36/36	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	N	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1104	-	-	0/0/0/0	0/0/0/0
4	7JA	P	1100	-	-	0/19/36/36	0/1/1/1
5	PO4	P	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1104	-	-	0/0/0/0	0/0/0/0

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1100	7JA	O14-C13	-2.79	1.17	1.23
4	D	1100	7JA	O14-C13	-2.72	1.17	1.23
4	B	1100	7JA	O08-C07	-2.67	1.17	1.21
4	B	1100	7JA	O14-C13	-2.49	1.18	1.23
4	H	1100	7JA	O14-C13	-2.47	1.18	1.23
5	F	1101	PO4	P-O2	-2.42	1.44	1.53
4	N	1100	7JA	O14-C13	-2.41	1.18	1.23
4	F	1100	7JA	O08-C07	-2.37	1.17	1.21
5	B	1101	PO4	P-O2	-2.32	1.45	1.53
4	L	1100	7JA	O14-C13	-2.29	1.18	1.23
4	J	1100	7JA	O14-C13	-2.26	1.18	1.23
4	J	1100	7JA	O08-C07	-2.17	1.17	1.21
5	D	1103	PO4	P-O2	-2.16	1.45	1.53
4	P	1100	7JA	O14-C13	-2.11	1.18	1.23
4	D	1100	7JA	O08-C07	-2.09	1.18	1.21
5	F	1102	PO4	P-O2	-2.06	1.46	1.53
5	H	1101	PO4	P-O2	-2.06	1.46	1.53
5	B	1103	PO4	P-O2	-2.02	1.46	1.53
5	B	1102	PO4	P-O2	-2.02	1.46	1.53
5	D	1101	PO4	P-O2	-2.01	1.46	1.53
4	P	1100	7JA	C09-C07	2.30	1.55	1.51
4	H	1100	7JA	C09-C07	2.42	1.55	1.51
4	N	1100	7JA	C09-C07	2.51	1.55	1.51
5	D	1101	PO4	P-O1	2.75	1.64	1.52
5	B	1103	PO4	P-O1	2.79	1.64	1.52
5	N	1101	PO4	P-O1	2.79	1.64	1.52
5	L	1103	PO4	P-O4	2.81	1.63	1.53
5	B	1101	PO4	P-O4	2.82	1.63	1.53
5	L	1101	PO4	P-O1	2.83	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1103	PO4	P-O4	2.85	1.63	1.53
5	J	1101	PO4	P-O1	2.87	1.65	1.52
5	D	1103	PO4	P-O1	2.88	1.65	1.52
5	H	1101	PO4	P-O1	2.89	1.65	1.52
5	B	1102	PO4	P-O3	2.91	1.63	1.53
5	H	1103	PO4	P-O1	2.92	1.65	1.52
5	J	1104	PO4	P-O3	2.92	1.63	1.53
5	F	1101	PO4	P-O1	2.93	1.65	1.52
5	H	1104	PO4	P-O1	2.93	1.65	1.52
5	D	1102	PO4	P-O3	2.93	1.63	1.53
5	F	1103	PO4	P-O4	2.94	1.64	1.53
5	F	1104	PO4	P-O1	2.94	1.65	1.52
5	F	1103	PO4	P-O1	2.96	1.65	1.52
5	L	1104	PO4	P-O1	2.97	1.65	1.52
5	L	1101	PO4	P-O4	2.98	1.64	1.53
5	N	1103	PO4	P-O1	3.00	1.65	1.52
5	B	1103	PO4	P-O4	3.01	1.64	1.53
5	B	1101	PO4	P-O1	3.01	1.65	1.52
5	B	1102	PO4	P-O1	3.01	1.65	1.52
5	P	1102	PO4	P-O1	3.01	1.65	1.52
5	L	1102	PO4	P-O1	3.02	1.65	1.52
5	J	1104	PO4	P-O4	3.02	1.64	1.53
5	D	1102	PO4	P-O1	3.03	1.65	1.52
5	F	1104	PO4	P-O4	3.03	1.64	1.53
5	F	1102	PO4	P-O3	3.04	1.64	1.53
5	F	1101	PO4	P-O4	3.04	1.64	1.53
5	B	1104	PO4	P-O1	3.05	1.65	1.52
5	J	1103	PO4	P-O3	3.08	1.64	1.53
5	P	1101	PO4	P-O1	3.08	1.65	1.52
5	J	1103	PO4	P-O1	3.08	1.65	1.52
5	D	1104	PO4	P-O1	3.09	1.65	1.52
5	N	1103	PO4	P-O3	3.12	1.64	1.53
5	P	1104	PO4	P-O3	3.12	1.64	1.53
5	L	1103	PO4	P-O1	3.13	1.66	1.52
5	N	1104	PO4	P-O1	3.15	1.66	1.52
5	B	1103	PO4	P-O3	3.15	1.64	1.53
5	F	1103	PO4	P-O3	3.16	1.64	1.53
5	J	1102	PO4	P-O1	3.18	1.66	1.52
5	N	1102	PO4	P-O1	3.18	1.66	1.52
5	H	1102	PO4	P-O1	3.21	1.66	1.52
5	P	1103	PO4	P-O3	3.22	1.65	1.53
5	P	1104	PO4	P-O1	3.25	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1101	PO4	P-O4	3.26	1.65	1.53
5	P	1103	PO4	P-O4	3.27	1.65	1.53
5	J	1104	PO4	P-O1	3.28	1.66	1.52
5	P	1103	PO4	P-O1	3.29	1.66	1.52
5	D	1104	PO4	P-O4	3.29	1.65	1.53
5	P	1104	PO4	P-O4	3.31	1.65	1.53
5	F	1102	PO4	P-O1	3.33	1.67	1.52
5	D	1101	PO4	P-O3	3.34	1.65	1.53
5	D	1101	PO4	P-O4	3.34	1.65	1.53
5	P	1101	PO4	P-O3	3.35	1.65	1.53
5	L	1101	PO4	P-O3	3.35	1.65	1.53
5	J	1102	PO4	P-O4	3.35	1.65	1.53
5	D	1103	PO4	P-O3	3.36	1.65	1.53
5	L	1102	PO4	P-O4	3.37	1.65	1.53
5	J	1103	PO4	P-O4	3.38	1.65	1.53
5	L	1104	PO4	P-O3	3.39	1.65	1.53
5	F	1101	PO4	P-O3	3.39	1.65	1.53
5	D	1104	PO4	P-O3	3.40	1.65	1.53
5	F	1102	PO4	P-O4	3.40	1.65	1.53
5	H	1104	PO4	P-O4	3.40	1.65	1.53
5	H	1102	PO4	P-O3	3.41	1.65	1.53
5	J	1101	PO4	P-O4	3.41	1.65	1.53
5	H	1103	PO4	P-O3	3.42	1.65	1.53
5	B	1102	PO4	P-O4	3.45	1.65	1.53
5	N	1103	PO4	P-O4	3.45	1.65	1.53
5	N	1102	PO4	P-O3	3.46	1.65	1.53
5	H	1103	PO4	P-O4	3.48	1.65	1.53
5	L	1104	PO4	P-O4	3.48	1.65	1.53
5	B	1104	PO4	P-O3	3.49	1.65	1.53
5	J	1101	PO4	P-O3	3.51	1.66	1.53
5	B	1104	PO4	P-O4	3.51	1.66	1.53
5	L	1102	PO4	P-O3	3.51	1.66	1.53
5	H	1101	PO4	P-O3	3.52	1.66	1.53
5	P	1102	PO4	P-O4	3.54	1.66	1.53
5	D	1102	PO4	P-O4	3.55	1.66	1.53
5	P	1101	PO4	P-O4	3.56	1.66	1.53
5	N	1104	PO4	P-O3	3.58	1.66	1.53
5	P	1102	PO4	P-O3	3.59	1.66	1.53
5	J	1102	PO4	P-O3	3.59	1.66	1.53
5	H	1102	PO4	P-O4	3.59	1.66	1.53
5	B	1101	PO4	P-O3	3.62	1.66	1.53
5	F	1104	PO4	P-O3	3.65	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1104	PO4	P-O4	3.69	1.66	1.53
5	N	1102	PO4	P-O4	3.72	1.66	1.53
5	L	1103	PO4	P-O3	3.79	1.67	1.53
5	H	1104	PO4	P-O3	3.82	1.67	1.53
5	N	1101	PO4	P-O3	3.87	1.67	1.53
5	H	1101	PO4	P-O4	3.90	1.67	1.53
4	H	1100	7JA	C13-N	4.82	1.43	1.34
4	N	1100	7JA	C13-N	4.83	1.43	1.34
4	D	1100	7JA	C13-N	4.89	1.43	1.34
4	L	1100	7JA	C13-N	5.14	1.44	1.34
4	P	1100	7JA	C13-N	5.40	1.44	1.34
4	F	1100	7JA	C13-N	5.42	1.45	1.34
4	J	1100	7JA	C13-N	5.43	1.45	1.34
4	B	1100	7JA	C13-N	5.63	1.45	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	1100	7JA	CB-CA-N	-5.79	98.25	111.12
4	J	1100	7JA	CB-CA-N	-5.25	99.44	111.12
4	D	1100	7JA	CB-CA-N	-5.24	99.46	111.12
4	B	1100	7JA	CB-CA-N	-5.22	99.51	111.12
4	F	1100	7JA	CB-CA-N	-5.06	99.86	111.12
4	P	1100	7JA	CB-CA-N	-4.78	100.48	111.12
4	L	1100	7JA	CB-CA-N	-4.63	100.81	111.12
4	F	1100	7JA	O14-C13-C12	-3.77	115.80	121.30
4	H	1100	7JA	CB-CA-N	-3.49	103.36	111.12
4	B	1100	7JA	O14-C13-C12	-3.42	116.31	121.30
4	H	1100	7JA	O14-C13-N	-3.16	117.66	123.01
4	N	1100	7JA	C10-C11-C12	-3.03	107.98	113.60
4	B	1100	7JA	C10-C09-C07	-2.88	102.50	105.45
4	P	1100	7JA	C10-C11-C12	-2.81	108.40	113.60
4	H	1100	7JA	CG1-CB-CA	-2.72	103.89	111.10
4	B	1100	7JA	C10-C11-C12	-2.51	108.94	113.60
4	D	1100	7JA	O14-C13-C12	-2.45	117.72	121.30
4	P	1100	7JA	O14-C13-C12	-2.43	117.75	121.30
4	D	1100	7JA	CG2-CB-CA	-2.43	104.60	111.17
4	J	1100	7JA	C10-C11-C12	-2.35	109.25	113.60
4	J	1100	7JA	O14-C13-C12	-2.24	118.04	121.30
4	D	1100	7JA	C02-C03-C04	-2.18	117.09	127.06
4	P	1100	7JA	C02-C03-C04	-2.12	117.36	127.06
4	F	1100	7JA	C02-C03-C04	-2.06	117.63	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1100	7JA	C10-C11-C12	-2.04	109.82	113.60
4	J	1100	7JA	C02-C03-C04	-2.01	117.87	127.06
4	H	1100	7JA	O08-C07-C09	2.11	128.43	125.67
4	H	1100	7JA	C10-C11-C06	2.84	107.58	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 158 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1100	7JA	16	0
5	B	1103	PO4	2	0
4	D	1100	7JA	15	0
5	D	1103	PO4	3	0
4	F	1100	7JA	19	0
5	F	1101	PO4	1	0
5	F	1103	PO4	3	0
4	H	1100	7JA	21	0
5	H	1103	PO4	3	0
4	J	1100	7JA	17	0
5	J	1103	PO4	2	0
4	L	1100	7JA	16	0
5	L	1101	PO4	1	0
5	L	1103	PO4	2	0
4	N	1100	7JA	17	0
5	N	1103	PO4	2	0
4	P	1100	7JA	15	0
5	P	1103	PO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	144/160 (90%)	0.30	4 (2%) 56 42	38, 87, 141, 157	0
1	C	144/160 (90%)	0.57	8 (5%) 28 15	40, 90, 140, 159	0
1	E	144/160 (90%)	0.06	1 (0%) 89 82	41, 85, 136, 157	0
1	G	144/160 (90%)	-0.07	0 100 100	37, 81, 136, 156	0
1	I	144/160 (90%)	0.37	8 (5%) 28 15	43, 88, 138, 160	0
1	K	144/160 (90%)	0.48	11 (7%) 17 9	43, 89, 140, 158	0
1	M	144/160 (90%)	0.64	20 (13%) 4 2	45, 89, 139, 163	0
1	O	144/160 (90%)	0.65	19 (13%) 4 3	43, 88, 138, 159	0
2	B	568/592 (95%)	-0.20	10 (1%) 71 58	31, 60, 122, 191	0
2	D	568/592 (95%)	-0.17	11 (1%) 70 55	33, 61, 124, 190	0
2	F	568/592 (95%)	-0.22	18 (3%) 51 36	32, 63, 125, 191	0
2	H	562/592 (94%)	-0.45	7 (1%) 81 69	29, 57, 106, 169	0
2	J	568/592 (95%)	-0.29	14 (2%) 61 46	33, 64, 124, 194	0
2	L	568/592 (95%)	-0.29	10 (1%) 71 58	33, 64, 125, 192	0
2	N	568/592 (95%)	0.11	28 (4%) 33 20	33, 69, 126, 194	0
2	P	568/592 (95%)	-0.16	20 (3%) 48 31	34, 68, 126, 192	0
3	Q	18/21 (85%)	-0.12	0 100 100	61, 77, 108, 128	0
3	R	18/21 (85%)	-0.09	1 (5%) 28 15	63, 78, 108, 131	0
3	S	18/21 (85%)	-0.27	0 100 100	64, 78, 109, 129	0
3	U	18/21 (85%)	-0.31	0 100 100	60, 80, 109, 130	0
3	V	18/21 (85%)	-0.16	1 (5%) 28 15	61, 81, 108, 132	0
3	W	18/21 (85%)	0.12	1 (5%) 28 15	66, 83, 110, 132	0
3	X	18/21 (85%)	-0.21	1 (5%) 28 15	65, 81, 109, 131	0
All	All	5816/6163 (94%)	-0.09	193 (3%) 50 34	29, 68, 128, 194	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	592	ILE	9.7
2	N	12	SER	8.8
2	P	12	SER	7.9
2	L	359	GLU	7.6
2	F	547	SER	7.3
2	D	360	ASP	7.1
2	D	12	SER	7.0
2	N	591	PRO	6.7
2	N	590	GLU	6.5
2	F	592	ILE	6.3
3	W	200	GLU	6.2
2	L	360	ASP	6.1
1	O	80	ASP	5.4
1	K	13	GLY	5.2
2	J	360	ASP	5.2
2	B	360	ASP	5.1
2	B	549	ARG	5.1
2	P	362	GLU	5.1
1	M	115	ASP	5.0
2	N	360	ASP	5.0
1	A	21	ALA	5.0
2	L	592	ILE	5.0
1	M	80	ASP	5.0
2	N	15	ALA	4.9
2	B	356	GLN	4.8
2	F	548	ARG	4.8
2	F	591	PRO	4.8
2	B	358	MET	4.7
2	J	12	SER	4.5
2	D	592	ILE	4.5
2	F	356	GLN	4.3
2	N	361	GLU	4.3
2	P	547	SER	4.2
2	N	359	GLU	4.1
2	L	362	GLU	4.1
2	D	361	GLU	4.1
1	C	115	ASP	4.0
2	F	546	PRO	4.0
2	J	592	ILE	4.0
1	C	13	GLY	4.0
2	H	353	ALA	4.0
2	P	592	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	356	GLN	3.8
2	P	546	PRO	3.8
2	F	590	GLU	3.8
2	P	548	ARG	3.7
1	M	17	GLU	3.7
2	N	355	GLU	3.7
2	N	358	MET	3.7
3	V	200	GLU	3.7
2	F	549	ARG	3.7
2	N	354	ASP	3.6
2	J	549	ARG	3.6
2	J	362	GLU	3.6
3	X	200	GLU	3.5
2	N	13	CYS	3.5
2	N	357	GLY	3.5
2	P	591	PRO	3.5
2	B	359	GLU	3.4
2	B	527	MET	3.4
2	D	358	MET	3.4
2	J	548	ARG	3.4
2	P	360	ASP	3.3
2	N	548	ARG	3.3
1	M	21	ALA	3.3
1	C	7	VAL	3.3
2	N	362	GLU	3.3
2	B	592	ILE	3.2
2	F	12	SER	3.2
2	F	358	MET	3.2
1	O	56	ILE	3.2
1	M	116	LEU	3.2
2	P	356	GLN	3.2
1	O	84	LYS	3.1
2	D	549	ARG	3.1
1	K	7	VAL	3.1
2	D	418	ARG	3.1
2	F	359	GLU	3.1
1	C	20	GLU	3.1
2	H	362	GLU	3.0
2	F	355	GLU	3.0
1	K	6	ILE	3.0
1	K	20	GLU	3.0
1	O	91	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	63	VAL	3.0
1	K	17	GLU	3.0
1	O	115	ASP	2.9
2	B	355	GLU	2.9
1	M	84	LYS	2.9
2	H	12	SER	2.9
2	P	549	ARG	2.9
1	I	38	VAL	2.9
1	O	52	LEU	2.8
1	M	6	ILE	2.8
2	N	527	MET	2.8
1	K	15	SER	2.8
2	N	356	GLN	2.7
1	I	20	GLU	2.7
1	O	89	ASP	2.7
2	N	588	LEU	2.7
2	J	359	GLU	2.7
1	M	35	ASP	2.7
1	I	47	VAL	2.6
2	D	548	ARG	2.6
3	R	200	GLU	2.6
1	K	63	VAL	2.6
1	K	67	ALA	2.6
2	P	590	GLU	2.6
2	P	418	ARG	2.6
2	J	591	PRO	2.6
1	A	20	GLU	2.6
2	D	22	GLU	2.5
1	I	39	ASP	2.5
2	N	363	GLY	2.5
2	N	314	ILE	2.5
2	B	548	ARG	2.5
2	F	361	GLU	2.5
2	N	547	SER	2.5
1	I	37	CYS	2.5
2	P	359	GLU	2.5
1	O	58	TYR	2.5
2	L	548	ARG	2.5
1	M	87	ASP	2.4
2	F	360	ASP	2.4
2	L	355	GLU	2.4
1	M	38	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	90	PHE	2.4
1	M	81	ASP	2.4
2	J	361	GLU	2.4
1	I	42	VAL	2.4
2	H	527	MET	2.4
2	J	355	GLU	2.4
2	F	354	ASP	2.4
2	F	527	MET	2.4
1	A	124	MET	2.3
2	L	258	GLY	2.3
2	N	402	LEU	2.3
2	P	370	LEU	2.3
1	O	19	GLU	2.3
1	C	66	ALA	2.3
1	I	84	LYS	2.3
1	A	59	CYS	2.3
1	M	82	ASP	2.3
1	O	22	VAL	2.3
2	D	357	GLY	2.3
2	N	546	PRO	2.3
2	P	361	GLU	2.3
2	F	258	GLY	2.3
1	C	118	CYS	2.3
2	P	527	MET	2.3
2	J	547	SER	2.3
1	M	16	PHE	2.2
2	N	398	ILE	2.2
2	P	589	LYS	2.2
2	L	591	PRO	2.2
2	H	355	GLU	2.2
2	F	357	GLY	2.2
1	M	91	MET	2.2
2	J	356	GLN	2.2
2	N	383	MET	2.2
1	K	114	LEU	2.2
2	L	12	SER	2.2
1	O	55	VAL	2.2
1	O	16	PHE	2.2
1	I	6	ILE	2.2
2	N	428	VAL	2.2
2	H	359	GLU	2.2
2	P	255	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	22	VAL	2.2
2	J	415	ARG	2.2
2	B	564	HIS	2.1
2	D	362	GLU	2.1
1	O	88	ALA	2.1
1	M	119	GLN	2.1
2	N	589	LYS	2.1
1	C	119	GLN	2.1
1	M	145	PRO	2.1
1	O	93	ILE	2.1
2	P	258	GLY	2.1
1	M	18	VAL	2.1
1	C	40	ASN	2.1
1	K	115	ASP	2.1
2	P	315	GLN	2.1
1	O	90	PHE	2.1
1	O	31	HIS	2.1
1	M	83	LEU	2.1
2	H	354	ASP	2.0
1	O	62	HIS	2.0
1	E	39	ASP	2.0
1	O	117	THR	2.0
1	M	126	LYS	2.0
2	J	590	GLU	2.0
2	N	14	VAL	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PO4	L	1102	5/5	0.96	0.30	11.19	64,67,83,96	0
5	PO4	L	1101	5/5	0.97	0.28	4.77	36,48,65,73	0
5	PO4	J	1102	5/5	0.96	0.24	4.69	53,74,83,101	0
5	PO4	J	1104	5/5	0.93	0.22	3.96	57,60,82,86	0
5	PO4	P	1104	5/5	0.94	0.22	3.81	50,58,89,93	0
5	PO4	P	1101	5/5	0.98	0.24	3.73	40,51,70,73	0
5	PO4	F	1101	5/5	0.98	0.22	3.53	40,41,55,77	0
5	PO4	N	1104	5/5	0.92	0.29	3.49	56,57,89,100	0
5	PO4	L	1103	5/5	0.97	0.25	2.92	45,48,58,71	0
5	PO4	L	1104	5/5	0.91	0.21	2.42	52,60,91,94	0
5	PO4	B	1102	5/5	0.91	0.24	2.40	49,75,81,91	0
4	7JA	J	1100	23/23	0.96	0.24	2.35	39,55,72,83	0
5	PO4	H	1104	5/5	0.92	0.23	2.31	57,64,69,95	0
4	7JA	H	1100	23/23	0.94	0.30	2.13	38,62,77,81	0
5	PO4	B	1103	5/5	0.98	0.24	1.96	41,45,51,66	0
4	7JA	F	1100	23/23	0.95	0.27	1.83	42,56,70,88	0
4	7JA	P	1100	23/23	0.95	0.25	1.76	47,59,73,85	0
5	PO4	F	1103	5/5	0.97	0.25	1.70	44,47,48,69	0
5	PO4	J	1103	5/5	0.97	0.23	1.69	42,45,52,68	0
5	PO4	D	1102	5/5	0.93	0.22	1.62	55,73,86,95	0
4	7JA	B	1100	23/23	0.95	0.27	1.57	34,55,70,87	0
5	PO4	N	1102	5/5	0.91	0.26	1.50	64,78,83,116	0
5	PO4	J	1101	5/5	0.97	0.20	1.48	37,45,66,73	0
5	PO4	F	1102	5/5	0.95	0.20	1.06	56,74,78,96	0
5	PO4	F	1104	5/5	0.95	0.20	1.01	48,54,80,83	0
4	7JA	D	1100	23/23	0.97	0.24	0.98	37,55,68,85	0
4	7JA	L	1100	23/23	0.95	0.23	0.96	42,58,72,86	0
5	PO4	D	1104	5/5	0.91	0.21	0.81	49,60,85,91	0
5	PO4	P	1102	5/5	0.95	0.19	0.72	63,72,83,106	0
5	PO4	D	1101	5/5	0.99	0.21	0.68	42,45,58,71	0
5	PO4	D	1103	5/5	0.99	0.23	0.66	38,46,52,75	0
5	PO4	N	1101	5/5	0.94	0.22	0.66	42,48,74,75	0
5	PO4	P	1103	5/5	0.93	0.21	0.41	47,55,70,76	0
5	PO4	N	1103	5/5	0.97	0.22	0.21	48,51,62,80	0
4	7JA	N	1100	23/23	0.94	0.23	-0.07	49,61,73,86	0
5	PO4	B	1101	5/5	0.97	0.20	-0.36	35,48,61,72	0
5	PO4	B	1104	5/5	0.94	0.16	-0.55	47,63,91,96	0
5	PO4	H	1102	5/5	0.90	0.18	-	72,73,108,121	0
5	PO4	H	1101	5/5	0.94	0.18	-	65,80,94,96	0
5	PO4	H	1103	5/5	0.96	0.16	-	35,56,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.