



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:56 PM UTC

PDB ID : 3OGM / pdb_00003ogm
Title : Structure of COI1-ASK1 in complex with coronatine and the JAZ1 degra
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 : 3.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

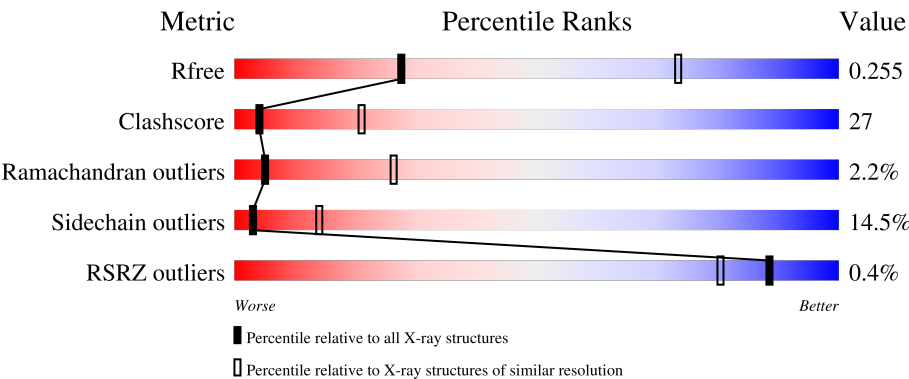
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	160	% 48% 36% 6% 10%
1	C	160	50% 32% 8% 10%
1	E	160	% 49% 34% 7% 10%
1	G	160	48% 36% 6% 10%
1	I	160	% 45% 37% 8% 10%

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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	OGK	H	4100	X	-	X	-
5	PO4	B	1101	-	X	-	-
5	PO4	B	1102	-	X	-	-
5	PO4	B	1103	-	X	-	-
5	PO4	B	1104	-	X	-	-
5	PO4	D	1101	-	X	-	-
5	PO4	D	1102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	D	1103	-	X	-	-
5	PO4	D	1104	-	X	-	-
5	PO4	F	1101	-	X	-	-
5	PO4	F	1102	-	X	-	-
5	PO4	F	1103	-	X	-	-
5	PO4	F	1104	-	X	-	-
5	PO4	H	1101	-	X	-	-
5	PO4	H	1102	-	X	-	-
5	PO4	H	1103	-	X	-	-
5	PO4	H	1104	-	X	-	-
5	PO4	J	1101	-	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	-	-
5	PO4	L	1104	-	X	-	-
5	PO4	N	1101	-	X	-	-
5	PO4	N	1102	-	X	-	-
5	PO4	N	1103	-	X	-	-
5	PO4	N	1104	-	X	-	-
5	PO4	P	1101	-	X	-	-
5	PO4	P	1102	-	X	-	-
5	PO4	P	1103	-	X	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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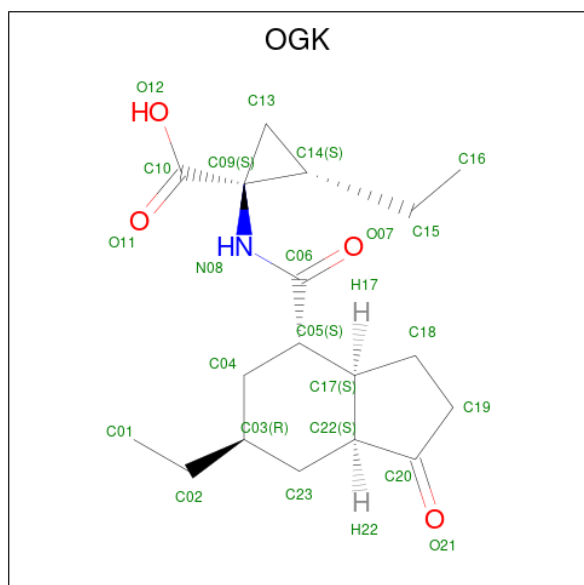
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	P	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

- Molecule 3 is a protein called JAZ1 degron peptide.

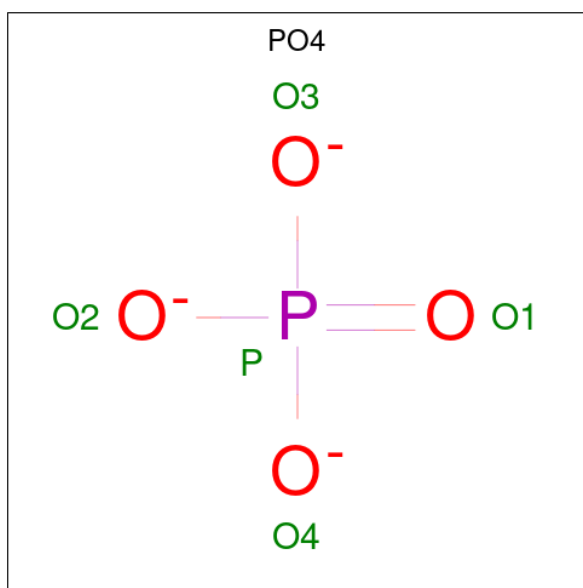
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156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

- Molecule 4 is (1S,2S)-2-ethyl-1-({[(3aS,4S,6R,7aS)-6-ethyl-1-oxooctahydro-1H-inden-4-yl]carbonyl}amino)cyclopropanecarboxylic acid (CCD ID: OGK) (formula: C₁₈H₂₇NO₄).



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 (CCD ID: 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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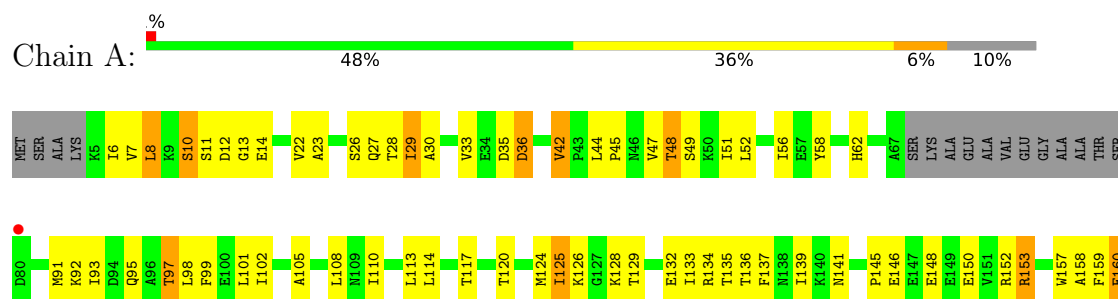
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		

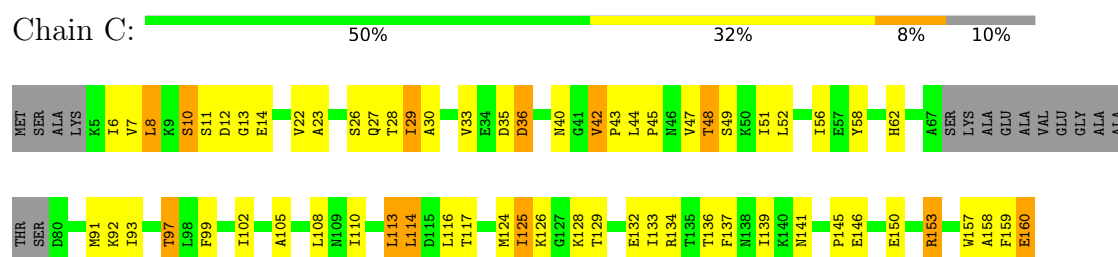
3 Residue-property plots

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

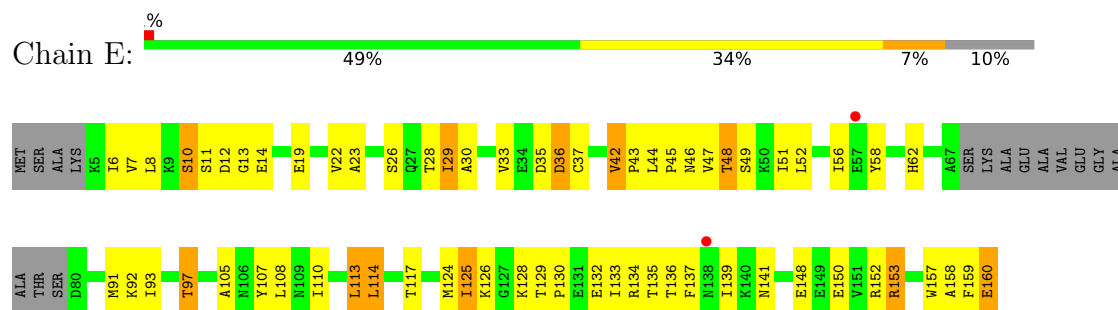
• Molecule 1: SKP1-like protein 1A



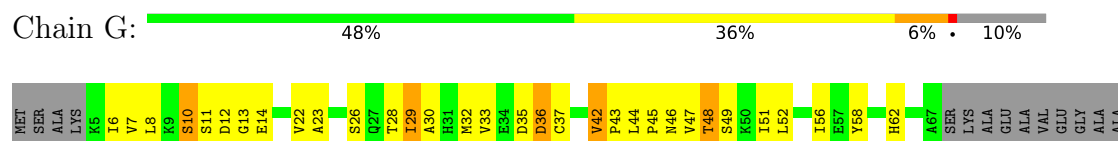
• Molecule 1: SKP1-like protein 1A



• Molecule 1: SKP1-like protein 1A

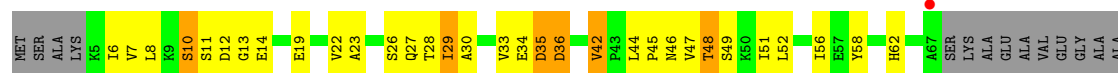
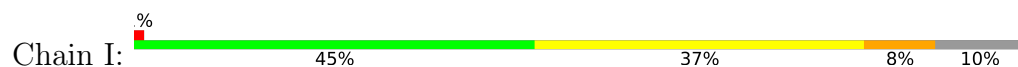


• Molecule 1: SKP1-like protein 1A





- Molecule 1: SKP1-like protein 1A



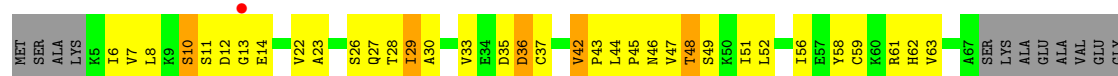
- Molecule 1: SKP1-like protein 1A



- Molecule 1: SKP1-like protein 1A

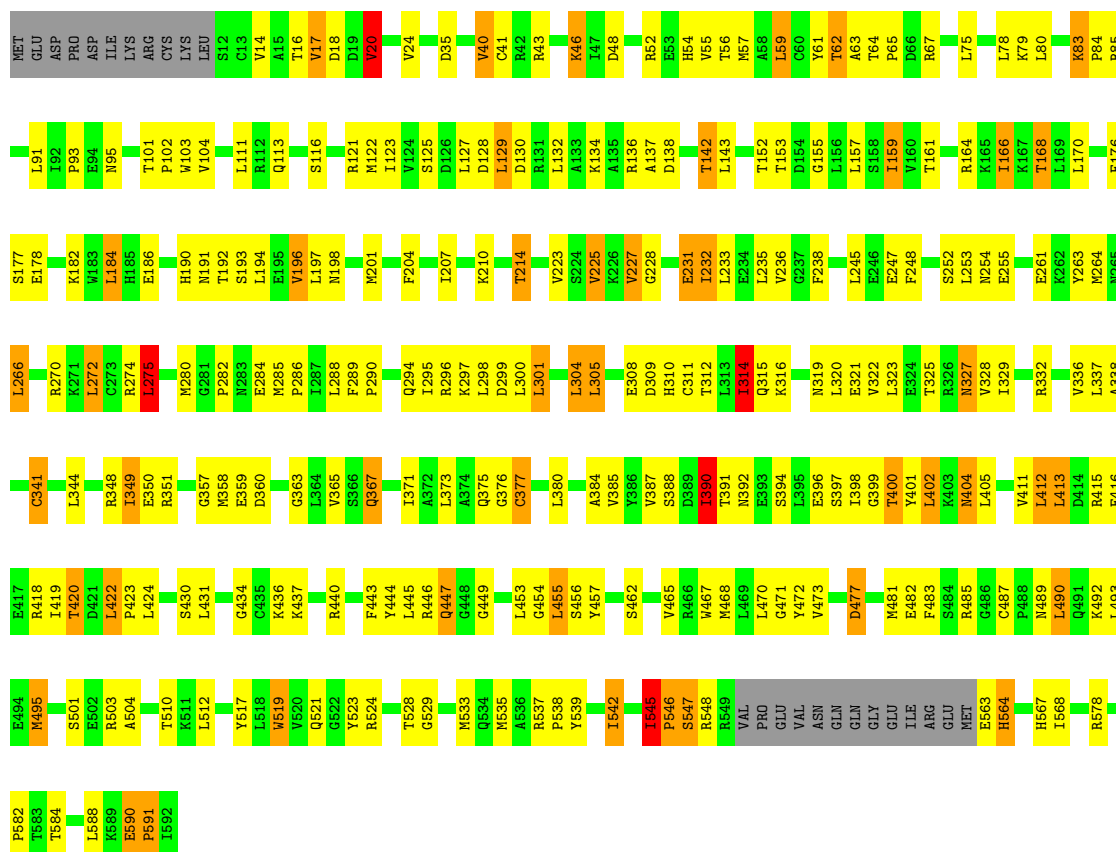


- Molecule 1: SKP1-like protein 1A



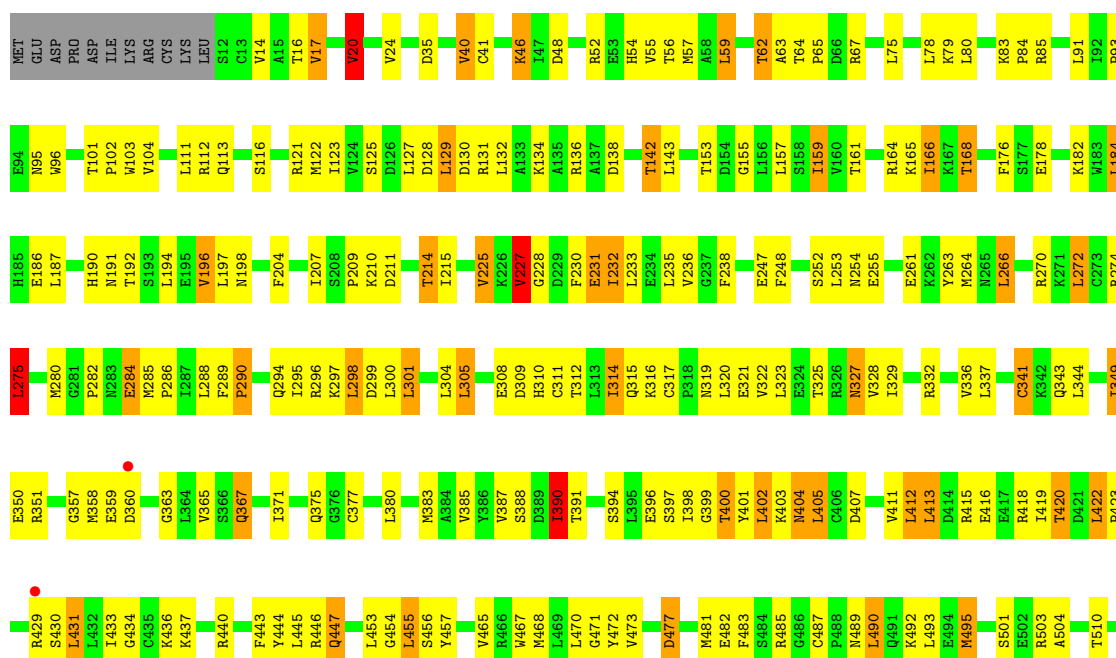
- Molecule 2: Coronatine-insensitive protein 1

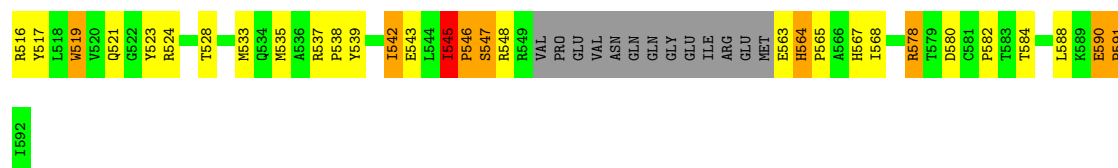




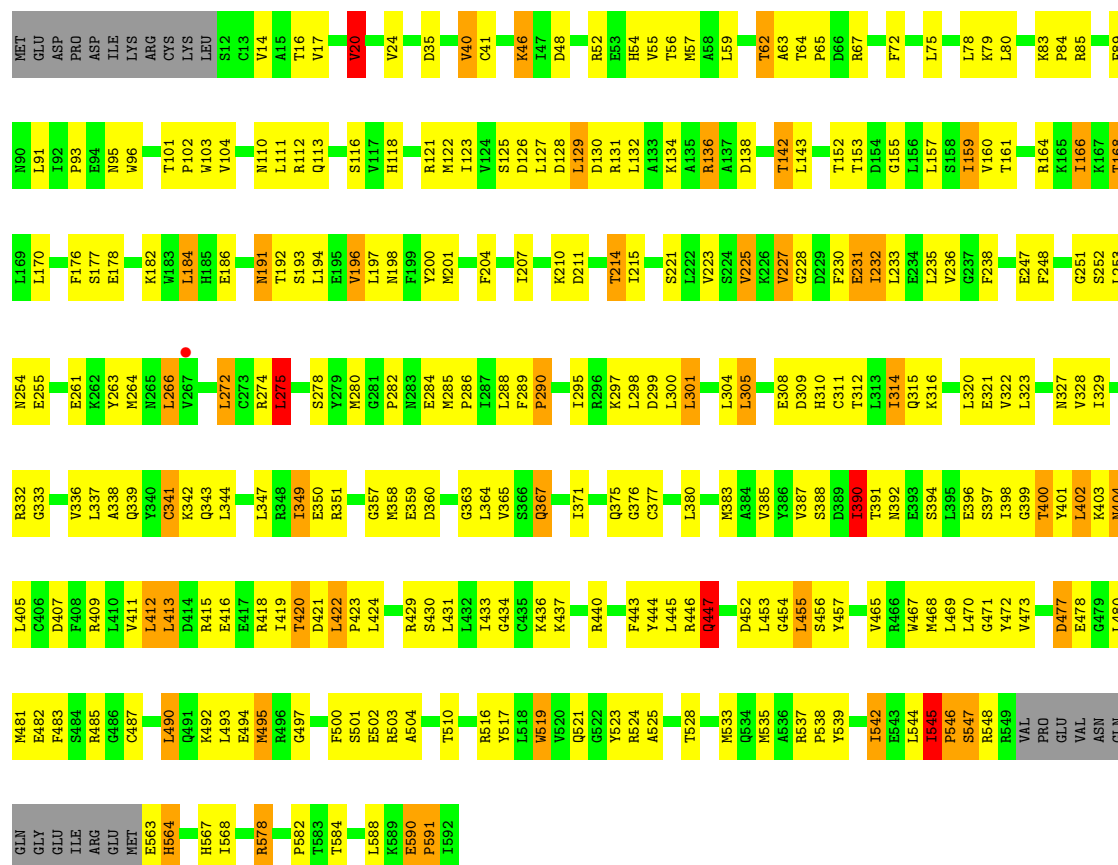
• Molecule 2: Coronatine-insensitive protein 1

Chain D: 52% 35% 8%

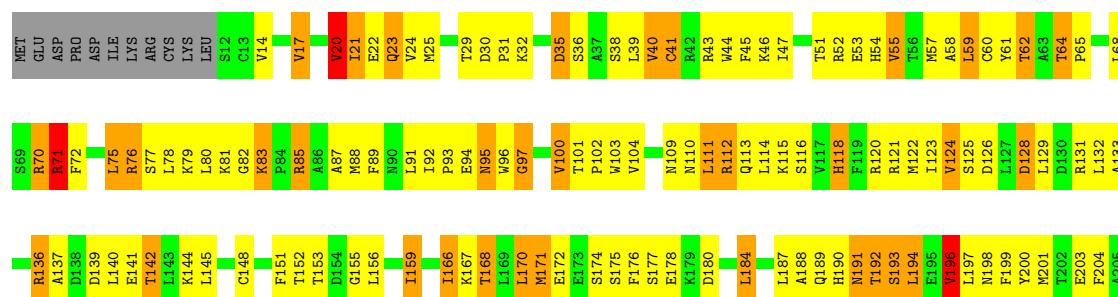


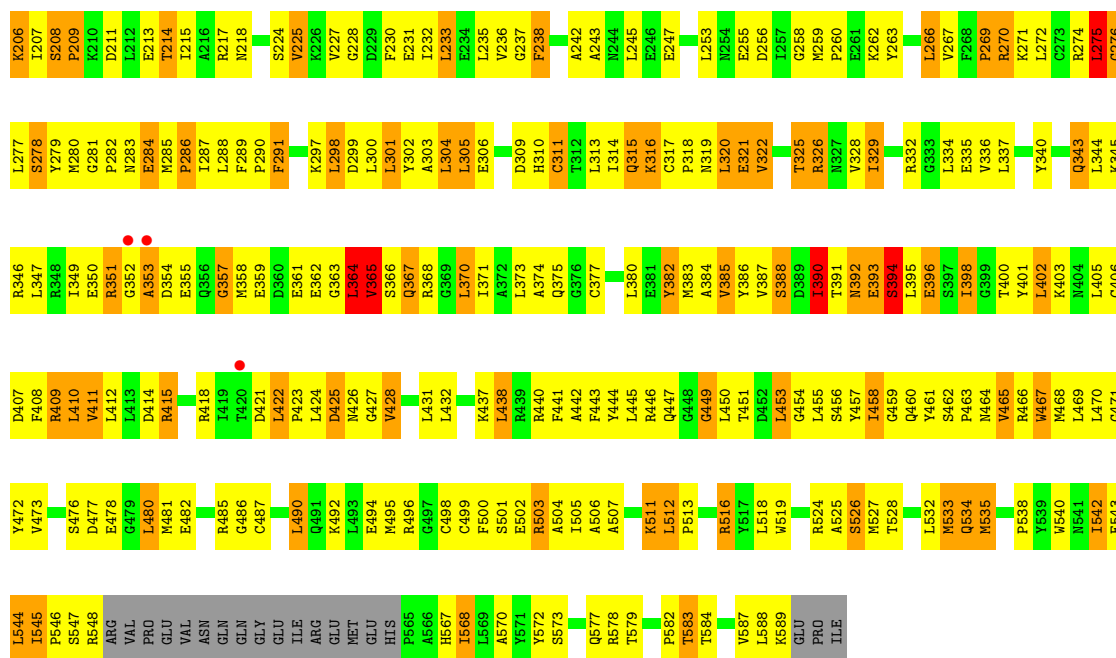


• Molecule 2: Coronatine-insensitive protein 1



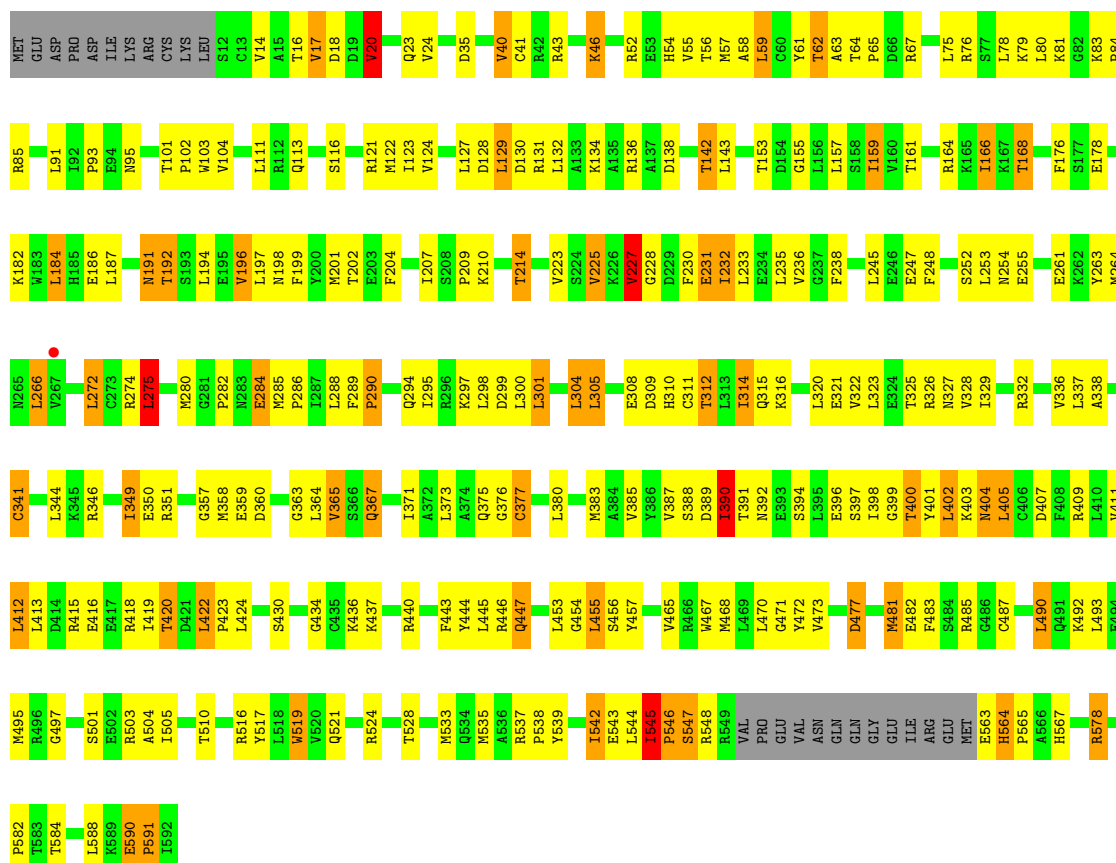
• Molecule 2: Coronatine-insensitive protein 1





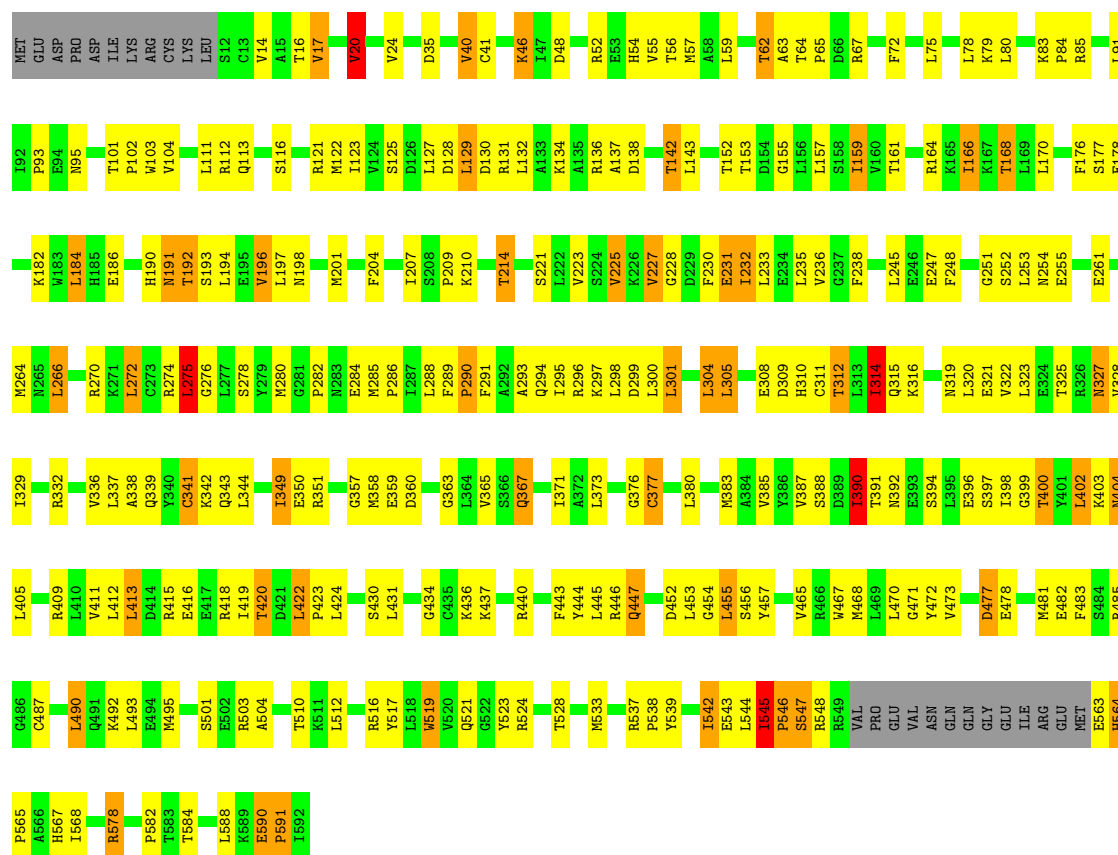
• Molecule 2: Coronatine-insensitive protein 1

Chain J: 51% 36% 9% . .



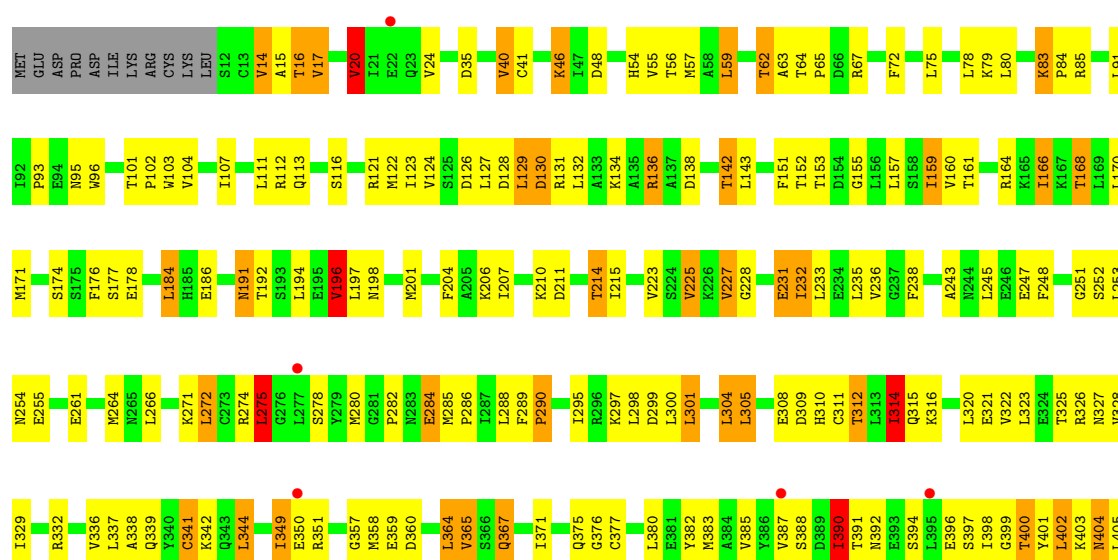
• Molecule 2: Coronatine-insensitive protein 1

Chain L: 



• Molecule 2: Coronatine-insensitive protein 1

Chain N: 





- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



- Molecule 3: JAZ1 degron peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.17Å 220.76Å 149.54Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	49.94 – 3.34 49.94 – 3.34	Depositor EDS
% Data completeness (in resolution range)	85.8 (49.94-3.34) 85.8 (49.94-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.226 , 0.270 0.214 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	46877	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, OGK

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	0.55	0/1162	0.86	0/1571
1	C	0.62	2/1162 (0.2%)	0.86	0/1571
1	E	0.57	1/1162 (0.1%)	0.93	2/1571 (0.1%)
1	G	0.64	0/1162	0.94	2/1571 (0.1%)
1	I	0.58	0/1162	0.88	2/1571 (0.1%)
1	K	0.58	0/1162	0.89	0/1571
1	M	0.60	0/1162	0.90	1/1571 (0.1%)
1	O	0.55	0/1162	0.88	2/1571 (0.1%)
2	B	0.63	0/4623	0.98	15/6238 (0.2%)
2	D	0.66	0/4623	0.96	11/6238 (0.2%)
2	F	0.59	0/4623	0.96	10/6238 (0.2%)
2	H	0.74	0/4566	1.19	29/6161 (0.5%)
2	J	0.63	0/4623	0.96	11/6238 (0.2%)
2	L	0.58	0/4623	0.96	14/6238 (0.2%)
2	N	0.69	0/4623	1.00	13/6238 (0.2%)
2	P	0.58	0/4623	0.96	15/6238 (0.2%)
3	Q	0.50	0/158	0.84	0/208
3	R	0.54	0/158	0.82	0/208
3	S	0.48	0/158	0.84	0/208
3	U	0.64	0/158	0.81	0/208
3	V	0.48	0/158	0.85	0/208
3	W	0.53	0/158	0.85	0/208
3	X	0.53	0/158	0.79	0/208
All	All	0.63	3/47329 (0.0%)	0.98	127/63851 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	LEU	C-N	6.15	1.41	1.33
1	C	114	LEU	N-CA	5.67	1.53	1.46
1	E	113	LEU	C-N	-5.60	1.26	1.33

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	83	LYS	CA-C-N	11.19	131.16	119.85
2	H	83	LYS	C-N-CA	11.19	131.16	119.85
1	G	159	PHE	N-CA-C	8.97	123.53	108.90
2	H	583	THR	N-CA-C	-8.45	103.16	113.97
1	E	114	LEU	N-CA-C	-8.37	103.20	113.41
2	F	390	ILE	N-CA-C	7.66	118.16	108.82
2	J	390	ILE	N-CA-C	7.54	118.02	108.82
2	H	275	LEU	N-CA-C	7.40	118.38	108.38
2	H	208	SER	CA-C-N	7.36	129.04	119.84
2	H	208	SER	C-N-CA	7.36	129.04	119.84
2	P	390	ILE	N-CA-C	7.36	117.80	108.82
2	D	390	ILE	N-CA-C	7.33	117.77	108.82
2	L	390	ILE	N-CA-C	7.19	117.59	108.82
2	J	275	LEU	N-CA-C	6.91	118.69	108.60
2	B	390	ILE	N-CA-C	6.89	117.22	108.82
2	F	275	LEU	N-CA-C	6.79	118.51	108.60
1	O	114	LEU	N-CA-C	-6.78	104.17	113.18
2	P	545	ILE	CA-C-N	6.50	127.96	119.84
2	P	545	ILE	C-N-CA	6.50	127.96	119.84
2	F	545	ILE	CA-C-N	6.37	127.80	119.84
2	F	545	ILE	C-N-CA	6.37	127.80	119.84
2	H	224	SER	N-CA-C	6.29	118.70	108.26
1	G	114	LEU	N-CA-C	-6.23	104.40	111.07
2	N	83	LYS	CA-C-N	6.23	126.58	119.92
2	N	83	LYS	C-N-CA	6.23	126.58	119.92
2	D	275	LEU	N-CA-C	6.11	117.52	108.60
2	N	275	LEU	N-CA-C	6.08	117.47	108.60
2	H	385	VAL	N-CA-C	6.07	117.03	108.17
2	H	355	GLU	N-CA-C	6.05	118.48	108.99
2	H	94	GLU	N-CA-C	-5.99	106.30	113.97
2	H	390	ILE	CB-CA-C	-5.99	101.47	111.29
2	N	390	ILE	N-CA-C	5.96	117.50	108.80
2	P	83	LYS	CA-C-N	5.86	126.19	119.92
2	P	83	LYS	C-N-CA	5.86	126.19	119.92
2	P	275	LEU	N-CA-C	5.86	117.16	108.60
2	B	83	LYS	CA-C-N	5.81	126.14	119.92
2	B	83	LYS	C-N-CA	5.81	126.14	119.92
2	J	76	ARG	N-CA-C	-5.81	106.73	113.88
2	B	275	LEU	N-CA-C	5.79	117.05	108.60
2	H	180	ASP	N-CA-C	5.78	116.21	108.23
2	L	564	HIS	CA-C-N	5.77	126.09	119.92
2	L	564	HIS	C-N-CA	5.77	126.09	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	130	ASP	N-CA-C	-5.71	105.14	111.36
2	L	512	LEU	CA-C-N	5.70	125.23	119.19
2	L	512	LEU	C-N-CA	5.70	125.23	119.19
2	P	317	CYS	CA-C-N	5.69	125.31	119.56
2	P	317	CYS	C-N-CA	5.69	125.31	119.56
2	H	465	VAL	N-CA-C	5.62	115.64	108.12
2	F	564	HIS	CA-C-N	5.61	125.92	119.92
2	F	564	HIS	C-N-CA	5.61	125.92	119.92
2	P	512	LEU	CA-C-N	5.60	125.12	119.19
2	P	512	LEU	C-N-CA	5.60	125.12	119.19
2	P	447	GLN	N-CA-C	5.59	117.07	110.97
2	H	535	MET	N-CA-C	-5.59	105.88	114.16
2	D	564	HIS	CA-C-N	5.58	125.89	119.92
2	D	564	HIS	C-N-CA	5.58	125.89	119.92
2	N	314	ILE	CB-CA-C	-5.55	104.76	112.04
2	D	545	ILE	CA-C-N	5.55	126.78	119.84
2	D	545	ILE	C-N-CA	5.55	126.78	119.84
2	D	317	CYS	CA-C-N	5.54	125.15	119.56
2	D	317	CYS	C-N-CA	5.54	125.15	119.56
1	I	114	LEU	N-CA-C	-5.53	105.15	111.07
2	B	137	ALA	CB-CA-C	-5.53	110.18	116.54
2	H	512	LEU	CA-C-N	5.50	126.71	119.84
2	H	512	LEU	C-N-CA	5.50	126.71	119.84
2	L	83	LYS	CA-C-N	5.45	125.75	119.92
2	L	83	LYS	C-N-CA	5.45	125.75	119.92
2	L	545	ILE	CA-C-N	5.41	126.60	119.84
2	L	545	ILE	C-N-CA	5.41	126.60	119.84
2	H	545	ILE	CA-C-N	5.40	126.59	119.84
2	H	545	ILE	C-N-CA	5.40	126.59	119.84
2	H	367	GLN	N-CA-C	-5.40	105.96	112.54
2	H	393	GLU	N-CA-C	5.40	116.85	110.97
2	B	512	LEU	CA-C-N	5.38	124.89	119.19
2	B	512	LEU	C-N-CA	5.38	124.89	119.19
1	O	159	PHE	N-CA-C	5.37	118.27	107.41
2	B	564	HIS	CA-C-N	5.36	125.66	119.92
2	B	564	HIS	C-N-CA	5.36	125.66	119.92
2	P	92	ILE	CA-C-N	5.34	125.34	119.89
2	P	92	ILE	C-N-CA	5.34	125.34	119.89
2	N	545	ILE	CA-C-N	5.33	126.50	119.84
2	N	545	ILE	C-N-CA	5.33	126.50	119.84
2	J	505	ILE	CB-CA-C	-5.31	105.17	111.81
2	H	351	ARG	N-CA-C	-5.30	100.53	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	462	SER	CA-C-N	5.29	124.98	119.64
2	B	462	SER	C-N-CA	5.29	124.98	119.64
2	H	126	ASP	N-CA-C	-5.28	105.64	111.71
2	H	480	LEU	N-CA-C	-5.28	106.34	112.89
2	L	275	LEU	N-CA-C	5.27	116.30	108.60
2	H	281	GLY	CA-C-N	5.27	124.90	119.05
2	H	281	GLY	C-N-CA	5.27	124.90	119.05
2	N	512	LEU	CA-C-N	5.26	124.59	118.85
2	N	512	LEU	C-N-CA	5.26	124.59	118.85
2	B	314	ILE	CB-CA-C	-5.26	105.15	112.04
1	I	159	PHE	N-CA-C	5.25	118.01	107.41
2	J	545	ILE	CA-C-N	5.23	126.38	119.84
2	J	545	ILE	C-N-CA	5.23	126.38	119.84
2	L	137	ALA	CB-CA-C	-5.23	110.53	116.54
2	L	72	PHE	CA-C-N	5.20	124.87	119.56
2	L	72	PHE	C-N-CA	5.20	124.87	119.56
2	B	545	ILE	CA-C-N	5.20	126.34	119.84
2	B	545	ILE	C-N-CA	5.20	126.34	119.84
2	D	227	VAL	N-CA-C	5.20	115.67	108.23
2	H	196	VAL	N-CA-C	5.18	115.44	107.77
2	J	83	LYS	CA-C-N	5.15	125.43	119.92
2	J	83	LYS	C-N-CA	5.15	125.43	119.92
2	H	573	SER	N-CA-C	5.14	116.55	107.61
1	E	114	LEU	N-CA-CB	-5.12	102.99	110.47
2	P	529	GLY	N-CA-C	-5.12	108.55	115.21
2	H	394	SER	N-CA-C	-5.12	105.39	110.97
2	H	124	VAL	N-CA-CB	-5.12	106.26	112.35
1	M	159	PHE	N-CA-C	5.11	117.73	107.41
2	N	196	VAL	N-CA-C	5.11	115.26	108.11
2	J	227	VAL	N-CA-C	5.10	115.53	108.23
2	P	314	ILE	CB-CA-C	-5.10	105.36	112.04
2	D	83	LYS	CA-C-N	5.08	125.36	119.92
2	D	83	LYS	C-N-CA	5.08	125.36	119.92
2	N	564	HIS	CA-C-N	5.07	125.35	119.92
2	N	564	HIS	C-N-CA	5.07	125.35	119.92
2	L	314	ILE	CB-CA-C	-5.05	105.42	112.04
2	F	83	LYS	CA-C-N	5.04	125.31	119.92
2	F	83	LYS	C-N-CA	5.04	125.31	119.92
2	F	447	GLN	N-CA-C	5.03	116.45	110.97
2	F	200	TYR	N-CA-C	5.02	116.45	110.97
2	J	564	HIS	CA-C-N	5.01	125.28	119.92
2	J	564	HIS	C-N-CA	5.01	125.28	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	529	GLY	N-CA-C	-5.01	108.70	115.21

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	63	0
1	C	1146	0	1117	60	0
1	E	1146	0	1117	73	0
1	G	1146	0	1117	67	0
1	I	1146	0	1117	71	0
1	K	1146	0	1117	58	0
1	M	1146	0	1117	91	0
1	O	1146	0	1117	72	0
2	B	4541	0	4583	230	0
2	D	4541	0	4583	234	0
2	F	4541	0	4583	229	0
2	H	4486	0	4534	459	0
2	J	4541	0	4583	237	0
2	L	4541	0	4583	237	0
2	N	4541	0	4583	281	0
2	P	4541	0	4583	234	0
3	Q	156	0	171	7	0
3	R	156	0	171	5	0
3	S	156	0	171	5	0
3	U	156	0	171	7	0
3	V	156	0	171	5	0
3	W	156	0	171	7	0
3	X	156	0	171	5	0
4	B	23	0	27	7	0
4	D	23	0	27	7	0
4	F	23	0	27	7	0
4	H	23	0	27	16	0
4	J	23	0	27	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	23	0	27	7	0
4	N	23	0	27	6	0
4	P	23	0	27	8	0
5	B	20	0	0	3	0
5	D	20	0	0	2	0
5	F	20	0	0	2	0
5	H	20	0	0	3	0
5	J	20	0	0	2	0
5	L	20	0	0	2	0
5	N	20	0	0	3	0
5	P	20	0	0	3	0
All	All	46877	0	46964	2577	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (2577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:116:SER:HB2	2:H:142:THR:HG23	1.35	1.09
2:P:168:THR:HB	2:P:196:VAL:HG13	1.35	1.08
2:D:168:THR:HB	2:D:196:VAL:HG13	1.35	1.08
2:J:168:THR:HB	2:J:196:VAL:HG13	1.35	1.06
2:L:168:THR:HB	2:L:196:VAL:HG13	1.35	1.06
2:L:542:ILE:HD11	2:L:588:LEU:HD12	1.35	1.06
2:B:168:THR:HB	2:B:196:VAL:HG13	1.37	1.05
2:N:168:THR:HB	2:N:196:VAL:HG13	1.38	1.05
2:N:142:THR:HB	2:N:168:THR:HG23	1.38	1.05
1:M:93:ILE:HD12	1:M:97:THR:HG22	1.40	1.04
2:H:78:LEU:HD12	2:H:79:LYS:H	1.22	1.04
2:H:311:CYS:HB3	2:H:336:VAL:HG21	1.34	1.04
2:F:142:THR:HB	2:F:168:THR:HG23	1.40	1.04
2:D:542:ILE:HD11	2:D:588:LEU:HD12	1.40	1.04
2:J:542:ILE:HD11	2:J:588:LEU:HD12	1.40	1.04
2:H:533:MET:HE3	2:H:588:LEU:HD13	1.36	1.03
1:A:93:ILE:HD12	1:A:97:THR:HG22	1.40	1.02
2:F:168:THR:HB	2:F:196:VAL:HG13	1.39	1.01
2:F:542:ILE:HD11	2:F:588:LEU:HD12	1.43	1.01
2:H:310:HIS:O	2:H:314:ILE:HG12	1.61	1.00
2:P:142:THR:HB	2:P:168:THR:HG23	1.43	1.00
2:N:542:ILE:HD11	2:N:588:LEU:HD12	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:542:ILE:HD11	2:P:588:LEU:HD12	1.45	0.98
2:F:93:PRO:HA	2:F:548:ARG:HB2	1.44	0.98
2:L:142:THR:HB	2:L:168:THR:HG23	1.46	0.98
2:P:357:GLY:HA2	2:P:415:ARG:HH22	1.29	0.97
2:L:93:PRO:HA	2:L:548:ARG:HB2	1.42	0.97
2:P:93:PRO:HA	2:P:548:ARG:HB2	1.44	0.97
2:F:357:GLY:HA2	2:F:415:ARG:HH22	1.30	0.96
1:M:159:PHE:O	1:M:160:GLU:HB2	1.63	0.96
2:H:392:ASN:O	2:H:396:GLU:HG2	1.66	0.96
2:B:357:GLY:HA2	2:B:415:ARG:HH22	1.31	0.96
1:K:93:ILE:HD12	1:K:97:THR:HG22	1.45	0.95
2:D:93:PRO:HA	2:D:548:ARG:HB2	1.48	0.95
2:H:152:THR:HG22	2:H:177:SER:HB2	1.47	0.95
1:O:93:ILE:HD12	1:O:97:THR:HG22	1.49	0.95
2:B:93:PRO:HA	2:B:548:ARG:HB2	1.48	0.94
2:J:93:PRO:HA	2:J:548:ARG:HB2	1.48	0.94
2:L:357:GLY:HA2	2:L:415:ARG:HH22	1.29	0.94
2:J:357:GLY:HA2	2:J:415:ARG:HH22	1.30	0.94
1:K:159:PHE:O	1:K:160:GLU:HB2	1.66	0.94
2:N:93:PRO:HA	2:N:548:ARG:HB2	1.50	0.94
1:E:93:ILE:HD12	1:E:97:THR:HG22	1.46	0.94
2:H:95:ASN:H	2:H:95:ASN:HD22	1.09	0.93
2:J:142:THR:HB	2:J:168:THR:HG23	1.49	0.93
2:B:142:THR:HB	2:B:168:THR:HG23	1.51	0.93
1:C:93:ILE:HD12	1:C:97:THR:HG22	1.49	0.93
1:I:93:ILE:HD12	1:I:97:THR:HG22	1.47	0.93
2:B:542:ILE:HD11	2:B:588:LEU:HD12	1.50	0.93
1:A:159:PHE:O	1:A:160:GLU:HB2	1.69	0.93
1:E:159:PHE:O	1:E:160:GLU:HB2	1.67	0.92
1:O:159:PHE:O	1:O:160:GLU:HB2	1.67	0.92
2:D:357:GLY:HA2	2:D:415:ARG:HH22	1.32	0.92
1:G:160:GLU:HG3	2:H:52:ARG:HH21	1.35	0.92
1:I:159:PHE:O	1:I:160:GLU:HB2	1.67	0.91
2:N:357:GLY:HA2	2:N:415:ARG:HH22	1.32	0.91
1:G:93:ILE:HD12	1:G:97:THR:HG22	1.52	0.91
2:H:286:PRO:HA	2:H:289:PHE:CE2	2.06	0.91
2:H:415:ARG:HH12	2:H:472:TYR:HE1	1.08	0.91
1:C:159:PHE:O	1:C:160:GLU:HB2	1.69	0.90
2:J:590:GLU:HB3	2:J:591:PRO:HD2	1.54	0.90
2:B:444:TYR:HA	2:B:471:GLY:HA3	1.54	0.90
2:B:210:LYS:O	2:B:214:THR:HG22	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:444:TYR:HA	2:D:471:GLY:HA3	1.53	0.89
2:F:590:GLU:HB3	2:F:591:PRO:HD2	1.54	0.89
2:L:590:GLU:HB3	2:L:591:PRO:HD2	1.54	0.89
2:D:590:GLU:HB3	2:D:591:PRO:HD2	1.55	0.89
2:J:419:ILE:HD13	2:J:446:ARG:HH12	1.38	0.88
2:N:444:TYR:HA	2:N:471:GLY:HA3	1.55	0.88
2:H:322:VAL:HG22	2:H:346:ARG:HB2	1.54	0.88
1:E:107:TYR:OH	2:L:294:GLN:NE2	2.07	0.88
2:P:590:GLU:HB3	2:P:591:PRO:HD2	1.53	0.88
2:N:590:GLU:HB3	2:N:591:PRO:HD2	1.54	0.87
2:B:590:GLU:HB3	2:B:591:PRO:HD2	1.54	0.87
2:F:444:TYR:HA	2:F:471:GLY:HA3	1.55	0.87
2:J:367:GLN:HB3	2:J:391:THR:HG22	1.58	0.86
2:L:444:TYR:HA	2:L:471:GLY:HA3	1.57	0.86
1:E:105:ALA:HB3	1:E:114:LEU:HD13	1.56	0.86
2:B:419:ILE:HD13	2:B:446:ARG:HH12	1.40	0.86
1:K:108:LEU:HD12	1:K:110:ILE:HD11	1.58	0.86
2:H:365:VAL:HG11	2:H:387:VAL:HG22	1.55	0.85
2:H:519:TRP:NE1	4:H:4100:OGK:H01	1.90	0.85
1:M:125:ILE:HG23	1:M:133:ILE:HD12	1.58	0.85
2:N:367:GLN:HB3	2:N:391:THR:HG22	1.57	0.85
2:J:444:TYR:HA	2:J:471:GLY:HA3	1.56	0.85
2:J:210:LYS:O	2:J:214:THR:HG22	1.77	0.85
2:L:349:ILE:HG13	2:L:385:VAL:HG22	1.57	0.85
1:E:43:PRO:HG2	2:L:319:ASN:ND2	1.92	0.85
2:P:286:PRO:HA	2:P:289:PHE:CE2	2.12	0.85
2:H:152:THR:CG2	2:H:177:SER:HB2	2.07	0.85
1:M:102:ILE:HD12	2:N:20:VAL:HG21	1.58	0.84
2:H:40:VAL:O	2:H:41:CYS:HB3	1.78	0.84
2:H:285:MET:HG2	2:H:286:PRO:HD3	1.57	0.84
2:H:415:ARG:NH1	2:H:472:TYR:CE1	2.46	0.84
2:H:440:ARG:HB3	2:H:467:TRP:HD1	1.43	0.84
1:G:153:ARG:HG3	1:G:157:TRP:CZ3	2.13	0.84
2:H:95:ASN:H	2:H:95:ASN:ND2	1.75	0.83
2:P:282:PRO:HA	2:P:285:MET:HE2	1.61	0.83
2:B:116:SER:HB2	2:B:142:THR:HG23	1.59	0.83
2:D:142:THR:HB	2:D:168:THR:HG23	1.58	0.83
2:H:199:PHE:CZ	2:H:227:VAL:HG23	2.13	0.83
1:I:125:ILE:HG23	1:I:133:ILE:HD12	1.58	0.83
2:N:328:VAL:HG22	2:N:359:GLU:HB2	1.61	0.82
2:D:210:LYS:O	2:D:214:THR:HG22	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:210:LYS:O	2:F:214:THR:HG22	1.79	0.82
2:L:210:LYS:O	2:L:214:THR:HG22	1.80	0.82
2:F:367:GLN:HB3	2:F:391:THR:HG22	1.61	0.82
2:L:367:GLN:HB3	2:L:391:THR:HG22	1.60	0.82
2:P:444:TYR:HA	2:P:471:GLY:HA3	1.61	0.82
2:D:116:SER:HB2	2:D:142:THR:HG23	1.62	0.82
1:I:108:LEU:HD12	1:I:110:ILE:HD11	1.62	0.81
1:M:108:LEU:HD12	1:M:110:ILE:HD11	1.62	0.81
2:H:387:VAL:HG11	2:H:390:ILE:HD13	1.60	0.81
1:A:108:LEU:HD12	1:A:110:ILE:HD11	1.61	0.81
2:D:367:GLN:HB3	2:D:391:THR:HG22	1.60	0.81
2:P:419:ILE:HD13	2:P:446:ARG:HH12	1.44	0.81
2:H:256:ASP:OD2	2:H:259:MET:HG2	1.80	0.81
2:J:286:PRO:HA	2:J:289:PHE:CE2	2.16	0.81
2:N:419:ILE:HD13	2:N:446:ARG:HH12	1.44	0.81
2:H:253:LEU:HD11	2:H:277:LEU:HD13	1.62	0.81
2:J:164:ARG:HE	2:N:112:ARG:CG	1.94	0.81
1:M:102:ILE:HG21	2:N:20:VAL:HG22	1.62	0.81
2:N:116:SER:HB2	2:N:142:THR:HG23	1.60	0.81
4:N:7100:OGK:H18A	4:N:7100:OGK:HN08	1.45	0.81
2:P:328:VAL:HG22	2:P:359:GLU:HB2	1.62	0.81
2:D:282:PRO:HA	2:D:285:MET:HE2	1.63	0.80
2:D:419:ILE:HD13	2:D:446:ARG:HH12	1.44	0.80
2:N:210:LYS:O	2:N:214:THR:HG22	1.81	0.80
2:P:210:LYS:O	2:P:214:THR:HG22	1.79	0.80
2:H:286:PRO:HA	2:H:289:PHE:CD2	2.15	0.80
2:L:286:PRO:HA	2:L:289:PHE:CE2	2.15	0.80
2:P:367:GLN:HB3	2:P:391:THR:HG22	1.63	0.80
2:H:361:GLU:HA	2:H:388:SER:OG	1.81	0.80
2:N:282:PRO:HA	2:N:285:MET:HE2	1.63	0.80
2:F:282:PRO:HA	2:F:285:MET:HE2	1.64	0.80
2:B:328:VAL:HG22	2:B:359:GLU:HB2	1.64	0.80
2:F:419:ILE:HD13	2:F:446:ARG:HH12	1.47	0.79
2:N:349:ILE:HG13	2:N:385:VAL:HG22	1.62	0.79
2:B:282:PRO:HA	2:B:285:MET:HE2	1.64	0.79
1:A:125:ILE:HG23	1:A:133:ILE:HD12	1.65	0.79
2:H:441:PHE:O	2:H:468:MET:HA	1.82	0.79
1:O:125:ILE:HG23	1:O:133:ILE:HD12	1.63	0.79
2:L:289:PHE:CD1	2:L:316:LYS:HD2	2.18	0.79
2:D:328:VAL:HG22	2:D:359:GLU:HB2	1.64	0.79
2:F:112:ARG:HG2	2:L:164:ARG:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:VAL:HG22	2:F:359:GLU:HB2	1.63	0.79
2:B:367:GLN:HB3	2:B:391:THR:HG22	1.63	0.79
2:H:364:LEU:HD13	2:H:388:SER:OG	1.81	0.79
4:B:1100:OGK:H18A	4:B:1100:OGK:HN08	1.48	0.78
2:F:116:SER:HB2	2:F:142:THR:HG23	1.65	0.78
2:B:286:PRO:HA	2:B:289:PHE:CE2	2.18	0.78
2:B:289:PHE:CD1	2:B:316:LYS:HD2	2.18	0.78
2:J:328:VAL:HG22	2:J:359:GLU:HB2	1.66	0.78
2:L:161:THR:HG22	2:L:186:GLU:HG2	1.65	0.78
2:P:116:SER:HB2	2:P:142:THR:HG23	1.65	0.78
2:J:349:ILE:HG13	2:J:385:VAL:HG22	1.64	0.78
2:H:283:ASN:O	2:H:286:PRO:HD2	1.83	0.78
2:L:282:PRO:HA	2:L:285:MET:HE2	1.66	0.78
2:L:419:ILE:HD13	2:L:446:ARG:HH12	1.49	0.78
1:M:96:ALA:HB1	2:N:14:VAL:HG12	1.65	0.78
2:D:349:ILE:HG13	2:D:385:VAL:HG22	1.63	0.77
2:H:411:VAL:HG13	2:H:444:TYR:HB3	1.66	0.77
2:D:289:PHE:CD1	2:D:316:LYS:HD2	2.19	0.77
2:H:519:TRP:HE1	4:H:4100:OGK:H01	1.46	0.77
2:L:116:SER:HB2	2:L:142:THR:HG23	1.64	0.77
2:F:286:PRO:HA	2:F:289:PHE:CE2	2.19	0.77
2:H:387:VAL:CG1	2:H:390:ILE:HD13	2.14	0.77
1:M:102:ILE:HG21	2:N:20:VAL:CG2	2.14	0.77
4:H:4100:OGK:H18A	4:H:4100:OGK:HN08	1.50	0.77
1:K:125:ILE:HG23	1:K:133:ILE:HD12	1.67	0.77
4:P:8100:OGK:H18A	4:P:8100:OGK:HN08	1.49	0.77
2:H:459:GLY:O	2:H:486:GLY:HA3	1.84	0.77
1:I:105:ALA:HB3	1:I:114:LEU:HD13	1.66	0.77
2:L:328:VAL:HG22	2:L:359:GLU:HB2	1.65	0.77
2:D:286:PRO:HA	2:D:289:PHE:CE2	2.20	0.77
2:N:492:LYS:HE3	2:N:517:TYR:CE2	2.20	0.77
2:N:286:PRO:HA	2:N:289:PHE:CE2	2.19	0.77
2:H:450:LEU:HD11	2:H:454:GLY:HA3	1.65	0.76
2:N:289:PHE:CD1	2:N:316:LYS:HD2	2.19	0.76
1:C:125:ILE:HG23	1:C:133:ILE:HD12	1.65	0.76
2:H:542:ILE:HD11	2:H:588:LEU:HB2	1.67	0.76
4:D:2100:OGK:H18A	4:D:2100:OGK:HN08	1.49	0.76
2:P:286:PRO:HA	2:P:289:PHE:CD2	2.20	0.76
2:J:164:ARG:HE	2:N:112:ARG:HG3	1.51	0.76
4:F:3100:OGK:H18A	4:F:3100:OGK:HN08	1.49	0.75
2:P:168:THR:HB	2:P:196:VAL:CG1	2.13	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:289:PHE:CD1	2:P:316:LYS:HD2	2.20	0.75
2:J:116:SER:HB2	2:J:142:THR:HG23	1.65	0.75
2:J:308:GLU:HG3	2:J:332:ARG:HH22	1.52	0.75
2:N:168:THR:HB	2:N:196:VAL:CG1	2.16	0.75
1:M:112:ASN:C	1:M:114:LEU:H	1.95	0.75
1:C:108:LEU:HD12	1:C:110:ILE:HD11	1.69	0.75
1:E:125:ILE:HG23	1:E:133:ILE:HD12	1.69	0.75
1:E:108:LEU:HD12	1:E:110:ILE:HD11	1.68	0.75
2:H:321:GLU:HA	2:H:344:LEU:HA	1.69	0.75
2:H:365:VAL:HG21	2:H:387:VAL:HG13	1.68	0.75
2:H:467:TRP:HH2	2:H:494:GLU:OE1	1.70	0.75
2:N:391:THR:HG23	2:N:394:SER:H	1.52	0.75
2:F:289:PHE:CD1	2:F:316:LYS:HD2	2.22	0.74
2:H:170:LEU:HD23	2:H:170:LEU:O	1.86	0.74
2:L:308:GLU:HG3	2:L:332:ARG:HH22	1.51	0.74
2:H:415:ARG:NH1	2:H:472:TYR:HE1	1.84	0.74
1:K:124:MET:O	1:K:128:LYS:HE2	1.87	0.74
2:B:270:ARG:HB3	1:O:107:TYR:CD1	2.22	0.74
2:H:298:LEU:HD22	2:H:300:LEU:HG	1.70	0.74
1:O:108:LEU:HD12	1:O:110:ILE:HD11	1.70	0.74
2:J:289:PHE:CD1	2:J:316:LYS:HD2	2.22	0.74
3:S:203:ILE:H	3:S:203:ILE:HD12	1.53	0.74
1:M:124:MET:O	1:M:128:LYS:HE2	1.88	0.74
1:E:43:PRO:CG	2:L:319:ASN:ND2	2.50	0.74
1:M:129:THR:O	1:M:133:ILE:HG12	1.86	0.74
2:F:472:TYR:OH	3:S:201:LEU:HB2	1.88	0.73
2:N:84:PRO:HB3	2:N:517:TYR:OH	1.87	0.73
2:B:161:THR:HG22	2:B:186:GLU:HG2	1.68	0.73
2:N:57:MET:HE3	2:N:62:THR:HG22	1.70	0.73
2:J:282:PRO:HA	2:J:285:MET:HE2	1.69	0.73
2:H:533:MET:CE	2:H:588:LEU:HD13	2.14	0.73
2:J:286:PRO:HA	2:J:289:PHE:CD2	2.24	0.73
4:L:6100:OGK:HN08	4:L:6100:OGK:H18A	1.52	0.73
2:B:391:THR:HG23	2:B:394:SER:H	1.53	0.73
2:F:308:GLU:HG3	2:F:332:ARG:HH22	1.53	0.73
2:J:164:ARG:HD2	2:N:112:ARG:HG2	1.70	0.73
2:L:168:THR:HB	2:L:196:VAL:CG1	2.16	0.73
1:E:124:MET:O	1:E:128:LYS:HE2	1.89	0.73
2:H:136:ARG:HA	2:H:136:ARG:NE	2.04	0.73
2:H:120:ARG:NH2	5:H:1102:PO4:O3	2.20	0.73
2:P:391:THR:HG23	2:P:394:SER:H	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:412:LEU:HD11	2:H:445:LEU:HD22	1.69	0.72
2:J:391:THR:HG23	2:J:394:SER:H	1.54	0.72
4:J:5100:OGK:H18A	4:J:5100:OGK:HN08	1.54	0.72
2:N:308:GLU:HG3	2:N:332:ARG:HH22	1.54	0.72
2:B:253:LEU:HD12	2:B:280:MET:HB2	1.72	0.72
2:D:440:ARG:HB3	2:D:467:TRP:HE3	1.54	0.72
1:K:129:THR:O	1:K:133:ILE:HG12	1.89	0.72
2:H:76:ARG:HG2	2:H:76:ARG:HH11	1.55	0.72
2:H:467:TRP:CH2	2:H:494:GLU:OE1	2.42	0.72
2:J:168:THR:HB	2:J:196:VAL:CG1	2.17	0.72
2:L:286:PRO:HA	2:L:289:PHE:CD2	2.24	0.72
2:B:349:ILE:HG13	2:B:385:VAL:HG22	1.71	0.72
1:I:124:MET:O	1:I:128:LYS:HE2	1.89	0.72
2:D:319:ASN:ND2	1:G:43:PRO:HG2	2.03	0.72
2:H:391:THR:OG1	2:H:393:GLU:HB2	1.90	0.72
3:W:203:ILE:H	3:W:203:ILE:HD12	1.55	0.72
2:P:308:GLU:HG3	2:P:332:ARG:HH22	1.53	0.72
2:D:308:GLU:HG3	2:D:332:ARG:HH22	1.55	0.71
1:G:108:LEU:HD12	1:G:110:ILE:HD11	1.72	0.71
2:H:78:LEU:HD12	2:H:79:LYS:N	2.01	0.71
2:P:161:THR:HG22	2:P:186:GLU:HG2	1.71	0.71
2:D:391:THR:HG23	2:D:394:SER:H	1.54	0.71
1:M:99:PHE:HD2	2:N:15:ALA:O	1.73	0.71
2:B:157:LEU:O	2:B:161:THR:HG23	1.91	0.71
2:H:334:LEU:CD2	2:H:373:LEU:HD22	2.21	0.71
2:B:308:GLU:HG3	2:B:332:ARG:HH22	1.56	0.71
2:F:286:PRO:HA	2:F:289:PHE:CD2	2.25	0.71
1:E:129:THR:O	1:E:133:ILE:HG12	1.89	0.71
3:V:203:ILE:HD12	3:V:203:ILE:H	1.55	0.71
2:P:349:ILE:HG13	2:P:385:VAL:HG22	1.72	0.71
2:D:57:MET:HE3	2:D:62:THR:HG22	1.73	0.71
2:H:540:TRP:CZ2	2:H:570:ALA:HB1	2.25	0.71
2:D:492:LYS:HE3	2:D:517:TYR:CE2	2.26	0.70
2:H:211:ASP:O	2:H:215:ILE:HG13	1.91	0.70
1:E:105:ALA:CB	1:E:114:LEU:HD13	2.21	0.70
2:N:55:VAL:HG23	2:N:75:LEU:HD21	1.72	0.70
2:J:161:THR:HG22	2:J:186:GLU:HG2	1.73	0.70
3:U:203:ILE:H	3:U:203:ILE:HD12	1.56	0.70
2:F:161:THR:HG22	2:F:186:GLU:HG2	1.72	0.70
2:H:76:ARG:HH11	2:H:76:ARG:CG	2.04	0.70
2:L:391:THR:HG23	2:L:394:SER:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:ARG:NH2	4:F:3100:OGK:O07	2.23	0.70
2:B:492:LYS:HE3	2:B:517:TYR:CE2	2.25	0.70
2:H:59:LEU:HD22	2:H:61:TYR:HB2	1.73	0.70
2:H:116:SER:CB	2:H:142:THR:HG23	2.16	0.70
2:H:311:CYS:CB	2:H:336:VAL:HG21	2.19	0.70
2:H:370:LEU:N	2:H:370:LEU:HD23	2.06	0.70
2:P:55:VAL:HG23	2:P:75:LEU:HD21	1.73	0.70
2:H:191:ASN:HD21	2:H:194:LEU:H	1.37	0.70
2:H:364:LEU:HD22	2:H:388:SER:H	1.54	0.70
2:H:118:HIS:CD2	2:H:144:LYS:HD3	2.26	0.70
1:C:124:MET:O	1:C:128:LYS:HE2	1.92	0.70
2:F:101:THR:HG22	2:F:128:ASP:OD1	1.91	0.70
2:H:450:LEU:CD1	2:H:454:GLY:HA3	2.22	0.69
2:J:419:ILE:HD13	2:J:446:ARG:NH1	2.07	0.69
2:D:286:PRO:HA	2:D:289:PHE:CD2	2.28	0.69
2:H:325:THR:O	2:H:349:ILE:HA	1.91	0.69
1:I:35:ASP:HB3	2:N:243:ALA:HB1	1.73	0.69
2:P:191:ASN:HD21	2:P:194:LEU:H	1.40	0.69
2:L:143:LEU:HD23	2:L:159:ILE:HD13	1.75	0.69
1:M:10:SER:HB2	1:M:52:LEU:HD23	1.74	0.69
2:B:101:THR:HG22	2:B:128:ASP:OD1	1.92	0.69
2:B:350:GLU:HB3	3:Q:209:LEU:HD21	1.74	0.69
2:F:295:ILE:HG21	2:F:298:LEU:HD13	1.74	0.69
2:D:161:THR:HG22	2:D:186:GLU:HG2	1.75	0.69
2:N:521:GLN:HG3	2:N:567:HIS:HD2	1.55	0.69
2:B:419:ILE:HD13	2:B:446:ARG:NH1	2.08	0.69
2:F:168:THR:HB	2:F:196:VAL:CG1	2.18	0.69
2:F:297:LYS:HG3	2:F:322:VAL:HB	1.75	0.69
2:F:349:ILE:HG13	2:F:385:VAL:HG22	1.73	0.69
2:H:176:PHE:CZ	2:H:204:PHE:CZ	2.80	0.69
2:H:367:GLN:O	2:H:371:ILE:HG13	1.93	0.69
2:B:286:PRO:HA	2:B:289:PHE:CD2	2.27	0.69
2:F:157:LEU:O	2:F:161:THR:HG23	1.92	0.69
2:H:286:PRO:C	2:H:288:LEU:H	2.00	0.69
3:R:203:ILE:H	3:R:203:ILE:HD12	1.56	0.69
2:H:116:SER:HB2	2:H:142:THR:CG2	2.18	0.69
2:H:133:ALA:HB2	2:H:159:ILE:HG22	1.75	0.69
1:M:93:ILE:HD12	1:M:97:THR:CG2	2.21	0.69
2:P:492:LYS:HE3	2:P:517:TYR:CE2	2.28	0.69
3:X:203:ILE:H	3:X:203:ILE:HD12	1.58	0.69
2:F:391:THR:HG23	2:F:394:SER:H	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:161:THR:HG22	2:N:186:GLU:HG2	1.76	0.68
2:H:414:ASP:HB3	2:H:446:ARG:NH2	2.08	0.68
2:N:286:PRO:HA	2:N:289:PHE:CD2	2.28	0.68
3:Q:203:ILE:HD12	3:Q:203:ILE:H	1.57	0.68
2:H:278:SER:O	2:H:280:MET:N	2.24	0.68
2:J:164:ARG:NE	2:N:112:ARG:CG	2.55	0.68
1:K:10:SER:HB2	1:K:52:LEU:HD23	1.76	0.68
1:A:124:MET:O	1:A:128:LYS:HE2	1.94	0.68
2:H:519:TRP:HH2	2:H:567:HIS:CE1	2.10	0.68
2:L:253:LEU:HD12	2:L:280:MET:HB2	1.74	0.68
2:N:519:TRP:HE1	4:N:7100:OGK:H01	1.57	0.68
2:P:101:THR:HG22	2:P:128:ASP:OD1	1.93	0.68
2:B:168:THR:HB	2:B:196:VAL:CG1	2.18	0.68
2:J:164:ARG:CD	2:N:112:ARG:HG2	2.24	0.68
4:N:7100:OGK:HN08	4:N:7100:OGK:C18	2.07	0.68
2:J:297:LYS:HG3	2:J:322:VAL:HB	1.75	0.68
1:M:100:GLU:HG2	2:N:15:ALA:HB2	1.76	0.68
2:L:468:MET:HE3	2:L:470:LEU:HD21	1.75	0.68
1:O:129:THR:O	1:O:133:ILE:HG12	1.94	0.68
2:P:547:SER:HB3	2:P:564:HIS:CB	2.24	0.67
2:B:143:LEU:HD23	2:B:159:ILE:HD13	1.75	0.67
2:H:357:GLY:C	2:H:359:GLU:H	2.02	0.67
2:B:547:SER:HB3	2:B:564:HIS:CB	2.25	0.67
2:H:444:TYR:HA	2:H:471:GLY:HA3	1.76	0.67
1:I:129:THR:O	1:I:133:ILE:HG12	1.94	0.67
2:J:101:THR:HG22	2:J:128:ASP:OD1	1.94	0.67
2:J:295:ILE:HG21	2:J:298:LEU:HD13	1.76	0.67
2:L:492:LYS:HE3	2:L:517:TYR:CE2	2.29	0.67
2:B:84:PRO:HB3	2:B:517:TYR:OH	1.94	0.67
2:H:81:LYS:HG2	2:H:120:ARG:HD3	1.77	0.67
2:J:547:SER:HB3	2:J:564:HIS:CB	2.24	0.67
1:C:40:ASN:HB3	1:K:13:GLY:O	1.94	0.67
2:J:337:LEU:HD12	2:J:341:CYS:SG	2.34	0.67
2:P:295:ILE:HG21	2:P:298:LEU:HD13	1.75	0.67
2:L:487:CYS:HB3	2:L:490:LEU:HB2	1.76	0.67
2:P:157:LEU:O	2:P:161:THR:HG23	1.93	0.67
2:P:468:MET:HE3	2:P:470:LEU:HD21	1.76	0.67
2:J:350:GLU:HB3	3:U:209:LEU:HD21	1.77	0.67
2:D:297:LYS:HG3	2:D:322:VAL:HB	1.77	0.67
1:I:91:MET:HA	1:I:91:MET:HE2	1.77	0.67
2:N:388:SER:O	2:N:416:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:ARG:NH1	2:H:72:PHE:CZ	2.63	0.67
2:L:547:SER:HB3	2:L:564:HIS:CB	2.25	0.67
2:D:547:SER:HB3	2:D:564:HIS:CB	2.25	0.66
2:H:85:ARG:NH2	4:H:4100:OGK:O07	2.29	0.66
1:O:105:ALA:HB3	1:O:114:LEU:HD13	1.77	0.66
2:F:57:MET:HE3	2:F:62:THR:HG22	1.76	0.66
2:D:295:ILE:HG21	2:D:298:LEU:HD13	1.78	0.66
2:N:157:LEU:O	2:N:161:THR:HG23	1.96	0.66
2:N:297:LYS:HG3	2:N:322:VAL:HB	1.78	0.66
2:H:59:LEU:CD2	2:H:61:TYR:HB2	2.25	0.66
2:J:440:ARG:HB3	2:J:467:TRP:HE3	1.59	0.66
1:M:52:LEU:O	1:M:56:ILE:HG13	1.96	0.66
2:H:57:MET:HE3	2:H:62:THR:HG22	1.77	0.66
2:H:398:ILE:HG23	2:H:402:LEU:HD11	1.76	0.66
2:P:253:LEU:HD12	2:P:280:MET:HB2	1.77	0.66
2:N:295:ILE:HG21	2:N:298:LEU:HD13	1.78	0.66
1:A:93:ILE:HD12	1:A:97:THR:CG2	2.22	0.66
2:F:455:LEU:HD22	2:F:483:PHE:HB2	1.78	0.66
2:J:492:LYS:HE3	2:J:517:TYR:CE2	2.30	0.66
2:N:101:THR:HG22	2:N:128:ASP:OD1	1.96	0.66
2:P:419:ILE:HD13	2:P:446:ARG:NH1	2.11	0.66
1:G:10:SER:HB2	1:G:52:LEU:HD23	1.77	0.66
2:H:461:TYR:C	2:H:463:PRO:HD3	2.20	0.66
2:J:157:LEU:O	2:J:161:THR:HG23	1.95	0.66
2:L:472:TYR:OH	3:V:201:LEU:HB2	1.96	0.66
2:H:546:PRO:HD2	2:H:584:THR:O	1.96	0.65
2:D:472:TYR:OH	3:R:201:LEU:HB2	1.96	0.65
2:J:487:CYS:HB3	2:J:490:LEU:HB2	1.79	0.65
2:B:487:CYS:HB3	2:B:490:LEU:HB2	1.77	0.65
2:H:492:LYS:NZ	2:H:516:ARG:HH11	1.93	0.65
1:I:105:ALA:HB3	1:I:114:LEU:CD1	2.26	0.65
2:L:57:MET:HE3	2:L:62:THR:HG22	1.77	0.65
2:P:57:MET:HE3	2:P:62:THR:HG22	1.77	0.65
2:B:85:ARG:NH2	4:B:1100:OGK:O07	2.28	0.65
2:B:590:GLU:HB3	2:B:591:PRO:CD	2.27	0.65
2:H:40:VAL:O	2:H:41:CYS:CB	2.43	0.65
2:J:138:ASP:OD2	2:J:164:ARG:HG3	1.96	0.65
2:N:547:SER:HB3	2:N:564:HIS:CB	2.26	0.65
2:H:304:LEU:HD13	2:H:304:LEU:O	1.96	0.65
2:H:375:GLN:HG2	2:H:401:TYR:CD1	2.31	0.65
2:N:129:LEU:HD21	2:N:155:GLY:HA3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:487:CYS:HB3	2:P:490:LEU:HB2	1.77	0.65
1:E:37:CYS:SG	2:L:296:ARG:NH2	2.69	0.65
2:H:95:ASN:HD22	2:H:95:ASN:N	1.78	0.65
2:H:109:ASN:C	2:H:110:ASN:HD22	2.05	0.65
2:J:164:ARG:NE	2:N:112:ARG:HG2	2.11	0.65
2:N:143:LEU:HD23	2:N:159:ILE:HD13	1.78	0.65
1:C:10:SER:HB2	1:C:52:LEU:HD23	1.79	0.65
2:F:84:PRO:HB3	2:F:517:TYR:OH	1.96	0.65
2:J:191:ASN:HD21	2:J:194:LEU:H	1.45	0.65
2:F:350:GLU:HB3	3:S:209:LEU:HD21	1.77	0.65
1:G:91:MET:HE2	1:G:91:MET:HA	1.78	0.65
2:N:487:CYS:HB3	2:N:490:LEU:HB2	1.77	0.65
2:B:440:ARG:HB3	2:B:467:TRP:HE3	1.61	0.64
2:H:545:ILE:HB	2:H:567:HIS:HB2	1.79	0.64
2:H:492:LYS:NZ	2:H:516:ARG:NH1	2.45	0.64
2:L:297:LYS:HG3	2:L:322:VAL:HB	1.80	0.64
2:N:399:GLY:O	2:N:434:GLY:HA3	1.97	0.64
2:B:295:ILE:HG21	2:B:298:LEU:HD13	1.79	0.64
1:C:113:LEU:O	1:C:117:THR:HG23	1.96	0.64
2:H:52:ARG:NH1	2:H:72:PHE:CE2	2.66	0.64
2:H:442:ALA:HB1	2:H:469:LEU:HB3	1.78	0.64
1:O:91:MET:HE2	1:O:91:MET:HA	1.80	0.64
2:P:440:ARG:HB3	2:P:467:TRP:HE3	1.62	0.64
2:D:101:THR:HG22	2:D:128:ASP:OD1	1.98	0.64
2:F:101:THR:OG1	2:F:102:PRO:HD3	1.96	0.64
1:I:26:SER:OG	1:I:108:LEU:HB3	1.98	0.64
2:B:468:MET:HE3	2:B:470:LEU:HD21	1.79	0.64
2:D:191:ASN:HD21	2:D:194:LEU:H	1.44	0.64
2:H:371:ILE:O	2:H:375:GLN:HG3	1.97	0.64
2:F:143:LEU:HD23	2:F:159:ILE:HD13	1.78	0.64
2:L:440:ARG:HB3	2:L:467:TRP:HE3	1.61	0.64
2:J:253:LEU:HD12	2:J:280:MET:HB2	1.80	0.64
1:O:10:SER:HB2	1:O:52:LEU:HD23	1.79	0.64
2:D:487:CYS:HB3	2:D:490:LEU:HB2	1.80	0.64
1:M:102:ILE:CD1	2:N:20:VAL:HG21	2.26	0.64
2:F:40:VAL:O	2:F:41:CYS:HB3	1.96	0.64
2:F:253:LEU:HD12	2:F:280:MET:HB2	1.79	0.64
2:H:104:VAL:HG21	2:H:128:ASP:HB2	1.80	0.64
2:H:384:ALA:HB2	2:H:409:ARG:HG3	1.79	0.64
2:H:409:ARG:HB2	4:H:4100:OGK:H16B	1.79	0.64
2:P:85:ARG:NH2	4:P:8100:OGK:O07	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:364:LEU:O	2:H:365:VAL:HG13	1.97	0.64
2:L:157:LEU:O	2:L:161:THR:HG23	1.98	0.64
1:M:91:MET:HE2	1:M:91:MET:HA	1.79	0.64
1:A:10:SER:HB2	1:A:52:LEU:HD23	1.78	0.63
1:I:10:SER:HB2	1:I:52:LEU:HD23	1.78	0.63
1:A:12:ASP:OD2	1:A:49:SER:HB2	1.98	0.63
2:B:521:GLN:HG3	2:B:567:HIS:HD2	1.63	0.63
2:D:388:SER:O	2:D:416:GLU:HG3	1.99	0.63
2:H:225:VAL:HG22	2:H:245:LEU:HD11	1.80	0.63
2:N:298:LEU:HD23	2:N:300:LEU:HD11	1.81	0.63
2:N:521:GLN:HG3	2:N:567:HIS:CD2	2.33	0.63
1:C:129:THR:O	1:C:133:ILE:HG12	1.99	0.63
2:L:191:ASN:HD21	2:L:194:LEU:H	1.46	0.63
1:O:124:MET:O	1:O:128:LYS:HE2	1.97	0.63
1:A:129:THR:O	1:A:133:ILE:HG12	1.98	0.63
1:M:96:ALA:HB1	2:N:14:VAL:CG1	2.28	0.63
1:C:91:MET:HE2	1:C:91:MET:HA	1.80	0.63
2:J:55:VAL:HG23	2:J:75:LEU:HD21	1.79	0.63
1:M:102:ILE:CG2	2:N:20:VAL:CG2	2.76	0.63
2:D:168:THR:HB	2:D:196:VAL:CG1	2.21	0.63
2:F:468:MET:HE3	2:F:470:LEU:HD21	1.79	0.63
2:F:521:GLN:HG3	2:F:567:HIS:HD2	1.64	0.63
1:K:102:ILE:HG12	1:K:117:THR:HB	1.80	0.63
1:M:12:ASP:OD2	1:M:49:SER:HB2	1.99	0.63
2:N:519:TRP:NE1	4:N:7100:OGK:H01	2.12	0.63
2:P:311:CYS:HB3	2:P:336:VAL:HG21	1.80	0.63
2:D:294:GLN:NE2	1:G:107:TYR:OH	2.32	0.63
1:I:102:ILE:HG23	1:I:118:CYS:SG	2.39	0.63
2:N:311:CYS:HB3	2:N:336:VAL:HG21	1.79	0.63
2:N:419:ILE:HD13	2:N:446:ARG:NH1	2.13	0.63
2:B:191:ASN:HD21	2:B:194:LEU:H	1.47	0.62
2:F:547:SER:HB3	2:F:564:HIS:CB	2.28	0.62
2:H:230:PHE:HB3	2:H:235:LEU:HD21	1.81	0.62
2:H:501:SER:HB3	2:H:524:ARG:NH1	2.14	0.62
2:J:590:GLU:HB3	2:J:591:PRO:CD	2.27	0.62
2:D:590:GLU:HB3	2:D:591:PRO:CD	2.28	0.62
1:E:10:SER:HB2	1:E:52:LEU:HD23	1.79	0.62
1:E:45:PRO:HB2	2:L:291:PHE:HA	1.81	0.62
2:F:492:LYS:HE3	2:F:517:TYR:CE2	2.34	0.62
2:H:366:SER:OG	2:H:368:ARG:HG2	1.99	0.62
2:N:85:ARG:NH2	4:N:7100:OGK:O07	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:HIS:CG	2:H:112:ARG:HH11	2.17	0.62
2:J:164:ARG:HE	2:N:112:ARG:HG2	1.64	0.62
2:N:310:HIS:O	2:N:314:ILE:HG12	2.00	0.62
2:F:590:GLU:HB3	2:F:591:PRO:CD	2.28	0.62
2:L:55:VAL:HG23	2:L:75:LEU:HD21	1.81	0.62
2:L:84:PRO:HB3	2:L:517:TYR:OH	1.99	0.62
2:L:138:ASP:OD2	2:L:164:ARG:HG3	1.98	0.62
2:L:295:ILE:HG21	2:L:298:LEU:HD13	1.79	0.62
2:L:455:LEU:HD22	2:L:483:PHE:HB2	1.81	0.62
2:N:63:ALA:HB1	2:N:67:ARG:HD2	1.82	0.62
2:N:253:LEU:HD12	2:N:280:MET:HB2	1.81	0.62
2:D:350:GLU:HB3	3:R:209:LEU:HD21	1.81	0.62
2:H:280:MET:HE1	2:H:288:LEU:HD11	1.81	0.62
2:H:544:LEU:O	2:H:546:PRO:HD3	2.00	0.62
2:J:521:GLN:HG3	2:J:567:HIS:HD2	1.65	0.62
2:F:440:ARG:HB3	2:F:467:TRP:HE3	1.65	0.62
2:B:388:SER:O	2:B:416:GLU:HG3	2.00	0.62
2:F:487:CYS:HB3	2:F:490:LEU:HB2	1.80	0.62
1:A:91:MET:HA	1:A:91:MET:HE2	1.82	0.62
2:D:419:ILE:HD13	2:D:446:ARG:NH1	2.13	0.62
2:H:101:THR:HG23	2:H:131:ARG:HH12	1.65	0.61
2:P:129:LEU:HD21	2:P:155:GLY:HA3	1.82	0.61
1:E:91:MET:HE2	1:E:91:MET:HA	1.82	0.61
2:H:442:ALA:CB	2:H:469:LEU:HB3	2.30	0.61
2:P:184:LEU:HD12	2:P:207:ILE:HB	1.81	0.61
2:F:365:VAL:HG23	2:F:387:VAL:HA	1.83	0.61
2:F:399:GLY:O	2:F:434:GLY:HA3	2.00	0.61
2:H:253:LEU:HD13	2:H:284:GLU:HG3	1.82	0.61
2:H:440:ARG:HB3	2:H:467:TRP:CD1	2.31	0.61
2:J:164:ARG:NE	2:N:112:ARG:HG3	2.15	0.61
2:N:455:LEU:HD22	2:N:483:PHE:HB2	1.82	0.61
1:A:99:PHE:HZ	1:A:137:PHE:HE1	1.46	0.61
2:D:253:LEU:HD12	2:D:280:MET:HB2	1.81	0.61
2:H:85:ARG:O	2:H:88:MET:HG2	2.01	0.61
1:K:52:LEU:O	1:K:56:ILE:HG13	2.01	0.61
2:N:101:THR:OG1	2:N:102:PRO:HD3	2.00	0.61
2:H:89:PHE:CE1	4:H:4100:OGK:H17	2.35	0.61
2:L:184:LEU:HD12	2:L:207:ILE:HB	1.82	0.61
2:L:419:ILE:HD13	2:L:446:ARG:NH1	2.15	0.61
1:M:137:PHE:CD1	2:N:17:VAL:HG21	2.36	0.61
1:E:48:THR:HG22	1:E:51:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:137:PHE:CD1	2:P:17:VAL:HG21	2.35	0.61
2:P:310:HIS:O	2:P:314:ILE:HG12	2.00	0.61
4:P:8100:OGK:HN08	4:P:8100:OGK:C18	2.13	0.61
2:D:227:VAL:CG1	2:D:228:GLY:N	2.64	0.61
2:F:419:ILE:HD13	2:F:446:ARG:NH1	2.16	0.61
2:H:412:LEU:HD12	2:H:445:LEU:HA	1.83	0.61
1:K:91:MET:HE2	1:K:91:MET:HA	1.82	0.61
1:M:26:SER:OG	1:M:108:LEU:HB3	2.00	0.61
2:N:285:MET:HE1	2:N:309:ASP:HB3	1.82	0.61
2:H:40:VAL:O	2:H:40:VAL:HG23	1.99	0.61
2:L:85:ARG:NH2	4:L:6100:OGK:O07	2.30	0.61
1:E:12:ASP:OD2	1:E:49:SER:HB2	2.00	0.61
2:J:129:LEU:HD21	2:J:155:GLY:HA3	1.82	0.61
2:P:455:LEU:HD22	2:P:483:PHE:HB2	1.81	0.61
2:P:590:GLU:HB3	2:P:591:PRO:CD	2.26	0.61
1:A:137:PHE:CD1	2:B:17:VAL:HG21	2.36	0.60
2:L:388:SER:O	2:L:416:GLU:HG3	2.01	0.60
2:L:590:GLU:HB3	2:L:591:PRO:CD	2.27	0.60
2:N:311:CYS:O	2:N:315:GLN:HB2	2.00	0.60
2:H:343:GLN:CD	2:H:343:GLN:H	2.09	0.60
2:H:428:VAL:HG11	2:H:443:PHE:CZ	2.36	0.60
2:J:101:THR:OG1	2:J:102:PRO:HD3	2.00	0.60
2:L:542:ILE:CD1	2:L:588:LEU:HD12	2.21	0.60
2:N:272:LEU:HD21	2:N:275:LEU:HB3	1.82	0.60
1:E:6:ILE:HD12	1:E:23:ALA:HB3	1.82	0.60
1:E:52:LEU:O	1:E:56:ILE:HG13	2.01	0.60
2:H:124:VAL:O	2:H:151:PHE:HB3	2.02	0.60
2:H:392:ASN:HD22	2:H:422:LEU:HD13	1.66	0.60
2:L:227:VAL:CG1	2:L:228:GLY:N	2.64	0.60
2:H:233:LEU:HA	2:H:236:VAL:HG23	1.82	0.60
2:J:547:SER:HB3	2:J:564:HIS:HB3	1.83	0.60
2:N:367:GLN:O	2:N:371:ILE:HG22	2.01	0.60
2:P:388:SER:O	2:P:416:GLU:HG3	2.00	0.60
2:P:565:PRO:HG2	3:X:201:LEU:HD21	1.83	0.60
2:F:130:ASP:OD1	2:F:134:LYS:HE3	2.00	0.60
1:G:52:LEU:O	1:G:56:ILE:HG13	2.02	0.60
1:I:52:LEU:O	1:I:56:ILE:HG13	2.01	0.60
2:J:519:TRP:HE1	4:J:5100:OGK:H01	1.66	0.60
2:L:521:GLN:HG3	2:L:567:HIS:HD2	1.64	0.60
2:B:311:CYS:O	2:B:315:GLN:HB2	2.01	0.60
2:B:365:VAL:HG23	2:B:387:VAL:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:LEU:O	2:D:567:HIS:HE1	1.83	0.60
2:F:285:MET:HE1	2:F:309:ASP:HB3	1.84	0.60
1:G:137:PHE:HB3	2:H:17:VAL:HG21	1.82	0.60
2:H:396:GLU:O	2:H:400:THR:HG23	2.01	0.60
2:H:425:ASP:OD2	2:H:451:THR:HG23	2.02	0.60
2:L:101:THR:HG22	2:L:128:ASP:OD1	2.01	0.60
1:A:58:TYR:CD2	1:A:113:LEU:HD13	2.37	0.60
2:D:84:PRO:HB3	2:D:517:TYR:OH	2.02	0.60
2:F:310:HIS:O	2:F:314:ILE:HG12	2.02	0.60
4:F:3100:OGK:HN08	4:F:3100:OGK:C18	2.15	0.60
2:L:227:VAL:HG13	2:L:228:GLY:N	2.16	0.60
2:B:443:PHE:CE2	2:B:445:LEU:HD11	2.37	0.60
2:D:101:THR:HG22	2:D:128:ASP:HB3	1.83	0.60
2:H:87:ALA:HB2	2:H:92:ILE:HG13	1.83	0.60
1:M:100:GLU:HG2	2:N:15:ALA:CB	2.31	0.60
2:B:298:LEU:HD23	2:B:300:LEU:HD11	1.84	0.60
2:D:367:GLN:HB3	2:D:391:THR:CG2	2.31	0.60
2:H:47:ILE:O	2:H:51:THR:HG23	2.02	0.60
2:H:445:LEU:HD12	2:H:473:VAL:HG12	1.83	0.60
2:H:469:LEU:HD12	2:H:494:GLU:O	2.01	0.60
2:J:519:TRP:NE1	4:J:5100:OGK:H01	2.17	0.60
2:P:547:SER:HB3	2:P:564:HIS:HB3	1.84	0.60
2:B:101:THR:OG1	2:B:102:PRO:HD3	2.02	0.60
1:G:30:ALA:O	1:G:33:VAL:HG22	2.01	0.60
2:H:76:ARG:CG	2:H:76:ARG:NH1	2.65	0.60
2:J:57:MET:HE3	2:J:62:THR:HG22	1.84	0.60
2:B:297:LYS:HG3	2:B:322:VAL:HB	1.83	0.59
2:D:157:LEU:O	2:D:161:THR:HG23	2.02	0.59
1:E:30:ALA:O	1:E:33:VAL:HG22	2.02	0.59
1:G:153:ARG:HG2	1:G:153:ARG:NH1	2.17	0.59
2:J:367:GLN:HB3	2:J:391:THR:CG2	2.31	0.59
2:J:468:MET:HE3	2:J:470:LEU:HD21	1.84	0.59
2:L:365:VAL:HG23	2:L:387:VAL:HA	1.84	0.59
1:M:48:THR:HG22	1:M:51:ILE:HB	1.84	0.59
1:M:99:PHE:HB2	2:N:15:ALA:CB	2.32	0.59
1:M:158:ALA:HA	2:N:62:THR:HG21	1.84	0.59
2:B:121:ARG:NH2	5:B:1103:PO4:O4	2.34	0.59
1:G:129:THR:HG23	1:G:132:GLU:CD	2.27	0.59
2:H:22:GLU:HG2	2:H:47:ILE:CD1	2.32	0.59
2:H:382:TYR:C	2:H:382:TYR:CD1	2.79	0.59
2:N:65:PRO:HB3	2:N:103:TRP:CE3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:91:LEU:O	2:N:567:HIS:HE1	1.85	0.59
2:N:275:LEU:HD11	2:N:288:LEU:HD21	1.83	0.59
2:H:230:PHE:CD1	2:H:235:LEU:HD21	2.37	0.59
2:J:388:SER:O	2:J:416:GLU:HG3	2.03	0.59
2:D:40:VAL:O	2:D:41:CYS:HB3	2.02	0.59
2:D:184:LEU:HD12	2:D:207:ILE:HB	1.84	0.59
2:P:298:LEU:HD23	2:P:300:LEU:HD11	1.84	0.59
2:D:101:THR:OG1	2:D:102:PRO:HD3	2.02	0.59
2:H:392:ASN:O	2:H:396:GLU:CG	2.45	0.59
1:O:93:ILE:HD12	1:O:97:THR:CG2	2.29	0.59
2:H:125:SER:HB2	2:H:128:ASP:H	1.67	0.59
2:H:444:TYR:OH	2:H:496:ARG:HD3	2.01	0.59
2:L:129:LEU:HD21	2:L:155:GLY:HA3	1.85	0.59
2:N:367:GLN:HB3	2:N:391:THR:CG2	2.30	0.59
2:P:357:GLY:HA2	2:P:415:ARG:NH2	2.11	0.59
2:B:227:VAL:CG1	2:B:228:GLY:N	2.65	0.59
2:D:311:CYS:O	2:D:315:GLN:HB2	2.03	0.59
1:G:130:PRO:HD3	2:H:36:SER:HB2	1.84	0.59
2:H:22:GLU:HG2	2:H:47:ILE:HD11	1.83	0.59
2:H:363:GLY:O	2:H:364:LEU:C	2.46	0.59
1:K:12:ASP:OD2	1:K:49:SER:HB2	2.01	0.59
1:A:52:LEU:O	1:A:56:ILE:HG13	2.01	0.59
1:E:158:ALA:HA	2:F:62:THR:HG21	1.84	0.59
2:J:285:MET:HE1	2:J:309:ASP:HB3	1.85	0.59
2:J:351:ARG:HG3	2:J:351:ARG:O	2.03	0.59
2:N:468:MET:HE3	2:N:470:LEU:HD21	1.83	0.59
2:H:280:MET:HE1	2:H:288:LEU:CD1	2.33	0.59
2:B:261:GLU:HG2	2:B:264:MET:HG3	1.85	0.59
2:D:261:GLU:HG2	2:D:264:MET:HG3	1.85	0.59
1:E:43:PRO:HG3	2:L:319:ASN:HD21	1.67	0.59
2:H:412:LEU:HD11	2:H:445:LEU:CD2	2.33	0.59
2:L:197:LEU:O	2:L:225:VAL:HA	2.02	0.59
1:M:99:PHE:CD2	2:N:16:THR:C	2.81	0.59
2:N:65:PRO:HA	2:N:103:TRP:CZ3	2.38	0.59
1:O:91:MET:HE1	1:O:117:THR:HG22	1.84	0.58
2:P:91:LEU:O	2:P:567:HIS:HE1	1.86	0.58
2:B:519:TRP:NE1	4:B:1100:OGK:H01	2.18	0.58
1:C:12:ASP:OD2	1:C:49:SER:HB2	2.03	0.58
1:I:93:ILE:HD12	1:I:97:THR:CG2	2.26	0.58
2:J:357:GLY:HA2	2:J:415:ARG:NH2	2.12	0.58
2:N:404:ASN:HA	2:N:437:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:O	1:C:56:ILE:HG13	2.02	0.58
2:D:319:ASN:ND2	1:G:43:PRO:CG	2.65	0.58
2:F:227:VAL:CG1	2:F:228:GLY:N	2.66	0.58
1:G:153:ARG:HG2	1:G:153:ARG:HH11	1.67	0.58
1:K:158:ALA:HA	2:L:62:THR:HG21	1.84	0.58
2:L:547:SER:HB3	2:L:564:HIS:HB3	1.86	0.58
1:M:105:ALA:HB2	1:M:113:LEU:HD23	1.83	0.58
2:P:311:CYS:O	2:P:315:GLN:HB2	2.04	0.58
1:E:137:PHE:CD1	2:F:17:VAL:HG21	2.39	0.58
2:F:80:LEU:HB2	2:F:122:MET:CE	2.33	0.58
2:J:233:LEU:O	2:J:236:VAL:HG23	2.04	0.58
2:P:197:LEU:O	2:P:225:VAL:HA	2.03	0.58
2:P:337:LEU:HD12	2:P:341:CYS:SG	2.44	0.58
2:B:63:ALA:HB1	2:B:67:ARG:HD2	1.85	0.58
2:B:533:MET:HE3	2:B:588:LEU:HD13	1.86	0.58
2:F:357:GLY:HA2	2:F:415:ARG:NH2	2.12	0.58
2:L:357:GLY:HA2	2:L:415:ARG:NH2	2.11	0.58
2:P:84:PRO:HB3	2:P:517:TYR:OH	2.04	0.58
2:B:227:VAL:HG13	2:B:228:GLY:N	2.19	0.58
2:F:388:SER:O	2:F:416:GLU:HG3	2.03	0.58
1:G:98:LEU:HD21	1:G:120:THR:HG22	1.85	0.58
2:H:311:CYS:HB3	2:H:336:VAL:CG2	2.22	0.58
2:J:91:LEU:O	2:J:567:HIS:HE1	1.87	0.58
4:J:5100:OGK:HN08	4:J:5100:OGK:C18	2.16	0.58
2:P:519:TRP:NE1	4:P:8100:OGK:H01	2.18	0.58
2:F:129:LEU:HD21	2:F:155:GLY:HA3	1.86	0.58
2:H:390:ILE:HD11	2:H:410:LEU:HD11	1.83	0.58
2:N:80:LEU:HB2	2:N:122:MET:CE	2.34	0.58
1:O:12:ASP:OD2	1:O:49:SER:HB2	2.04	0.58
2:J:40:VAL:O	2:J:41:CYS:HB3	2.03	0.58
2:P:272:LEU:HD21	2:P:275:LEU:HB3	1.84	0.58
2:P:519:TRP:HE1	4:P:8100:OGK:H01	1.67	0.58
2:D:440:ARG:HB3	2:D:467:TRP:CE3	2.37	0.58
1:E:158:ALA:HA	2:F:62:THR:CG2	2.34	0.58
1:G:12:ASP:OD2	1:G:49:SER:HB2	2.04	0.58
2:H:25:MET:HG2	2:H:47:ILE:HG22	1.86	0.58
2:H:305:LEU:HD23	2:H:305:LEU:H	1.69	0.58
2:H:519:TRP:CH2	2:H:567:HIS:CE1	2.92	0.58
2:P:399:GLY:O	2:P:434:GLY:HA3	2.03	0.58
2:B:444:TYR:HA	2:B:471:GLY:CA	2.30	0.58
2:D:129:LEU:HD21	2:D:155:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:VAL:HG13	2:D:228:GLY:N	2.19	0.58
2:D:547:SER:HB3	2:D:564:HIS:HB3	1.85	0.58
1:K:137:PHE:CD1	2:L:17:VAL:HG21	2.39	0.58
2:L:130:ASP:OD1	2:L:134:LYS:HE3	2.03	0.58
2:L:285:MET:HE1	2:L:309:ASP:HB3	1.85	0.58
2:L:367:GLN:HB3	2:L:391:THR:CG2	2.32	0.58
2:B:129:LEU:HD21	2:B:155:GLY:HA3	1.85	0.57
2:B:477:ASP:OD2	2:B:504:ALA:HB2	2.04	0.57
2:F:446:ARG:HG2	2:F:447:GLN:H	1.69	0.57
2:H:38:SER:O	2:H:45:PHE:HB2	2.04	0.57
1:I:134:ARG:HB2	1:I:139:ILE:O	2.04	0.57
2:F:396:GLU:O	2:F:400:THR:HB	2.04	0.57
2:H:111:LEU:C	2:H:113:GLN:H	2.10	0.57
2:N:184:LEU:HD12	2:N:207:ILE:HB	1.86	0.57
2:P:101:THR:HG22	2:P:128:ASP:HB3	1.84	0.57
2:B:396:GLU:O	2:B:400:THR:HB	2.04	0.57
1:G:159:PHE:CE2	2:H:68:LEU:HD13	2.39	0.57
2:H:468:MET:HE2	2:H:470:LEU:HD21	1.86	0.57
2:H:519:TRP:HE1	4:H:4100:OGK:C01	2.16	0.57
1:M:158:ALA:HA	2:N:62:THR:CG2	2.34	0.57
1:O:91:MET:SD	1:O:117:THR:HG22	2.44	0.57
2:H:444:TYR:CD1	2:H:471:GLY:HA2	2.39	0.57
2:J:197:LEU:O	2:J:225:VAL:HA	2.04	0.57
1:M:112:ASN:C	1:M:114:LEU:N	2.62	0.57
1:O:134:ARG:HB2	1:O:139:ILE:O	2.04	0.57
2:B:91:LEU:O	2:B:567:HIS:HE1	1.87	0.57
2:J:184:LEU:HD12	2:J:207:ILE:HB	1.86	0.57
2:B:101:THR:HG22	2:B:128:ASP:HB3	1.85	0.57
2:B:270:ARG:CB	1:O:107:TYR:CD1	2.88	0.57
2:B:519:TRP:HE1	4:B:1100:OGK:H01	1.70	0.57
2:D:233:LEU:O	2:D:236:VAL:HG23	2.04	0.57
2:F:55:VAL:HG23	2:F:75:LEU:HD21	1.87	0.57
2:D:365:VAL:HG23	2:D:387:VAL:HA	1.85	0.57
2:H:587:VAL:O	2:H:587:VAL:HG12	2.04	0.57
1:I:105:ALA:CB	1:I:114:LEU:HD13	2.33	0.57
2:N:590:GLU:HB3	2:N:591:PRO:CD	2.27	0.57
2:P:297:LYS:HG3	2:P:322:VAL:HB	1.85	0.57
2:B:547:SER:HB3	2:B:564:HIS:HB3	1.86	0.57
2:H:395:LEU:HB3	2:H:427:GLY:O	2.04	0.57
1:M:134:ARG:HB2	1:M:139:ILE:O	2.04	0.57
2:B:138:ASP:OD2	2:B:164:ARG:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:ASP:OD1	2:D:134:LYS:HE3	2.04	0.57
2:H:121:ARG:NH2	5:H:1103:PO4:O4	2.38	0.57
2:J:101:THR:CG2	2:J:128:ASP:OD1	2.53	0.57
2:J:344:LEU:HD23	2:J:380:LEU:HD21	1.87	0.57
2:L:93:PRO:HA	2:L:548:ARG:CB	2.26	0.57
2:N:191:ASN:HD21	2:N:194:LEU:H	1.50	0.57
1:O:48:THR:HG22	1:O:51:ILE:HB	1.87	0.57
1:O:158:ALA:HA	2:P:62:THR:HG21	1.87	0.57
2:H:95:ASN:ND2	2:H:95:ASN:N	2.44	0.57
2:J:84:PRO:HB3	2:J:517:TYR:OH	2.05	0.57
2:N:261:GLU:HG2	2:N:264:MET:HG3	1.87	0.57
2:P:40:VAL:O	2:P:41:CYS:HB3	2.02	0.57
1:A:48:THR:HG22	1:A:51:ILE:HB	1.86	0.56
1:E:134:ARG:HB2	1:E:139:ILE:O	2.05	0.56
2:H:170:LEU:HD23	2:H:170:LEU:C	2.30	0.56
2:H:407:ASP:OD1	2:H:440:ARG:HD2	2.05	0.56
2:H:542:ILE:CD1	2:H:588:LEU:HB2	2.35	0.56
1:I:160:GLU:HA	1:I:160:GLU:OE2	2.05	0.56
2:J:143:LEU:HD23	2:J:159:ILE:HD13	1.87	0.56
1:K:6:ILE:HD12	1:K:23:ALA:HB3	1.86	0.56
2:L:311:CYS:O	2:L:315:GLN:HB2	2.04	0.56
2:P:396:GLU:O	2:P:400:THR:HB	2.04	0.56
2:D:396:GLU:O	2:D:400:THR:HB	2.05	0.56
1:E:160:GLU:OE2	1:E:160:GLU:HA	2.05	0.56
2:F:91:LEU:O	2:F:567:HIS:HE1	1.88	0.56
2:F:227:VAL:HG13	2:F:228:GLY:N	2.19	0.56
2:H:225:VAL:HG21	2:H:238:PHE:HZ	1.70	0.56
2:J:101:THR:HG22	2:J:128:ASP:HB3	1.86	0.56
1:M:102:ILE:HD12	2:N:20:VAL:CG2	2.31	0.56
2:P:533:MET:HE3	2:P:588:LEU:HD13	1.87	0.56
2:B:233:LEU:O	2:B:236:VAL:HG23	2.04	0.56
2:D:519:TRP:HE1	4:D:2100:OGK:H01	1.69	0.56
2:F:261:GLU:HG2	2:F:264:MET:HG3	1.87	0.56
2:F:311:CYS:O	2:F:315:GLN:HB2	2.06	0.56
2:F:443:PHE:CE2	2:F:445:LEU:HD11	2.40	0.56
1:G:130:PRO:O	1:G:134:ARG:HG3	2.05	0.56
2:H:365:VAL:CG2	2:H:387:VAL:HG13	2.34	0.56
2:J:272:LEU:HD21	2:J:275:LEU:HB3	1.88	0.56
2:J:565:PRO:HG2	3:U:201:LEU:HD21	1.86	0.56
1:K:30:ALA:O	1:K:33:VAL:HG22	2.05	0.56
2:L:357:GLY:CA	2:L:415:ARG:HH22	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:519:TRP:NE1	4:L:6100:OGK:H01	2.20	0.56
2:N:223:VAL:O	2:N:245:LEU:HD12	2.06	0.56
2:N:547:SER:HB3	2:N:564:HIS:HB3	1.86	0.56
1:O:52:LEU:O	1:O:56:ILE:HG13	2.05	0.56
2:P:350:GLU:HB3	3:X:209:LEU:HD21	1.86	0.56
2:P:521:GLN:HG3	2:P:567:HIS:HD2	1.69	0.56
1:M:58:TYR:CD2	1:M:113:LEU:HD13	2.40	0.56
2:P:54:HIS:HE1	2:P:56:THR:OG1	1.88	0.56
2:P:227:VAL:CG1	2:P:228:GLY:N	2.68	0.56
2:D:121:ARG:NH2	5:D:1103:PO4:O4	2.37	0.56
2:D:298:LEU:HD23	2:D:300:LEU:HD11	1.87	0.56
1:E:43:PRO:HG2	2:L:319:ASN:HD22	1.68	0.56
2:F:101:THR:CG2	2:F:128:ASP:OD1	2.54	0.56
2:H:82:GLY:HA3	2:H:122:MET:HG2	1.88	0.56
2:H:276:GLY:HA3	2:H:299:ASP:HB3	1.87	0.56
2:H:411:VAL:CG1	2:H:444:TYR:HB3	2.35	0.56
2:L:311:CYS:HB3	2:L:336:VAL:HG21	1.88	0.56
2:B:472:TYR:OH	3:Q:201:LEU:HB2	2.05	0.56
1:C:48:THR:HG22	1:C:51:ILE:HB	1.86	0.56
2:D:357:GLY:HA2	2:D:415:ARG:NH2	2.14	0.56
2:D:404:ASN:HA	2:D:437:LYS:HD2	1.86	0.56
2:F:482:GLU:O	2:F:485:ARG:HG2	2.05	0.56
2:H:282:PRO:HA	2:H:285:MET:HE3	1.87	0.56
2:H:334:LEU:HD22	2:H:373:LEU:HD22	1.85	0.56
2:H:447:GLN:O	2:H:447:GLN:HG3	2.05	0.56
1:I:30:ALA:O	1:I:33:VAL:HG22	2.06	0.56
2:N:40:VAL:O	2:N:41:CYS:HB3	2.04	0.56
2:N:396:GLU:O	2:N:400:THR:HB	2.05	0.56
2:N:477:ASP:OD2	2:N:504:ALA:HB2	2.05	0.56
2:P:93:PRO:HA	2:P:548:ARG:CB	2.29	0.56
2:P:404:ASN:HA	2:P:437:LYS:HD2	1.88	0.56
2:B:57:MET:HE3	2:B:62:THR:HG22	1.86	0.56
2:D:444:TYR:HA	2:D:471:GLY:CA	2.31	0.56
2:H:199:PHE:CE1	2:H:227:VAL:HG23	2.41	0.56
2:H:384:ALA:CB	2:H:409:ARG:HG3	2.35	0.56
2:L:337:LEU:HD12	2:L:341:CYS:SG	2.46	0.56
2:L:519:TRP:HE1	4:L:6100:OGK:H01	1.71	0.56
2:P:443:PHE:CE2	2:P:445:LEU:HD11	2.40	0.56
1:C:158:ALA:HA	2:D:62:THR:CG2	2.36	0.56
2:D:80:LEU:HB2	2:D:122:MET:HE1	1.87	0.56
2:D:138:ASP:OD2	2:D:164:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:275:LEU:HD11	2:F:288:LEU:HD21	1.88	0.56
1:G:48:THR:HG22	1:G:51:ILE:HB	1.88	0.56
2:H:326:ARG:HA	2:H:350:GLU:O	2.05	0.56
2:J:365:VAL:HG23	2:J:387:VAL:HA	1.87	0.56
2:F:191:ASN:HD21	2:F:194:LEU:H	1.53	0.56
2:H:278:SER:C	2:H:280:MET:H	2.13	0.56
2:H:285:MET:CG	2:H:286:PRO:HD3	2.34	0.56
2:H:469:LEU:HD21	4:H:4100:OGK:H05	1.88	0.56
2:L:396:GLU:O	2:L:400:THR:HB	2.06	0.56
2:N:321:GLU:HA	2:N:344:LEU:HA	1.87	0.56
2:N:344:LEU:HD23	2:N:380:LEU:HD21	1.86	0.56
2:P:367:GLN:O	2:P:371:ILE:HG22	2.05	0.56
1:A:134:ARG:HB2	1:A:139:ILE:O	2.06	0.56
2:B:310:HIS:O	2:B:314:ILE:HG12	2.05	0.56
2:D:411:VAL:HG22	2:D:444:TYR:HB3	1.87	0.56
2:F:93:PRO:HA	2:F:548:ARG:CB	2.29	0.56
2:F:184:LEU:HD12	2:F:207:ILE:HB	1.88	0.56
2:F:519:TRP:NE1	4:F:3100:OGK:H01	2.21	0.56
2:H:291:PHE:H	2:H:291:PHE:HD2	1.53	0.56
2:H:462:SER:N	2:H:463:PRO:HD3	2.20	0.56
1:I:12:ASP:OD2	1:I:49:SER:HB2	2.05	0.56
1:K:158:ALA:HA	2:L:62:THR:CG2	2.35	0.56
1:M:96:ALA:CB	2:N:14:VAL:HG12	2.34	0.56
2:N:80:LEU:HB2	2:N:122:MET:HE1	1.88	0.56
2:B:55:VAL:HG23	2:B:75:LEU:HD21	1.88	0.55
1:C:30:ALA:O	1:C:33:VAL:HG22	2.05	0.55
1:G:125:ILE:HD11	2:H:44:TRP:HH2	1.71	0.55
2:H:390:ILE:HD12	2:H:410:LEU:HD21	1.88	0.55
2:L:272:LEU:HD21	2:L:275:LEU:HB3	1.87	0.55
2:L:399:GLY:O	2:L:434:GLY:HA3	2.06	0.55
2:N:546:PRO:HD3	2:N:584:THR:O	2.06	0.55
2:P:351:ARG:O	2:P:351:ARG:HG3	2.06	0.55
2:B:397:SER:O	2:B:400:THR:HG22	2.06	0.55
2:D:519:TRP:NE1	4:D:2100:OGK:H01	2.20	0.55
2:H:76:ARG:O	2:H:114:LEU:HD12	2.07	0.55
2:J:396:GLU:O	2:J:400:THR:HB	2.05	0.55
2:L:40:VAL:O	2:L:41:CYS:HB3	2.06	0.55
2:L:411:VAL:HG22	2:L:444:TYR:HB3	1.88	0.55
2:P:397:SER:O	2:P:400:THR:HG22	2.06	0.55
1:E:45:PRO:HG3	2:L:293:ALA:HB3	1.87	0.55
1:G:153:ARG:HH11	1:G:153:ARG:CG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:366:SER:HB3	2:H:368:ARG:HG3	1.88	0.55
2:H:477:ASP:O	2:H:481:MET:HG2	2.06	0.55
4:L:6100:OGK:HN08	4:L:6100:OGK:C18	2.17	0.55
4:N:7100:OGK:C18	4:N:7100:OGK:N08	2.69	0.55
1:O:153:ARG:NH2	2:P:539:TYR:CE1	2.74	0.55
2:F:519:TRP:HE1	4:F:3100:OGK:H01	1.71	0.55
1:G:26:SER:OG	1:G:108:LEU:HB3	2.06	0.55
2:J:261:GLU:HG2	2:J:264:MET:HG3	1.89	0.55
1:A:158:ALA:HA	2:B:62:THR:HG21	1.88	0.55
1:E:45:PRO:CD	2:L:294:GLN:HB2	2.37	0.55
1:I:6:ILE:HD12	1:I:23:ALA:HB3	1.88	0.55
2:L:101:THR:HG22	2:L:128:ASP:HB3	1.88	0.55
2:L:398:ILE:HG23	2:L:402:LEU:HD11	1.89	0.55
1:A:6:ILE:HD12	1:A:23:ALA:HB3	1.87	0.55
2:B:296:ARG:NH2	1:O:37:CYS:SG	2.80	0.55
2:D:143:LEU:HD23	2:D:159:ILE:HD13	1.89	0.55
4:D:2100:OGK:HN08	4:D:2100:OGK:C18	2.19	0.55
2:F:80:LEU:HB2	2:F:122:MET:HE1	1.88	0.55
2:F:310:HIS:O	2:F:314:ILE:CG1	2.55	0.55
2:J:95:ASN:O	2:J:582:PRO:HG3	2.06	0.55
2:J:446:ARG:HG2	2:J:447:GLN:H	1.71	0.55
1:K:48:THR:HG22	1:K:51:ILE:HB	1.88	0.55
2:P:101:THR:CG2	2:P:128:ASP:OD1	2.54	0.55
1:A:30:ALA:O	1:A:33:VAL:HG22	2.06	0.55
1:C:102:ILE:HG12	1:C:117:THR:HB	1.89	0.55
2:F:367:GLN:HB3	2:F:391:THR:CG2	2.34	0.55
2:H:232:ILE:HG13	2:H:253:LEU:HD21	1.89	0.55
2:H:286:PRO:C	2:H:288:LEU:N	2.62	0.55
2:H:374:ALA:HB2	2:H:398:ILE:HD12	1.88	0.55
2:J:311:CYS:O	2:J:315:GLN:HB2	2.06	0.55
1:O:105:ALA:CB	1:O:114:LEU:HD13	2.37	0.55
2:P:261:GLU:HG2	2:P:264:MET:HG3	1.89	0.55
2:P:310:HIS:O	2:P:314:ILE:CG1	2.55	0.55
2:B:197:LEU:O	2:B:225:VAL:HA	2.07	0.55
2:D:80:LEU:HB2	2:D:122:MET:CE	2.37	0.55
1:G:6:ILE:HD12	1:G:23:ALA:HB3	1.89	0.55
2:H:280:MET:HE2	2:H:285:MET:HA	1.89	0.55
1:M:30:ALA:O	1:M:33:VAL:HG22	2.07	0.55
1:M:102:ILE:HB	2:N:20:VAL:HG21	1.89	0.55
1:O:48:THR:HG22	1:O:51:ILE:CG1	2.37	0.55
1:A:91:MET:O	1:A:93:ILE:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:547:SER:HB3	2:B:564:HIS:CG	2.42	0.55
2:J:130:ASP:OD1	2:J:134:LYS:HE3	2.06	0.55
2:J:444:TYR:HA	2:J:471:GLY:CA	2.32	0.55
2:N:365:VAL:HG23	2:N:387:VAL:HA	1.88	0.55
2:N:440:ARG:HB3	2:N:467:TRP:HE3	1.72	0.55
2:B:20:VAL:O	2:B:24:VAL:HG23	2.07	0.55
2:B:40:VAL:O	2:B:41:CYS:HB3	2.06	0.55
2:B:311:CYS:HB3	2:B:336:VAL:HG21	1.89	0.55
2:D:197:LEU:O	2:D:225:VAL:HA	2.06	0.55
2:D:285:MET:HE1	2:D:309:ASP:HB3	1.88	0.55
2:D:319:ASN:HD22	1:G:43:PRO:HG2	1.71	0.55
2:H:232:ILE:HG13	2:H:253:LEU:CD2	2.37	0.55
2:H:362:GLU:C	2:H:364:LEU:N	2.61	0.55
2:J:298:LEU:HD23	2:J:300:LEU:HD11	1.88	0.55
2:N:397:SER:O	2:N:400:THR:HG22	2.07	0.55
1:O:30:ALA:O	1:O:33:VAL:HG22	2.06	0.55
2:B:101:THR:CG2	2:B:128:ASP:OD1	2.55	0.54
2:H:201:MET:HG3	2:H:302:TYR:CE1	2.41	0.54
2:L:63:ALA:HB1	2:L:67:ARG:HD2	1.87	0.54
2:L:444:TYR:HA	2:L:471:GLY:CA	2.34	0.54
1:M:6:ILE:HD12	1:M:23:ALA:HB3	1.89	0.54
2:P:547:SER:HB3	2:P:564:HIS:CG	2.42	0.54
2:B:404:ASN:HA	2:B:437:LYS:HD2	1.89	0.54
2:F:298:LEU:HD23	2:F:300:LEU:HD11	1.88	0.54
2:H:104:VAL:HG21	2:H:128:ASP:CB	2.37	0.54
2:H:367:GLN:CD	2:H:367:GLN:N	2.65	0.54
1:K:26:SER:OG	1:K:108:LEU:HB3	2.07	0.54
2:N:444:TYR:HA	2:N:471:GLY:CA	2.31	0.54
1:O:26:SER:OG	1:O:108:LEU:HB3	2.07	0.54
2:P:365:VAL:HG23	2:P:387:VAL:HA	1.89	0.54
2:D:468:MET:HE3	2:D:470:LEU:HD21	1.88	0.54
2:F:357:GLY:CA	2:F:415:ARG:HH22	2.12	0.54
1:I:137:PHE:CD1	2:J:17:VAL:HG21	2.43	0.54
2:N:95:ASN:O	2:N:582:PRO:HG3	2.07	0.54
2:P:454:GLY:O	2:P:457:TYR:HB2	2.08	0.54
1:C:134:ARG:HB2	1:C:139:ILE:O	2.07	0.54
2:L:91:LEU:O	2:L:567:HIS:HE1	1.89	0.54
1:A:158:ALA:HA	2:B:62:THR:CG2	2.37	0.54
1:E:52:LEU:O	1:E:52:LEU:HD12	2.06	0.54
2:H:54:HIS:ND1	2:H:55:VAL:N	2.56	0.54
2:H:375:GLN:HG2	2:H:401:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:455:LEU:HD22	2:J:483:PHE:HB2	1.88	0.54
2:J:477:ASP:OD2	2:J:504:ALA:HB2	2.08	0.54
2:L:350:GLU:HB3	3:V:209:LEU:HD21	1.89	0.54
2:N:314:ILE:HD11	2:N:329:ILE:HD11	1.90	0.54
2:N:465:VAL:HG11	2:N:468:MET:HG3	1.89	0.54
1:A:145:PRO:HB2	2:D:539:TYR:CE2	2.42	0.54
2:F:547:SER:HB3	2:F:564:HIS:HB3	1.88	0.54
2:H:428:VAL:HG11	2:H:443:PHE:CE2	2.42	0.54
2:J:367:GLN:HG3	2:J:390:ILE:HA	1.89	0.54
2:L:547:SER:HB3	2:L:564:HIS:CG	2.43	0.54
2:P:227:VAL:HG13	2:P:228:GLY:N	2.22	0.54
2:P:285:MET:HE1	2:P:309:ASP:HB3	1.90	0.54
2:P:357:GLY:CA	2:P:415:ARG:HH22	2.12	0.54
1:A:58:TYR:CE1	1:A:62:HIS:CE1	2.96	0.54
2:F:519:TRP:CZ3	2:F:567:HIS:CG	2.95	0.54
2:H:357:GLY:C	2:H:359:GLU:N	2.66	0.54
2:H:506:ALA:HB1	2:H:535:MET:HB2	1.88	0.54
2:J:440:ARG:HB3	2:J:467:TRP:CE3	2.43	0.54
1:M:159:PHE:O	1:M:160:GLU:CB	2.47	0.54
1:M:160:GLU:OE2	1:M:160:GLU:HA	2.08	0.54
2:N:211:ASP:O	2:N:215:ILE:HG13	2.08	0.54
2:N:446:ARG:HG2	2:N:447:GLN:H	1.73	0.54
2:P:121:ARG:NH2	5:P:1103:PO4:O4	2.40	0.54
2:P:152:THR:HG22	2:P:177:SER:HB2	1.90	0.54
2:P:344:LEU:HD23	2:P:380:LEU:HD21	1.90	0.54
2:P:367:GLN:HB3	2:P:391:THR:CG2	2.34	0.54
1:A:137:PHE:HD1	2:B:17:VAL:HG21	1.72	0.54
2:H:153:THR:CG2	2:H:178:GLU:HA	2.38	0.54
2:H:266:LEU:HD13	2:H:267:VAL:N	2.22	0.54
2:N:78:LEU:HD12	2:N:79:LYS:H	1.72	0.54
2:P:248:PHE:C	2:P:248:PHE:CD2	2.86	0.54
1:A:160:GLU:HA	1:A:160:GLU:OE2	2.08	0.54
2:H:478:GLU:O	2:H:482:GLU:HG2	2.06	0.54
2:J:357:GLY:CA	2:J:415:ARG:HH22	2.13	0.54
2:L:153:THR:HG23	2:L:178:GLU:HA	1.90	0.54
2:N:55:VAL:CG2	2:N:75:LEU:HD21	2.37	0.54
2:B:285:MET:HE1	2:B:309:ASP:HB3	1.90	0.54
1:C:93:ILE:HD12	1:C:97:THR:CG2	2.32	0.54
2:D:521:GLN:HG3	2:D:567:HIS:HD2	1.71	0.54
1:E:128:LYS:HB3	1:E:132:GLU:HB2	1.91	0.54
2:L:261:GLU:HG2	2:L:264:MET:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:490:LEU:HD11	2:L:493:LEU:HD13	1.90	0.54
2:N:54:HIS:HE1	2:N:56:THR:OG1	1.91	0.54
2:N:170:LEU:C	2:N:170:LEU:HD23	2.33	0.54
2:J:227:VAL:CG1	2:J:228:GLY:N	2.71	0.53
2:L:54:HIS:HE1	2:L:56:THR:OG1	1.90	0.53
2:N:320:LEU:HD21	2:N:323:LEU:HB2	1.90	0.53
2:N:357:GLY:CA	2:N:415:ARG:HH22	2.14	0.53
2:P:143:LEU:HD23	2:P:159:ILE:HD13	1.90	0.53
2:B:521:GLN:HG3	2:B:567:HIS:CD2	2.43	0.53
1:C:6:ILE:HD12	1:C:23:ALA:HB3	1.90	0.53
1:I:48:THR:HG22	1:I:51:ILE:HB	1.91	0.53
2:P:221:SER:O	2:P:223:VAL:HG23	2.08	0.53
1:E:105:ALA:HB3	1:E:114:LEU:CD1	2.32	0.53
2:F:65:PRO:HA	2:F:103:TRP:CZ3	2.44	0.53
2:J:201:MET:HB3	3:U:211:ARG:HH12	1.74	0.53
1:K:134:ARG:HB2	1:K:139:ILE:O	2.09	0.53
2:L:101:THR:OG1	2:L:102:PRO:HD3	2.08	0.53
2:L:314:ILE:HD11	2:L:329:ILE:HD11	1.90	0.53
2:N:143:LEU:CD2	2:N:159:ILE:HD13	2.38	0.53
1:A:98:LEU:HD21	1:A:120:THR:HG22	1.90	0.53
2:B:501:SER:HA	2:B:524:ARG:HB2	1.91	0.53
1:C:48:THR:HG22	1:C:51:ILE:CG1	2.38	0.53
2:D:270:ARG:HB3	1:G:107:TYR:CD1	2.43	0.53
2:F:85:ARG:NH1	5:F:1101:PO4:O3	2.41	0.53
2:H:526:SER:O	2:H:527:MET:C	2.52	0.53
1:I:6:ILE:HG22	1:I:7:VAL:N	2.24	0.53
1:K:113:LEU:O	1:K:117:THR:HG23	2.08	0.53
2:N:468:MET:HE1	2:N:483:PHE:CE1	2.44	0.53
2:B:294:GLN:NE2	1:O:107:TYR:OH	2.42	0.53
2:B:298:LEU:HB2	2:B:320:LEU:HD11	1.90	0.53
2:D:55:VAL:HG23	2:D:75:LEU:HD21	1.91	0.53
2:F:404:ASN:HA	2:F:437:LYS:HD2	1.89	0.53
2:H:43:ARG:HH21	2:H:47:ILE:HD11	1.73	0.53
2:J:399:GLY:O	2:J:434:GLY:HA3	2.08	0.53
2:J:547:SER:HB3	2:J:564:HIS:CG	2.44	0.53
1:K:91:MET:O	1:K:93:ILE:N	2.40	0.53
2:L:465:VAL:HG11	2:L:468:MET:HG3	1.91	0.53
1:M:91:MET:O	1:M:93:ILE:N	2.40	0.53
2:N:367:GLN:HG3	2:N:390:ILE:HA	1.90	0.53
2:N:454:GLY:O	2:N:457:TYR:HB2	2.09	0.53
2:B:184:LEU:HD12	2:B:207:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:GLN:HB3	2:B:391:THR:CG2	2.34	0.53
1:C:91:MET:O	1:C:93:ILE:N	2.41	0.53
2:F:444:TYR:HA	2:F:471:GLY:CA	2.32	0.53
1:I:153:ARG:HG2	1:I:157:TRP:CZ3	2.44	0.53
2:L:121:ARG:NH2	5:L:1103:PO4:O4	2.42	0.53
1:M:87:ASP:OD2	1:M:116:LEU:HD22	2.09	0.53
1:C:134:ARG:HH11	2:D:40:VAL:HA	1.74	0.53
2:D:63:ALA:HB1	2:D:67:ARG:HD2	1.91	0.53
2:F:367:GLN:HG3	2:F:390:ILE:HA	1.91	0.53
2:F:397:SER:O	2:F:400:THR:HG22	2.08	0.53
2:H:364:LEU:HD22	2:H:388:SER:N	2.24	0.53
2:H:423:PRO:HB3	2:H:425:ASP:OD2	2.09	0.53
2:H:476:SER:C	2:H:478:GLU:H	2.16	0.53
2:H:486:GLY:O	2:H:487:CYS:C	2.51	0.53
2:L:367:GLN:HG3	2:L:390:ILE:HA	1.89	0.53
1:A:159:PHE:O	1:A:160:GLU:CB	2.52	0.53
2:D:101:THR:CG2	2:D:128:ASP:OD1	2.56	0.53
2:D:533:MET:HE3	2:D:588:LEU:HD13	1.90	0.53
2:F:153:THR:HG23	2:F:178:GLU:HA	1.91	0.53
2:F:311:CYS:HB3	2:F:336:VAL:HG21	1.91	0.53
2:H:391:THR:C	2:H:393:GLU:N	2.67	0.53
2:P:325:THR:O	2:P:349:ILE:HA	2.09	0.53
1:A:48:THR:HG22	1:A:51:ILE:CG1	2.39	0.53
2:B:170:LEU:HD23	2:B:170:LEU:C	2.34	0.53
2:D:443:PHE:CE2	2:D:445:LEU:HD11	2.44	0.53
2:D:455:LEU:HD22	2:D:483:PHE:HB2	1.90	0.53
1:E:11:SER:HA	1:E:45:PRO:HA	1.90	0.53
1:E:26:SER:OG	1:E:108:LEU:HB3	2.09	0.53
2:F:547:SER:HB3	2:F:564:HIS:CG	2.44	0.53
2:H:97:GLY:HA3	2:H:123:ILE:CD1	2.38	0.53
4:H:4100:OGK:HN08	4:H:4100:OGK:C18	2.21	0.53
1:K:160:GLU:HA	1:K:160:GLU:OE2	2.09	0.53
2:L:440:ARG:HB3	2:L:467:TRP:CE3	2.43	0.53
1:M:102:ILE:HB	2:N:20:VAL:CG2	2.39	0.53
2:N:519:TRP:CZ3	2:N:567:HIS:CG	2.97	0.53
2:B:367:GLN:HG3	2:B:390:ILE:HA	1.90	0.53
2:B:419:ILE:HD11	2:B:446:ARG:HH22	1.74	0.53
2:H:65:PRO:HG3	2:H:103:TRP:CD2	2.44	0.53
2:H:214:THR:HA	2:H:217:ARG:HG2	1.91	0.53
2:J:227:VAL:HG13	2:J:228:GLY:N	2.23	0.53
1:K:93:ILE:HD12	1:K:97:THR:CG2	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:80:LEU:HB2	2:L:122:MET:CE	2.39	0.53
1:M:134:ARG:CZ	1:M:141:ASN:HD22	2.22	0.53
2:N:59:LEU:O	2:N:62:THR:HB	2.08	0.53
2:N:93:PRO:HA	2:N:548:ARG:CB	2.33	0.53
2:N:197:LEU:O	2:N:225:VAL:HA	2.09	0.53
1:O:158:ALA:HA	2:P:62:THR:CG2	2.39	0.53
2:B:93:PRO:HA	2:B:548:ARG:CB	2.32	0.52
2:B:275:LEU:HD11	2:B:288:LEU:HD21	1.89	0.52
1:G:160:GLU:HB3	2:H:31:PRO:HB3	1.90	0.52
2:H:111:LEU:O	2:H:113:GLN:N	2.42	0.52
2:H:184:LEU:HD12	2:H:207:ILE:HB	1.91	0.52
2:H:187:LEU:HB3	2:H:215:ILE:HD11	1.90	0.52
1:I:58:TYR:CD2	1:I:113:LEU:HD13	2.44	0.52
2:J:422:LEU:HB3	2:J:423:PRO:HD3	1.90	0.52
2:B:399:GLY:O	2:B:434:GLY:HA3	2.09	0.52
2:H:535:MET:CE	2:H:542:ILE:HG21	2.39	0.52
2:J:533:MET:HE3	2:J:588:LEU:HD13	1.91	0.52
2:L:542:ILE:HD11	2:L:588:LEU:CD1	2.24	0.52
1:O:6:ILE:HD12	1:O:23:ALA:HB3	1.90	0.52
1:O:58:TYR:CD2	1:O:113:LEU:HD13	2.44	0.52
2:F:454:GLY:O	2:F:457:TYR:HB2	2.09	0.52
2:H:492:LYS:HZ3	2:H:516:ARG:HH11	1.57	0.52
2:H:494:GLU:HG2	2:H:519:TRP:HB3	1.91	0.52
1:I:134:ARG:CZ	1:I:141:ASN:HD22	2.23	0.52
2:L:397:SER:O	2:L:400:THR:HG22	2.08	0.52
1:M:52:LEU:O	1:M:52:LEU:HD12	2.09	0.52
2:N:101:THR:HG22	2:N:128:ASP:HB3	1.90	0.52
2:N:138:ASP:OD2	2:N:164:ARG:HG3	2.09	0.52
2:P:411:VAL:HG22	2:P:444:TYR:HB3	1.91	0.52
1:C:11:SER:HA	1:C:45:PRO:HA	1.90	0.52
2:D:54:HIS:HE1	2:D:56:THR:OG1	1.92	0.52
2:D:190:HIS:ND1	2:H:112:ARG:HD2	2.24	0.52
2:D:235:LEU:O	2:D:238:PHE:HB3	2.10	0.52
2:F:337:LEU:HD12	2:F:341:CYS:SG	2.49	0.52
2:H:192:THR:HG22	2:H:218:ASN:O	2.10	0.52
2:H:354:ASP:O	2:H:354:ASP:OD2	2.28	0.52
1:I:159:PHE:O	1:I:160:GLU:CB	2.49	0.52
2:J:456:SER:HB2	2:J:482:GLU:HB3	1.91	0.52
2:L:344:LEU:HD23	2:L:380:LEU:HD21	1.91	0.52
1:M:99:PHE:HB2	2:N:15:ALA:HB3	1.90	0.52
1:M:102:ILE:CD1	2:N:20:VAL:CG2	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:233:LEU:O	2:N:236:VAL:HG23	2.08	0.52
2:P:546:PRO:HD3	2:P:584:THR:O	2.08	0.52
1:C:160:GLU:HA	1:C:160:GLU:OE2	2.09	0.52
2:D:412:LEU:C	2:D:412:LEU:HD12	2.35	0.52
2:D:519:TRP:CZ3	2:D:567:HIS:CG	2.97	0.52
2:F:289:PHE:HB2	2:F:290:PRO:HD3	1.91	0.52
1:G:48:THR:HG22	1:G:51:ILE:CG1	2.39	0.52
2:H:64:THR:O	2:H:65:PRO:C	2.51	0.52
2:H:365:VAL:HG21	2:H:387:VAL:CA	2.39	0.52
2:H:402:LEU:HD13	2:H:405:LEU:HG	1.92	0.52
2:J:232:ILE:HD12	2:J:252:SER:H	1.74	0.52
2:P:55:VAL:CG2	2:P:75:LEU:HD21	2.37	0.52
2:P:170:LEU:HD23	2:P:170:LEU:C	2.34	0.52
2:B:248:PHE:C	2:B:248:PHE:CD2	2.87	0.52
1:C:26:SER:OG	1:C:108:LEU:HB3	2.10	0.52
2:D:547:SER:HB3	2:D:564:HIS:CG	2.43	0.52
2:L:446:ARG:HG2	2:L:447:GLN:H	1.74	0.52
2:N:248:PHE:C	2:N:248:PHE:CD2	2.87	0.52
2:N:547:SER:HB3	2:N:564:HIS:CG	2.44	0.52
1:O:137:PHE:HD1	2:P:17:VAL:HG21	1.72	0.52
1:O:160:GLU:HA	1:O:160:GLU:OE2	2.10	0.52
2:P:275:LEU:HD11	2:P:288:LEU:HD21	1.91	0.52
2:P:501:SER:HA	2:P:524:ARG:HB2	1.92	0.52
2:D:446:ARG:HG2	2:D:447:GLN:H	1.74	0.52
1:I:158:ALA:HA	2:J:62:THR:HG21	1.90	0.52
2:J:380:LEU:HD12	2:J:383:MET:HE2	1.92	0.52
2:L:235:LEU:O	2:L:238:PHE:HB3	2.10	0.52
2:L:545:ILE:HG22	2:L:546:PRO:CD	2.40	0.52
2:N:325:THR:O	2:N:349:ILE:HA	2.09	0.52
2:N:472:TYR:OH	3:W:201:LEU:HB2	2.10	0.52
2:P:446:ARG:HG2	2:P:447:GLN:H	1.74	0.52
2:B:454:GLY:O	2:B:457:TYR:HB2	2.10	0.52
2:D:275:LEU:HD11	2:D:288:LEU:HD21	1.92	0.52
2:D:375:GLN:HG2	2:D:401:TYR:CE1	2.45	0.52
2:F:521:GLN:HG3	2:F:567:HIS:CD2	2.45	0.52
2:H:269:PRO:O	2:H:270:ARG:C	2.52	0.52
1:K:153:ARG:NH2	2:L:539:TYR:CE1	2.78	0.52
2:L:521:GLN:HG3	2:L:567:HIS:CD2	2.44	0.52
2:N:130:ASP:OD1	2:N:134:LYS:HE3	2.09	0.52
2:N:456:SER:HB2	2:N:482:GLU:HB3	1.92	0.52
2:B:54:HIS:HE1	2:B:56:THR:OG1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:ARG:NH2	4:D:2100:OGK:O07	2.35	0.52
2:D:311:CYS:HB3	2:D:336:VAL:HG21	1.91	0.52
2:D:367:GLN:HG3	2:D:390:ILE:HA	1.92	0.52
2:F:411:VAL:HG22	2:F:444:TYR:HB3	1.92	0.52
2:H:225:VAL:CG2	2:H:245:LEU:HD11	2.40	0.52
2:J:275:LEU:HD11	2:J:288:LEU:HD21	1.90	0.52
2:J:305:LEU:HD23	2:J:305:LEU:O	2.10	0.52
2:J:465:VAL:HG11	2:J:468:MET:HG3	1.91	0.52
2:J:521:GLN:HG3	2:J:567:HIS:CD2	2.45	0.52
2:P:419:ILE:CD1	2:P:446:ARG:HH22	2.23	0.52
2:B:337:LEU:HD12	2:B:341:CYS:SG	2.50	0.52
4:B:1100:OGK:HN08	4:B:1100:OGK:C18	2.19	0.52
1:C:137:PHE:CD1	2:D:17:VAL:HG21	2.45	0.52
2:F:422:LEU:HB3	2:F:423:PRO:HD3	1.92	0.52
2:H:306:GLU:O	2:H:310:HIS:HD2	1.92	0.52
2:H:328:VAL:HG12	2:H:359:GLU:HG2	1.92	0.52
2:J:80:LEU:HB2	2:J:122:MET:CE	2.39	0.52
2:J:85:ARG:NH2	4:J:5100:OGK:O07	2.33	0.52
2:J:93:PRO:HA	2:J:548:ARG:CB	2.33	0.52
2:L:404:ASN:HA	2:L:437:LYS:HD2	1.92	0.52
2:N:298:LEU:HB2	2:N:320:LEU:HD11	1.92	0.52
2:P:407:ASP:OD1	2:P:440:ARG:HD2	2.10	0.52
2:D:191:ASN:ND2	2:D:194:LEU:H	2.07	0.51
2:D:519:TRP:CZ3	2:D:567:HIS:ND1	2.79	0.51
1:E:93:ILE:HD12	1:E:97:THR:CG2	2.29	0.51
2:F:235:LEU:O	2:F:238:PHE:HB3	2.10	0.51
1:G:151:VAL:CG1	2:H:39:LEU:HD21	2.40	0.51
2:H:302:TYR:N	2:H:302:TYR:CD2	2.74	0.51
2:H:532:LEU:HD11	2:H:568:ILE:HD13	1.92	0.51
2:J:398:ILE:C	2:J:400:THR:H	2.17	0.51
1:M:137:PHE:HD1	2:N:17:VAL:HG21	1.74	0.51
2:N:101:THR:CG2	2:N:128:ASP:OD1	2.58	0.51
2:N:310:HIS:O	2:N:314:ILE:CG1	2.58	0.51
2:P:80:LEU:HB2	2:P:122:MET:CE	2.40	0.51
2:P:367:GLN:HG3	2:P:390:ILE:HA	1.92	0.51
2:P:456:SER:HB2	2:P:482:GLU:HB3	1.92	0.51
2:B:367:GLN:O	2:B:371:ILE:HG22	2.09	0.51
2:H:411:VAL:CG2	4:H:4100:OGK:H16A	2.40	0.51
2:L:477:ASP:OD2	2:L:504:ALA:HB2	2.10	0.51
2:N:456:SER:CB	2:N:482:GLU:HB3	2.40	0.51
2:P:233:LEU:O	2:P:236:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:251:GLY:O	2:P:278:SER:HB2	2.10	0.51
2:B:446:ARG:HG2	2:B:447:GLN:H	1.75	0.51
1:C:114:LEU:C	1:C:116:LEU:H	2.17	0.51
2:F:233:LEU:O	2:F:236:VAL:HG23	2.09	0.51
2:P:101:THR:OG1	2:P:102:PRO:HD3	2.10	0.51
2:P:398:ILE:HG23	2:P:402:LEU:HD11	1.92	0.51
1:A:11:SER:HA	1:A:45:PRO:HA	1.92	0.51
2:B:455:LEU:HD22	2:B:483:PHE:HB2	1.91	0.51
1:C:158:ALA:HA	2:D:62:THR:HG21	1.91	0.51
2:D:298:LEU:HB2	2:D:320:LEU:HD11	1.93	0.51
2:F:63:ALA:HB1	2:F:67:ARG:HD2	1.91	0.51
2:H:406:CYS:HA	2:H:438:LEU:HA	1.92	0.51
2:H:418:ARG:HG2	2:H:446:ARG:NH1	2.25	0.51
2:H:455:LEU:HD21	2:H:473:VAL:CG2	2.40	0.51
2:J:235:LEU:O	2:J:238:PHE:HB3	2.10	0.51
1:M:87:ASP:HB3	1:M:116:LEU:HD21	1.92	0.51
2:B:143:LEU:CD2	2:B:159:ILE:HD13	2.40	0.51
2:D:93:PRO:HA	2:D:548:ARG:CB	2.32	0.51
1:E:48:THR:HG22	1:E:51:ILE:CG1	2.40	0.51
2:H:65:PRO:HA	2:H:103:TRP:CZ3	2.44	0.51
2:H:424:LEU:O	2:H:426:ASN:N	2.43	0.51
2:N:153:THR:HG23	2:N:178:GLU:HA	1.93	0.51
2:N:337:LEU:HD12	2:N:341:CYS:SG	2.51	0.51
1:O:48:THR:CG2	1:O:51:ILE:HG12	2.41	0.51
1:A:52:LEU:O	1:A:52:LEU:HD12	2.10	0.51
1:A:105:ALA:HB2	1:A:113:LEU:HD23	1.92	0.51
2:B:590:GLU:O	2:B:591:PRO:C	2.54	0.51
2:F:255:GLU:HG3	2:F:255:GLU:O	2.11	0.51
2:F:546:PRO:HD3	2:F:584:THR:O	2.08	0.51
2:H:382:TYR:CD2	2:H:407:ASP:HB3	2.46	0.51
1:I:48:THR:HG22	1:I:51:ILE:CG1	2.40	0.51
2:J:311:CYS:HB3	2:J:336:VAL:HG21	1.91	0.51
1:M:48:THR:HG22	1:M:51:ILE:CG1	2.40	0.51
2:N:542:ILE:CD1	2:N:588:LEU:HD12	2.28	0.51
1:A:134:ARG:HH11	2:B:40:VAL:HA	1.75	0.51
1:A:153:ARG:NH2	2:B:539:TYR:CE1	2.79	0.51
2:D:422:LEU:HB3	2:D:423:PRO:HD3	1.93	0.51
2:H:496:ARG:HD2	4:H:4100:OGK:H23A	1.92	0.51
2:J:501:SER:HA	2:J:524:ARG:HB2	1.92	0.51
2:P:63:ALA:HB1	2:P:67:ARG:HD2	1.91	0.51
2:P:247:GLU:HA	2:P:274:ARG:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:298:LEU:HB2	2:F:320:LEU:HD11	1.92	0.51
2:H:306:GLU:HA	2:H:306:GLU:OE2	2.09	0.51
1:K:48:THR:HG22	1:K:51:ILE:CG1	2.41	0.51
1:K:137:PHE:HD1	2:L:17:VAL:HG21	1.76	0.51
2:L:78:LEU:HD12	2:L:79:LYS:H	1.76	0.51
2:L:519:TRP:HH2	2:L:567:HIS:CE1	2.29	0.51
2:P:191:ASN:ND2	2:P:194:LEU:H	2.06	0.51
2:P:232:ILE:HD12	2:P:252:SER:H	1.76	0.51
2:D:310:HIS:O	2:D:314:ILE:HG12	2.11	0.51
2:F:367:GLN:O	2:F:371:ILE:HG22	2.10	0.51
1:O:91:MET:CE	1:O:117:THR:HG22	2.41	0.51
2:P:78:LEU:HD12	2:P:79:LYS:H	1.74	0.51
2:B:272:LEU:HD21	2:B:275:LEU:HB3	1.93	0.51
2:F:272:LEU:HD21	2:F:275:LEU:HB3	1.92	0.51
2:F:305:LEU:O	2:F:305:LEU:HD23	2.11	0.51
2:F:501:SER:HA	2:F:524:ARG:HB2	1.93	0.51
1:G:26:SER:C	1:G:28:THR:H	2.19	0.51
2:H:414:ASP:HB3	2:H:446:ARG:HH21	1.76	0.51
2:L:198:ASN:C	2:L:198:ASN:OD1	2.53	0.51
2:N:422:LEU:HB3	2:N:423:PRO:HD3	1.93	0.51
1:O:11:SER:HA	1:O:45:PRO:HA	1.92	0.51
1:O:91:MET:O	1:O:93:ILE:N	2.44	0.51
2:B:153:THR:HG23	2:B:178:GLU:HA	1.92	0.50
2:B:255:GLU:HG3	2:B:255:GLU:O	2.11	0.50
2:B:305:LEU:HD23	2:B:305:LEU:O	2.11	0.50
2:B:320:LEU:HD21	2:B:323:LEU:HB2	1.93	0.50
2:B:519:TRP:HH2	2:B:567:HIS:CE1	2.29	0.50
2:B:546:PRO:HD3	2:B:584:THR:O	2.11	0.50
2:D:272:LEU:HD21	2:D:275:LEU:HB3	1.92	0.50
2:H:365:VAL:HG21	2:H:387:VAL:CG1	2.39	0.50
2:H:390:ILE:HD11	2:H:412:LEU:CD2	2.41	0.50
2:H:409:ARG:HD2	4:H:4100:OGK:H13A	1.92	0.50
1:M:153:ARG:HG2	1:M:157:TRP:CZ3	2.46	0.50
2:B:482:GLU:O	2:B:485:ARG:HG2	2.11	0.50
1:C:134:ARG:NH1	2:D:40:VAL:HA	2.26	0.50
2:F:143:LEU:CD2	2:F:159:ILE:HD13	2.41	0.50
2:F:542:ILE:CD1	2:F:588:LEU:HD12	2.30	0.50
2:N:533:MET:HE3	2:N:588:LEU:HD13	1.91	0.50
2:B:357:GLY:CA	2:B:415:ARG:HH22	2.12	0.50
2:F:110:ASN:HA	2:L:190:HIS:HE1	1.77	0.50
2:F:398:ILE:O	2:F:402:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:291:PHE:N	2:H:291:PHE:CD2	2.79	0.50
2:H:370:LEU:HB2	2:H:394:SER:HB3	1.93	0.50
2:L:248:PHE:C	2:L:248:PHE:CD2	2.89	0.50
2:L:482:GLU:O	2:L:485:ARG:HG2	2.11	0.50
2:L:533:MET:HE3	2:L:588:LEU:HD13	1.91	0.50
2:P:65:PRO:HA	2:P:103:TRP:CZ3	2.46	0.50
2:P:153:THR:HG23	2:P:178:GLU:HA	1.92	0.50
2:P:289:PHE:HB2	2:P:290:PRO:HD3	1.92	0.50
1:C:91:MET:O	1:C:93:ILE:HG12	2.12	0.50
2:D:456:SER:HB2	2:D:482:GLU:HB3	1.94	0.50
2:F:95:ASN:O	2:F:582:PRO:HG3	2.12	0.50
2:H:87:ALA:HB2	2:H:92:ILE:HB	1.93	0.50
2:H:230:PHE:CB	2:H:235:LEU:HD21	2.41	0.50
2:H:432:LEU:HD11	2:H:458:ILE:HD13	1.93	0.50
1:I:158:ALA:HA	2:J:62:THR:CG2	2.41	0.50
1:K:128:LYS:HB3	1:K:132:GLU:HB2	1.93	0.50
2:P:159:ILE:HD12	2:P:166:ILE:HD11	1.93	0.50
2:B:80:LEU:HB2	2:B:122:MET:CE	2.41	0.50
2:B:130:ASP:OD1	2:B:134:LYS:HE3	2.12	0.50
2:B:440:ARG:HB3	2:B:467:TRP:CE3	2.45	0.50
2:F:170:LEU:C	2:F:170:LEU:HD23	2.36	0.50
2:H:145:LEU:O	2:H:171:MET:HA	2.10	0.50
2:J:519:TRP:HH2	2:J:567:HIS:CE1	2.30	0.50
2:L:233:LEU:O	2:L:236:VAL:HG23	2.11	0.50
2:N:523:TYR:CE2	2:N:568:ILE:HD11	2.47	0.50
2:D:20:VAL:O	2:D:24:VAL:HG23	2.11	0.50
2:H:464:ASN:O	2:H:466:ARG:HD2	2.11	0.50
2:J:419:ILE:HD11	2:J:446:ARG:HH22	1.75	0.50
1:K:105:ALA:HB2	1:K:113:LEU:HD23	1.93	0.50
2:P:422:LEU:HB3	2:P:423:PRO:HD3	1.93	0.50
1:A:128:LYS:HB3	1:A:132:GLU:HB2	1.94	0.50
2:B:159:ILE:HD12	2:B:166:ILE:HD11	1.94	0.50
1:E:48:THR:HG22	1:E:51:ILE:CB	2.41	0.50
2:F:477:ASP:OD2	2:F:504:ALA:HB2	2.12	0.50
2:J:289:PHE:HB2	2:J:290:PRO:HD3	1.93	0.50
2:P:289:PHE:HD1	2:P:316:LYS:HD2	1.73	0.50
2:F:465:VAL:HG11	2:F:468:MET:HG3	1.93	0.50
2:H:392:ASN:ND2	2:H:422:LEU:HD13	2.26	0.50
1:I:128:LYS:HB3	1:I:132:GLU:HB2	1.94	0.50
2:J:398:ILE:HG23	2:J:402:LEU:HD11	1.94	0.50
1:K:26:SER:HB3	1:K:29:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:ILE:HD12	2:B:252:SER:H	1.76	0.50
2:F:197:LEU:O	2:F:225:VAL:HA	2.12	0.50
2:F:232:ILE:HD12	2:F:252:SER:H	1.76	0.50
1:G:113:LEU:O	1:G:117:THR:HG23	2.11	0.50
2:H:243:ALA:C	2:H:245:LEU:H	2.20	0.50
2:H:282:PRO:HB3	2:H:309:ASP:OD2	2.11	0.50
2:H:289:PHE:N	2:H:290:PRO:CD	2.74	0.50
2:H:496:ARG:HB2	4:H:4100:OGK:H01A	1.94	0.50
2:L:320:LEU:HD21	2:L:323:LEU:HB2	1.93	0.50
1:M:130:PRO:O	1:M:134:ARG:HG2	2.12	0.50
2:N:227:VAL:CG1	2:N:228:GLY:N	2.74	0.50
2:P:482:GLU:O	2:P:485:ARG:HG2	2.12	0.50
2:B:310:HIS:O	2:B:314:ILE:CG1	2.58	0.49
2:D:248:PHE:C	2:D:248:PHE:CD2	2.90	0.49
2:D:310:HIS:O	2:D:314:ILE:CG1	2.60	0.49
2:D:407:ASP:OD1	2:D:440:ARG:HD2	2.12	0.49
1:G:11:SER:HA	1:G:45:PRO:HA	1.94	0.49
2:H:191:ASN:ND2	2:H:194:LEU:H	2.08	0.49
2:H:516:ARG:HA	2:H:572:TYR:HD1	1.75	0.49
2:J:54:HIS:HE1	2:J:56:THR:OG1	1.95	0.49
2:J:164:ARG:HH21	2:N:136:ARG:HH21	1.60	0.49
1:K:91:MET:O	1:K:93:ILE:HG12	2.12	0.49
1:O:113:LEU:O	1:O:113:LEU:HG	2.12	0.49
2:P:419:ILE:HD11	2:P:446:ARG:HH22	1.75	0.49
2:P:465:VAL:HG11	2:P:468:MET:HG3	1.94	0.49
2:D:398:ILE:HG23	2:D:402:LEU:HD11	1.94	0.49
2:H:97:GLY:CA	2:H:123:ILE:HD11	2.42	0.49
2:H:191:ASN:ND2	2:H:193:SER:H	2.10	0.49
2:H:289:PHE:N	2:H:290:PRO:HD2	2.27	0.49
2:J:198:ASN:C	2:J:198:ASN:OD1	2.55	0.49
2:L:310:HIS:O	2:L:314:ILE:HG12	2.12	0.49
1:M:102:ILE:CB	2:N:20:VAL:CG2	2.90	0.49
2:N:565:PRO:HG2	3:W:201:LEU:HD21	1.94	0.49
1:O:134:ARG:CZ	1:O:141:ASN:HD22	2.25	0.49
2:P:477:ASP:OD2	2:P:504:ALA:HB2	2.12	0.49
1:C:114:LEU:C	1:C:116:LEU:N	2.68	0.49
1:C:134:ARG:CZ	1:C:141:ASN:HD22	2.24	0.49
1:E:91:MET:O	1:E:93:ILE:N	2.45	0.49
2:F:533:MET:HE3	2:F:588:LEU:HD13	1.95	0.49
2:H:387:VAL:HG11	2:H:390:ILE:CD1	2.39	0.49
2:J:519:TRP:CZ3	2:J:567:HIS:CG	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:132:GLU:O	1:K:136:THR:HG23	2.12	0.49
2:P:138:ASP:OD2	2:P:164:ARG:HG3	2.12	0.49
1:A:134:ARG:NH1	2:B:40:VAL:HA	2.27	0.49
2:B:350:GLU:HB3	3:Q:209:LEU:CD2	2.40	0.49
1:C:58:TYR:CE1	1:C:62:HIS:CE1	3.00	0.49
2:D:65:PRO:HA	2:D:103:TRP:CZ3	2.48	0.49
2:L:519:TRP:CZ3	2:L:567:HIS:CG	3.00	0.49
2:N:357:GLY:HA2	2:N:415:ARG:NH2	2.14	0.49
2:P:159:ILE:HG13	2:P:160:VAL:N	2.26	0.49
2:P:468:MET:CE	2:P:470:LEU:HD11	2.42	0.49
1:A:91:MET:O	1:A:93:ILE:HG12	2.13	0.49
2:B:519:TRP:CZ3	2:B:567:HIS:CG	3.00	0.49
2:D:358:MET:HE3	2:D:363:GLY:O	2.13	0.49
2:H:156:LEU:HD11	2:H:171:MET:HE3	1.93	0.49
2:H:400:THR:C	2:H:403:LYS:HE2	2.37	0.49
2:H:487:CYS:HB3	2:H:490:LEU:HB2	1.95	0.49
2:H:492:LYS:HZ3	2:H:516:ARG:NH1	2.09	0.49
1:I:91:MET:O	1:I:93:ILE:N	2.42	0.49
2:N:116:SER:CB	2:N:142:THR:HG23	2.36	0.49
2:B:412:LEU:C	2:B:412:LEU:HD12	2.37	0.49
2:B:419:ILE:CD1	2:B:446:ARG:HH22	2.26	0.49
2:D:211:ASP:O	2:D:215:ILE:HG13	2.12	0.49
2:D:398:ILE:C	2:D:400:THR:H	2.20	0.49
1:G:10:SER:OG	1:G:11:SER:N	2.46	0.49
2:H:275:LEU:C	2:H:275:LEU:HD12	2.37	0.49
2:H:428:VAL:CG1	2:H:443:PHE:CZ	2.96	0.49
2:J:159:ILE:HD12	2:J:166:ILE:HD11	1.94	0.49
2:J:404:ASN:HA	2:J:437:LYS:HD2	1.94	0.49
2:J:411:VAL:HG22	2:J:444:TYR:HB3	1.93	0.49
2:J:419:ILE:O	2:J:420:THR:C	2.55	0.49
2:J:443:PHE:CE2	2:J:445:LEU:HD11	2.48	0.49
1:K:134:ARG:HH11	2:L:40:VAL:HA	1.76	0.49
1:M:48:THR:HG22	1:M:51:ILE:CB	2.42	0.49
2:N:159:ILE:HG13	2:N:160:VAL:N	2.27	0.49
2:N:375:GLN:HG2	2:N:401:TYR:CE1	2.48	0.49
1:A:26:SER:OG	1:A:108:LEU:HB3	2.13	0.49
1:C:128:LYS:HB3	1:C:132:GLU:HB2	1.95	0.49
2:D:519:TRP:HH2	2:D:567:HIS:CE1	2.31	0.49
2:F:295:ILE:HG21	2:F:298:LEU:CD1	2.41	0.49
2:F:407:ASP:OD1	2:F:440:ARG:HD2	2.12	0.49
2:H:83:LYS:O	2:H:121:ARG:NH1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:223:VAL:O	2:L:245:LEU:HD12	2.13	0.49
2:N:235:LEU:O	2:N:238:PHE:HB3	2.12	0.49
2:N:289:PHE:HB2	2:N:290:PRO:HD3	1.94	0.49
1:O:128:LYS:HB3	1:O:132:GLU:HB2	1.94	0.49
2:P:320:LEU:HD21	2:P:323:LEU:HB2	1.93	0.49
2:B:546:PRO:O	2:B:547:SER:HB2	2.13	0.49
2:H:332:ARG:O	2:H:336:VAL:HG23	2.13	0.49
2:H:431:LEU:HD23	2:H:432:LEU:N	2.27	0.49
2:H:450:LEU:HD11	2:H:454:GLY:CA	2.39	0.49
2:H:450:LEU:CG	2:H:454:GLY:HA3	2.43	0.49
2:J:482:GLU:O	2:J:485:ARG:HG2	2.13	0.49
2:J:490:LEU:HD11	2:J:493:LEU:HD13	1.94	0.49
2:L:227:VAL:HG13	2:L:228:GLY:H	1.76	0.49
2:L:255:GLU:HG3	2:L:255:GLU:O	2.13	0.49
2:L:412:LEU:C	2:L:412:LEU:HD12	2.37	0.49
2:N:400:THR:O	2:N:403:LYS:HE2	2.12	0.49
1:O:10:SER:OG	1:O:11:SER:N	2.46	0.49
1:O:153:ARG:HG2	1:O:157:TRP:CZ3	2.48	0.49
2:P:255:GLU:HG3	2:P:255:GLU:O	2.13	0.49
2:D:247:GLU:HA	2:D:274:ARG:O	2.12	0.49
2:D:482:GLU:O	2:D:485:ARG:HG2	2.12	0.49
2:F:409:ARG:HD3	4:F:3100:OGK:H13A	1.93	0.49
2:H:153:THR:HG23	2:H:178:GLU:HA	1.95	0.49
1:I:134:ARG:HH11	2:J:40:VAL:HA	1.77	0.49
2:L:275:LEU:HD11	2:L:288:LEU:HD21	1.93	0.49
2:N:469:LEU:HA	2:N:494:GLU:O	2.11	0.49
2:P:130:ASP:OD1	2:P:134:LYS:HE3	2.12	0.49
2:D:419:ILE:O	2:D:420:THR:C	2.56	0.49
2:F:490:LEU:HD11	2:F:493:LEU:HD13	1.95	0.49
2:H:57:MET:HB2	2:H:80:LEU:HD23	1.95	0.49
2:H:259:MET:N	2:H:260:PRO:HD3	2.28	0.49
2:H:385:VAL:HG12	2:H:387:VAL:HG23	1.95	0.49
2:J:153:THR:HG23	2:J:178:GLU:HA	1.94	0.49
2:L:298:LEU:HB2	2:L:320:LEU:HD11	1.94	0.49
2:N:311:CYS:CB	2:N:336:VAL:HG21	2.43	0.49
2:P:419:ILE:O	2:P:420:THR:C	2.56	0.49
2:B:321:GLU:HA	2:B:344:LEU:HA	1.94	0.48
2:D:153:THR:HG23	2:D:178:GLU:HA	1.95	0.48
2:F:538:PRO:O	2:F:539:TYR:HB2	2.13	0.48
2:H:43:ARG:NH2	2:H:47:ILE:HD11	2.28	0.48
2:H:275:LEU:C	2:H:275:LEU:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:397:SER:O	2:J:400:THR:HG22	2.13	0.48
1:K:134:ARG:NH1	2:L:40:VAL:HA	2.28	0.48
1:K:159:PHE:O	1:K:160:GLU:CB	2.50	0.48
2:N:96:TRP:O	2:N:578:ARG:NH2	2.41	0.48
2:N:152:THR:HG22	2:N:177:SER:HB2	1.95	0.48
2:N:419:ILE:O	2:N:420:THR:C	2.56	0.48
2:N:546:PRO:O	2:N:547:SER:HB2	2.12	0.48
2:F:419:ILE:O	2:F:420:THR:C	2.56	0.48
2:J:400:THR:O	2:J:403:LYS:HE2	2.13	0.48
1:K:58:TYR:CD2	1:K:113:LEU:HD13	2.47	0.48
2:L:501:SER:HA	2:L:524:ARG:HB2	1.95	0.48
2:L:546:PRO:HD3	2:L:584:THR:O	2.11	0.48
2:N:482:GLU:O	2:N:485:ARG:HG2	2.13	0.48
1:A:48:THR:CG2	1:A:51:ILE:HG12	2.43	0.48
2:B:176:PHE:CZ	2:B:204:PHE:CZ	3.01	0.48
2:D:255:GLU:HG3	2:D:255:GLU:O	2.13	0.48
2:F:247:GLU:HA	2:F:274:ARG:O	2.13	0.48
2:F:519:TRP:CZ3	2:F:567:HIS:ND1	2.81	0.48
2:H:85:ARG:NH1	5:H:1101:PO4:O2	2.45	0.48
2:H:122:MET:HE2	2:H:122:MET:HB3	1.66	0.48
2:H:326:ARG:O	2:H:329:ILE:HG22	2.12	0.48
2:J:255:GLU:HG3	2:J:255:GLU:O	2.12	0.48
2:L:419:ILE:CD1	2:L:446:ARG:HH22	2.27	0.48
2:P:398:ILE:C	2:P:400:THR:H	2.20	0.48
2:P:519:TRP:CZ3	2:P:567:HIS:CG	3.01	0.48
2:B:247:GLU:HA	2:B:274:ARG:O	2.14	0.48
2:B:419:ILE:O	2:B:420:THR:C	2.56	0.48
2:D:397:SER:O	2:D:400:THR:HG22	2.13	0.48
2:D:399:GLY:O	2:D:434:GLY:HA3	2.13	0.48
1:E:134:ARG:HH11	2:F:40:VAL:HA	1.78	0.48
2:F:46:LYS:HE3	2:F:46:LYS:HB2	1.61	0.48
2:F:152:THR:HG22	2:F:177:SER:HB2	1.95	0.48
2:F:231:GLU:HG2	2:F:254:ASN:HD22	1.78	0.48
2:H:189:GLN:C	2:H:190:HIS:ND1	2.71	0.48
2:H:454:GLY:O	2:H:457:TYR:HB2	2.12	0.48
2:J:546:PRO:HD3	2:J:584:THR:O	2.14	0.48
2:L:519:TRP:CZ3	2:L:567:HIS:ND1	2.82	0.48
2:L:578:ARG:H	2:L:578:ARG:HG3	1.44	0.48
1:M:128:LYS:HB2	1:M:133:ILE:CD1	2.43	0.48
2:N:419:ILE:CD1	2:N:446:ARG:HH22	2.26	0.48
1:O:48:THR:HG22	1:O:51:ILE:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:456:SER:CB	2:P:482:GLU:HB3	2.43	0.48
2:B:539:TYR:OH	1:C:146:GLU:HA	2.13	0.48
1:C:153:ARG:NH2	2:D:539:TYR:CE1	2.81	0.48
2:D:296:ARG:NH2	1:G:37:CYS:SG	2.87	0.48
2:D:305:LEU:O	2:D:305:LEU:HD23	2.13	0.48
2:D:454:GLY:O	2:D:457:TYR:HB2	2.14	0.48
2:F:590:GLU:O	2:F:591:PRO:C	2.57	0.48
1:I:111:LYS:O	1:I:115:ASP:HB2	2.12	0.48
2:J:454:GLY:O	2:J:457:TYR:HB2	2.14	0.48
2:J:519:TRP:CZ3	2:J:567:HIS:ND1	2.82	0.48
2:L:85:ARG:NH1	5:L:1101:PO4:O3	2.46	0.48
2:L:454:GLY:O	2:L:457:TYR:HB2	2.13	0.48
2:N:159:ILE:HD12	2:N:166:ILE:HD11	1.95	0.48
2:N:501:SER:HA	2:N:524:ARG:HB2	1.95	0.48
1:G:48:THR:CG2	1:G:51:ILE:HG12	2.44	0.48
1:G:137:PHE:HB3	2:H:17:VAL:CG2	2.43	0.48
2:H:364:LEU:HD21	2:H:386:TYR:O	2.13	0.48
2:J:57:MET:CE	2:J:62:THR:HG22	2.43	0.48
2:J:295:ILE:HG21	2:J:298:LEU:CD1	2.43	0.48
2:J:546:PRO:O	2:J:547:SER:HB2	2.13	0.48
2:L:398:ILE:O	2:L:402:LEU:HD12	2.12	0.48
2:N:398:ILE:C	2:N:400:THR:H	2.20	0.48
2:D:546:PRO:HD3	2:D:584:THR:O	2.13	0.48
1:E:153:ARG:HG2	1:E:157:TRP:CZ3	2.49	0.48
2:F:101:THR:HG22	2:F:128:ASP:HB3	1.95	0.48
2:F:127:LEU:HD21	2:F:131:ARG:NH2	2.28	0.48
2:F:248:PHE:C	2:F:248:PHE:CD2	2.91	0.48
2:F:446:ARG:HG2	2:F:447:GLN:N	2.28	0.48
2:H:316:LYS:O	2:H:318:PRO:HD3	2.14	0.48
2:H:431:LEU:CD2	2:H:432:LEU:HD23	2.43	0.48
2:J:456:SER:CB	2:J:482:GLU:HB3	2.43	0.48
1:A:105:ALA:HB3	1:A:114:LEU:HD13	1.94	0.48
2:B:519:TRP:CD1	2:B:519:TRP:C	2.90	0.48
2:D:465:VAL:HG11	2:D:468:MET:HG3	1.96	0.48
2:H:21:ILE:HD12	2:H:24:VAL:HB	1.95	0.48
2:H:542:ILE:HD11	2:H:588:LEU:HD12	1.96	0.48
1:I:26:SER:HB3	1:I:29:ILE:HG13	1.96	0.48
2:J:121:ARG:NH2	5:J:1103:PO4:O4	2.47	0.48
2:L:289:PHE:HD1	2:L:316:LYS:HD2	1.73	0.48
2:L:398:ILE:C	2:L:400:THR:H	2.22	0.48
2:L:456:SER:HB2	2:L:482:GLU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:477:ASP:N	2:L:477:ASP:OD1	2.47	0.48
1:M:11:SER:HA	1:M:45:PRO:HA	1.96	0.48
2:N:419:ILE:HD11	2:N:446:ARG:HH22	1.79	0.48
2:N:545:ILE:HG22	2:N:546:PRO:CD	2.44	0.48
2:P:176:PHE:CZ	2:P:204:PHE:CZ	3.02	0.48
2:D:176:PHE:CZ	2:D:204:PHE:CZ	3.01	0.48
1:E:134:ARG:CZ	1:E:141:ASN:HD22	2.26	0.48
2:H:492:LYS:HZ1	2:H:516:ARG:NH1	2.10	0.48
2:L:251:GLY:O	2:L:278:SER:HB2	2.13	0.48
2:L:538:PRO:O	2:L:539:TYR:HB2	2.13	0.48
2:N:380:LEU:HD12	2:N:383:MET:HE2	1.94	0.48
2:N:392:ASN:HD21	2:N:424:LEU:HA	1.77	0.48
1:A:48:THR:HG22	1:A:51:ILE:CB	2.43	0.48
2:B:398:ILE:C	2:B:400:THR:H	2.22	0.48
2:D:321:GLU:HA	2:D:344:LEU:HA	1.96	0.48
2:F:96:TRP:O	2:F:578:ARG:NH2	2.42	0.48
2:F:523:TYR:CE2	2:F:568:ILE:HD11	2.49	0.48
1:G:6:ILE:HG22	1:G:7:VAL:N	2.28	0.48
2:H:170:LEU:HB2	2:H:198:ASN:HB3	1.95	0.48
2:H:365:VAL:HG21	2:H:387:VAL:HA	1.95	0.48
2:H:477:ASP:OD2	2:H:501:SER:OG	2.23	0.48
2:H:542:ILE:HD12	2:H:542:ILE:C	2.39	0.48
1:K:11:SER:HA	1:K:45:PRO:HA	1.95	0.48
2:L:127:LEU:HD21	2:L:131:ARG:NH2	2.29	0.48
2:L:419:ILE:HD11	2:L:446:ARG:HH22	1.79	0.48
2:N:387:VAL:O	2:N:413:LEU:HD22	2.14	0.48
2:P:521:GLN:HG3	2:P:567:HIS:CD2	2.48	0.48
2:B:519:TRP:CZ3	2:B:567:HIS:ND1	2.82	0.47
2:D:367:GLN:O	2:D:371:ILE:HG22	2.14	0.47
1:E:45:PRO:CB	2:L:291:PHE:HA	2.44	0.47
1:E:48:THR:HG23	1:E:51:ILE:H	1.79	0.47
2:H:318:PRO:C	2:H:320:LEU:H	2.22	0.47
2:H:412:LEU:HD12	2:H:445:LEU:CA	2.44	0.47
2:J:545:ILE:HG22	2:J:546:PRO:CD	2.43	0.47
2:L:80:LEU:HB2	2:L:122:MET:HE1	1.96	0.47
2:L:298:LEU:HD23	2:L:300:LEU:HD11	1.95	0.47
2:L:367:GLN:O	2:L:371:ILE:HG22	2.14	0.47
2:L:419:ILE:O	2:L:420:THR:C	2.56	0.47
2:N:191:ASN:ND2	2:N:194:LEU:H	2.12	0.47
2:N:443:PHE:CE2	2:N:445:LEU:HD11	2.48	0.47
1:O:134:ARG:HH11	2:P:40:VAL:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:468:MET:HE1	2:P:483:PHE:CE1	2.49	0.47
2:B:227:VAL:HG13	2:B:228:GLY:H	1.78	0.47
2:D:295:ILE:HG21	2:D:298:LEU:CD1	2.43	0.47
2:H:247:GLU:HA	2:H:274:ARG:O	2.14	0.47
2:H:364:LEU:HD22	2:H:365:VAL:HG22	1.96	0.47
1:I:48:THR:CG2	1:I:51:ILE:HG12	2.43	0.47
2:J:164:ARG:HD2	2:N:112:ARG:CZ	2.45	0.47
2:J:298:LEU:HB2	2:J:320:LEU:HD11	1.96	0.47
2:L:456:SER:CB	2:L:482:GLU:HB3	2.44	0.47
2:N:289:PHE:HD1	2:N:316:LYS:HD2	1.76	0.47
2:N:351:ARG:HG3	2:N:351:ARG:O	2.14	0.47
2:N:519:TRP:CZ3	2:N:567:HIS:ND1	2.82	0.47
1:C:48:THR:CG2	1:C:51:ILE:HG12	2.44	0.47
2:D:232:ILE:HD12	2:D:252:SER:H	1.79	0.47
2:D:477:ASP:OD2	2:D:504:ALA:HB2	2.12	0.47
2:D:590:GLU:O	2:D:591:PRO:C	2.56	0.47
1:G:120:THR:O	1:G:124:MET:HG3	2.14	0.47
2:H:114:LEU:O	2:H:136:ARG:NH1	2.48	0.47
2:H:204:PHE:O	2:H:206:LYS:N	2.47	0.47
2:J:63:ALA:HB1	2:J:67:ARG:HD2	1.96	0.47
2:J:247:GLU:HA	2:J:274:ARG:O	2.14	0.47
2:J:248:PHE:C	2:J:248:PHE:CD2	2.92	0.47
1:M:48:THR:CG2	1:M:51:ILE:HG12	2.45	0.47
2:N:171:MET:O	2:N:174:SER:HB2	2.14	0.47
2:N:176:PHE:CZ	2:N:204:PHE:CZ	3.02	0.47
2:N:490:LEU:HD11	2:N:493:LEU:HD13	1.96	0.47
2:D:501:SER:HA	2:D:524:ARG:HB2	1.96	0.47
2:D:565:PRO:HG2	3:R:201:LEU:HD21	1.97	0.47
2:F:297:LYS:HE3	2:F:297:LYS:HB2	1.65	0.47
2:H:280:MET:O	2:H:280:MET:HG2	2.14	0.47
1:I:11:SER:HA	1:I:45:PRO:HA	1.95	0.47
2:J:446:ARG:HG2	2:J:447:GLN:N	2.29	0.47
2:L:545:ILE:HG22	2:L:546:PRO:N	2.30	0.47
2:N:247:GLU:HA	2:N:274:ARG:O	2.14	0.47
2:N:297:LYS:HB2	2:N:297:LYS:HE3	1.62	0.47
2:P:440:ARG:HB3	2:P:467:TRP:CE3	2.45	0.47
2:B:198:ASN:C	2:B:198:ASN:OD1	2.57	0.47
2:B:422:LEU:HB3	2:B:423:PRO:HD3	1.96	0.47
2:B:465:VAL:HG11	2:B:468:MET:HG3	1.95	0.47
2:D:289:PHE:HD1	2:D:316:LYS:HD2	1.73	0.47
1:E:105:ALA:HB2	1:E:113:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLU:O	1:E:136:THR:HG23	2.15	0.47
2:F:138:ASP:OD2	2:F:164:ARG:HG3	2.14	0.47
2:F:198:ASN:C	2:F:198:ASN:OD1	2.56	0.47
2:H:89:PHE:CE2	4:H:4100:OGK:H04A	2.50	0.47
2:H:315:GLN:HG3	2:H:340:TYR:CE1	2.50	0.47
1:K:26:SER:C	1:K:28:THR:H	2.21	0.47
1:K:134:ARG:CZ	1:K:141:ASN:HD22	2.28	0.47
2:N:412:LEU:C	2:N:412:LEU:HD12	2.40	0.47
2:F:375:GLN:HG2	2:F:401:TYR:CE1	2.49	0.47
2:H:53:GLU:O	2:H:75:LEU:HD22	2.15	0.47
2:H:262:LYS:HD2	2:H:263:TYR:CE1	2.49	0.47
2:H:316:LYS:C	2:H:318:PRO:HD3	2.40	0.47
1:I:52:LEU:O	1:I:52:LEU:HD12	2.14	0.47
2:P:477:ASP:OD1	2:P:477:ASP:N	2.48	0.47
2:P:543:GLU:OE2	2:P:578:ARG:HD3	2.13	0.47
1:C:26:SER:HB3	1:C:29:ILE:HG13	1.96	0.47
1:C:52:LEU:O	1:C:52:LEU:HD12	2.14	0.47
2:D:95:ASN:O	2:D:582:PRO:HG3	2.15	0.47
2:D:299:ASP:C	2:D:301:LEU:H	2.23	0.47
2:D:320:LEU:HD21	2:D:323:LEU:HB2	1.97	0.47
2:D:468:MET:HE1	2:D:483:PHE:CE1	2.50	0.47
2:H:52:ARG:NH1	2:H:72:PHE:HZ	2.11	0.47
2:H:153:THR:HG23	2:H:177:SER:O	2.15	0.47
2:H:505:ILE:C	2:H:507:ALA:N	2.73	0.47
2:H:532:LEU:O	2:H:534:GLN:N	2.48	0.47
2:J:285:MET:N	2:J:286:PRO:CD	2.78	0.47
2:J:590:GLU:O	2:J:591:PRO:C	2.57	0.47
2:L:247:GLU:HA	2:L:274:ARG:O	2.13	0.47
2:L:339:GLN:HA	2:L:342:LYS:HE2	1.96	0.47
2:L:543:GLU:OE2	2:L:578:ARG:HD3	2.15	0.47
2:P:398:ILE:O	2:P:402:LEU:HD12	2.14	0.47
2:P:431:LEU:C	2:P:431:LEU:HD12	2.39	0.47
2:P:546:PRO:O	2:P:547:SER:HB2	2.15	0.47
2:B:80:LEU:HB2	2:B:122:MET:HE1	1.97	0.47
2:B:272:LEU:C	2:B:272:LEU:CD2	2.88	0.47
2:B:468:MET:CE	2:B:470:LEU:HD11	2.45	0.47
1:E:26:SER:C	1:E:28:THR:H	2.22	0.47
1:E:26:SER:HB3	1:E:29:ILE:HG13	1.97	0.47
2:F:113:GLN:HE22	2:L:192:THR:HG21	1.80	0.47
1:G:105:ALA:HB2	1:G:113:LEU:HD23	1.97	0.47
2:H:352:GLY:O	2:H:353:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:367:GLN:OE1	2:H:367:GLN:CA	2.62	0.47
1:I:35:ASP:CB	2:N:243:ALA:HB1	2.42	0.47
2:J:223:VAL:O	2:J:245:LEU:HD12	2.14	0.47
2:J:472:TYR:CD2	2:J:497:GLY:O	2.68	0.47
2:L:519:TRP:CD1	2:L:519:TRP:C	2.90	0.47
2:P:298:LEU:HB2	2:P:320:LEU:HD11	1.96	0.47
2:P:321:GLU:HA	2:P:344:LEU:HA	1.97	0.47
2:P:444:TYR:HA	2:P:471:GLY:CA	2.37	0.47
1:C:48:THR:HG22	1:C:51:ILE:CB	2.44	0.47
2:D:190:HIS:HE1	2:H:110:ASN:HA	1.80	0.47
2:D:289:PHE:HB2	2:D:290:PRO:HD3	1.97	0.47
2:F:400:THR:O	2:F:403:LYS:HE2	2.15	0.47
1:G:58:TYR:CE1	1:G:62:HIS:CE1	3.03	0.47
2:H:168:THR:HB	2:H:196:VAL:HG13	1.96	0.47
2:H:187:LEU:HA	2:H:187:LEU:HD23	1.72	0.47
2:H:468:MET:HG3	2:H:490:LEU:HD21	1.96	0.47
2:J:289:PHE:HD1	2:J:316:LYS:HD2	1.77	0.47
2:J:325:THR:O	2:J:349:ILE:HA	2.15	0.47
1:M:132:GLU:O	1:M:136:THR:HG23	2.14	0.47
2:N:20:VAL:O	2:N:24:VAL:HG23	2.15	0.47
2:F:440:ARG:HB3	2:F:467:TRP:CE3	2.48	0.47
2:H:58:ALA:HA	2:H:81:LYS:HD2	1.97	0.47
1:I:134:ARG:NH1	2:J:40:VAL:HA	2.30	0.47
2:J:310:HIS:O	2:J:314:ILE:CG1	2.63	0.47
2:L:297:LYS:HB2	2:L:297:LYS:HE3	1.64	0.47
2:P:80:LEU:HB2	2:P:122:MET:HE1	1.97	0.47
2:D:477:ASP:OD1	2:D:477:ASP:N	2.47	0.46
2:F:320:LEU:HD21	2:F:323:LEU:HB2	1.96	0.46
1:G:134:ARG:HH11	2:H:40:VAL:HA	1.80	0.46
2:H:197:LEU:O	2:H:225:VAL:HA	2.15	0.46
2:H:230:PHE:HD1	2:H:235:LEU:HD21	1.78	0.46
2:H:284:GLU:O	2:H:287:ILE:HG23	2.15	0.46
1:I:91:MET:O	1:I:93:ILE:HG12	2.14	0.46
2:J:80:LEU:HB2	2:J:122:MET:HE1	1.97	0.46
2:J:191:ASN:ND2	2:J:194:LEU:H	2.11	0.46
2:L:523:TYR:CE2	2:L:568:ILE:HD11	2.50	0.46
2:L:546:PRO:O	2:L:547:SER:HB2	2.15	0.46
1:M:137:PHE:HD1	2:N:17:VAL:CG2	2.27	0.46
2:B:357:GLY:HA2	2:B:415:ARG:NH2	2.12	0.46
2:D:431:LEU:C	2:D:431:LEU:HD12	2.39	0.46
2:F:159:ILE:HG13	2:F:160:VAL:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:PRO:O	2:H:35:ASP:HB2	2.16	0.46
2:H:78:LEU:CD1	2:H:79:LYS:H	2.11	0.46
2:H:92:ILE:HG23	2:H:93:PRO:HD2	1.97	0.46
2:J:533:MET:HE2	2:J:533:MET:HA	1.97	0.46
1:K:108:LEU:HD12	1:K:110:ILE:CD1	2.40	0.46
1:M:128:LYS:HB3	1:M:132:GLU:HB2	1.96	0.46
2:P:519:TRP:CZ3	2:P:567:HIS:ND1	2.83	0.46
2:P:519:TRP:HH2	2:P:567:HIS:CE1	2.32	0.46
1:E:6:ILE:HG22	1:E:7:VAL:N	2.30	0.46
2:F:380:LEU:HD12	2:F:383:MET:HE2	1.97	0.46
2:F:396:GLU:HG2	2:F:430:SER:OG	2.15	0.46
2:H:495:MET:HE3	2:H:498:CYS:CB	2.44	0.46
2:J:396:GLU:HG2	2:J:430:SER:OG	2.16	0.46
2:L:65:PRO:HA	2:L:103:TRP:CZ3	2.50	0.46
2:P:85:ARG:NH1	5:P:1101:PO4:O3	2.48	0.46
2:P:311:CYS:CB	2:P:336:VAL:HG21	2.46	0.46
2:P:373:LEU:HD12	2:P:377:CYS:SG	2.54	0.46
2:B:456:SER:HB2	2:B:482:GLU:HB3	1.98	0.46
2:B:545:ILE:HG22	2:B:546:PRO:CD	2.45	0.46
2:D:380:LEU:HD12	2:D:383:MET:HE2	1.98	0.46
1:E:137:PHE:HD1	2:F:17:VAL:HG21	1.79	0.46
2:F:266:LEU:HD13	2:F:266:LEU:HA	1.81	0.46
1:G:91:MET:O	1:G:93:ILE:N	2.47	0.46
2:H:148:CYS:O	2:H:174:SER:HA	2.16	0.46
2:H:469:LEU:HA	2:H:494:GLU:O	2.14	0.46
2:J:358:MET:HE3	2:J:363:GLY:O	2.16	0.46
1:M:58:TYR:CE1	1:M:62:HIS:CE1	3.04	0.46
2:N:227:VAL:HG13	2:N:228:GLY:N	2.30	0.46
2:N:338:ALA:O	2:N:376:GLY:HA3	2.15	0.46
2:N:490:LEU:O	2:N:514:SER:HB2	2.14	0.46
2:P:285:MET:N	2:P:286:PRO:CD	2.79	0.46
2:B:85:ARG:NH1	5:B:1101:PO4:O3	2.49	0.46
1:C:159:PHE:O	1:C:160:GLU:CB	2.52	0.46
1:E:42:VAL:O	1:E:42:VAL:HG22	2.15	0.46
1:G:48:THR:HG22	1:G:51:ILE:CB	2.45	0.46
1:G:48:THR:HG23	1:G:51:ILE:H	1.80	0.46
2:H:450:LEU:HD21	2:H:455:LEU:N	2.30	0.46
2:J:310:HIS:O	2:J:314:ILE:HG12	2.16	0.46
2:J:373:LEU:HD12	2:J:377:CYS:SG	2.55	0.46
2:L:143:LEU:CD2	2:L:159:ILE:HD13	2.43	0.46
2:L:232:ILE:HD12	2:L:252:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:310:HIS:O	2:L:314:ILE:CG1	2.64	0.46
2:L:422:LEU:HB3	2:L:423:PRO:HD3	1.97	0.46
2:L:446:ARG:HG2	2:L:447:GLN:N	2.31	0.46
1:M:99:PHE:CB	2:N:15:ALA:HB1	2.45	0.46
2:N:398:ILE:O	2:N:402:LEU:HD12	2.16	0.46
2:N:468:MET:CE	2:N:470:LEU:HD11	2.46	0.46
2:N:590:GLU:O	2:N:591:PRO:C	2.57	0.46
2:P:235:LEU:O	2:P:238:PHE:HB3	2.14	0.46
2:B:270:ARG:O	1:O:107:TYR:HE1	1.98	0.46
1:C:153:ARG:HG2	1:C:157:TRP:CZ3	2.50	0.46
2:D:285:MET:N	2:D:286:PRO:CD	2.79	0.46
2:F:191:ASN:ND2	2:F:194:LEU:H	2.13	0.46
4:F:3100:OGK:C18	4:F:3100:OGK:N08	2.77	0.46
1:G:125:ILE:HD11	2:H:44:TRP:CH2	2.51	0.46
2:H:29:THR:HG23	2:H:30:ASP:N	2.31	0.46
2:H:298:LEU:HD13	2:H:300:LEU:HD11	1.96	0.46
2:H:395:LEU:HB3	2:H:427:GLY:C	2.40	0.46
1:I:106:ASN:ND2	2:J:23:GLN:NE2	2.63	0.46
2:J:419:ILE:CD1	2:J:446:ARG:HH22	2.28	0.46
2:L:46:LYS:HE3	2:L:46:LYS:HB2	1.60	0.46
2:D:299:ASP:OD2	2:D:301:LEU:HB2	2.16	0.46
2:F:344:LEU:HD23	2:F:380:LEU:HD21	1.98	0.46
2:F:456:SER:CB	2:F:482:GLU:HB3	2.46	0.46
1:G:160:GLU:HG3	2:H:52:ARG:NH2	2.18	0.46
2:J:46:LYS:HE3	2:J:46:LYS:HB2	1.55	0.46
2:L:367:GLN:CB	2:L:391:THR:HG22	2.39	0.46
2:B:367:GLN:CB	2:B:391:THR:HG22	2.41	0.46
2:B:539:TYR:CE2	1:C:145:PRO:HB2	2.51	0.46
1:E:91:MET:HE1	1:E:117:THR:HG22	1.98	0.46
2:J:294:GLN:NE2	1:M:107:TYR:OH	2.49	0.46
2:J:367:GLN:O	2:J:371:ILE:HG22	2.15	0.46
1:K:52:LEU:O	1:K:52:LEU:HD12	2.16	0.46
2:L:590:GLU:O	2:L:591:PRO:C	2.57	0.46
1:M:46:ASN:HB2	1:M:107:TYR:CZ	2.51	0.46
1:O:134:ARG:NH1	2:P:40:VAL:HA	2.31	0.46
2:B:191:ASN:ND2	2:B:194:LEU:H	2.11	0.46
2:B:253:LEU:CD1	2:B:280:MET:HB2	2.42	0.46
2:B:289:PHE:N	2:B:290:PRO:CD	2.79	0.46
2:B:398:ILE:O	2:B:402:LEU:HD12	2.16	0.46
1:C:137:PHE:HD1	2:D:17:VAL:HG21	1.79	0.46
2:D:419:ILE:HD11	2:D:446:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:101:THR:N	2:F:102:PRO:CD	2.79	0.46
2:F:121:ARG:NH2	5:F:1103:PO4:O4	2.48	0.46
2:H:291:PHE:HD2	2:H:291:PHE:N	2.11	0.46
2:J:412:LEU:C	2:J:412:LEU:HD12	2.41	0.46
2:L:101:THR:CG2	2:L:128:ASP:OD1	2.63	0.46
2:L:431:LEU:C	2:L:431:LEU:HD12	2.41	0.46
2:P:545:ILE:HG22	2:P:546:PRO:CD	2.45	0.46
2:F:392:ASN:HD21	2:F:424:LEU:HA	1.80	0.46
2:H:253:LEU:HD12	2:H:280:MET:HB2	1.97	0.46
2:H:390:ILE:CD1	2:H:410:LEU:HD11	2.45	0.46
2:H:501:SER:HB2	2:H:503:ARG:NH2	2.31	0.46
2:J:538:PRO:O	2:J:539:TYR:HB2	2.16	0.46
2:L:325:THR:O	2:L:349:ILE:HA	2.16	0.46
1:O:159:PHE:O	1:O:160:GLU:CB	2.51	0.46
2:P:198:ASN:C	2:P:198:ASN:OD1	2.59	0.46
2:P:446:ARG:HG2	2:P:447:GLN:N	2.31	0.46
2:D:412:LEU:HD12	2:D:412:LEU:O	2.15	0.45
2:F:468:MET:CE	2:F:470:LEU:HD11	2.46	0.45
1:G:26:SER:HB3	1:G:29:ILE:HG13	1.97	0.45
2:H:80:LEU:HD11	2:H:103:TRP:CD2	2.51	0.45
2:H:129:LEU:HD23	2:H:155:GLY:HA3	1.98	0.45
2:H:233:LEU:HD21	2:H:262:LYS:HG2	1.97	0.45
2:H:408:PHE:C	2:H:409:ARG:HG2	2.41	0.45
1:I:102:ILE:CG2	1:I:118:CYS:SG	3.03	0.45
2:J:20:VAL:O	2:J:24:VAL:HG23	2.16	0.45
2:N:339:GLN:HA	2:N:342:LYS:HE2	1.98	0.45
2:N:545:ILE:HG22	2:N:546:PRO:HD2	1.98	0.45
2:N:546:PRO:HB2	2:N:547:SER:H	1.67	0.45
2:P:542:ILE:CD1	2:P:588:LEU:HD12	2.32	0.45
2:P:590:GLU:O	2:P:591:PRO:C	2.58	0.45
2:B:289:PHE:HD1	2:B:316:LYS:HD2	1.75	0.45
2:B:327:ASN:HD22	2:B:327:ASN:N	2.13	0.45
2:B:351:ARG:O	2:B:351:ARG:HG3	2.16	0.45
2:B:436:LYS:HE2	2:B:436:LYS:HB3	1.72	0.45
2:D:116:SER:CB	2:D:142:THR:HG23	2.40	0.45
2:F:398:ILE:HG23	2:F:402:LEU:HD11	1.97	0.45
2:H:111:LEU:C	2:H:113:GLN:N	2.74	0.45
2:H:365:VAL:CG2	2:H:388:SER:H	2.29	0.45
1:I:58:TYR:CE1	1:I:62:HIS:CE1	3.04	0.45
2:N:496:ARG:NH2	3:W:201:LEU:HD22	2.31	0.45
1:O:26:SER:C	1:O:28:THR:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:468:MET:CE	2:D:470:LEU:HD11	2.46	0.45
2:F:387:VAL:O	2:F:413:LEU:HD22	2.17	0.45
2:F:436:LYS:HE2	2:F:436:LYS:HB3	1.72	0.45
1:G:52:LEU:O	1:G:52:LEU:HD12	2.16	0.45
1:G:130:PRO:HG3	2:H:39:LEU:HB2	1.98	0.45
2:J:176:PHE:CZ	2:J:204:PHE:CZ	3.04	0.45
2:J:519:TRP:CD1	2:J:519:TRP:C	2.92	0.45
5:N:1102:PO4:O3	3:W:206:ARG:NH2	2.45	0.45
2:P:409:ARG:HD3	4:P:8100:OGK:H13A	1.98	0.45
1:A:141:ASN:C	1:A:141:ASN:OD1	2.58	0.45
2:B:101:THR:HG22	2:B:128:ASP:CB	2.46	0.45
1:C:26:SER:C	1:C:28:THR:H	2.25	0.45
2:D:96:TRP:O	2:D:578:ARG:NH2	2.42	0.45
1:E:159:PHE:O	1:E:160:GLU:CB	2.51	0.45
2:F:351:ARG:HG3	2:F:351:ARG:O	2.15	0.45
2:F:490:LEU:HD23	2:F:490:LEU:HA	1.74	0.45
1:G:93:ILE:HD12	1:G:97:THR:CG2	2.36	0.45
2:J:533:MET:C	2:J:535:MET:H	2.24	0.45
2:L:305:LEU:O	2:L:305:LEU:HD23	2.16	0.45
2:L:358:MET:HE3	2:L:363:GLY:O	2.16	0.45
2:L:380:LEU:HD12	2:L:383:MET:HE2	1.97	0.45
4:L:6100:OGK:C18	4:L:6100:OGK:N08	2.79	0.45
2:P:387:VAL:O	2:P:413:LEU:HD22	2.17	0.45
1:A:26:SER:C	1:A:28:THR:H	2.24	0.45
2:B:65:PRO:HA	2:B:103:TRP:CZ3	2.52	0.45
2:B:338:ALA:O	2:B:376:GLY:HA3	2.17	0.45
2:D:456:SER:CB	2:D:482:GLU:HB3	2.47	0.45
2:D:533:MET:C	2:D:535:MET:H	2.25	0.45
1:E:19:GLU:OE1	1:E:19:GLU:N	2.47	0.45
1:E:58:TYR:CE1	1:E:62:HIS:CE1	3.04	0.45
2:F:118:HIS:C	2:F:118:HIS:CD2	2.94	0.45
2:F:367:GLN:CB	2:F:391:THR:HG22	2.41	0.45
2:F:472:TYR:CD2	2:F:497:GLY:O	2.70	0.45
2:F:495:MET:HE3	2:F:495:MET:HB2	1.77	0.45
2:H:418:ARG:HB3	2:H:421:ASP:HB2	1.99	0.45
2:H:487:CYS:HB2	2:H:512:LEU:CD2	2.46	0.45
2:H:503:ARG:HG2	2:H:504:ALA:N	2.31	0.45
2:J:546:PRO:O	2:J:547:SER:CB	2.65	0.45
1:K:114:LEU:C	1:K:116:LEU:H	2.25	0.45
1:M:6:ILE:HG22	1:M:7:VAL:N	2.31	0.45
1:M:91:MET:SD	1:M:117:THR:HG22	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:137:PHE:CD1	2:N:17:VAL:CG2	2.99	0.45
2:N:255:GLU:HG3	2:N:255:GLU:O	2.16	0.45
2:P:523:TYR:CE2	2:P:568:ILE:HD11	2.52	0.45
1:E:10:SER:OG	1:E:11:SER:N	2.48	0.45
1:E:48:THR:CG2	1:E:51:ILE:HG12	2.46	0.45
1:E:134:ARG:NH1	2:F:40:VAL:HA	2.32	0.45
2:F:398:ILE:C	2:F:400:THR:H	2.25	0.45
2:F:519:TRP:HH2	2:F:567:HIS:CE1	2.34	0.45
2:L:159:ILE:HD12	2:L:166:ILE:HD11	1.98	0.45
1:M:91:MET:O	1:M:93:ILE:HG12	2.16	0.45
1:O:48:THR:HG23	1:O:51:ILE:H	1.82	0.45
1:O:91:MET:O	1:O:93:ILE:HG12	2.17	0.45
1:C:42:VAL:HA	1:C:43:PRO:HD3	1.79	0.45
2:D:127:LEU:HB2	2:N:126:ASP:HB3	1.99	0.45
2:D:327:ASN:HD22	2:D:327:ASN:N	2.15	0.45
2:D:446:ARG:HG2	2:D:447:GLN:N	2.32	0.45
2:F:456:SER:HB2	2:F:482:GLU:HB3	1.98	0.45
2:F:468:MET:HE1	2:F:483:PHE:CE1	2.52	0.45
2:H:351:ARG:HG3	2:H:359:GLU:OE2	2.16	0.45
1:I:125:ILE:HG23	1:I:133:ILE:CD1	2.39	0.45
2:J:127:LEU:HD21	2:J:131:ARG:NH2	2.32	0.45
2:L:563:GLU:HG3	2:L:563:GLU:O	2.17	0.45
2:N:440:ARG:HB3	2:N:467:TRP:CE3	2.51	0.45
2:N:446:ARG:HG2	2:N:447:GLN:N	2.32	0.45
2:P:285:MET:N	2:P:286:PRO:HD2	2.32	0.45
2:P:358:MET:HE3	2:P:363:GLY:O	2.15	0.45
2:B:289:PHE:HB2	2:B:290:PRO:HD3	1.97	0.45
2:B:351:ARG:HD3	2:B:413:LEU:HD11	1.98	0.45
2:B:545:ILE:HB	2:B:567:HIS:HB2	1.98	0.45
2:D:357:GLY:CA	2:D:415:ARG:HH22	2.14	0.45
2:D:400:THR:O	2:D:403:LYS:HE2	2.17	0.45
2:H:191:ASN:HD22	2:H:191:ASN:C	2.24	0.45
2:H:387:VAL:HG12	2:H:390:ILE:HD13	1.95	0.45
1:I:46:ASN:HB2	1:I:107:TYR:CZ	2.52	0.45
1:I:102:ILE:HG12	1:I:117:THR:CB	2.47	0.45
2:J:187:LEU:HD23	2:J:187:LEU:HA	1.82	0.45
1:K:6:ILE:HG22	1:K:7:VAL:N	2.32	0.45
2:L:419:ILE:O	2:L:420:THR:O	2.34	0.45
1:M:102:ILE:CB	2:N:20:VAL:HG21	2.47	0.45
2:N:468:MET:HE1	2:N:483:PHE:HE1	1.81	0.45
3:X:201:LEU:HD23	3:X:201:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:MET:HE3	2:B:363:GLY:O	2.17	0.45
2:D:289:PHE:N	2:D:290:PRO:CD	2.80	0.45
2:D:523:TYR:CE2	2:D:568:ILE:HD11	2.52	0.45
1:G:42:VAL:O	1:G:42:VAL:HG22	2.17	0.45
2:H:91:LEU:O	2:H:567:HIS:HE1	2.00	0.45
2:H:343:GLN:CD	2:H:343:GLN:N	2.74	0.45
2:H:362:GLU:C	2:H:364:LEU:H	2.25	0.45
1:I:102:ILE:HG12	1:I:117:THR:HB	1.99	0.45
2:N:407:ASP:OD1	2:N:440:ARG:HD2	2.17	0.45
1:O:137:PHE:HD1	2:P:17:VAL:CG2	2.29	0.45
2:B:477:ASP:OD1	2:B:477:ASP:N	2.46	0.45
1:C:6:ILE:HG22	1:C:7:VAL:N	2.32	0.45
2:D:159:ILE:HD12	2:D:166:ILE:HD11	1.99	0.45
2:D:351:ARG:HG3	2:D:351:ARG:O	2.16	0.45
2:F:89:PHE:CD1	3:S:206:ARG:HA	2.52	0.45
2:F:546:PRO:O	2:F:547:SER:HB2	2.17	0.45
1:G:42:VAL:HA	1:G:43:PRO:HD3	1.79	0.45
2:H:53:GLU:O	2:H:75:LEU:CD2	2.65	0.45
2:H:96:TRP:HE3	2:H:97:GLY:N	2.15	0.45
2:H:362:GLU:O	2:H:363:GLY:C	2.60	0.45
1:I:26:SER:C	1:I:28:THR:H	2.25	0.45
2:L:55:VAL:CG2	2:L:75:LEU:HD21	2.44	0.45
2:L:544:LEU:HD11	2:L:588:LEU:HD11	1.99	0.45
1:M:99:PHE:CZ	2:N:17:VAL:HG22	2.52	0.45
2:N:429:ARG:O	2:N:433:ILE:HD12	2.17	0.45
1:O:6:ILE:HG22	1:O:7:VAL:N	2.32	0.45
2:P:380:LEU:HD12	2:P:383:MET:HE2	1.98	0.45
2:B:311:CYS:CB	2:B:336:VAL:HG21	2.47	0.44
2:D:490:LEU:HD11	2:D:493:LEU:HD13	1.98	0.44
2:D:546:PRO:O	2:D:547:SER:HB2	2.16	0.44
2:D:578:ARG:H	2:D:578:ARG:HG3	1.46	0.44
2:F:20:VAL:O	2:F:24:VAL:HG23	2.18	0.44
2:F:251:GLY:O	2:F:278:SER:HB2	2.17	0.44
2:H:110:ASN:C	2:H:111:LEU:HD23	2.43	0.44
2:H:467:TRP:HZ3	2:H:494:GLU:HG3	1.82	0.44
2:J:285:MET:N	2:J:286:PRO:HD2	2.32	0.44
2:J:490:LEU:HD23	2:J:490:LEU:HA	1.79	0.44
1:K:42:VAL:HA	1:K:43:PRO:HD3	1.81	0.44
1:K:48:THR:CG2	1:K:51:ILE:HG12	2.48	0.44
2:N:367:GLN:CB	2:N:391:THR:HG22	2.37	0.44
2:N:398:ILE:HG23	2:N:402:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:120:ARG:NH2	5:P:1103:PO4:O4	2.48	0.44
2:P:339:GLN:HA	2:P:342:LYS:HE2	1.99	0.44
2:B:59:LEU:O	2:B:62:THR:HB	2.17	0.44
2:B:392:ASN:HD21	2:B:424:LEU:HA	1.82	0.44
2:B:419:ILE:O	2:B:420:THR:O	2.35	0.44
2:B:533:MET:CE	2:B:588:LEU:HD13	2.47	0.44
1:E:153:ARG:NH2	2:F:539:TYR:CE1	2.85	0.44
2:F:544:LEU:HD11	2:F:588:LEU:HD11	2.00	0.44
2:H:97:GLY:HA3	2:H:123:ILE:HD11	1.98	0.44
2:J:321:GLU:HA	2:J:344:LEU:HA	1.99	0.44
2:L:373:LEU:HD12	2:L:377:CYS:SG	2.57	0.44
2:L:443:PHE:CE2	2:L:445:LEU:HD11	2.52	0.44
2:L:468:MET:CE	2:L:470:LEU:HD11	2.48	0.44
2:N:46:LYS:HB2	2:N:46:LYS:HE3	1.54	0.44
3:W:201:LEU:HA	3:W:202:PRO:HD3	1.83	0.44
2:P:367:GLN:CB	2:P:391:THR:HG22	2.42	0.44
2:P:375:GLN:HG2	2:P:401:TYR:CE1	2.52	0.44
2:D:419:ILE:CD1	2:D:446:ARG:HH22	2.29	0.44
2:D:521:GLN:HG3	2:D:567:HIS:CD2	2.50	0.44
2:F:545:ILE:HG22	2:F:546:PRO:CD	2.47	0.44
2:H:87:ALA:HB2	2:H:92:ILE:CG1	2.47	0.44
2:H:409:ARG:HA	2:H:442:ALA:O	2.18	0.44
2:H:410:LEU:HD13	2:H:411:VAL:O	2.18	0.44
2:H:495:MET:HE2	2:H:495:MET:HB3	1.83	0.44
2:N:519:TRP:HH2	2:N:567:HIS:CE1	2.35	0.44
1:O:26:SER:HB3	1:O:29:ILE:HG13	1.98	0.44
1:O:58:TYR:CE1	1:O:62:HIS:CE1	3.05	0.44
2:P:96:TRP:O	2:P:578:ARG:NH2	2.44	0.44
2:P:412:LEU:C	2:P:412:LEU:HD12	2.42	0.44
2:P:545:ILE:HG22	2:P:546:PRO:HD2	1.99	0.44
2:B:546:PRO:HB2	2:B:547:SER:H	1.68	0.44
2:D:351:ARG:HD3	2:D:413:LEU:HD11	1.98	0.44
2:D:545:ILE:HB	2:D:567:HIS:HB2	1.99	0.44
4:D:2100:OGK:H18A	4:D:2100:OGK:N08	2.26	0.44
1:E:107:TYR:CD1	2:L:270:ARG:HB3	2.52	0.44
2:F:419:ILE:CD1	2:F:446:ARG:HH22	2.31	0.44
2:H:423:PRO:HA	2:H:449:GLY:O	2.18	0.44
2:J:380:LEU:HD23	2:J:380:LEU:HA	1.79	0.44
2:L:191:ASN:ND2	2:L:194:LEU:H	2.12	0.44
2:L:338:ALA:O	2:L:376:GLY:HA3	2.17	0.44
2:L:400:THR:O	2:L:403:LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:198:ASN:C	2:N:198:ASN:OD1	2.60	0.44
2:P:101:THR:HG22	2:P:128:ASP:CB	2.47	0.44
2:P:168:THR:CB	2:P:196:VAL:HG13	2.26	0.44
2:P:396:GLU:HG2	2:P:430:SER:OG	2.16	0.44
2:D:533:MET:CE	2:D:588:LEU:HD13	2.47	0.44
2:H:97:GLY:CA	2:H:123:ILE:CD1	2.96	0.44
2:H:101:THR:HB	2:H:102:PRO:HD3	1.98	0.44
2:H:208:SER:HA	2:H:209:PRO:HD2	1.82	0.44
1:I:148:GLU:HG2	1:I:152:ARG:HH12	1.83	0.44
2:J:304:LEU:HD12	2:J:304:LEU:HA	1.71	0.44
2:J:338:ALA:O	2:J:376:GLY:HA3	2.17	0.44
2:J:419:ILE:O	2:J:420:THR:O	2.36	0.44
2:J:539:TYR:OH	1:K:146:GLU:HA	2.18	0.44
1:K:114:LEU:C	1:K:116:LEU:N	2.73	0.44
2:N:57:MET:CE	2:N:62:THR:HG22	2.43	0.44
1:O:137:PHE:CD1	2:P:17:VAL:CG2	3.01	0.44
2:B:111:LEU:C	2:B:113:GLN:H	2.26	0.44
2:D:297:LYS:HB2	2:D:297:LYS:HE3	1.68	0.44
2:D:344:LEU:HD23	2:D:380:LEU:HD21	1.98	0.44
1:E:141:ASN:OD1	1:E:141:ASN:C	2.61	0.44
2:H:511:LYS:HB2	2:H:511:LYS:HE2	1.66	0.44
2:H:535:MET:HG2	2:H:535:MET:O	2.17	0.44
2:J:85:ARG:NH1	5:J:1101:PO4:O3	2.50	0.44
2:J:299:ASP:OD2	2:J:301:LEU:HB2	2.18	0.44
2:J:392:ASN:HD21	2:J:424:LEU:HA	1.82	0.44
4:J:5100:OGK:C18	4:J:5100:OGK:N08	2.79	0.44
2:N:231:GLU:HG2	2:N:254:ASN:HD22	1.82	0.44
2:P:65:PRO:HB3	2:P:103:TRP:CE3	2.52	0.44
2:P:314:ILE:HD11	2:P:329:ILE:HD11	1.99	0.44
2:P:538:PRO:O	2:P:539:TYR:HB2	2.18	0.44
1:A:137:PHE:HD1	2:B:17:VAL:CG2	2.31	0.44
2:B:299:ASP:C	2:B:301:LEU:H	2.25	0.44
2:D:75:LEU:HD23	2:D:75:LEU:HA	1.81	0.44
2:F:55:VAL:CG2	2:F:75:LEU:HD21	2.48	0.44
2:H:225:VAL:HG21	2:H:238:PHE:CZ	2.53	0.44
2:H:423:PRO:CB	2:H:425:ASP:OD2	2.65	0.44
1:I:153:ARG:NH2	2:J:539:TYR:CE1	2.86	0.44
2:J:263:TYR:O	2:J:266:LEU:HD23	2.18	0.44
1:K:48:THR:HG22	1:K:51:ILE:CB	2.47	0.44
2:L:321:GLU:HA	2:L:344:LEU:HA	1.98	0.44
2:L:545:ILE:HG22	2:L:546:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:96:ALA:CB	2:N:14:VAL:CG1	2.95	0.44
1:M:99:PHE:HB2	2:N:15:ALA:HB1	2.00	0.44
2:N:83:LYS:O	2:N:121:ARG:NH1	2.46	0.44
2:N:382:TYR:CD2	2:N:407:ASP:HB3	2.53	0.44
2:P:419:ILE:O	2:P:420:THR:O	2.36	0.44
4:P:8100:OGK:C18	4:P:8100:OGK:N08	2.75	0.44
2:B:545:ILE:HG22	2:B:546:PRO:HD2	2.00	0.44
2:D:46:LYS:HB2	2:D:46:LYS:HE3	1.55	0.44
2:D:127:LEU:HD21	2:D:131:ARG:NH2	2.33	0.44
2:D:266:LEU:HA	2:D:266:LEU:HD13	1.80	0.44
2:D:319:ASN:HD21	1:G:43:PRO:HG3	1.82	0.44
1:E:129:THR:HB	1:E:130:PRO:HD2	2.00	0.44
2:F:230:PHE:O	2:F:252:SER:HB3	2.18	0.44
1:G:148:GLU:HG3	1:G:152:ARG:NH1	2.33	0.44
2:H:159:ILE:C	2:H:159:ILE:HD12	2.43	0.44
2:J:78:LEU:HD12	2:J:79:LYS:H	1.83	0.44
2:J:543:GLU:OE2	2:J:578:ARG:HD3	2.16	0.44
2:L:276:GLY:HA3	2:L:299:ASP:HB3	2.00	0.44
2:N:85:ARG:NH1	5:N:1101:PO4:O3	2.51	0.44
2:N:101:THR:N	2:N:102:PRO:CD	2.81	0.44
1:A:95:GLN:HG2	1:A:124:MET:HE1	1.99	0.44
1:C:58:TYR:CD2	1:C:113:LEU:HD13	2.52	0.44
2:D:57:MET:CE	2:D:62:THR:HG22	2.43	0.44
2:H:101:THR:N	2:H:102:PRO:CD	2.81	0.44
2:H:289:PHE:CE1	2:H:316:LYS:HD3	2.53	0.44
2:H:519:TRP:CH2	2:H:567:HIS:ND1	2.86	0.44
1:I:34:GLU:O	2:N:271:LYS:HE3	2.18	0.44
2:J:468:MET:CE	2:J:470:LEU:HD11	2.48	0.44
2:L:75:LEU:HD23	2:L:75:LEU:HA	1.83	0.44
2:L:176:PHE:CZ	2:L:204:PHE:CZ	3.06	0.44
1:O:52:LEU:O	1:O:52:LEU:HD12	2.17	0.44
2:B:18:ASP:OD2	2:B:43:ARG:HD2	2.17	0.43
2:B:446:ARG:HG2	2:B:447:GLN:N	2.33	0.43
1:C:48:THR:HG23	1:C:51:ILE:H	1.83	0.43
2:D:165:LYS:NZ	2:H:139:ASP:OD1	2.43	0.43
2:D:328:VAL:O	2:D:329:ILE:C	2.60	0.43
2:D:538:PRO:O	2:D:539:TYR:HB2	2.18	0.43
2:H:70:ARG:O	2:H:71:ARG:C	2.61	0.43
2:H:390:ILE:HD11	2:H:412:LEU:HD21	2.00	0.43
2:H:411:VAL:HG13	2:H:444:TYR:CB	2.40	0.43
1:I:108:LEU:HD12	1:I:110:ILE:CD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:545:ILE:HG22	2:J:546:PRO:HD2	1.99	0.43
2:N:184:LEU:HD23	2:N:184:LEU:HA	1.86	0.43
2:N:251:GLY:O	2:N:278:SER:HB2	2.18	0.43
2:N:305:LEU:O	2:N:305:LEU:HD23	2.18	0.43
2:N:436:LYS:HB3	2:N:436:LYS:HE2	1.75	0.43
2:P:125:SER:O	2:P:129:LEU:HD22	2.18	0.43
2:B:57:MET:CE	2:B:62:THR:HG22	2.48	0.43
2:B:373:LEU:HD12	2:B:377:CYS:SG	2.58	0.43
2:D:209:PRO:HD3	2:D:230:PHE:HE2	1.83	0.43
2:D:233:LEU:HD23	2:D:233:LEU:HA	1.78	0.43
2:F:111:LEU:C	2:F:113:GLN:H	2.27	0.43
2:F:419:ILE:O	2:F:420:THR:O	2.36	0.43
2:H:166:ILE:CG2	2:H:167:LYS:N	2.80	0.43
2:H:380:LEU:HD13	2:H:383:MET:HE2	1.99	0.43
2:H:501:SER:O	2:H:502:GLU:C	2.60	0.43
2:H:512:LEU:HA	2:H:513:PRO:HD3	1.71	0.43
1:I:10:SER:OG	1:I:11:SER:N	2.50	0.43
1:I:48:THR:HG22	1:I:51:ILE:CB	2.48	0.43
2:J:320:LEU:HD21	2:J:323:LEU:HB2	1.99	0.43
1:A:27:GLN:HA	1:A:30:ALA:HB3	2.00	0.43
2:F:578:ARG:H	2:F:578:ARG:HG3	1.51	0.43
2:H:76:ARG:C	2:H:114:LEU:HD12	2.43	0.43
2:H:196:VAL:O	2:H:196:VAL:HG22	2.17	0.43
2:H:243:ALA:C	2:H:245:LEU:N	2.76	0.43
2:H:266:LEU:HD13	2:H:267:VAL:H	1.82	0.43
1:K:137:PHE:HD1	2:L:17:VAL:CG2	2.31	0.43
2:L:116:SER:CB	2:L:142:THR:HG23	2.43	0.43
2:L:392:ASN:HD21	2:L:424:LEU:HA	1.84	0.43
1:M:26:SER:C	1:M:28:THR:H	2.25	0.43
2:N:519:TRP:HA	2:N:568:ILE:O	2.18	0.43
1:A:146:GLU:HA	2:D:539:TYR:OH	2.18	0.43
2:B:125:SER:O	2:B:129:LEU:HD22	2.19	0.43
2:B:235:LEU:O	2:B:238:PHE:HB3	2.18	0.43
4:B:1100:OGK:C18	4:B:1100:OGK:N08	2.79	0.43
2:D:85:ARG:NH1	5:D:1101:PO4:O3	2.51	0.43
2:H:542:ILE:HD12	2:H:543:GLU:N	2.33	0.43
1:M:26:SER:HB3	1:M:29:ILE:HG13	2.00	0.43
1:M:101:LEU:HD23	1:M:101:LEU:HA	1.80	0.43
2:N:431:LEU:HD12	2:N:431:LEU:C	2.43	0.43
2:N:546:PRO:O	2:N:547:SER:CB	2.66	0.43
1:A:6:ILE:HG22	1:A:7:VAL:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:THR:O	2:B:349:ILE:HA	2.19	0.43
4:B:1100:OGK:H18A	4:B:1100:OGK:N08	2.24	0.43
1:C:113:LEU:O	1:C:117:THR:CG2	2.65	0.43
3:R:201:LEU:HD23	3:R:201:LEU:HA	1.85	0.43
2:F:176:PHE:CZ	2:F:204:PHE:CZ	3.07	0.43
2:F:321:GLU:HA	2:F:344:LEU:HA	1.99	0.43
1:I:141:ASN:C	1:I:141:ASN:OD1	2.60	0.43
2:J:18:ASP:OD2	2:J:43:ARG:HD2	2.19	0.43
2:J:55:VAL:CG2	2:J:75:LEU:HD21	2.47	0.43
2:J:231:GLU:HG2	2:J:254:ASN:HD22	1.83	0.43
2:L:95:ASN:O	2:L:582:PRO:HG3	2.18	0.43
2:L:351:ARG:O	2:L:351:ARG:HG3	2.19	0.43
2:N:282:PRO:HA	2:N:285:MET:CE	2.43	0.43
2:N:289:PHE:N	2:N:290:PRO:CD	2.81	0.43
1:O:42:VAL:O	1:O:42:VAL:HG22	2.18	0.43
1:O:101:LEU:HD23	1:O:101:LEU:HA	1.88	0.43
1:O:128:LYS:HB2	1:O:133:ILE:CD1	2.49	0.43
2:P:289:PHE:N	2:P:290:PRO:CD	2.81	0.43
2:P:343:GLN:NE2	2:P:343:GLN:HA	2.33	0.43
2:B:59:LEU:HD22	2:B:61:TYR:H	1.83	0.43
2:D:227:VAL:HG13	2:D:228:GLY:H	1.80	0.43
2:D:485:ARG:HE	2:D:485:ARG:HB3	1.69	0.43
2:D:563:GLU:HG3	2:D:563:GLU:O	2.19	0.43
2:F:545:ILE:HG22	2:F:546:PRO:HD2	2.00	0.43
2:H:57:MET:HE2	2:H:60:CYS:HA	2.01	0.43
2:H:444:TYR:CD1	2:H:471:GLY:CA	3.01	0.43
2:J:308:GLU:O	2:J:312:THR:HG23	2.18	0.43
2:J:468:MET:HE1	2:J:483:PHE:CE1	2.53	0.43
1:K:58:TYR:CE1	1:K:62:HIS:CE1	3.06	0.43
2:L:152:THR:HG22	2:L:177:SER:HB2	2.01	0.43
2:L:311:CYS:CB	2:L:336:VAL:HG21	2.48	0.43
2:N:304:LEU:HD12	2:N:304:LEU:HA	1.71	0.43
2:B:157:LEU:O	2:B:157:LEU:HD12	2.19	0.43
1:C:8:LEU:HD23	1:C:42:VAL:CG1	2.49	0.43
2:D:542:ILE:CD1	2:D:588:LEU:HD12	2.29	0.43
2:D:546:PRO:O	2:D:547:SER:CB	2.67	0.43
1:E:107:TYR:HE1	2:L:270:ARG:O	2.02	0.43
2:F:358:MET:HE3	2:F:363:GLY:O	2.19	0.43
2:F:412:LEU:C	2:F:412:LEU:HD12	2.44	0.43
2:F:419:ILE:HD11	2:F:446:ARG:HH22	1.84	0.43
2:F:502:GLU:HG3	2:F:525:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:201:LEU:HD23	3:S:201:LEU:HA	1.79	0.43
2:H:207:ILE:H	2:H:207:ILE:HG12	1.59	0.43
2:H:301:LEU:HB3	2:H:302:TYR:CD2	2.53	0.43
2:H:367:GLN:OE1	2:H:367:GLN:HA	2.18	0.43
2:J:266:LEU:HA	2:J:266:LEU:HD13	1.79	0.43
2:J:407:ASP:OD1	2:J:440:ARG:HD2	2.19	0.43
2:L:304:LEU:HD12	2:L:304:LEU:HA	1.75	0.43
2:L:351:ARG:HD3	2:L:413:LEU:HD11	2.00	0.43
1:M:42:VAL:HA	1:M:43:PRO:HD3	1.79	0.43
1:A:48:THR:HG23	1:A:51:ILE:H	1.84	0.43
2:B:116:SER:CB	2:B:142:THR:HG23	2.40	0.43
2:D:59:LEU:O	2:D:62:THR:HB	2.18	0.43
2:D:519:TRP:HZ3	2:D:567:HIS:ND1	2.15	0.43
2:F:125:SER:O	2:F:128:ASP:OD2	2.37	0.43
2:H:129:LEU:HA	2:H:129:LEU:HD12	1.69	0.43
2:H:335:GLU:C	2:H:337:LEU:N	2.73	0.43
2:H:424:LEU:O	2:H:425:ASP:C	2.62	0.43
2:H:444:TYR:CE1	2:H:471:GLY:HA2	2.54	0.43
2:H:480:LEU:HD22	2:H:500:PHE:CD1	2.53	0.43
2:J:59:LEU:HD22	2:J:61:TYR:H	1.84	0.43
2:J:299:ASP:C	2:J:301:LEU:H	2.26	0.43
1:M:148:GLU:HG2	1:M:152:ARG:HH12	1.83	0.43
2:N:411:VAL:HG22	2:N:444:TYR:HB3	1.99	0.43
2:N:412:LEU:HD12	2:N:412:LEU:O	2.18	0.43
2:N:490:LEU:HD23	2:N:490:LEU:HA	1.82	0.43
2:P:46:LYS:HB2	2:P:46:LYS:HE3	1.54	0.43
1:A:108:LEU:HD12	1:A:110:ILE:CD1	2.42	0.43
2:B:190:HIS:HE1	2:P:110:ASN:HA	1.84	0.43
2:B:201:MET:HB3	3:Q:211:ARG:HH12	1.82	0.43
2:B:233:LEU:HD23	2:B:233:LEU:HA	1.80	0.43
2:B:411:VAL:HG22	2:B:444:TYR:HB3	2.01	0.43
5:B:1102:PO4:O3	3:Q:206:ARG:NH2	2.49	0.43
2:D:111:LEU:C	2:D:113:GLN:H	2.27	0.43
2:D:190:HIS:CD2	2:H:112:ARG:NH1	2.86	0.43
2:F:65:PRO:HB3	2:F:103:TRP:CE3	2.54	0.43
2:F:136:ARG:HH21	2:L:164:ARG:HH21	1.65	0.43
2:F:431:LEU:HD12	2:F:431:LEU:C	2.44	0.43
2:H:298:LEU:HD22	2:H:300:LEU:CG	2.45	0.43
2:H:385:VAL:CG1	2:H:387:VAL:HG23	2.48	0.43
2:H:412:LEU:CD1	2:H:445:LEU:CD2	2.97	0.43
1:I:132:GLU:O	1:I:136:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:233:LEU:HD23	2:J:233:LEU:HA	1.81	0.43
2:J:542:ILE:CD1	2:J:588:LEU:HD12	2.29	0.43
3:U:201:LEU:HA	3:U:201:LEU:HD23	1.85	0.43
1:M:134:ARG:HH11	2:N:40:VAL:HA	1.82	0.43
1:M:153:ARG:CG	1:M:157:TRP:CZ3	3.02	0.43
2:N:380:LEU:HD23	2:N:380:LEU:HA	1.77	0.43
2:N:396:GLU:HG2	2:N:430:SER:OG	2.18	0.43
2:N:472:TYR:CD2	2:N:497:GLY:O	2.71	0.43
2:P:227:VAL:HG13	2:P:228:GLY:H	1.82	0.43
2:B:55:VAL:CG2	2:B:75:LEU:HD21	2.49	0.43
2:B:375:GLN:HG2	2:B:401:TYR:CE1	2.53	0.43
2:B:538:PRO:O	2:B:539:TYR:HB2	2.19	0.43
2:D:580:ASP:HA	2:N:206:LYS:HE3	2.01	0.43
1:E:42:VAL:HA	1:E:43:PRO:HD3	1.79	0.43
1:E:91:MET:O	1:E:93:ILE:HG12	2.18	0.43
1:E:128:LYS:HB2	1:E:133:ILE:CD1	2.49	0.43
2:F:311:CYS:CB	2:F:336:VAL:HG21	2.49	0.43
1:G:58:TYR:CD2	1:G:113:LEU:HD13	2.54	0.43
2:H:97:GLY:HA3	2:H:123:ILE:HD12	1.99	0.43
2:H:362:GLU:O	2:H:364:LEU:N	2.52	0.43
2:H:431:LEU:HD23	2:H:431:LEU:C	2.44	0.43
2:H:535:MET:HE3	2:H:542:ILE:HG21	2.01	0.43
2:J:58:ALA:O	2:J:81:LYS:HB2	2.19	0.43
2:L:565:PRO:HG2	3:V:201:LEU:HD21	1.99	0.43
1:M:42:VAL:O	1:M:42:VAL:HG22	2.18	0.43
2:N:351:ARG:HD3	2:N:413:LEU:HD11	2.00	0.43
2:N:519:TRP:CD1	2:N:519:TRP:C	2.95	0.43
1:A:95:GLN:NE2	1:A:124:MET:CE	2.82	0.42
2:D:263:TYR:O	2:D:266:LEU:HD23	2.19	0.42
2:D:343:GLN:HA	2:D:343:GLN:NE2	2.34	0.42
2:D:546:PRO:HB2	2:D:547:SER:H	1.72	0.42
2:F:519:TRP:CH2	2:F:567:HIS:CG	3.07	0.42
2:H:213:GLU:CD	2:H:237:GLY:HA3	2.44	0.42
2:H:437:LYS:HB3	2:H:437:LYS:HE2	1.80	0.42
2:H:450:LEU:HG	2:H:454:GLY:HA3	2.01	0.42
1:I:27:GLN:HA	1:I:30:ALA:HB3	2.01	0.42
1:I:42:VAL:O	1:I:42:VAL:HG22	2.18	0.42
2:J:308:GLU:HG3	2:J:332:ARG:NH2	2.28	0.42
2:J:545:ILE:HG22	2:J:546:PRO:N	2.34	0.42
2:L:231:GLU:HG2	2:L:254:ASN:HD22	1.83	0.42
1:O:141:ASN:OD1	1:O:141:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:578:ARG:H	2:P:578:ARG:HG3	1.44	0.42
1:A:26:SER:HB3	1:A:29:ILE:HG13	2.01	0.42
2:B:46:LYS:HB2	2:B:46:LYS:HE3	1.51	0.42
2:B:344:LEU:HD23	2:B:380:LEU:HD21	2.01	0.42
2:B:523:TYR:CE2	2:B:568:ILE:HD11	2.54	0.42
2:D:311:CYS:CB	2:D:336:VAL:HG21	2.50	0.42
1:E:45:PRO:HD2	2:L:294:GLN:HB2	2.01	0.42
2:H:303:ALA:O	2:H:326:ARG:NH2	2.52	0.42
2:H:304:LEU:HD22	2:H:304:LEU:HA	1.48	0.42
2:H:310:HIS:O	2:H:314:ILE:CG1	2.49	0.42
2:H:476:SER:C	2:H:478:GLU:N	2.75	0.42
2:J:544:LEU:HD11	2:J:588:LEU:HD11	2.01	0.42
1:K:141:ASN:C	1:K:141:ASN:OD1	2.61	0.42
2:P:338:ALA:O	2:P:376:GLY:HA3	2.19	0.42
2:B:396:GLU:HG2	2:B:430:SER:OG	2.19	0.42
1:C:27:GLN:HA	1:C:30:ALA:HB3	2.00	0.42
2:D:78:LEU:HD12	2:D:79:LYS:H	1.85	0.42
2:D:198:ASN:C	2:D:198:ASN:OD1	2.62	0.42
2:D:231:GLU:HG2	2:D:254:ASN:HD22	1.84	0.42
2:D:380:LEU:HA	2:D:380:LEU:HD23	1.71	0.42
1:G:46:ASN:HB2	1:G:107:TYR:CZ	2.54	0.42
1:G:102:ILE:HG12	1:G:117:THR:OG1	2.18	0.42
2:H:20:VAL:O	2:H:24:VAL:HG23	2.20	0.42
2:H:168:THR:CG2	2:H:196:VAL:HG13	2.50	0.42
2:J:101:THR:N	2:J:102:PRO:CD	2.82	0.42
2:J:289:PHE:N	2:J:290:PRO:CD	2.82	0.42
2:J:297:LYS:HB2	2:J:297:LYS:HE3	1.62	0.42
2:L:299:ASP:OD2	2:L:301:LEU:HB2	2.18	0.42
2:N:465:VAL:CG1	2:N:468:MET:HG3	2.48	0.42
1:A:148:GLU:HG2	1:A:152:ARG:HH12	1.84	0.42
2:B:398:ILE:HG23	2:B:402:LEU:HD11	2.02	0.42
2:B:519:TRP:CH2	2:B:567:HIS:CE1	3.07	0.42
4:D:2100:OGK:C18	4:D:2100:OGK:N08	2.81	0.42
1:E:46:ASN:HB2	1:E:107:TYR:CZ	2.54	0.42
2:F:452:ASP:OD1	2:F:478:GLU:HB2	2.19	0.42
2:H:208:SER:O	2:H:211:ASP:N	2.50	0.42
2:H:335:GLU:O	2:H:336:VAL:C	2.59	0.42
2:H:350:GLU:CB	2:H:386:TYR:CD1	3.02	0.42
2:J:367:GLN:CB	2:J:391:THR:HG22	2.37	0.42
3:V:201:LEU:HA	3:V:202:PRO:HD3	1.82	0.42
1:M:87:ASP:HB3	1:M:116:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:232:ILE:HD12	2:N:252:SER:H	1.83	0.42
2:N:477:ASP:N	2:N:477:ASP:OD1	2.52	0.42
2:N:544:LEU:HD11	2:N:588:LEU:CD1	2.50	0.42
2:P:20:VAL:O	2:P:24:VAL:HG23	2.19	0.42
2:P:546:PRO:O	2:P:547:SER:CB	2.67	0.42
4:P:8100:OGK:H18A	4:P:8100:OGK:N08	2.25	0.42
2:B:95:ASN:O	2:B:582:PRO:HG3	2.20	0.42
1:E:137:PHE:CD1	2:F:17:VAL:CG2	3.02	0.42
2:F:221:SER:O	2:F:223:VAL:HG23	2.20	0.42
2:F:299:ASP:C	2:F:301:LEU:H	2.27	0.42
2:F:519:TRP:CD1	2:F:519:TRP:C	2.95	0.42
2:F:542:ILE:CG1	2:F:588:LEU:HB2	2.49	0.42
2:F:544:LEU:HD11	2:F:588:LEU:CD1	2.50	0.42
2:H:136:ARG:O	2:H:139:ASP:HB2	2.19	0.42
2:H:325:THR:OG1	2:H:326:ARG:N	2.51	0.42
2:H:412:LEU:O	2:H:414:ASP:N	2.53	0.42
1:I:48:THR:HG23	1:I:51:ILE:H	1.85	0.42
2:J:284:GLU:C	2:J:286:PRO:HD2	2.44	0.42
2:J:563:GLU:O	2:J:563:GLU:HG3	2.19	0.42
1:K:48:THR:HG23	1:K:51:ILE:H	1.85	0.42
2:L:20:VAL:O	2:L:24:VAL:HG23	2.19	0.42
2:L:221:SER:O	2:L:223:VAL:HG23	2.18	0.42
1:M:134:ARG:NE	1:M:141:ASN:HB2	2.34	0.42
2:N:111:LEU:C	2:N:113:GLN:H	2.28	0.42
2:N:127:LEU:HD21	2:N:131:ARG:NH2	2.34	0.42
1:A:134:ARG:CZ	1:A:141:ASN:HD22	2.32	0.42
2:B:295:ILE:HG21	2:B:298:LEU:CD1	2.47	0.42
2:B:456:SER:CB	2:B:482:GLU:HB3	2.49	0.42
2:B:490:LEU:HD11	2:B:493:LEU:HD13	2.01	0.42
2:D:125:SER:O	2:D:129:LEU:HD22	2.20	0.42
2:D:436:LYS:HB3	2:D:436:LYS:HE2	1.74	0.42
2:F:227:VAL:HG13	2:F:228:GLY:H	1.84	0.42
2:H:194:LEU:HA	2:H:194:LEU:HD12	1.77	0.42
2:H:242:ALA:HB1	2:H:245:LEU:HB2	2.02	0.42
2:H:258:GLY:C	2:H:260:PRO:HD3	2.45	0.42
2:H:362:GLU:HB3	2:H:363:GLY:H	1.52	0.42
2:H:518:LEU:HB3	2:H:570:ALA:HB3	2.02	0.42
1:I:137:PHE:HD1	2:J:17:VAL:HG21	1.83	0.42
2:J:65:PRO:HA	2:J:103:TRP:CZ3	2.54	0.42
2:J:350:GLU:HB3	3:U:209:LEU:CD2	2.46	0.42
1:K:26:SER:C	1:K:28:THR:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:431:LEU:HD12	2:L:431:LEU:O	2.19	0.42
1:M:48:THR:HG23	1:M:51:ILE:H	1.84	0.42
1:M:124:MET:HE2	1:M:137:PHE:CZ	2.54	0.42
1:A:98:LEU:CD2	1:A:120:THR:HG22	2.49	0.42
1:A:137:PHE:CD1	2:B:17:VAL:CG2	3.03	0.42
1:A:153:ARG:HG2	1:A:157:TRP:CZ3	2.54	0.42
2:B:299:ASP:OD2	2:B:301:LEU:HB2	2.19	0.42
1:C:132:GLU:O	1:C:136:THR:HG23	2.20	0.42
2:F:339:GLN:HA	2:F:342:LYS:HE2	2.01	0.42
2:F:347:LEU:HD11	2:F:349:ILE:HD11	2.01	0.42
2:F:469:LEU:HA	2:F:494:GLU:O	2.19	0.42
2:F:563:GLU:HG3	2:F:563:GLU:O	2.20	0.42
2:H:115:LYS:O	2:H:141:GLU:N	2.51	0.42
2:H:320:LEU:HD12	2:H:321:GLU:H	1.84	0.42
1:I:101:LEU:HB3	1:I:117:THR:HG21	2.01	0.42
1:I:128:LYS:HB2	1:I:133:ILE:CD1	2.50	0.42
2:J:59:LEU:O	2:J:62:THR:HB	2.20	0.42
2:J:101:THR:HG22	2:J:128:ASP:CB	2.48	0.42
3:U:214:GLU:C	3:U:216:ARG:H	2.28	0.42
2:L:253:LEU:CD1	2:L:280:MET:HB2	2.46	0.42
2:L:308:GLU:O	2:L:312:THR:HG23	2.20	0.42
2:L:452:ASP:OD1	2:L:478:GLU:HB2	2.20	0.42
2:N:299:ASP:OD2	2:N:301:LEU:HB2	2.19	0.42
1:O:48:THR:HG22	1:O:51:ILE:HG12	2.01	0.42
2:P:59:LEU:O	2:P:62:THR:HB	2.19	0.42
2:P:231:GLU:HG2	2:P:254:ASN:HD22	1.84	0.42
2:P:431:LEU:HD12	2:P:431:LEU:O	2.20	0.42
2:B:270:ARG:CB	1:O:107:TYR:HD1	2.31	0.42
2:B:282:PRO:HA	2:B:285:MET:CE	2.44	0.42
2:D:101:THR:HG22	2:D:128:ASP:CB	2.48	0.42
2:D:495:MET:HB2	2:D:495:MET:HE3	1.69	0.42
2:F:78:LEU:HD12	2:F:79:LYS:H	1.84	0.42
2:F:159:ILE:HD12	2:F:166:ILE:HD11	2.00	0.42
2:F:211:ASP:O	2:F:215:ILE:HG13	2.19	0.42
1:G:91:MET:O	1:G:93:ILE:HG12	2.19	0.42
1:G:101:LEU:HA	1:G:101:LEU:HD23	1.82	0.42
2:H:503:ARG:HE	2:H:503:ARG:H	1.66	0.42
2:J:199:PHE:O	2:J:202:THR:OG1	2.35	0.42
2:J:325:THR:OG1	2:J:326:ARG:N	2.53	0.42
2:L:299:ASP:C	2:L:301:LEU:H	2.27	0.42
1:M:10:SER:OG	1:M:11:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HD23	1:A:42:VAL:CG1	2.50	0.42
1:A:10:SER:OG	1:A:11:SER:N	2.52	0.42
2:B:546:PRO:O	2:B:547:SER:CB	2.66	0.42
2:F:289:PHE:HD1	2:F:316:LYS:HD2	1.76	0.42
2:H:213:GLU:HA	2:H:238:PHE:HB2	2.01	0.42
2:H:390:ILE:H	2:H:390:ILE:HG12	1.64	0.42
2:J:477:ASP:OD1	2:J:477:ASP:N	2.53	0.42
1:K:135:THR:HG22	1:K:136:THR:N	2.34	0.42
2:L:412:LEU:HD12	2:L:412:LEU:O	2.19	0.42
2:N:284:GLU:C	2:N:286:PRO:HD2	2.45	0.42
2:N:429:ARG:HG2	2:N:433:ILE:HD12	2.02	0.42
1:O:59:CYS:O	1:O:63:VAL:HG23	2.19	0.42
2:P:533:MET:HE2	2:P:533:MET:HA	2.01	0.42
2:P:563:GLU:HG3	2:P:563:GLU:O	2.20	0.42
2:B:533:MET:C	2:B:535:MET:H	2.27	0.42
2:F:380:LEU:HD23	2:F:380:LEU:HA	1.74	0.42
2:H:285:MET:O	2:H:287:ILE:N	2.53	0.42
2:H:462:SER:HB2	2:H:465:VAL:HB	2.02	0.42
2:L:170:LEU:HD23	2:L:170:LEU:C	2.44	0.42
1:M:99:PHE:CE2	2:N:17:VAL:N	2.88	0.42
2:N:419:ILE:O	2:N:420:THR:O	2.37	0.42
2:P:392:ASN:ND2	2:P:421:ASP:OD1	2.48	0.42
1:A:102:ILE:HG12	1:A:117:THR:HB	2.02	0.41
2:B:300:LEU:HD12	2:B:323:LEU:HD11	2.02	0.41
2:D:296:ARG:HH12	1:G:32:MET:HG3	1.85	0.41
2:D:396:GLU:HG2	2:D:430:SER:OG	2.20	0.41
2:D:419:ILE:O	2:D:420:THR:O	2.38	0.41
2:D:543:GLU:OE2	2:D:578:ARG:HD3	2.20	0.41
2:F:314:ILE:HD11	2:F:329:ILE:HD11	2.01	0.41
2:H:100:VAL:O	2:H:100:VAL:HG13	2.19	0.41
2:H:188:ALA:HB1	2:H:214:THR:OG1	2.20	0.41
2:H:284:GLU:CD	2:H:284:GLU:H	2.28	0.41
2:J:111:LEU:C	2:J:113:GLN:H	2.28	0.41
2:L:396:GLU:HG2	2:L:430:SER:OG	2.19	0.41
2:L:546:PRO:O	2:L:547:SER:CB	2.67	0.41
1:M:134:ARG:NH1	2:N:40:VAL:HA	2.35	0.41
2:N:326:ARG:HA	2:N:350:GLU:O	2.20	0.41
1:A:48:THR:HG22	1:A:51:ILE:HG12	2.03	0.41
2:B:54:HIS:C	2:B:54:HIS:ND1	2.78	0.41
2:B:223:VAL:O	2:B:245:LEU:HD12	2.20	0.41
3:Q:201:LEU:HD23	3:Q:201:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:LEU:HD12	2:D:341:CYS:SG	2.60	0.41
2:F:285:MET:N	2:F:286:PRO:CD	2.81	0.41
2:H:184:LEU:HD23	2:H:184:LEU:HA	1.69	0.41
2:H:213:GLU:HG3	2:H:237:GLY:C	2.45	0.41
2:H:458:ILE:C	2:H:460:GLN:H	2.27	0.41
1:I:101:LEU:HD23	1:I:101:LEU:HA	1.83	0.41
2:J:143:LEU:CD2	2:J:159:ILE:HD13	2.50	0.41
2:J:314:ILE:HD11	2:J:329:ILE:HD11	2.01	0.41
2:L:285:MET:N	2:L:286:PRO:CD	2.83	0.41
2:L:308:GLU:HG3	2:L:332:ARG:NH2	2.26	0.41
2:P:253:LEU:CD1	2:P:280:MET:HB2	2.49	0.41
2:P:519:TRP:CD1	2:P:519:TRP:C	2.95	0.41
2:B:348:ARG:HG3	2:B:384:ALA:HB3	2.02	0.41
2:B:563:GLU:O	2:B:563:GLU:HG3	2.21	0.41
1:E:134:ARG:NE	1:E:141:ASN:HB2	2.35	0.41
2:H:87:ALA:HB2	2:H:92:ILE:CB	2.50	0.41
1:I:19:GLU:OE1	1:I:19:GLU:N	2.51	0.41
1:I:106:ASN:HB2	1:I:114:LEU:HD11	2.02	0.41
1:I:129:THR:HB	1:I:130:PRO:HD2	2.03	0.41
2:J:75:LEU:HD23	2:J:75:LEU:HA	1.83	0.41
2:J:322:VAL:HG13	2:J:346:ARG:HB2	2.01	0.41
1:K:46:ASN:HB2	1:K:107:TYR:CZ	2.55	0.41
2:L:209:PRO:HD3	2:L:230:PHE:HE2	1.84	0.41
1:M:27:GLN:HA	1:M:30:ALA:HB3	2.02	0.41
2:N:107:ILE:HA	2:N:111:LEU:HB2	2.02	0.41
2:N:299:ASP:C	2:N:301:LEU:H	2.28	0.41
2:N:358:MET:HG3	2:N:364:LEU:HG	2.01	0.41
2:N:502:GLU:HG3	2:N:525:ALA:HA	2.03	0.41
2:N:544:LEU:HD11	2:N:588:LEU:HD11	2.01	0.41
1:O:105:ALA:HB2	1:O:113:LEU:HD23	2.02	0.41
1:O:125:ILE:HG23	1:O:133:ILE:CD1	2.44	0.41
1:C:105:ALA:HB2	1:C:113:LEU:HD23	2.02	0.41
2:D:325:THR:O	2:D:349:ILE:HA	2.20	0.41
2:F:343:GLN:HA	2:F:343:GLN:NE2	2.35	0.41
2:F:533:MET:C	2:F:535:MET:H	2.28	0.41
2:H:96:TRP:NE1	2:H:578:ARG:HH12	2.18	0.41
2:H:347:LEU:CD2	2:H:373:LEU:HD21	2.50	0.41
2:H:533:MET:C	2:H:535:MET:H	2.28	0.41
2:L:125:SER:O	2:L:129:LEU:HD22	2.20	0.41
2:L:289:PHE:N	2:L:290:PRO:CD	2.82	0.41
2:P:83:LYS:HA	2:P:84:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:495:MET:HE3	2:P:495:MET:HB2	1.76	0.41
1:A:132:GLU:O	1:A:136:THR:HG23	2.20	0.41
2:B:266:LEU:HD13	2:B:266:LEU:HA	1.83	0.41
2:D:187:LEU:HD23	2:D:187:LEU:HA	1.88	0.41
2:F:54:HIS:HE1	2:F:56:THR:OG1	2.03	0.41
2:H:124:VAL:CG1	2:H:129:LEU:HD13	2.51	0.41
2:H:411:VAL:HG23	4:H:4100:OGK:H16A	2.02	0.41
1:K:137:PHE:CD1	2:L:17:VAL:CG2	3.03	0.41
2:L:289:PHE:HB2	2:L:290:PRO:HD3	2.01	0.41
1:M:125:ILE:HG23	1:M:133:ILE:CD1	2.39	0.41
2:N:519:TRP:HZ3	2:N:567:HIS:ND1	2.18	0.41
1:O:102:ILE:HD12	2:P:20:VAL:HG21	2.02	0.41
2:P:89:PHE:CD1	3:X:206:ARG:HA	2.56	0.41
2:P:308:GLU:O	2:P:312:THR:HG23	2.21	0.41
2:P:328:VAL:CG2	2:P:359:GLU:HB2	2.43	0.41
2:P:436:LYS:HE2	2:P:436:LYS:HB3	1.74	0.41
2:P:490:LEU:HD11	2:P:493:LEU:HD13	2.03	0.41
1:A:101:LEU:HB3	1:A:117:THR:HG21	2.01	0.41
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.97	0.41
2:B:468:MET:HE1	2:B:483:PHE:CE1	2.55	0.41
2:D:285:MET:N	2:D:286:PRO:HD2	2.36	0.41
2:F:311:CYS:SG	2:F:333:GLY:HA2	2.60	0.41
2:H:54:HIS:O	2:H:55:VAL:HG23	2.20	0.41
2:H:365:VAL:HG21	2:H:387:VAL:CB	2.50	0.41
2:L:519:TRP:CH2	2:L:567:HIS:CE1	3.08	0.41
1:O:153:ARG:NH2	2:P:539:TYR:HE1	2.19	0.41
2:B:231:GLU:HG2	2:B:254:ASN:HD22	1.86	0.41
2:H:315:GLN:HG3	2:H:340:TYR:CZ	2.55	0.41
1:I:134:ARG:NE	1:I:141:ASN:HB2	2.36	0.41
2:J:209:PRO:HD3	2:J:230:PHE:HE2	1.85	0.41
2:J:409:ARG:HD3	4:J:5100:OGK:H13A	2.01	0.41
2:J:481:MET:HE2	2:J:481:MET:HB3	1.97	0.41
1:K:8:LEU:HD23	1:K:42:VAL:CG1	2.50	0.41
1:M:99:PHE:CE2	2:N:16:THR:C	2.98	0.41
2:N:308:GLU:HG3	2:N:332:ARG:NH2	2.30	0.41
2:P:545:ILE:HB	2:P:567:HIS:HB2	2.01	0.41
1:C:137:PHE:HD1	2:D:17:VAL:CG2	2.34	0.41
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.88	0.41
2:D:429:ARG:HG2	2:D:433:ILE:HD12	2.02	0.41
2:D:519:TRP:CD1	2:D:519:TRP:C	2.97	0.41
2:H:52:ARG:HH11	2:H:72:PHE:HE2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:THR:HG22	2:H:196:VAL:HG13	2.01	0.41
2:J:124:VAL:CG1	2:J:129:LEU:HD13	2.50	0.41
2:L:101:THR:N	2:L:102:PRO:CD	2.84	0.41
2:N:121:ARG:NH2	5:N:1103:PO4:O4	2.54	0.41
2:N:496:ARG:HA	2:N:521:GLN:O	2.19	0.41
2:N:586:ARG:NH2	2:N:588:LEU:HD21	2.35	0.41
2:P:272:LEU:C	2:P:272:LEU:CD2	2.93	0.41
2:P:490:LEU:HD23	2:P:490:LEU:HA	1.72	0.41
2:B:78:LEU:HD12	2:B:79:LYS:H	1.86	0.41
2:B:314:ILE:HD11	2:B:329:ILE:HD11	2.03	0.41
2:B:328:VAL:CG2	2:B:359:GLU:HB2	2.45	0.41
2:B:519:TRP:HA	2:B:568:ILE:O	2.21	0.41
1:C:99:PHE:CE2	2:D:17:VAL:HG22	2.56	0.41
1:C:141:ASN:OD1	1:C:141:ASN:C	2.63	0.41
2:D:545:ILE:HG22	2:D:546:PRO:CD	2.51	0.41
2:F:338:ALA:O	2:F:376:GLY:HA3	2.21	0.41
1:G:129:THR:OG1	1:G:132:GLU:HG3	2.21	0.41
1:G:148:GLU:HG3	1:G:152:ARG:HH11	1.85	0.41
2:H:59:LEU:O	2:H:62:THR:HB	2.21	0.41
2:H:92:ILE:HD11	2:H:519:TRP:CZ3	2.56	0.41
2:H:170:LEU:HA	2:H:198:ASN:O	2.20	0.41
2:H:391:THR:O	2:H:393:GLU:N	2.54	0.41
2:H:455:LEU:HD21	2:H:473:VAL:HG21	2.03	0.41
2:J:191:ASN:ND2	2:J:192:THR:N	2.68	0.41
2:J:328:VAL:O	2:J:329:ILE:C	2.64	0.41
2:J:405:LEU:HD23	2:J:405:LEU:HA	1.85	0.41
2:J:545:ILE:HB	2:J:567:HIS:HB2	2.03	0.41
2:L:490:LEU:HD23	2:L:490:LEU:HA	1.77	0.41
2:L:533:MET:CE	2:L:588:LEU:HD13	2.51	0.41
2:N:308:GLU:O	2:N:312:THR:HG23	2.21	0.41
2:N:398:ILE:HG22	2:N:431:LEU:HD13	2.02	0.41
1:O:46:ASN:HB2	1:O:107:TYR:CZ	2.56	0.41
2:P:299:ASP:C	2:P:301:LEU:H	2.28	0.41
2:P:392:ASN:HD21	2:P:424:LEU:HA	1.85	0.41
2:B:495:MET:HE3	2:B:495:MET:HB2	1.74	0.41
1:C:125:ILE:HG23	1:C:133:ILE:CD1	2.44	0.41
2:D:489:ASN:HD22	2:D:489:ASN:HA	1.65	0.41
2:F:480:LEU:HB2	2:F:500:PHE:CE2	2.56	0.41
1:G:129:THR:O	1:G:130:PRO:C	2.63	0.41
1:G:147:GLU:H	1:G:147:GLU:HG3	1.60	0.41
2:H:21:ILE:C	2:H:23:GLN:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:ARG:O	2:H:72:PHE:N	2.54	0.41
2:H:352:GLY:O	2:H:353:ALA:CB	2.69	0.41
2:H:584:THR:O	2:H:584:THR:HG22	2.21	0.41
2:J:328:VAL:CG2	2:J:359:GLU:HB2	2.45	0.41
2:J:367:GLN:NE2	2:J:389:ASP:OD1	2.54	0.41
2:L:436:LYS:HB3	2:L:436:LYS:HE2	1.70	0.41
1:M:141:ASN:OD1	1:M:141:ASN:C	2.64	0.41
1:O:114:LEU:HD12	1:O:114:LEU:HA	1.91	0.41
2:B:152:THR:HG22	2:B:177:SER:HB2	2.03	0.40
1:C:10:SER:OG	1:C:11:SER:N	2.54	0.40
1:C:158:ALA:HA	2:D:62:THR:HG23	2.03	0.40
2:D:284:GLU:C	2:D:286:PRO:HD2	2.45	0.40
2:D:404:ASN:HB3	2:D:437:LYS:HD2	2.03	0.40
2:F:263:TYR:O	2:F:266:LEU:HD23	2.20	0.40
1:G:130:PRO:HD3	2:H:36:SER:CB	2.50	0.40
2:H:120:ARG:O	2:H:122:MET:HG3	2.20	0.40
2:H:502:GLU:CD	2:H:526:SER:HB2	2.47	0.40
2:L:266:LEU:HA	2:L:266:LEU:HD13	1.83	0.40
2:L:327:ASN:N	2:L:327:ASN:HD22	2.18	0.40
2:L:409:ARG:HD3	4:L:6100:OGK:H13A	2.03	0.40
2:N:380:LEU:CD1	2:N:383:MET:HE2	2.51	0.40
2:N:563:GLU:HG3	2:N:563:GLU:O	2.21	0.40
2:P:101:THR:N	2:P:102:PRO:CD	2.84	0.40
2:P:266:LEU:HD13	2:P:266:LEU:HA	1.86	0.40
2:P:276:GLY:HA3	2:P:299:ASP:HB3	2.02	0.40
2:P:305:LEU:HD23	2:P:305:LEU:O	2.19	0.40
2:P:399:GLY:HA3	2:P:431:LEU:HA	2.04	0.40
2:B:127:LEU:HB2	2:F:126:ASP:HB3	2.03	0.40
2:B:304:LEU:HA	2:B:304:LEU:HD12	1.72	0.40
2:B:447:GLN:C	2:B:449:GLY:H	2.30	0.40
2:B:489:ASN:HD22	2:B:489:ASN:HA	1.66	0.40
2:D:490:LEU:HD23	2:D:490:LEU:HA	1.74	0.40
1:E:130:PRO:O	1:E:134:ARG:HG2	2.20	0.40
2:F:55:VAL:HG21	2:F:72:PHE:CD1	2.56	0.40
2:F:392:ASN:ND2	2:F:421:ASP:OD1	2.54	0.40
2:F:429:ARG:HG2	2:F:433:ILE:HD12	2.04	0.40
2:H:32:LYS:HA	2:H:32:LYS:HD3	1.81	0.40
2:H:274:ARG:HA	2:H:297:LYS:HB3	2.03	0.40
2:H:391:THR:O	2:H:392:ASN:C	2.65	0.40
2:J:436:LYS:HB3	2:J:436:LYS:HE2	1.77	0.40
2:L:111:LEU:C	2:L:113:GLN:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:55:VAL:HG21	2:N:72:PHE:CD1	2.56	0.40
2:N:285:MET:N	2:N:286:PRO:CD	2.85	0.40
2:N:545:ILE:HG22	2:N:546:PRO:N	2.36	0.40
3:W:201:LEU:HA	3:W:201:LEU:HD23	1.81	0.40
2:P:95:ASN:O	2:P:582:PRO:HG3	2.21	0.40
2:P:232:ILE:O	2:P:235:LEU:HB2	2.21	0.40
2:B:83:LYS:HA	2:B:84:PRO:HD3	1.86	0.40
2:B:263:TYR:O	2:B:266:LEU:HD23	2.21	0.40
2:B:545:ILE:HG22	2:B:546:PRO:N	2.36	0.40
1:E:26:SER:C	1:E:28:THR:N	2.79	0.40
2:F:289:PHE:N	2:F:290:PRO:CD	2.84	0.40
1:I:146:GLU:HA	2:L:539:TYR:OH	2.22	0.40
1:I:153:ARG:CG	1:I:157:TRP:CZ3	3.04	0.40
2:L:519:TRP:HZ3	2:L:567:HIS:ND1	2.20	0.40
2:N:328:VAL:CG2	2:N:359:GLU:HB2	2.41	0.40
2:N:501:SER:O	2:N:505:ILE:HG12	2.21	0.40
2:P:100:VAL:HG11	2:P:124:VAL:HG22	2.03	0.40
2:P:107:ILE:HA	2:P:111:LEU:HB2	2.03	0.40
2:P:184:LEU:HD23	2:P:184:LEU:HA	1.85	0.40
2:P:187:LEU:HD23	2:P:187:LEU:HA	1.85	0.40
2:P:284:GLU:C	2:P:286:PRO:HD2	2.46	0.40
2:P:327:ASN:N	2:P:327:ASN:HD22	2.20	0.40
2:P:351:ARG:HD3	2:P:413:LEU:HD11	2.03	0.40
2:P:519:TRP:HZ3	2:P:567:HIS:ND1	2.20	0.40
2:B:319:ASN:ND2	1:O:43:PRO:HG2	2.36	0.40
1:E:26:SER:CB	1:E:29:ILE:HG13	2.51	0.40
2:F:308:GLU:HG3	2:F:332:ARG:NH2	2.28	0.40
1:G:135:THR:HG22	1:G:136:THR:HG23	2.04	0.40
2:H:191:ASN:ND2	2:H:193:SER:N	2.70	0.40
4:H:4100:OGK:C18	4:H:4100:OGK:N08	2.84	0.40
1:K:26:SER:CB	1:K:29:ILE:HG13	2.50	0.40
2:L:343:GLN:NE2	2:L:343:GLN:HA	2.36	0.40
2:N:124:VAL:O	2:N:151:PHE:HB3	2.20	0.40
2:N:538:PRO:O	2:N:539:TYR:HB2	2.21	0.40
1:O:132:GLU:O	1:O:136:THR:HG23	2.22	0.40
1:O:148:GLU:HG2	1:O:152:ARG:HH12	1.85	0.40
2:P:57:MET:CE	2:P:62:THR:HG22	2.46	0.40
2:P:263:TYR:O	2:P:266:LEU:HD23	2.21	0.40
2:B:285:MET:N	2:B:286:PRO:CD	2.85	0.40
1:E:148:GLU:HG2	1:E:152:ARG:HH12	1.86	0.40
2:F:398:ILE:HG22	2:F:431:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:519:TRP:HZ3	2:F:567:HIS:ND1	2.17	0.40
2:H:80:LEU:CD1	2:H:103:TRP:CG	3.05	0.40
2:H:374:ALA:CB	2:H:398:ILE:HD12	2.49	0.40
2:H:453:LEU:O	2:H:456:SER:HB3	2.21	0.40
2:J:253:LEU:CD1	2:J:280:MET:HB2	2.49	0.40
2:J:375:GLN:HG2	2:J:401:TYR:CE1	2.56	0.40
2:N:289:PHE:N	2:N:290:PRO:HD2	2.37	0.40
2:N:398:ILE:CG2	2:N:431:LEU:HD13	2.52	0.40
2:N:492:LYS:HG3	2:N:517:TYR:CD2	2.57	0.40
1:O:61:ARG:HA	1:O:61:ARG:HD2	1.97	0.40
2:P:289:PHE:N	2:P:290:PRO:HD2	2.37	0.40
2:P:358:MET:HG3	2:P:364:LEU:HG	2.03	0.40
2:P:400:THR:O	2:P:403:LYS:HE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	2	18
1	C	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	2	18
1	E	140/160 (88%)	118 (84%)	17 (12%)	5 (4%)	2	18
1	G	140/160 (88%)	113 (81%)	21 (15%)	6 (4%)	2	14
1	I	140/160 (88%)	117 (84%)	17 (12%)	6 (4%)	2	14
1	K	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	2	18
1	M	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	2	18
1	O	140/160 (88%)	115 (82%)	19 (14%)	6 (4%)	2	14
2	B	564/592 (95%)	501 (89%)	57 (10%)	6 (1%)	11	40
2	D	564/592 (95%)	503 (89%)	53 (9%)	8 (1%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	10	37
2	H	558/592 (94%)	426 (76%)	95 (17%)	37 (7%)	1	7
2	J	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	10	37
2	L	564/592 (95%)	501 (89%)	55 (10%)	8 (1%)	9	34
2	N	564/592 (95%)	502 (89%)	55 (10%)	7 (1%)	10	37
2	P	564/592 (95%)	500 (89%)	58 (10%)	6 (1%)	11	40
3	Q	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	R	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	S	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	U	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	V	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	W	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	X	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
All	All	5738/6163 (93%)	4968 (87%)	641 (11%)	129 (2%)	5	26

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
2	B	420	THR
2	B	546	PRO
2	D	420	THR
2	D	546	PRO
2	F	420	THR
2	F	546	PRO
2	H	41	CYS
2	H	71	ARG
2	H	172	GLU
2	H	200	TYR
2	H	270	ARG
2	H	278	SER
2	H	357	GLY
2	H	364	LEU
2	H	425	ASP
2	H	525	ALA
2	H	526	SER
2	J	420	THR

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Mol	Chain	Res	Type
2	J	546	PRO
1	K	92	LYS
2	L	420	THR
2	L	546	PRO
2	N	420	THR
2	N	546	PRO
2	P	420	THR
2	P	546	PRO
1	A	10	SER
1	A	13	GLY
1	A	36	ASP
1	A	126	LYS
2	B	547	SER
1	C	10	SER
1	C	13	GLY
1	C	36	ASP
1	C	92	LYS
1	C	126	LYS
2	D	547	SER
1	E	10	SER
1	E	13	GLY
1	E	36	ASP
1	E	92	LYS
1	E	126	LYS
1	G	10	SER
1	G	13	GLY
1	G	36	ASP
1	G	92	LYS
1	G	128	LYS
2	H	97	GLY
2	H	228	GLY
2	H	271	LYS
2	H	279	TYR
2	H	353	ALA
2	H	365	VAL
2	H	392	ASN
2	H	449	GLY
2	H	528	THR
1	I	10	SER
1	I	13	GLY
1	I	36	ASP
1	I	92	LYS

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Mol	Chain	Res	Type
1	I	126	LYS
2	J	547	SER
1	K	10	SER
1	K	36	ASP
1	K	126	LYS
2	L	547	SER
1	M	10	SER
1	M	13	GLY
1	M	36	ASP
1	M	92	LYS
1	M	126	LYS
1	O	10	SER
1	O	36	ASP
1	O	92	LYS
1	O	126	LYS
2	P	547	SER
2	B	590	GLU
2	D	590	GLU
2	F	20	VAL
2	F	547	SER
2	F	590	GLU
2	H	70	ARG
2	H	319	ASN
2	H	499	CYS
2	H	533	MET
2	H	577	GLN
2	H	582	PRO
2	J	590	GLU
1	K	13	GLY
2	L	590	GLU
2	N	547	SER
2	N	590	GLU
1	O	13	GLY
2	P	590	GLU
2	B	20	VAL
2	D	20	VAL
2	D	112	ARG
2	H	112	ARG
2	H	137	ALA
2	H	269	PRO
2	H	305	LEU
2	H	358	MET

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Mol	Chain	Res	Type
2	H	538	PRO
2	L	112	ARG
2	N	290	PRO
2	P	20	VAL
2	D	290	PRO
2	H	206	LYS
1	I	137	PHE
2	J	20	VAL
2	J	290	PRO
2	L	20	VAL
2	L	290	PRO
2	N	20	VAL
1	O	27	GLN
2	P	290	PRO
2	F	290	PRO
1	G	153	ARG
2	H	209	PRO
2	H	276	GLY
2	H	20	VAL
2	H	286	PRO
2	B	591	PRO
2	D	591	PRO
2	N	591	PRO
2	F	591	PRO
2	J	591	PRO
2	L	591	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/137 (93%)	111 (87%)	16 (13%)	4	19
1	C	127/137 (93%)	112 (88%)	15 (12%)	5	21
1	E	127/137 (93%)	111 (87%)	16 (13%)	4	19
1	G	127/137 (93%)	109 (86%)	18 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	127/137 (93%)	111 (87%)	16 (13%)	4	19
1	K	127/137 (93%)	112 (88%)	15 (12%)	5	21
1	M	127/137 (93%)	110 (87%)	17 (13%)	4	16
1	O	127/137 (93%)	112 (88%)	15 (12%)	5	21
2	B	500/523 (96%)	428 (86%)	72 (14%)	3	14
2	D	500/523 (96%)	427 (85%)	73 (15%)	3	14
2	F	500/523 (96%)	426 (85%)	74 (15%)	3	13
2	H	494/523 (94%)	393 (80%)	101 (20%)	1	5
2	J	500/523 (96%)	427 (85%)	73 (15%)	3	14
2	L	500/523 (96%)	427 (85%)	73 (15%)	3	14
2	N	500/523 (96%)	426 (85%)	74 (15%)	3	13
2	P	500/523 (96%)	427 (85%)	73 (15%)	3	14
3	Q	16/19 (84%)	16 (100%)	0	100	100
3	R	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	S	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	U	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	V	16/19 (84%)	15 (94%)	1 (6%)	16	45
3	W	16/19 (84%)	16 (100%)	0	100	100
3	X	16/19 (84%)	16 (100%)	0	100	100
All	All	5122/5413 (95%)	4377 (86%)	745 (14%)	3	14

All (745) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	14	GLU
1	A	22	VAL
1	A	29	ILE
1	A	35	ASP
1	A	36	ASP
1	A	42	VAL
1	A	44	LEU
1	A	47	VAL
1	A	48	THR
1	A	97	THR

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Mol	Chain	Res	Type
1	A	125	ILE
1	A	135	THR
1	A	150	GLU
1	A	153	ARG
1	A	160	GLU
2	B	14	VAL
2	B	16	THR
2	B	17	VAL
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	104	VAL
2	B	123	ILE
2	B	129	LEU
2	B	132	LEU
2	B	136	ARG
2	B	142	THR
2	B	159	ILE
2	B	166	ILE
2	B	168	THR
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	225	VAL
2	B	227	VAL
2	B	231	GLU
2	B	232	ILE
2	B	266	LEU
2	B	272	LEU
2	B	275	LEU
2	B	284	GLU
2	B	301	LEU
2	B	304	LEU

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Mol	Chain	Res	Type
2	B	305	LEU
2	B	312	THR
2	B	314	ILE
2	B	327	ASN
2	B	341	CYS
2	B	349	ILE
2	B	360	ASP
2	B	367	GLN
2	B	377	CYS
2	B	390	ILE
2	B	400	THR
2	B	402	LEU
2	B	404	ASN
2	B	405	LEU
2	B	412	LEU
2	B	413	LEU
2	B	418	ARG
2	B	422	LEU
2	B	431	LEU
2	B	447	GLN
2	B	453	LEU
2	B	455	LEU
2	B	473	VAL
2	B	477	ASP
2	B	481	MET
2	B	490	LEU
2	B	495	MET
2	B	503	ARG
2	B	510	THR
2	B	519	TRP
2	B	528	THR
2	B	537	ARG
2	B	542	ILE
2	B	545	ILE
2	B	578	ARG
1	C	8	LEU
1	C	14	GLU
1	C	22	VAL
1	C	29	ILE
1	C	35	ASP
1	C	36	ASP
1	C	42	VAL

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Mol	Chain	Res	Type
1	C	44	LEU
1	C	47	VAL
1	C	48	THR
1	C	97	THR
1	C	125	ILE
1	C	150	GLU
1	C	153	ARG
1	C	160	GLU
2	D	14	VAL
2	D	16	THR
2	D	17	VAL
2	D	20	VAL
2	D	35	ASP
2	D	40	VAL
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	104	VAL
2	D	123	ILE
2	D	129	LEU
2	D	132	LEU
2	D	136	ARG
2	D	142	THR
2	D	159	ILE
2	D	166	ILE
2	D	168	THR
2	D	182	LYS
2	D	184	LEU
2	D	192	THR
2	D	196	VAL
2	D	214	THR
2	D	225	VAL
2	D	227	VAL
2	D	231	GLU
2	D	232	ILE
2	D	266	LEU
2	D	272	LEU
2	D	275	LEU
2	D	284	GLU

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Mol	Chain	Res	Type
2	D	298	LEU
2	D	301	LEU
2	D	304	LEU
2	D	305	LEU
2	D	312	THR
2	D	314	ILE
2	D	327	ASN
2	D	341	CYS
2	D	349	ILE
2	D	360	ASP
2	D	367	GLN
2	D	377	CYS
2	D	390	ILE
2	D	400	THR
2	D	402	LEU
2	D	404	ASN
2	D	405	LEU
2	D	412	LEU
2	D	413	LEU
2	D	418	ARG
2	D	422	LEU
2	D	431	LEU
2	D	447	GLN
2	D	453	LEU
2	D	455	LEU
2	D	473	VAL
2	D	477	ASP
2	D	481	MET
2	D	490	LEU
2	D	495	MET
2	D	503	ARG
2	D	510	THR
2	D	516	ARG
2	D	519	TRP
2	D	528	THR
2	D	537	ARG
2	D	542	ILE
2	D	545	ILE
2	D	578	ARG
3	R	217	LYS
1	E	8	LEU
1	E	14	GLU

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Mol	Chain	Res	Type
1	E	22	VAL
1	E	29	ILE
1	E	35	ASP
1	E	36	ASP
1	E	42	VAL
1	E	44	LEU
1	E	47	VAL
1	E	48	THR
1	E	97	THR
1	E	125	ILE
1	E	135	THR
1	E	150	GLU
1	E	153	ARG
1	E	160	GLU
2	F	14	VAL
2	F	16	THR
2	F	20	VAL
2	F	35	ASP
2	F	40	VAL
2	F	46	LYS
2	F	48	ASP
2	F	52	ARG
2	F	59	LEU
2	F	62	THR
2	F	64	THR
2	F	104	VAL
2	F	123	ILE
2	F	129	LEU
2	F	132	LEU
2	F	136	ARG
2	F	142	THR
2	F	159	ILE
2	F	166	ILE
2	F	168	THR
2	F	182	LYS
2	F	184	LEU
2	F	191	ASN
2	F	192	THR
2	F	193	SER
2	F	196	VAL
2	F	201	MET
2	F	214	THR

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Mol	Chain	Res	Type
2	F	225	VAL
2	F	227	VAL
2	F	231	GLU
2	F	232	ILE
2	F	266	LEU
2	F	272	LEU
2	F	275	LEU
2	F	284	GLU
2	F	301	LEU
2	F	304	LEU
2	F	305	LEU
2	F	312	THR
2	F	314	ILE
2	F	327	ASN
2	F	341	CYS
2	F	349	ILE
2	F	360	ASP
2	F	364	LEU
2	F	367	GLN
2	F	377	CYS
2	F	390	ILE
2	F	400	THR
2	F	402	LEU
2	F	404	ASN
2	F	405	LEU
2	F	412	LEU
2	F	413	LEU
2	F	418	ARG
2	F	422	LEU
2	F	447	GLN
2	F	453	LEU
2	F	455	LEU
2	F	473	VAL
2	F	477	ASP
2	F	481	MET
2	F	490	LEU
2	F	495	MET
2	F	503	ARG
2	F	510	THR
2	F	516	ARG
2	F	519	TRP
2	F	528	THR

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Mol	Chain	Res	Type
2	F	537	ARG
2	F	542	ILE
2	F	545	ILE
2	F	578	ARG
3	S	217	LYS
1	G	8	LEU
1	G	14	GLU
1	G	22	VAL
1	G	29	ILE
1	G	35	ASP
1	G	36	ASP
1	G	42	VAL
1	G	44	LEU
1	G	47	VAL
1	G	48	THR
1	G	97	THR
1	G	114	LEU
1	G	129	THR
1	G	133	ILE
1	G	135	THR
1	G	144	THR
1	G	150	GLU
1	G	153	ARG
2	H	14	VAL
2	H	17	VAL
2	H	20	VAL
2	H	21	ILE
2	H	23	GLN
2	H	35	ASP
2	H	40	VAL
2	H	46	LYS
2	H	55	VAL
2	H	59	LEU
2	H	62	THR
2	H	64	THR
2	H	71	ARG
2	H	75	LEU
2	H	76	ARG
2	H	77	SER
2	H	85	ARG
2	H	95	ASN
2	H	100	VAL

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Mol	Chain	Res	Type
2	H	111	LEU
2	H	118	HIS
2	H	128	ASP
2	H	132	LEU
2	H	136	ARG
2	H	140	LEU
2	H	142	THR
2	H	159	ILE
2	H	166	ILE
2	H	168	THR
2	H	170	LEU
2	H	171	MET
2	H	175	SER
2	H	184	LEU
2	H	191	ASN
2	H	192	THR
2	H	193	SER
2	H	194	LEU
2	H	196	VAL
2	H	203	GLU
2	H	214	THR
2	H	225	VAL
2	H	231	GLU
2	H	233	LEU
2	H	238	PHE
2	H	255	GLU
2	H	266	LEU
2	H	272	LEU
2	H	275	LEU
2	H	284	GLU
2	H	291	PHE
2	H	298	LEU
2	H	301	LEU
2	H	304	LEU
2	H	311	CYS
2	H	313	LEU
2	H	315	GLN
2	H	316	LYS
2	H	317	CYS
2	H	320	LEU
2	H	321	GLU
2	H	322	VAL

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Mol	Chain	Res	Type
2	H	325	THR
2	H	326	ARG
2	H	329	ILE
2	H	343	GLN
2	H	345	LYS
2	H	364	LEU
2	H	365	VAL
2	H	370	LEU
2	H	377	CYS
2	H	382	TYR
2	H	388	SER
2	H	390	ILE
2	H	394	SER
2	H	396	GLU
2	H	398	ILE
2	H	402	LEU
2	H	409	ARG
2	H	410	LEU
2	H	411	VAL
2	H	415	ARG
2	H	422	LEU
2	H	428	VAL
2	H	438	LEU
2	H	453	LEU
2	H	458	ILE
2	H	467	TRP
2	H	485	ARG
2	H	490	LEU
2	H	503	ARG
2	H	511	LYS
2	H	516	ARG
2	H	534	GLN
2	H	542	ILE
2	H	544	LEU
2	H	547	SER
2	H	548	ARG
2	H	568	ILE
2	H	579	THR
2	H	583	THR
2	H	589	LYS
1	I	8	LEU
1	I	14	GLU

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Mol	Chain	Res	Type
1	I	22	VAL
1	I	29	ILE
1	I	35	ASP
1	I	36	ASP
1	I	42	VAL
1	I	44	LEU
1	I	47	VAL
1	I	48	THR
1	I	97	THR
1	I	125	ILE
1	I	135	THR
1	I	150	GLU
1	I	153	ARG
1	I	160	GLU
2	J	14	VAL
2	J	16	THR
2	J	17	VAL
2	J	20	VAL
2	J	35	ASP
2	J	40	VAL
2	J	46	LYS
2	J	52	ARG
2	J	59	LEU
2	J	62	THR
2	J	64	THR
2	J	104	VAL
2	J	123	ILE
2	J	129	LEU
2	J	132	LEU
2	J	136	ARG
2	J	142	THR
2	J	159	ILE
2	J	166	ILE
2	J	168	THR
2	J	182	LYS
2	J	184	LEU
2	J	191	ASN
2	J	192	THR
2	J	196	VAL
2	J	214	THR
2	J	225	VAL
2	J	227	VAL

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Mol	Chain	Res	Type
2	J	231	GLU
2	J	232	ILE
2	J	266	LEU
2	J	272	LEU
2	J	275	LEU
2	J	284	GLU
2	J	301	LEU
2	J	304	LEU
2	J	305	LEU
2	J	312	THR
2	J	314	ILE
2	J	327	ASN
2	J	341	CYS
2	J	349	ILE
2	J	360	ASP
2	J	364	LEU
2	J	365	VAL
2	J	367	GLN
2	J	377	CYS
2	J	390	ILE
2	J	400	THR
2	J	402	LEU
2	J	404	ASN
2	J	405	LEU
2	J	412	LEU
2	J	413	LEU
2	J	418	ARG
2	J	422	LEU
2	J	447	GLN
2	J	453	LEU
2	J	455	LEU
2	J	473	VAL
2	J	477	ASP
2	J	481	MET
2	J	490	LEU
2	J	495	MET
2	J	503	ARG
2	J	510	THR
2	J	516	ARG
2	J	519	TRP
2	J	528	THR
2	J	537	ARG

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Mol	Chain	Res	Type
2	J	542	ILE
2	J	545	ILE
2	J	578	ARG
3	U	217	LYS
1	K	8	LEU
1	K	14	GLU
1	K	22	VAL
1	K	29	ILE
1	K	35	ASP
1	K	36	ASP
1	K	42	VAL
1	K	44	LEU
1	K	47	VAL
1	K	48	THR
1	K	97	THR
1	K	125	ILE
1	K	150	GLU
1	K	153	ARG
1	K	160	GLU
2	L	14	VAL
2	L	16	THR
2	L	17	VAL
2	L	20	VAL
2	L	35	ASP
2	L	40	VAL
2	L	46	LYS
2	L	48	ASP
2	L	52	ARG
2	L	59	LEU
2	L	62	THR
2	L	64	THR
2	L	104	VAL
2	L	123	ILE
2	L	129	LEU
2	L	132	LEU
2	L	136	ARG
2	L	142	THR
2	L	159	ILE
2	L	166	ILE
2	L	168	THR
2	L	182	LYS
2	L	184	LEU

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Mol	Chain	Res	Type
2	L	191	ASN
2	L	192	THR
2	L	193	SER
2	L	196	VAL
2	L	201	MET
2	L	214	THR
2	L	225	VAL
2	L	227	VAL
2	L	231	GLU
2	L	232	ILE
2	L	266	LEU
2	L	272	LEU
2	L	275	LEU
2	L	284	GLU
2	L	301	LEU
2	L	304	LEU
2	L	305	LEU
2	L	312	THR
2	L	314	ILE
2	L	327	ASN
2	L	341	CYS
2	L	349	ILE
2	L	360	ASP
2	L	367	GLN
2	L	377	CYS
2	L	390	ILE
2	L	400	THR
2	L	402	LEU
2	L	404	ASN
2	L	405	LEU
2	L	413	LEU
2	L	418	ARG
2	L	422	LEU
2	L	447	GLN
2	L	453	LEU
2	L	455	LEU
2	L	473	VAL
2	L	477	ASP
2	L	481	MET
2	L	490	LEU
2	L	495	MET
2	L	503	ARG

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Mol	Chain	Res	Type
2	L	510	THR
2	L	516	ARG
2	L	519	TRP
2	L	528	THR
2	L	537	ARG
2	L	542	ILE
2	L	545	ILE
2	L	578	ARG
3	V	217	LYS
1	M	8	LEU
1	M	14	GLU
1	M	22	VAL
1	M	29	ILE
1	M	35	ASP
1	M	36	ASP
1	M	42	VAL
1	M	44	LEU
1	M	47	VAL
1	M	48	THR
1	M	97	THR
1	M	114	LEU
1	M	125	ILE
1	M	135	THR
1	M	150	GLU
1	M	153	ARG
1	M	160	GLU
2	N	14	VAL
2	N	16	THR
2	N	17	VAL
2	N	20	VAL
2	N	35	ASP
2	N	40	VAL
2	N	46	LYS
2	N	48	ASP
2	N	59	LEU
2	N	62	THR
2	N	64	THR
2	N	104	VAL
2	N	123	ILE
2	N	129	LEU
2	N	132	LEU
2	N	136	ARG

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Mol	Chain	Res	Type
2	N	142	THR
2	N	159	ILE
2	N	166	ILE
2	N	168	THR
2	N	184	LEU
2	N	191	ASN
2	N	192	THR
2	N	196	VAL
2	N	201	MET
2	N	214	THR
2	N	225	VAL
2	N	227	VAL
2	N	231	GLU
2	N	232	ILE
2	N	266	LEU
2	N	272	LEU
2	N	275	LEU
2	N	284	GLU
2	N	301	LEU
2	N	304	LEU
2	N	305	LEU
2	N	312	THR
2	N	314	ILE
2	N	327	ASN
2	N	341	CYS
2	N	344	LEU
2	N	349	ILE
2	N	360	ASP
2	N	364	LEU
2	N	365	VAL
2	N	367	GLN
2	N	377	CYS
2	N	390	ILE
2	N	400	THR
2	N	402	LEU
2	N	404	ASN
2	N	405	LEU
2	N	412	LEU
2	N	413	LEU
2	N	418	ARG
2	N	422	LEU
2	N	447	GLN

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Mol	Chain	Res	Type
2	N	453	LEU
2	N	455	LEU
2	N	473	VAL
2	N	477	ASP
2	N	481	MET
2	N	490	LEU
2	N	495	MET
2	N	503	ARG
2	N	510	THR
2	N	516	ARG
2	N	519	TRP
2	N	528	THR
2	N	537	ARG
2	N	542	ILE
2	N	545	ILE
2	N	578	ARG
1	O	8	LEU
1	O	14	GLU
1	O	22	VAL
1	O	29	ILE
1	O	35	ASP
1	O	36	ASP
1	O	42	VAL
1	O	44	LEU
1	O	47	VAL
1	O	48	THR
1	O	97	THR
1	O	125	ILE
1	O	150	GLU
1	O	153	ARG
1	O	160	GLU
2	P	14	VAL
2	P	16	THR
2	P	20	VAL
2	P	35	ASP
2	P	40	VAL
2	P	46	LYS
2	P	48	ASP
2	P	59	LEU
2	P	62	THR
2	P	64	THR
2	P	104	VAL

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Mol	Chain	Res	Type
2	P	123	ILE
2	P	129	LEU
2	P	132	LEU
2	P	136	ARG
2	P	142	THR
2	P	159	ILE
2	P	166	ILE
2	P	168	THR
2	P	182	LYS
2	P	184	LEU
2	P	191	ASN
2	P	193	SER
2	P	196	VAL
2	P	214	THR
2	P	225	VAL
2	P	227	VAL
2	P	231	GLU
2	P	232	ILE
2	P	266	LEU
2	P	272	LEU
2	P	275	LEU
2	P	284	GLU
2	P	301	LEU
2	P	304	LEU
2	P	305	LEU
2	P	312	THR
2	P	314	ILE
2	P	327	ASN
2	P	341	CYS
2	P	349	ILE
2	P	360	ASP
2	P	364	LEU
2	P	367	GLN
2	P	377	CYS
2	P	390	ILE
2	P	400	THR
2	P	402	LEU
2	P	404	ASN
2	P	405	LEU
2	P	412	LEU
2	P	413	LEU
2	P	418	ARG

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Mol	Chain	Res	Type
2	P	422	LEU
2	P	431	LEU
2	P	447	GLN
2	P	453	LEU
2	P	455	LEU
2	P	473	VAL
2	P	477	ASP
2	P	481	MET
2	P	490	LEU
2	P	495	MET
2	P	503	ARG
2	P	510	THR
2	P	516	ARG
2	P	519	TRP
2	P	528	THR
2	P	537	ARG
2	P	542	ILE
2	P	545	ILE
2	P	578	ARG
2	P	587	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	46	ASN
1	A	62	HIS
1	A	95	GLN
1	A	156	GLN
2	B	54	HIS
2	B	74	ASN
2	B	109	ASN
2	B	185	HIS
2	B	191	ASN
2	B	254	ASN
2	B	294	GLN
2	B	319	ASN
2	B	327	ASN
2	B	343	GLN
2	B	392	ASN
2	B	460	GLN
2	B	489	ASN

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Mol	Chain	Res	Type
2	B	564	HIS
1	C	46	ASN
1	C	62	HIS
1	C	109	ASN
1	C	119	GLN
1	C	141	ASN
2	D	54	HIS
2	D	74	ASN
2	D	109	ASN
2	D	185	HIS
2	D	190	HIS
2	D	191	ASN
2	D	254	ASN
2	D	294	GLN
2	D	319	ASN
2	D	327	ASN
2	D	343	GLN
2	D	460	GLN
2	D	489	ASN
2	D	491	GLN
2	D	564	HIS
2	D	567	HIS
1	E	46	ASN
1	E	62	HIS
1	E	141	ASN
1	E	156	GLN
2	F	23	GLN
2	F	54	HIS
2	F	74	ASN
2	F	109	ASN
2	F	110	ASN
2	F	113	GLN
2	F	118	HIS
2	F	191	ASN
2	F	254	ASN
2	F	327	ASN
2	F	343	GLN
2	F	460	GLN
2	F	489	ASN
2	F	564	HIS
2	F	567	HIS
1	G	27	GLN

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Mol	Chain	Res	Type
1	G	46	ASN
1	G	62	HIS
1	G	119	GLN
2	H	23	GLN
2	H	74	ASN
2	H	95	ASN
2	H	110	ASN
2	H	191	ASN
2	H	265	ASN
2	H	310	HIS
2	H	343	GLN
2	H	375	GLN
2	H	392	ASN
2	H	447	GLN
2	H	460	GLN
2	H	489	ASN
2	H	577	GLN
1	I	46	ASN
1	I	62	HIS
1	I	106	ASN
1	I	141	ASN
2	J	23	GLN
2	J	54	HIS
2	J	74	ASN
2	J	109	ASN
2	J	118	HIS
2	J	185	HIS
2	J	191	ASN
2	J	254	ASN
2	J	294	GLN
2	J	327	ASN
2	J	343	GLN
2	J	460	GLN
2	J	489	ASN
2	J	491	GLN
2	J	564	HIS
1	K	46	ASN
1	K	62	HIS
1	K	109	ASN
1	K	119	GLN
1	K	141	ASN
1	K	156	GLN

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Mol	Chain	Res	Type
2	L	54	HIS
2	L	74	ASN
2	L	109	ASN
2	L	118	HIS
2	L	190	HIS
2	L	191	ASN
2	L	254	ASN
2	L	294	GLN
2	L	319	ASN
2	L	327	ASN
2	L	343	GLN
2	L	460	GLN
2	L	489	ASN
2	L	491	GLN
2	L	564	HIS
1	M	46	ASN
1	M	62	HIS
1	M	141	ASN
2	N	54	HIS
2	N	74	ASN
2	N	109	ASN
2	N	191	ASN
2	N	244	ASN
2	N	254	ASN
2	N	327	ASN
2	N	343	GLN
2	N	460	GLN
2	N	489	ASN
2	N	564	HIS
2	N	567	HIS
1	O	27	GLN
1	O	46	ASN
1	O	62	HIS
1	O	109	ASN
1	O	141	ASN
2	P	54	HIS
2	P	74	ASN
2	P	109	ASN
2	P	110	ASN
2	P	118	HIS
2	P	191	ASN
2	P	254	ASN

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Mol	Chain	Res	Type
2	P	327	ASN
2	P	343	GLN
2	P	460	GLN
2	P	489	ASN
2	P	491	GLN
2	P	564	HIS
2	P	567	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
5	PO4	H	1101	-	4,4,4	4.52	4 (100%)	6,6,6	0.66	0
5	PO4	F	1101	-	4,4,4	4.30	4 (100%)	6,6,6	1.28	0
5	PO4	L	1103	-	4,4,4	4.32	4 (100%)	6,6,6	0.79	0
4	OGK	B	1100	-	25,25,25	6.97	11 (44%)	31,38,38	2.47	14 (45%)
5	PO4	N	1101	-	4,4,4	4.59	3 (75%)	6,6,6	1.52	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OGK	F	3100	-	25,25,25	6.97	11 (44%)	31,38,38	2.45	12 (38%)
5	PO4	P	1104	-	4,4,4	4.34	4 (100%)	6,6,6	0.76	0
5	PO4	B	1104	-	4,4,4	4.29	4 (100%)	6,6,6	0.71	0
5	PO4	J	1101	-	4,4,4	4.21	4 (100%)	6,6,6	1.02	0
5	PO4	J	1102	-	4,4,4	4.38	4 (100%)	6,6,6	0.61	0
5	PO4	P	1101	-	4,4,4	4.26	4 (100%)	6,6,6	0.86	0
4	OGK	D	2100	-	25,25,25	7.09	11 (44%)	31,38,38	2.55	14 (45%)
4	OGK	J	5100	-	25,25,25	7.09	12 (48%)	31,38,38	2.50	14 (45%)
5	PO4	D	1103	-	4,4,4	4.42	4 (100%)	6,6,6	0.75	0
4	OGK	H	4100	-	25,25,25	6.90	11 (44%)	31,38,38	2.59	15 (48%)
5	PO4	L	1101	-	4,4,4	4.33	4 (100%)	6,6,6	0.90	0
5	PO4	D	1102	-	4,4,4	4.30	4 (100%)	6,6,6	0.34	0
5	PO4	N	1102	-	4,4,4	4.42	4 (100%)	6,6,6	0.55	0
5	PO4	N	1104	-	4,4,4	4.41	4 (100%)	6,6,6	0.72	0
5	PO4	N	1103	-	4,4,4	4.28	3 (75%)	6,6,6	1.40	1 (16%)
5	PO4	H	1104	-	4,4,4	4.46	4 (100%)	6,6,6	1.15	1 (16%)
5	PO4	F	1102	-	4,4,4	4.67	4 (100%)	6,6,6	0.58	0
5	PO4	F	1104	-	4,4,4	4.58	4 (100%)	6,6,6	0.71	0
5	PO4	H	1102	-	4,4,4	4.41	4 (100%)	6,6,6	0.83	0
5	PO4	B	1101	-	4,4,4	4.21	4 (100%)	6,6,6	0.85	0
5	PO4	F	1103	-	4,4,4	4.32	4 (100%)	6,6,6	0.79	0
5	PO4	J	1103	-	4,4,4	4.26	4 (100%)	6,6,6	0.67	0
5	PO4	P	1103	-	4,4,4	4.25	4 (100%)	6,6,6	0.76	0
5	PO4	J	1104	-	4,4,4	4.35	4 (100%)	6,6,6	0.69	0
5	PO4	L	1102	-	4,4,4	4.36	4 (100%)	6,6,6	0.36	0
5	PO4	L	1104	-	4,4,4	4.50	4 (100%)	6,6,6	0.60	0
5	PO4	P	1102	-	4,4,4	4.32	4 (100%)	6,6,6	0.60	0
4	OGK	P	8100	-	25,25,25	7.06	11 (44%)	31,38,38	2.47	12 (38%)
4	OGK	L	6100	-	25,25,25	6.92	11 (44%)	31,38,38	2.44	13 (41%)
5	PO4	B	1102	-	4,4,4	4.35	4 (100%)	6,6,6	0.60	0
5	PO4	B	1103	-	4,4,4	4.31	4 (100%)	6,6,6	0.49	0
4	OGK	N	7100	-	25,25,25	6.69	11 (44%)	31,38,38	2.50	10 (32%)
5	PO4	D	1101	-	4,4,4	4.07	4 (100%)	6,6,6	1.09	0
5	PO4	H	1103	-	4,4,4	4.59	4 (100%)	6,6,6	0.64	0
5	PO4	D	1104	-	4,4,4	4.33	4 (100%)	6,6,6	0.83	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	OGK	D	2100	-	-	9/19/52/52	0/3/3/3
4	OGK	J	5100	-	-	9/19/52/52	0/3/3/3
4	OGK	B	1100	-	-	10/19/52/52	0/3/3/3
4	OGK	P	8100	-	-	9/19/52/52	0/3/3/3
4	OGK	L	6100	-	-	9/19/52/52	0/3/3/3
4	OGK	H	4100	-	1/1/9/10	10/19/52/52	0/3/3/3
4	OGK	F	3100	-	-	10/19/52/52	0/3/3/3
4	OGK	N	7100	-	-	10/19/52/52	0/3/3/3

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5100	OGK	C13-C09	-22.76	1.27	1.51
4	D	2100	OGK	C13-C09	-22.66	1.27	1.51
4	P	8100	OGK	C13-C09	-22.40	1.28	1.51
4	F	3100	OGK	C13-C09	-22.34	1.28	1.51
4	B	1100	OGK	C13-C09	-22.09	1.28	1.51
4	L	6100	OGK	C13-C09	-22.08	1.28	1.51
4	H	4100	OGK	C13-C09	-21.85	1.28	1.51
4	N	7100	OGK	C13-C09	-21.06	1.29	1.51
4	P	8100	OGK	C09-C14	-17.95	1.33	1.52
4	D	2100	OGK	C09-C14	-17.77	1.33	1.52
4	J	5100	OGK	C09-C14	-17.54	1.34	1.52
4	F	3100	OGK	C09-C14	-17.45	1.34	1.52
4	B	1100	OGK	C09-C14	-17.35	1.34	1.52
4	L	6100	OGK	C09-C14	-17.22	1.34	1.52
4	H	4100	OGK	C09-C14	-17.19	1.34	1.52
4	N	7100	OGK	C09-C14	-16.45	1.35	1.52
4	J	5100	OGK	C09-C10	-16.21	1.13	1.52
4	D	2100	OGK	C09-C10	-16.10	1.13	1.52
4	P	8100	OGK	C09-C10	-16.07	1.14	1.52
4	L	6100	OGK	C09-C10	-15.79	1.14	1.52
4	B	1100	OGK	C09-C10	-15.59	1.15	1.52
4	F	3100	OGK	C09-C10	-15.55	1.15	1.52
4	H	4100	OGK	C09-C10	-15.32	1.15	1.52
4	N	7100	OGK	C09-C10	-15.27	1.15	1.52
4	B	1100	OGK	C13-C14	-7.84	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2100	OGK	C13-C14	-7.68	1.32	1.50
4	H	4100	OGK	C13-C14	-7.55	1.32	1.50
4	J	5100	OGK	C13-C14	-7.49	1.32	1.50
4	L	6100	OGK	C13-C14	-7.43	1.32	1.50
4	B	1100	OGK	C06-N08	7.39	1.49	1.34
4	F	3100	OGK	C13-C14	-7.34	1.33	1.50
4	F	3100	OGK	C06-N08	7.25	1.49	1.34
4	P	8100	OGK	C13-C14	-7.24	1.33	1.50
4	P	8100	OGK	C06-N08	7.20	1.49	1.34
5	F	1102	PO4	P-O1	7.05	1.66	1.50
4	N	7100	OGK	C13-C14	-6.95	1.33	1.50
4	N	7100	OGK	C06-N08	6.95	1.48	1.34
4	D	2100	OGK	C06-N08	6.90	1.48	1.34
5	F	1104	PO4	P-O1	6.88	1.66	1.50
5	J	1104	PO4	P-O1	6.87	1.66	1.50
5	L	1104	PO4	P-O1	6.74	1.66	1.50
5	H	1103	PO4	P-O1	6.66	1.66	1.50
5	B	1102	PO4	P-O1	6.56	1.65	1.50
4	J	5100	OGK	C06-N08	6.55	1.47	1.34
5	N	1102	PO4	P-O1	6.53	1.65	1.50
5	N	1103	PO4	P-O1	6.52	1.65	1.50
5	J	1103	PO4	P-O1	6.51	1.65	1.50
4	L	6100	OGK	C06-N08	6.50	1.47	1.34
5	L	1103	PO4	P-O1	6.49	1.65	1.50
5	D	1103	PO4	P-O1	6.49	1.65	1.50
4	H	4100	OGK	C06-N08	6.48	1.47	1.34
5	P	1104	PO4	P-O1	6.47	1.65	1.50
5	D	1102	PO4	P-O1	6.43	1.65	1.50
5	N	1101	PO4	P-O1	6.42	1.65	1.50
5	H	1102	PO4	P-O1	6.41	1.65	1.50
5	N	1104	PO4	P-O1	6.40	1.65	1.50
5	P	1103	PO4	P-O1	6.39	1.65	1.50
5	J	1102	PO4	P-O1	6.38	1.65	1.50
5	F	1101	PO4	P-O1	6.38	1.65	1.50
5	F	1103	PO4	P-O1	6.38	1.65	1.50
5	D	1104	PO4	P-O1	6.38	1.65	1.50
5	B	1104	PO4	P-O1	6.35	1.65	1.50
5	P	1102	PO4	P-O1	6.34	1.65	1.50
5	H	1104	PO4	P-O1	6.34	1.65	1.50
5	H	1101	PO4	P-O1	6.34	1.65	1.50
5	B	1103	PO4	P-O1	6.33	1.65	1.50
5	P	1101	PO4	P-O1	6.32	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1102	PO4	P-O1	6.29	1.65	1.50
5	B	1101	PO4	P-O1	6.15	1.64	1.50
5	J	1101	PO4	P-O1	6.07	1.64	1.50
5	L	1101	PO4	P-O1	6.03	1.64	1.50
5	D	1101	PO4	P-O1	5.84	1.64	1.50
4	H	4100	OGK	C23-C22	5.04	1.61	1.53
5	N	1101	PO4	P-O3	4.80	1.68	1.54
4	N	7100	OGK	C23-C22	4.42	1.60	1.53
5	H	1104	PO4	P-O3	4.25	1.67	1.54
5	N	1101	PO4	P-O4	4.16	1.66	1.54
5	N	1104	PO4	P-O4	4.16	1.66	1.54
5	H	1103	PO4	P-O3	4.08	1.66	1.54
4	N	7100	OGK	O12-C10	4.08	1.45	1.30
5	H	1101	PO4	P-O3	4.05	1.66	1.54
5	L	1104	PO4	P-O4	4.04	1.66	1.54
5	B	1103	PO4	P-O3	3.99	1.66	1.54
5	H	1104	PO4	P-O4	3.96	1.66	1.54
5	H	1101	PO4	P-O4	3.96	1.66	1.54
5	H	1102	PO4	P-O4	3.95	1.66	1.54
5	F	1103	PO4	P-O4	3.92	1.66	1.54
4	H	4100	OGK	O12-C10	3.92	1.44	1.30
5	L	1101	PO4	P-O3	3.90	1.66	1.54
5	N	1102	PO4	P-O4	3.90	1.66	1.54
5	F	1102	PO4	P-O3	3.89	1.66	1.54
5	P	1102	PO4	P-O3	3.88	1.65	1.54
5	J	1102	PO4	P-O3	3.87	1.65	1.54
5	F	1104	PO4	P-O4	3.86	1.65	1.54
5	F	1104	PO4	P-O3	3.85	1.65	1.54
5	D	1104	PO4	P-O3	3.85	1.65	1.54
5	J	1101	PO4	P-O4	3.84	1.65	1.54
5	L	1101	PO4	P-O4	3.84	1.65	1.54
5	H	1103	PO4	P-O4	3.83	1.65	1.54
5	L	1102	PO4	P-O3	3.80	1.65	1.54
5	B	1101	PO4	P-O3	3.80	1.65	1.54
5	N	1103	PO4	P-O3	3.79	1.65	1.54
5	N	1104	PO4	P-O3	3.79	1.65	1.54
5	N	1102	PO4	P-O3	3.74	1.65	1.54
4	F	3100	OGK	C18-C17	-3.72	1.44	1.54
5	P	1104	PO4	P-O4	3.72	1.65	1.54
5	J	1101	PO4	P-O3	3.71	1.65	1.54
5	L	1103	PO4	P-O3	3.71	1.65	1.54
5	F	1102	PO4	P-O4	3.69	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1104	PO4	P-O3	3.68	1.65	1.54
5	D	1102	PO4	P-O4	3.67	1.65	1.54
5	F	1103	PO4	P-O3	3.67	1.65	1.54
5	B	1102	PO4	P-O4	3.67	1.65	1.54
4	P	8100	OGK	C23-C22	3.67	1.59	1.53
5	D	1104	PO4	P-O4	3.66	1.65	1.54
4	B	1100	OGK	C18-C17	-3.66	1.44	1.54
4	B	1100	OGK	O12-C10	3.65	1.43	1.30
5	P	1104	PO4	P-O3	3.62	1.65	1.54
5	J	1102	PO4	P-O4	3.61	1.65	1.54
5	P	1103	PO4	P-O4	3.61	1.65	1.54
5	P	1101	PO4	P-O3	3.60	1.65	1.54
5	P	1103	PO4	P-O3	3.60	1.65	1.54
5	J	1104	PO4	P-O3	3.59	1.65	1.54
5	H	1102	PO4	P-O3	3.58	1.65	1.54
5	P	1102	PO4	P-O4	3.57	1.65	1.54
5	B	1104	PO4	P-O3	3.57	1.65	1.54
4	P	8100	OGK	C18-C17	-3.57	1.45	1.54
4	F	3100	OGK	O12-C10	3.57	1.43	1.30
5	N	1103	PO4	P-O4	3.57	1.65	1.54
5	D	1101	PO4	P-O4	3.56	1.65	1.54
5	L	1102	PO4	P-O4	3.56	1.65	1.54
5	D	1103	PO4	P-O3	3.54	1.65	1.54
4	J	5100	OGK	C18-C17	-3.53	1.45	1.54
4	L	6100	OGK	C23-C22	3.53	1.59	1.53
5	B	1102	PO4	P-O3	3.49	1.64	1.54
5	J	1103	PO4	P-O3	3.48	1.64	1.54
5	F	1101	PO4	P-O3	3.48	1.64	1.54
4	L	6100	OGK	O12-C10	3.47	1.42	1.30
5	D	1103	PO4	P-O4	3.46	1.64	1.54
5	B	1104	PO4	P-O4	3.45	1.64	1.54
5	P	1101	PO4	P-O4	3.44	1.64	1.54
5	F	1101	PO4	P-O4	3.43	1.64	1.54
4	D	2100	OGK	C18-C17	-3.43	1.45	1.54
4	P	8100	OGK	O12-C10	3.41	1.42	1.30
4	B	1100	OGK	C23-C22	3.40	1.58	1.53
4	H	4100	OGK	C18-C17	-3.40	1.45	1.54
5	D	1103	PO4	P-O2	-3.40	1.44	1.54
4	N	7100	OGK	C18-C17	-3.39	1.45	1.54
4	D	2100	OGK	O12-C10	3.39	1.42	1.30
4	J	5100	OGK	O12-C10	3.38	1.42	1.30
5	D	1101	PO4	P-O3	3.35	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2100	OGK	C23-C22	3.31	1.58	1.53
4	J	5100	OGK	C23-C22	3.29	1.58	1.53
5	J	1104	PO4	P-O4	3.26	1.64	1.54
5	L	1103	PO4	P-O4	3.18	1.63	1.54
5	J	1103	PO4	P-O4	3.17	1.63	1.54
4	L	6100	OGK	C18-C17	-3.17	1.46	1.54
5	D	1102	PO4	P-O3	3.15	1.63	1.54
5	B	1103	PO4	P-O4	3.14	1.63	1.54
4	B	1100	OGK	C09-N08	3.09	1.50	1.45
4	N	7100	OGK	C09-N08	3.08	1.50	1.45
5	H	1101	PO4	P-O2	-3.07	1.45	1.54
5	B	1101	PO4	P-O2	-3.06	1.45	1.54
5	D	1102	PO4	P-O2	-3.06	1.45	1.54
5	B	1101	PO4	P-O4	3.05	1.63	1.54
5	F	1101	PO4	P-O2	-3.05	1.45	1.54
5	L	1102	PO4	P-O2	-3.05	1.45	1.54
4	L	6100	OGK	C09-N08	2.97	1.50	1.45
5	H	1103	PO4	P-O2	-2.96	1.46	1.54
5	F	1102	PO4	P-O2	-2.96	1.46	1.54
5	L	1101	PO4	P-O2	-2.95	1.46	1.54
5	B	1104	PO4	P-O2	-2.95	1.46	1.54
5	B	1103	PO4	P-O2	-2.92	1.46	1.54
4	J	5100	OGK	C05-C06	2.91	1.56	1.51
4	D	2100	OGK	C05-C06	2.91	1.56	1.51
5	L	1103	PO4	P-O2	-2.91	1.46	1.54
5	D	1101	PO4	P-O2	-2.90	1.46	1.54
4	F	3100	OGK	C09-N08	2.88	1.50	1.45
4	F	3100	OGK	C23-C22	2.88	1.58	1.53
5	H	1102	PO4	P-O2	-2.87	1.46	1.54
4	J	5100	OGK	C09-N08	2.85	1.50	1.45
5	J	1103	PO4	P-O2	-2.82	1.46	1.54
5	P	1101	PO4	P-O2	-2.82	1.46	1.54
4	L	6100	OGK	C05-C06	2.82	1.56	1.51
5	J	1102	PO4	P-O2	-2.82	1.46	1.54
4	H	4100	OGK	C05-C06	2.73	1.56	1.51
5	B	1102	PO4	P-O2	-2.64	1.46	1.54
4	H	4100	OGK	C09-N08	2.62	1.50	1.45
5	F	1104	PO4	P-O2	-2.62	1.47	1.54
4	P	8100	OGK	C05-C06	2.61	1.56	1.51
5	P	1102	PO4	P-O2	-2.58	1.47	1.54
4	J	5100	OGK	O07-C06	-2.58	1.18	1.23
5	P	1104	PO4	P-O2	-2.57	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1102	PO4	P-O2	-2.55	1.47	1.54
4	D	2100	OGK	O07-C06	-2.54	1.18	1.23
5	D	1104	PO4	P-O2	-2.47	1.47	1.54
4	H	4100	OGK	O07-C06	-2.46	1.18	1.23
5	L	1104	PO4	P-O2	-2.40	1.47	1.54
4	L	6100	OGK	O07-C06	-2.39	1.18	1.23
5	H	1104	PO4	P-O2	-2.37	1.47	1.54
4	F	3100	OGK	C05-C06	2.35	1.55	1.51
5	J	1101	PO4	P-O2	-2.35	1.47	1.54
5	P	1103	PO4	P-O2	-2.33	1.47	1.54
4	B	1100	OGK	O07-C06	-2.29	1.19	1.23
5	N	1104	PO4	P-O2	-2.28	1.48	1.54
4	P	8100	OGK	C09-N08	2.27	1.49	1.45
5	F	1103	PO4	P-O2	-2.25	1.48	1.54
5	J	1104	PO4	P-O2	-2.19	1.48	1.54
4	N	7100	OGK	C05-C06	2.19	1.55	1.51
4	D	2100	OGK	C09-N08	2.15	1.49	1.45
4	N	7100	OGK	O07-C06	-2.06	1.19	1.23
4	B	1100	OGK	C05-C06	2.06	1.55	1.51
4	F	3100	OGK	O07-C06	-2.05	1.19	1.23
4	J	5100	OGK	O21-C20	-2.04	1.18	1.21
4	P	8100	OGK	O07-C06	-2.02	1.19	1.23

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	7100	OGK	C04-C05-C17	6.09	121.81	110.06
4	J	5100	OGK	C13-C14-C09	-5.99	57.22	60.30
4	F	3100	OGK	C13-C14-C09	-5.78	57.33	60.30
4	P	8100	OGK	C13-C14-C09	-5.70	57.37	60.30
4	B	1100	OGK	C04-C05-C17	5.68	121.01	110.06
4	P	8100	OGK	C04-C05-C17	5.65	120.95	110.06
4	D	2100	OGK	C13-C14-C09	-5.58	57.43	60.30
4	J	5100	OGK	C04-C05-C17	5.58	120.82	110.06
4	L	6100	OGK	C13-C14-C09	-5.54	57.45	60.30
4	F	3100	OGK	C04-C05-C17	5.47	120.60	110.06
4	L	6100	OGK	C04-C05-C17	5.45	120.58	110.06
4	N	7100	OGK	C13-C14-C09	-5.43	57.51	60.30
4	D	2100	OGK	C04-C05-C17	5.34	120.35	110.06
4	L	6100	OGK	C05-C04-C03	5.26	119.91	109.20
4	H	4100	OGK	C13-C14-C09	-5.20	57.63	60.30
4	H	4100	OGK	C23-C03-C02	5.12	121.43	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	8100	OGK	C05-C04-C03	5.12	119.63	109.20
4	B	1100	OGK	C13-C14-C09	-5.05	57.70	60.30
4	D	2100	OGK	C05-C04-C03	5.02	119.42	109.20
4	H	4100	OGK	C14-C09-C10	4.85	128.15	117.69
4	D	2100	OGK	C14-C09-C10	4.75	127.92	117.69
4	J	5100	OGK	C05-C04-C03	4.73	118.84	109.20
4	B	1100	OGK	C05-C04-C03	4.68	118.74	109.20
4	F	3100	OGK	C05-C04-C03	4.59	118.55	109.20
4	B	1100	OGK	C14-C09-C10	4.54	127.46	117.69
4	N	7100	OGK	C14-C09-C10	4.52	127.44	117.69
4	N	7100	OGK	C18-C17-C22	4.52	109.22	103.97
4	N	7100	OGK	C05-C04-C03	4.36	118.08	109.20
4	F	3100	OGK	C14-C09-C10	4.32	127.00	117.69
4	P	8100	OGK	C14-C09-C10	4.21	126.76	117.69
4	L	6100	OGK	C14-C09-C10	4.16	126.66	117.69
4	B	1100	OGK	O07-C06-C05	-4.16	116.69	121.67
4	H	4100	OGK	C13-C09-N08	-4.11	112.35	117.77
4	P	8100	OGK	C13-C09-C14	3.99	61.17	59.12
4	J	5100	OGK	C14-C09-C10	3.97	126.24	117.69
4	H	4100	OGK	C04-C05-C17	3.87	117.52	110.06
4	F	3100	OGK	C18-C17-C22	3.86	108.46	103.97
4	J	5100	OGK	C18-C17-C22	3.82	108.41	103.97
4	H	4100	OGK	C22-C23-C03	3.54	116.40	109.20
4	D	2100	OGK	C13-C09-N08	-3.51	113.14	117.77
4	F	3100	OGK	C13-C09-C14	3.44	60.89	59.12
4	D	2100	OGK	C18-C17-C22	3.36	107.87	103.97
4	J	5100	OGK	C13-C09-C14	3.35	60.84	59.12
4	H	4100	OGK	C23-C03-C04	3.31	115.98	109.69
4	H	4100	OGK	C14-C09-N08	-3.30	108.61	117.62
4	F	3100	OGK	C13-C09-N08	-3.20	113.54	117.77
4	H	4100	OGK	C18-C17-C22	3.19	107.68	103.97
4	N	7100	OGK	C13-C09-C14	3.19	60.76	59.12
4	D	2100	OGK	C04-C03-C02	-3.17	106.58	112.25
4	F	3100	OGK	C14-C09-N08	-3.09	109.17	117.62
4	D	2100	OGK	C14-C09-N08	-3.09	109.19	117.62
4	B	1100	OGK	C05-C06-N08	3.07	120.19	116.18
4	P	8100	OGK	C18-C17-C22	3.04	107.50	103.97
4	P	8100	OGK	C13-C09-N08	-3.02	113.79	117.77
4	L	6100	OGK	C13-C09-N08	-3.01	113.80	117.77
4	D	2100	OGK	C13-C09-C14	2.98	60.65	59.12
4	L	6100	OGK	C13-C09-C14	2.98	60.65	59.12
4	P	8100	OGK	C14-C09-N08	-2.90	109.70	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	7100	OGK	C13-C09-N08	-2.88	113.97	117.77
4	L	6100	OGK	C18-C17-C22	2.85	107.28	103.97
4	J	5100	OGK	C14-C09-N08	-2.84	109.85	117.62
4	L	6100	OGK	C14-C09-N08	-2.84	109.88	117.62
4	B	1100	OGK	C13-C09-N08	-2.83	114.03	117.77
4	J	5100	OGK	C04-C03-C02	-2.82	107.20	112.25
4	N	7100	OGK	C14-C09-N08	-2.82	109.93	117.62
4	L	6100	OGK	C04-C03-C02	-2.81	107.22	112.25
4	J	5100	OGK	C13-C09-N08	-2.81	114.07	117.77
4	B	1100	OGK	C14-C09-N08	-2.79	110.00	117.62
4	J	5100	OGK	C05-C06-N08	2.79	119.82	116.18
4	H	4100	OGK	C05-C04-C03	2.76	114.82	109.20
5	N	1103	PO4	O4-P-O1	-2.74	101.28	110.95
4	D	2100	OGK	C05-C06-N08	2.68	119.69	116.18
4	B	1100	OGK	C15-C14-C13	-2.65	117.56	121.32
4	P	8100	OGK	O07-C06-C05	-2.65	118.50	121.67
4	H	4100	OGK	C13-C09-C14	2.57	60.44	59.12
4	P	8100	OGK	C04-C03-C02	-2.56	107.67	112.25
4	B	1100	OGK	C09-C13-C14	2.53	62.10	60.84
4	J	5100	OGK	O07-C06-N08	-2.53	117.86	123.15
4	L	6100	OGK	C05-C06-N08	2.50	119.44	116.18
4	F	3100	OGK	O07-C06-C05	-2.46	118.73	121.67
4	H	4100	OGK	O12-C10-C09	2.46	120.18	113.66
4	B	1100	OGK	C04-C03-C02	-2.46	107.86	112.25
4	L	6100	OGK	O07-C06-N08	-2.31	118.33	123.15
4	D	2100	OGK	C15-C14-C13	-2.29	118.07	121.32
4	P	8100	OGK	C05-C06-N08	2.25	119.12	116.18
4	B	1100	OGK	C18-C17-C22	2.24	106.57	103.97
4	L	6100	OGK	O12-C10-C09	2.23	119.58	113.66
4	J	5100	OGK	C09-C13-C14	2.22	61.94	60.84
4	D	2100	OGK	O12-C10-C09	2.21	119.53	113.66
4	P	8100	OGK	O12-C10-C09	2.21	119.51	113.66
4	H	4100	OGK	C09-C13-C14	2.20	61.93	60.84
4	F	3100	OGK	O12-C10-C09	2.18	119.43	113.66
5	N	1101	PO4	O3-P-O2	2.17	114.68	107.91
4	D	2100	OGK	C09-C13-C14	2.17	61.92	60.84
4	N	7100	OGK	C22-C23-C03	2.16	113.60	109.20
4	H	4100	OGK	C19-C20-C22	-2.15	105.53	109.06
4	J	5100	OGK	O12-C10-C09	2.14	119.34	113.66
4	F	3100	OGK	C05-C06-N08	2.14	118.97	116.18
4	L	6100	OGK	C09-C13-C14	2.13	61.90	60.84
4	J	5100	OGK	C22-C23-C03	2.10	113.48	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1100	OGK	C13-C09-C14	2.10	60.20	59.12
4	F	3100	OGK	C04-C03-C02	-2.09	108.52	112.25
4	N	7100	OGK	O07-C06-C05	-2.04	119.23	121.67
4	D	2100	OGK	O07-C06-N08	-2.04	118.90	123.15
5	H	1104	PO4	O4-P-O3	2.03	114.23	107.91
4	B	1100	OGK	O12-C10-C09	2.03	119.03	113.66
4	H	4100	OGK	C05-C06-N08	2.02	118.82	116.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	4100	OGK	C03

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1100	OGK	C17-C05-C06-O07
4	B	1100	OGK	C17-C05-C06-N08
4	B	1100	OGK	N08-C09-C10-O11
4	B	1100	OGK	N08-C09-C10-O12
4	B	1100	OGK	C14-C09-C10-O11
4	B	1100	OGK	C14-C09-C10-O12
4	D	2100	OGK	C17-C05-C06-O07
4	D	2100	OGK	C17-C05-C06-N08
4	D	2100	OGK	N08-C09-C10-O12
4	D	2100	OGK	C14-C09-C10-O11
4	D	2100	OGK	C14-C09-C10-O12
4	F	3100	OGK	C17-C05-C06-O07
4	F	3100	OGK	C17-C05-C06-N08
4	F	3100	OGK	N08-C09-C10-O11
4	F	3100	OGK	N08-C09-C10-O12
4	F	3100	OGK	C14-C09-C10-O11
4	F	3100	OGK	C14-C09-C10-O12
4	H	4100	OGK	C17-C05-C06-O07
4	H	4100	OGK	C17-C05-C06-N08
4	H	4100	OGK	N08-C09-C10-O11
4	H	4100	OGK	N08-C09-C10-O12
4	H	4100	OGK	C14-C09-C10-O11
4	H	4100	OGK	C14-C09-C10-O12
4	J	5100	OGK	C17-C05-C06-O07
4	J	5100	OGK	C17-C05-C06-N08
4	J	5100	OGK	N08-C09-C10-O11

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Mol	Chain	Res	Type	Atoms
4	J	5100	OGK	N08-C09-C10-O12
4	J	5100	OGK	C14-C09-C10-O11
4	J	5100	OGK	C14-C09-C10-O12
4	L	6100	OGK	C17-C05-C06-O07
4	L	6100	OGK	C17-C05-C06-N08
4	L	6100	OGK	N08-C09-C10-O11
4	L	6100	OGK	N08-C09-C10-O12
4	L	6100	OGK	C14-C09-C10-O11
4	L	6100	OGK	C14-C09-C10-O12
4	N	7100	OGK	C17-C05-C06-O07
4	N	7100	OGK	C17-C05-C06-N08
4	N	7100	OGK	N08-C09-C10-O11
4	N	7100	OGK	N08-C09-C10-O12
4	N	7100	OGK	C14-C09-C10-O11
4	N	7100	OGK	C14-C09-C10-O12
4	P	8100	OGK	C17-C05-C06-O07
4	P	8100	OGK	C17-C05-C06-N08
4	P	8100	OGK	N08-C09-C10-O11
4	P	8100	OGK	N08-C09-C10-O12
4	P	8100	OGK	C14-C09-C10-O11
4	P	8100	OGK	C14-C09-C10-O12
4	H	4100	OGK	C01-C02-C03-C23
4	D	2100	OGK	N08-C09-C10-O11
4	B	1100	OGK	C01-C02-C03-C04
4	B	1100	OGK	C01-C02-C03-C23
4	D	2100	OGK	C01-C02-C03-C23
4	F	3100	OGK	C01-C02-C03-C04
4	F	3100	OGK	C01-C02-C03-C23
4	J	5100	OGK	C01-C02-C03-C23
4	L	6100	OGK	C01-C02-C03-C23
4	N	7100	OGK	C01-C02-C03-C04
4	N	7100	OGK	C01-C02-C03-C23
4	P	8100	OGK	C01-C02-C03-C23
4	B	1100	OGK	C13-C14-C15-C16
4	D	2100	OGK	C13-C14-C15-C16
4	F	3100	OGK	C13-C14-C15-C16
4	H	4100	OGK	C13-C14-C15-C16
4	J	5100	OGK	C13-C14-C15-C16
4	L	6100	OGK	C13-C14-C15-C16
4	N	7100	OGK	C13-C14-C15-C16
4	P	8100	OGK	C13-C14-C15-C16
4	H	4100	OGK	C04-C05-C06-N08

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Mol	Chain	Res	Type	Atoms
4	B	1100	OGK	C13-C09-C10-O11
4	D	2100	OGK	C13-C09-C10-O11
4	F	3100	OGK	C13-C09-C10-O11
4	H	4100	OGK	C13-C09-C10-O11
4	J	5100	OGK	C13-C09-C10-O11
4	L	6100	OGK	C13-C09-C10-O11
4	N	7100	OGK	C13-C09-C10-O11
4	P	8100	OGK	C13-C09-C10-O11

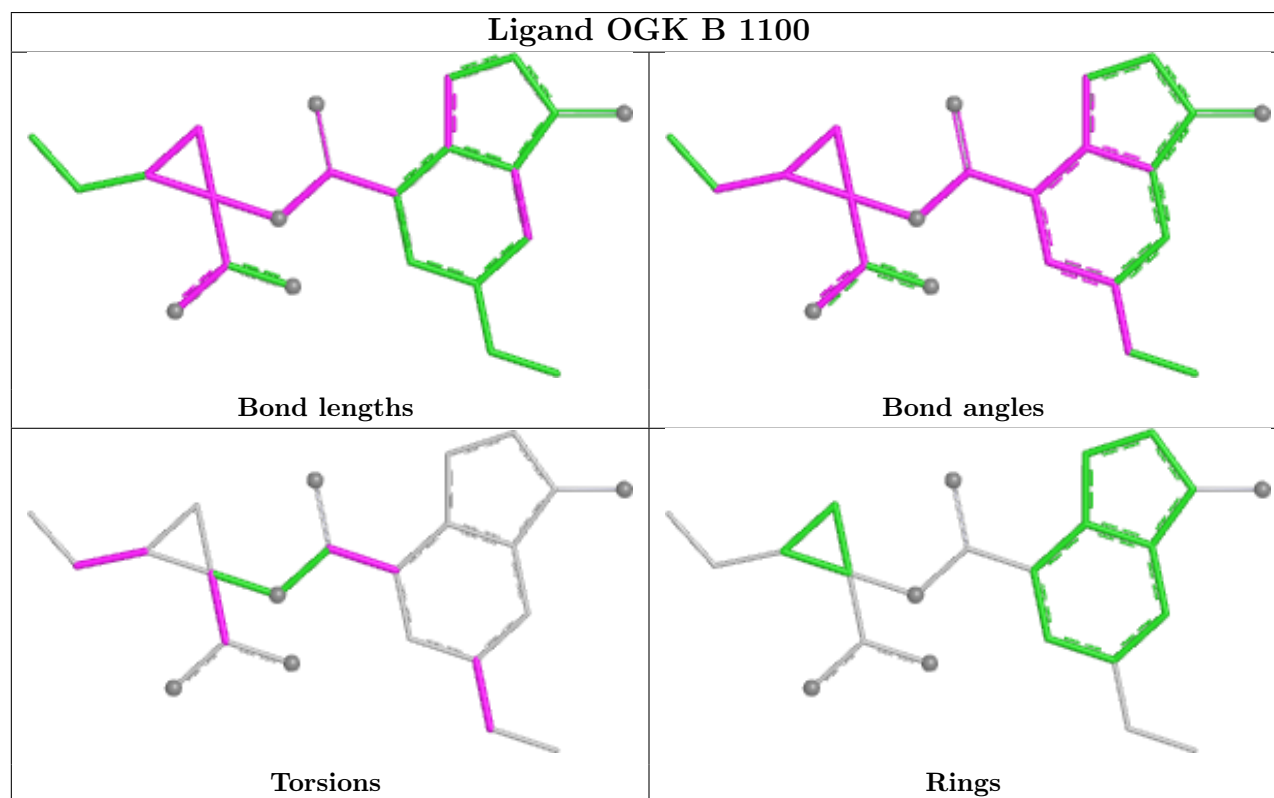
There are no ring outliers.

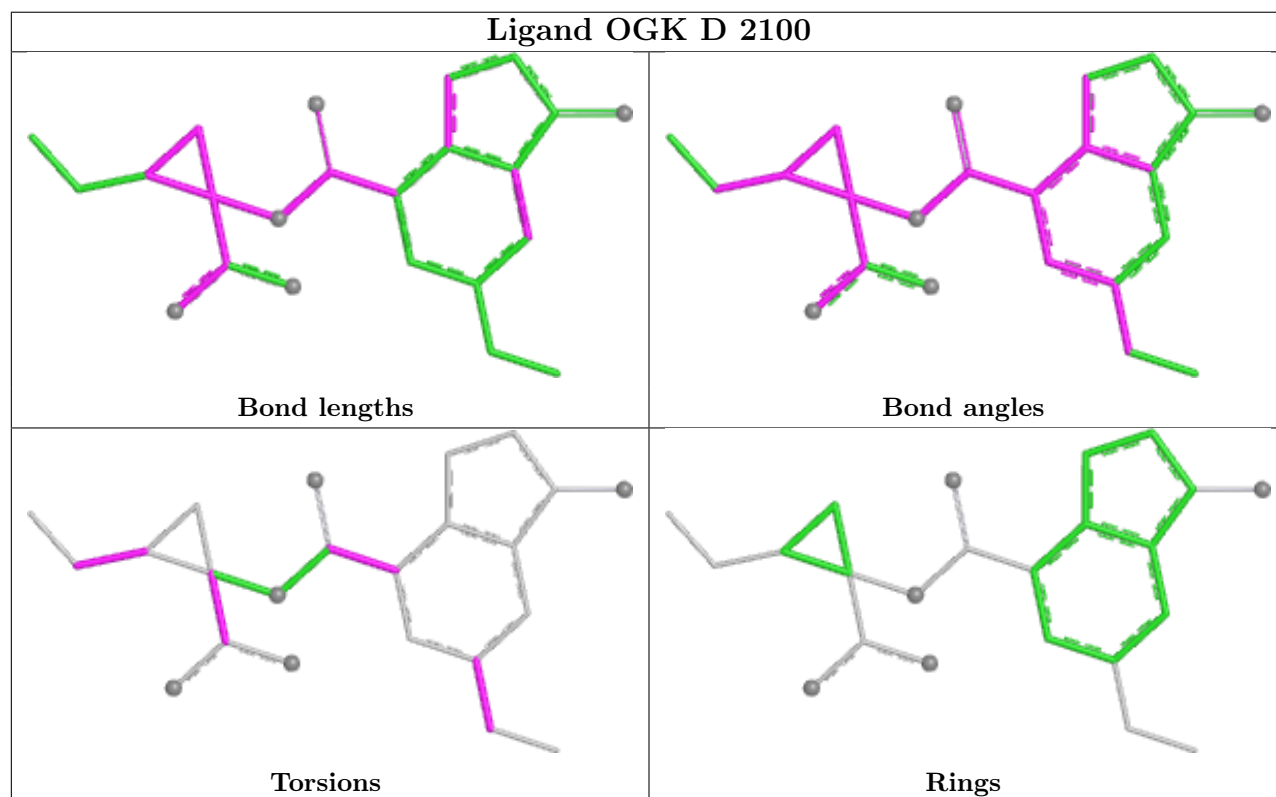
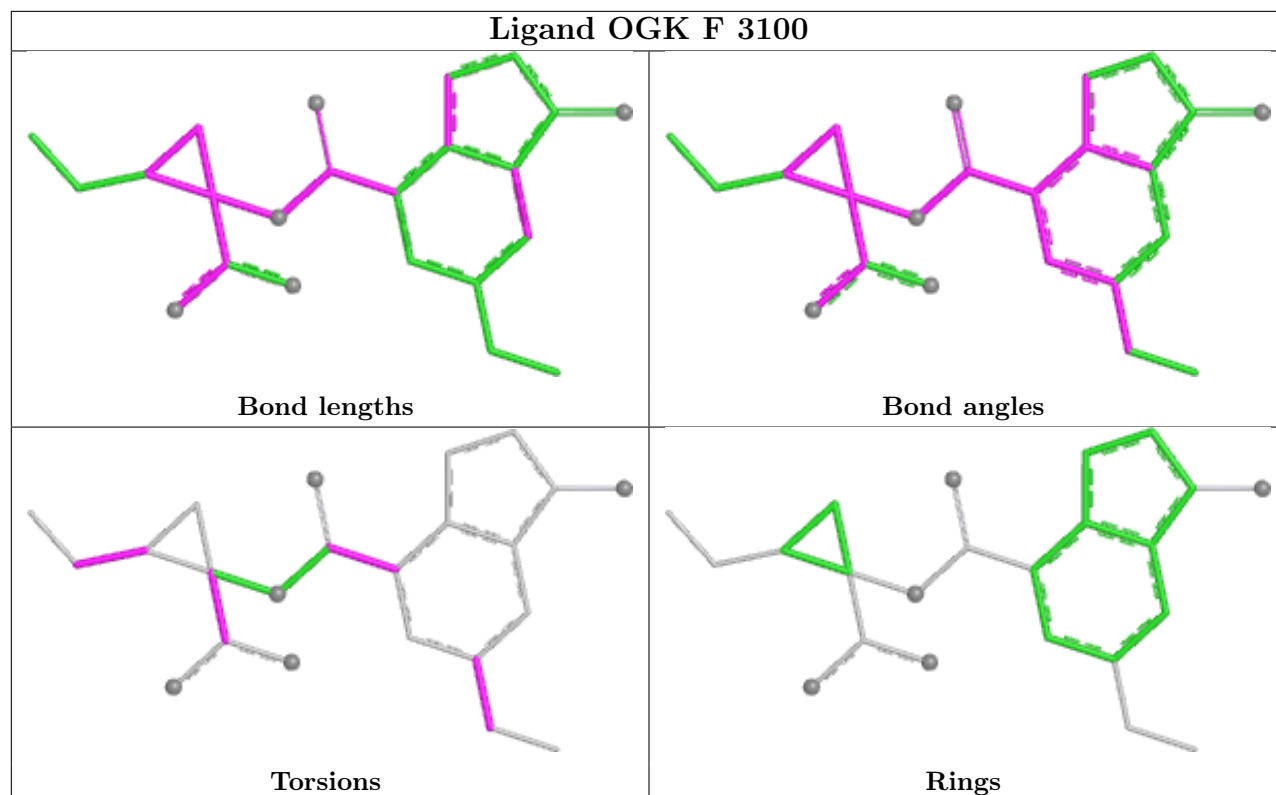
27 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1101	PO4	1	0
5	F	1101	PO4	1	0
5	L	1103	PO4	1	0
4	B	1100	OGK	7	0
5	N	1101	PO4	1	0
4	F	3100	OGK	7	0
5	J	1101	PO4	1	0
5	P	1101	PO4	1	0
4	D	2100	OGK	7	0
4	J	5100	OGK	7	0
5	D	1103	PO4	1	0
4	H	4100	OGK	16	0
5	L	1101	PO4	1	0
5	N	1102	PO4	1	0
5	N	1103	PO4	1	0
5	H	1102	PO4	1	0
5	B	1101	PO4	1	0
5	F	1103	PO4	1	0
5	J	1103	PO4	1	0
5	P	1103	PO4	2	0
4	P	8100	OGK	8	0
4	L	6100	OGK	7	0
5	B	1102	PO4	1	0
5	B	1103	PO4	1	0
4	N	7100	OGK	6	0
5	D	1101	PO4	1	0
5	H	1103	PO4	1	0

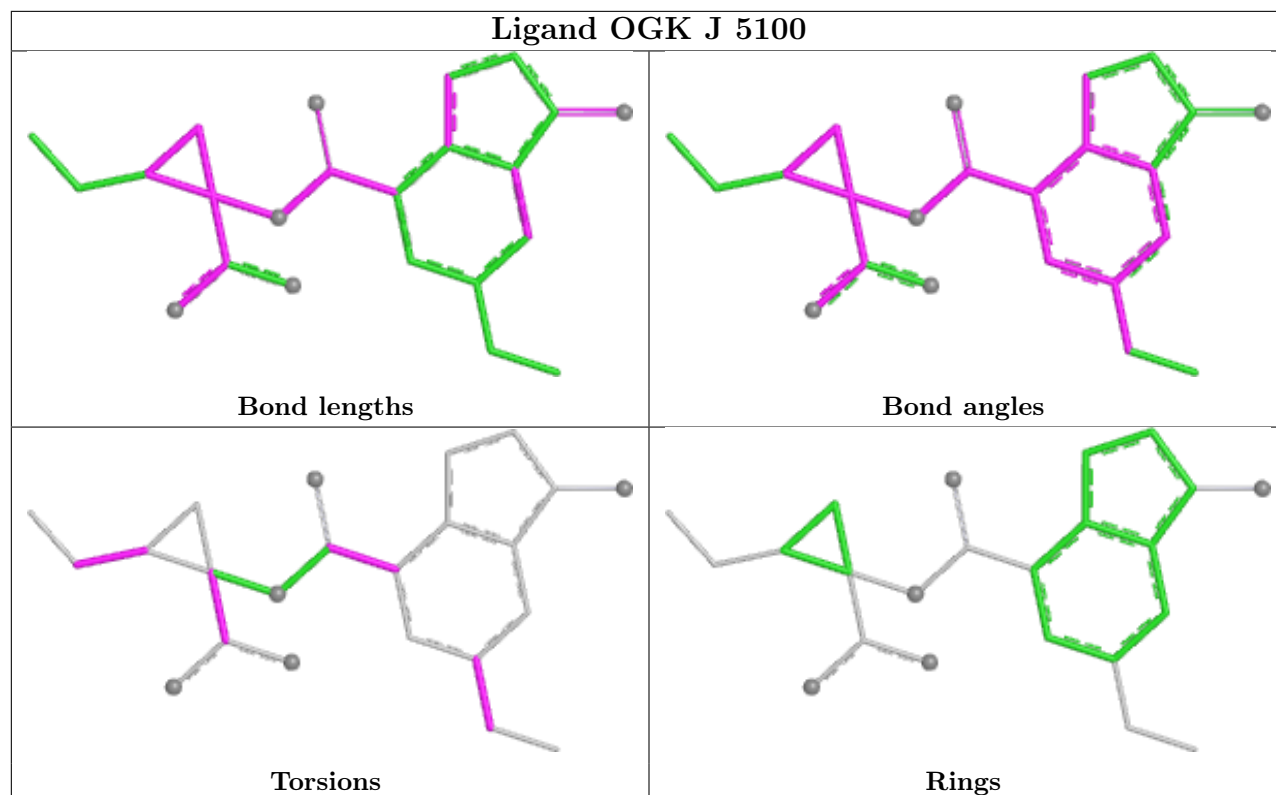
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

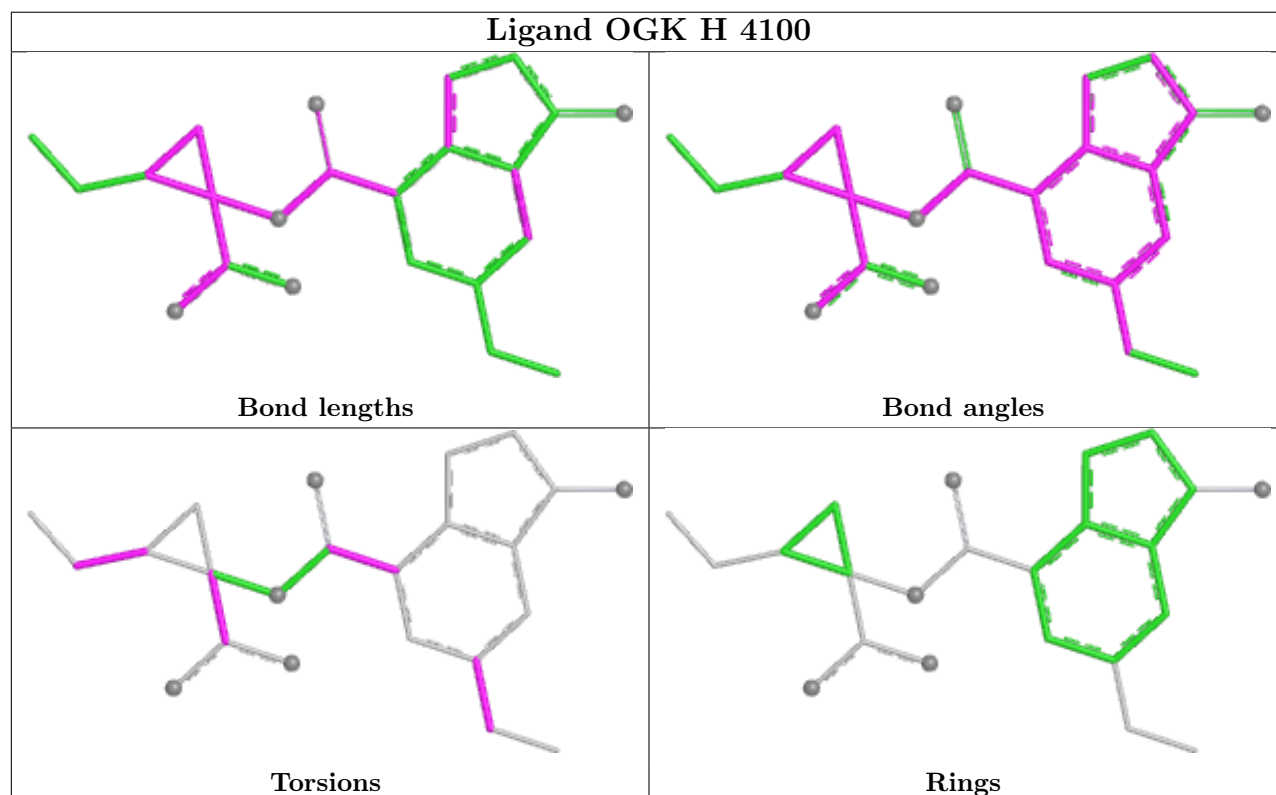




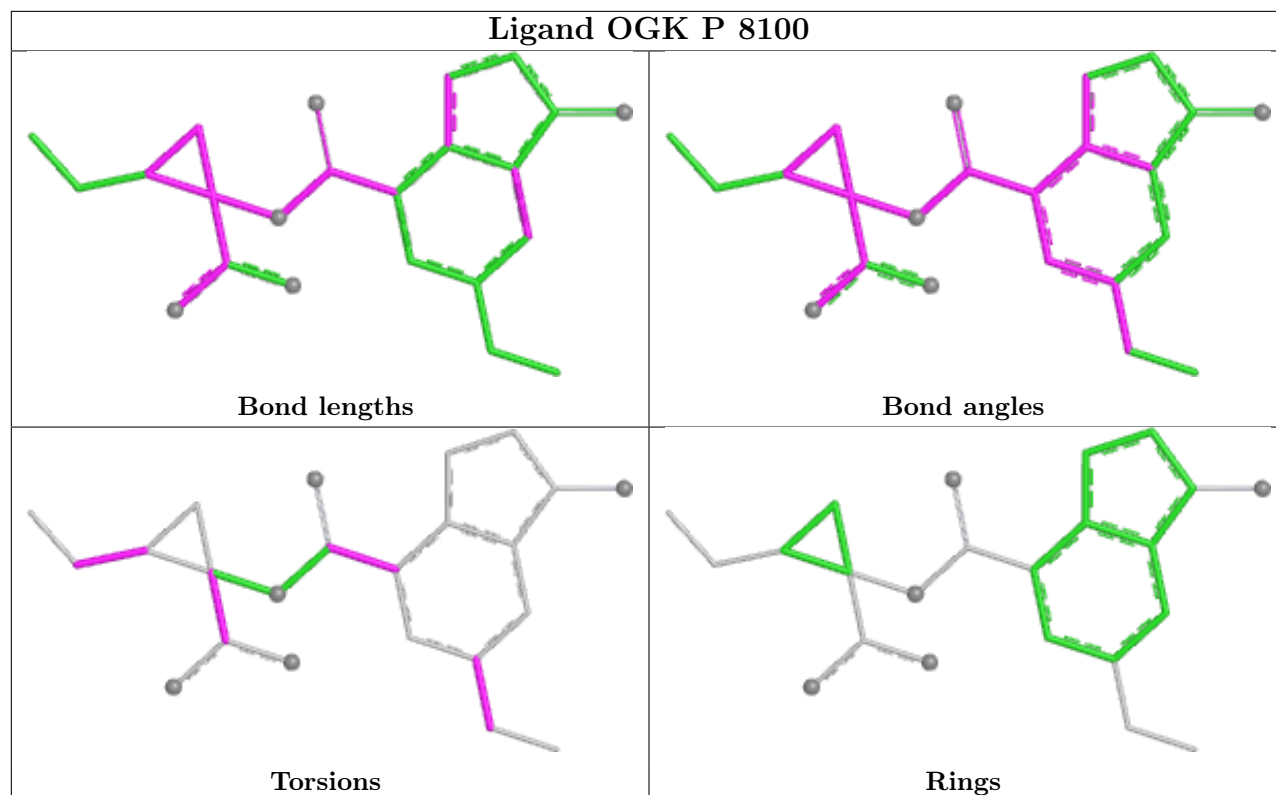
Ligand OGK J 5100



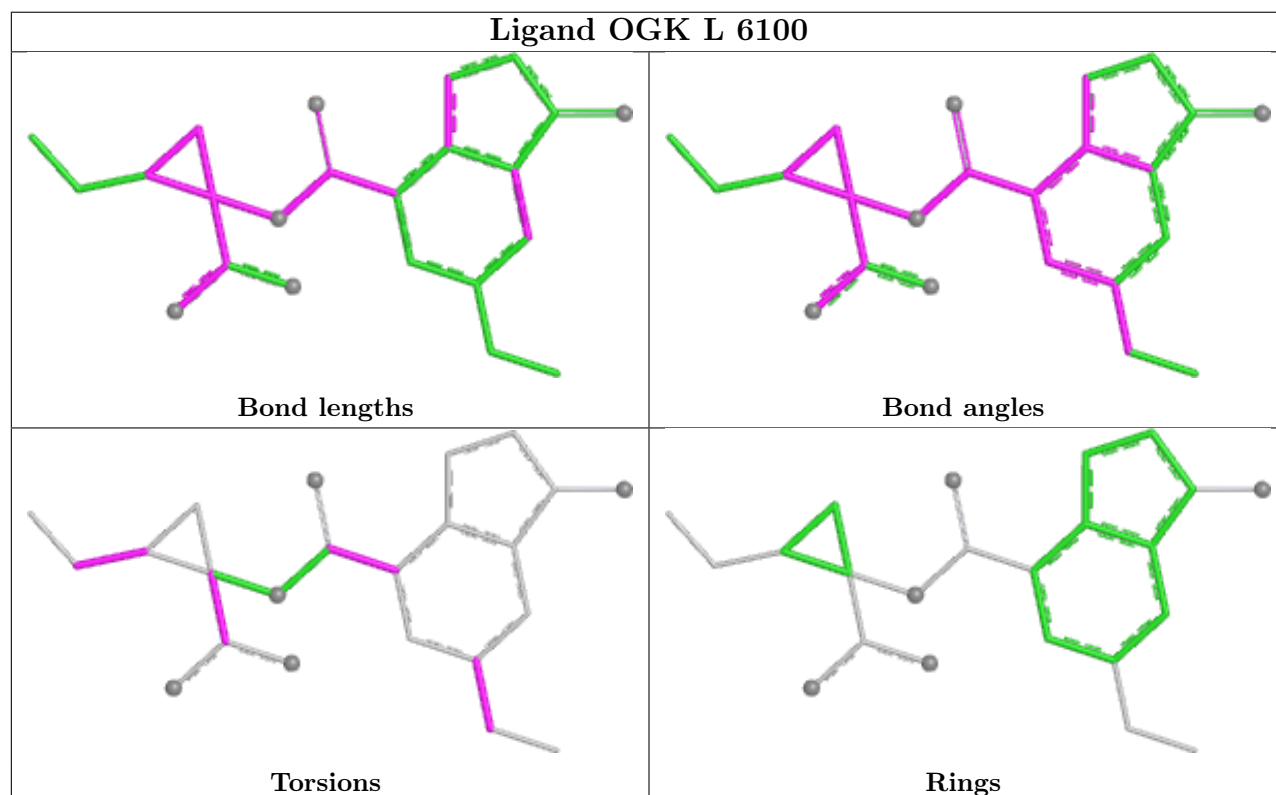
Ligand OGK H 4100

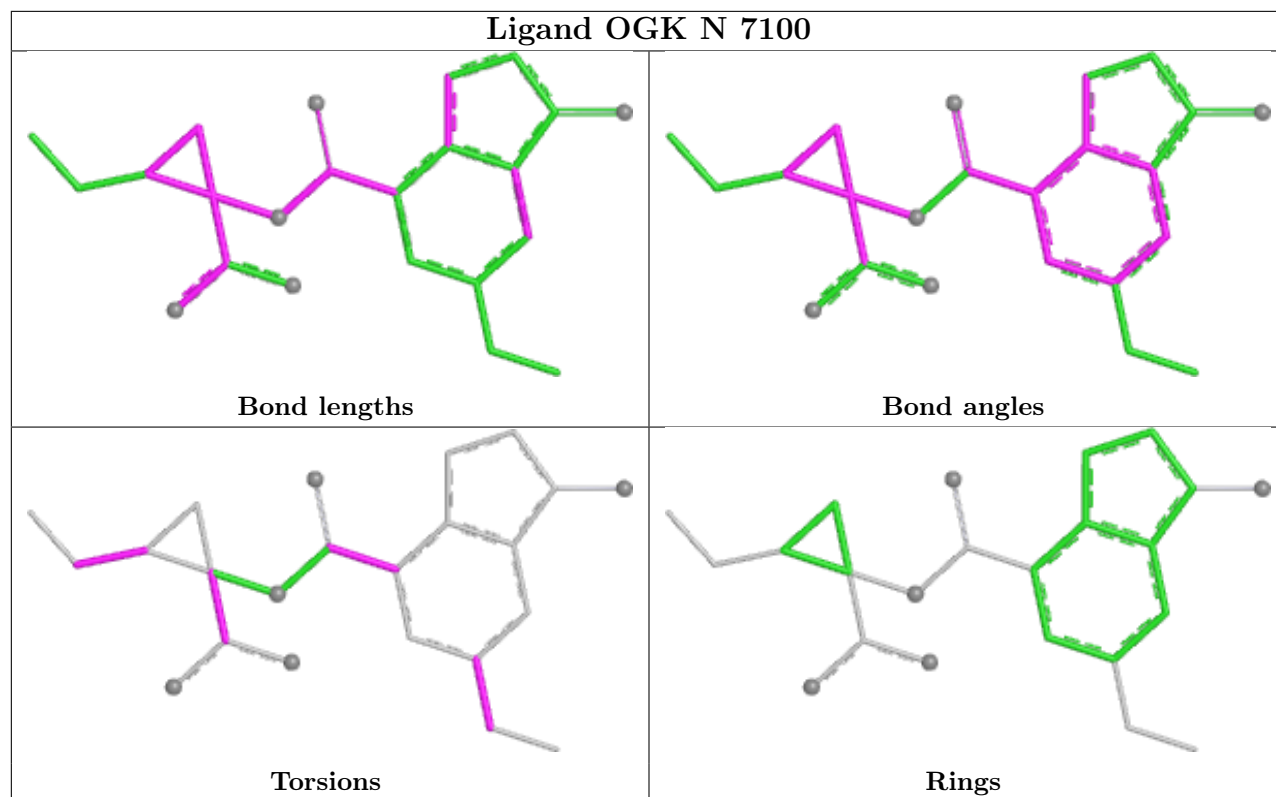


Ligand OGK P 8100



Ligand OGK L 6100





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	144/160 (90%)	-0.02	1 (0%) 84 71	50, 100, 151, 168	0
1	C	144/160 (90%)	-0.08	0 100 100	50, 102, 153, 170	0
1	E	144/160 (90%)	0.11	2 (1%) 73 56	54, 101, 151, 171	0
1	G	144/160 (90%)	-0.13	0 100 100	49, 96, 149, 170	0
1	I	144/160 (90%)	0.10	1 (0%) 84 71	50, 100, 150, 170	0
1	K	144/160 (90%)	-0.12	0 100 100	53, 102, 152, 170	0
1	M	144/160 (90%)	0.24	0 100 100	55, 102, 152, 175	0
1	O	144/160 (90%)	-0.10	1 (0%) 84 71	51, 101, 151, 173	0
2	B	568/592 (95%)	-0.22	0 100 100	38, 76, 136, 201	0
2	D	568/592 (95%)	-0.10	2 (0%) 88 80	38, 75, 135, 200	0
2	F	568/592 (95%)	-0.19	1 (0%) 91 87	40, 79, 136, 202	0
2	H	562/592 (94%)	-0.53	3 (0%) 87 77	34, 73, 127, 191	0
2	J	568/592 (95%)	-0.20	1 (0%) 91 87	39, 77, 136, 204	0
2	L	568/592 (95%)	-0.30	0 100 100	41, 79, 135, 202	0
2	N	568/592 (95%)	0.39	12 (2%) 63 45	41, 82, 137, 206	0
2	P	568/592 (95%)	-0.24	1 (0%) 91 87	40, 80, 138, 204	0
3	Q	18/21 (85%)	-0.09	0 100 100	72, 93, 116, 143	0
3	R	18/21 (85%)	0.15	0 100 100	71, 88, 115, 145	0
3	S	18/21 (85%)	-0.22	0 100 100	73, 93, 117, 143	0
3	U	18/21 (85%)	0.06	0 100 100	71, 88, 112, 143	0
3	V	18/21 (85%)	-0.16	0 100 100	75, 93, 115, 143	0
3	W	18/21 (85%)	0.42	0 100 100	80, 96, 119, 143	0
3	X	18/21 (85%)	-0.27	0 100 100	76, 91, 119, 143	0
All	All	5816/6163 (94%)	-0.13	25 (0%) 88 80	34, 82, 141, 206	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	462	SER	3.9
2	H	353	ALA	3.6
2	H	352	GLY	3.4
2	N	428	VAL	3.2
1	E	138	ASN	3.1
2	N	277	LEU	2.8
2	D	360	ASP	2.5
1	E	57	GLU	2.4
2	N	487	CYS	2.4
2	N	590	GLU	2.4
1	O	13	GLY	2.4
2	F	267	VAL	2.3
2	N	387	VAL	2.3
2	N	513	PRO	2.2
2	N	395	LEU	2.2
2	N	434	GLY	2.2
2	P	547	SER	2.2
1	I	67	ALA	2.2
2	J	267	VAL	2.2
2	N	350	GLU	2.1
1	A	80	ASP	2.1
2	D	429	ARG	2.1
2	N	22	GLU	2.1
2	N	495	MET	2.0
2	H	420	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

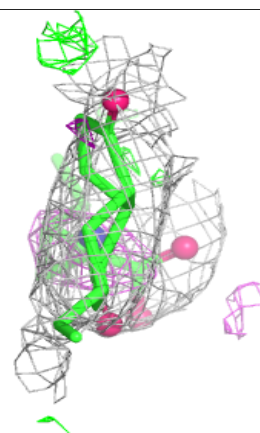
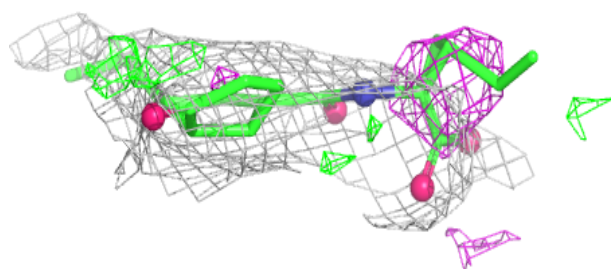
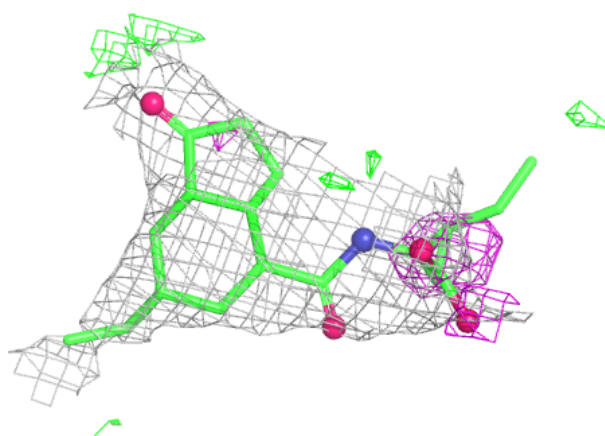
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	N	1104	5/5	0.81	0.12	82,83,118,122	0
5	PO4	N	1103	5/5	0.82	0.12	56,56,74,85	0
5	PO4	P	1102	5/5	0.85	0.17	72,87,98,108	0
5	PO4	N	1102	5/5	0.86	0.09	78,90,92,113	0
4	OGK	N	7100	23/23	0.86	0.18	65,79,100,104	0
5	PO4	F	1104	5/5	0.87	0.11	72,81,117,120	0
5	PO4	H	1104	5/5	0.87	0.09	54,57,114,134	0
5	PO4	F	1102	5/5	0.88	0.12	64,90,96,109	0
5	PO4	N	1101	5/5	0.88	0.09	51,59,80,82	0
5	PO4	B	1102	5/5	0.89	0.10	70,84,93,100	0
5	PO4	D	1102	5/5	0.91	0.11	66,79,93,93	0
5	PO4	D	1104	5/5	0.91	0.10	72,73,107,122	0
5	PO4	L	1104	5/5	0.91	0.09	76,78,119,123	0
5	PO4	B	1104	5/5	0.91	0.09	68,79,102,119	0
5	PO4	P	1103	5/5	0.91	0.07	50,58,73,85	0
5	PO4	J	1102	5/5	0.92	0.06	67,86,95,104	0
5	PO4	P	1104	5/5	0.92	0.08	73,75,110,121	0
4	OGK	H	4100	23/23	0.93	0.10	44,71,85,98	0
5	PO4	F	1101	5/5	0.93	0.10	52,58,68,88	0
4	OGK	B	1100	23/23	0.94	0.11	62,73,87,93	0
5	PO4	J	1101	5/5	0.94	0.07	50,55,74,79	0
4	OGK	J	5100	23/23	0.94	0.11	59,67,88,93	0
5	PO4	L	1102	5/5	0.94	0.07	73,82,96,100	0
4	OGK	P	8100	23/23	0.95	0.12	64,75,88,90	0
4	OGK	F	3100	23/23	0.95	0.11	64,72,91,94	0
5	PO4	B	1103	5/5	0.96	0.08	54,54,61,76	0
5	PO4	B	1101	5/5	0.96	0.06	58,59,65,75	0
5	PO4	D	1101	5/5	0.96	0.07	51,55,63,80	0
5	PO4	J	1104	5/5	0.96	0.08	76,81,112,117	0
5	PO4	P	1101	5/5	0.96	0.07	57,62,74,75	0
4	OGK	D	2100	23/23	0.96	0.12	60,72,81,86	0
5	PO4	L	1103	5/5	0.96	0.06	52,56,69,89	0
5	PO4	H	1102	5/5	0.96	0.05	58,59,72,88	0
5	PO4	J	1103	5/5	0.97	0.05	53,53,64,77	0
4	OGK	L	6100	23/23	0.97	0.09	62,71,90,92	0
5	PO4	L	1101	5/5	0.97	0.04	48,58,74,76	0
5	PO4	H	1103	5/5	0.97	0.05	38,47,52,77	0
5	PO4	F	1103	5/5	0.97	0.06	53,57,73,86	0
5	PO4	D	1103	5/5	0.97	0.06	48,52,55,81	0
5	PO4	H	1101	5/5	0.97	0.05	36,45,63,88	0

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

orientation to approximate a three-dimensional view.

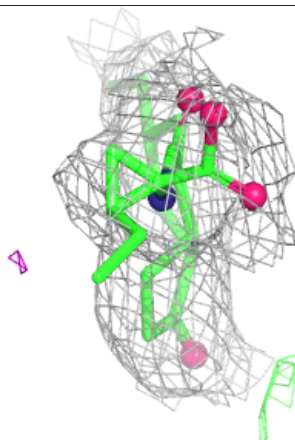
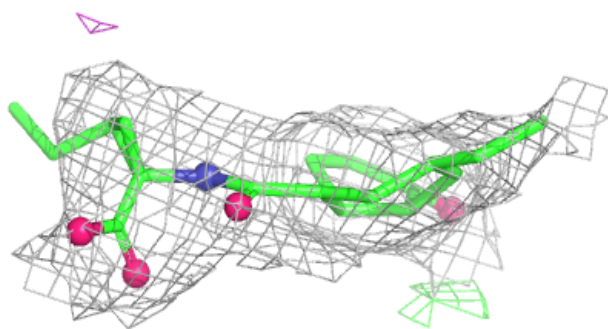
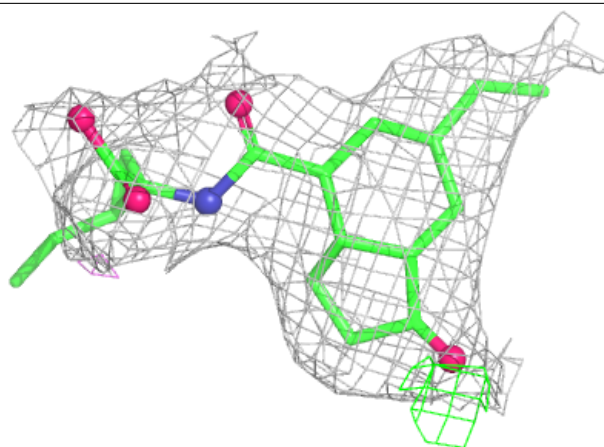
Electron density around OGK N 7100:

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

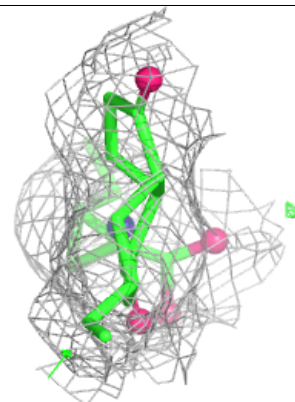
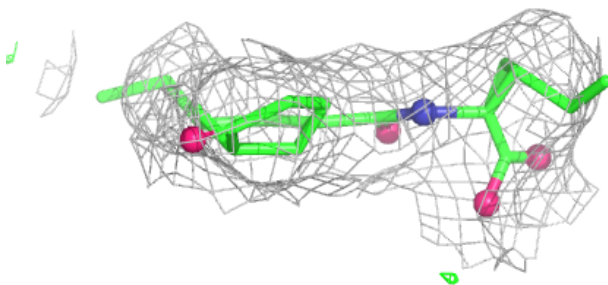
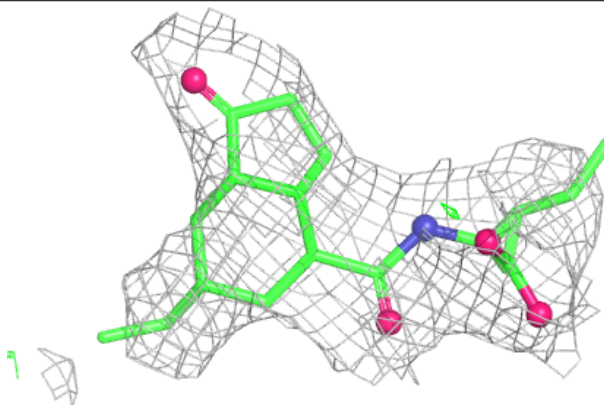


Electron density around OGK H 4100:

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

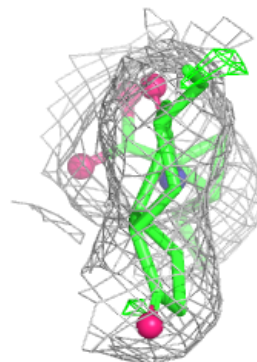
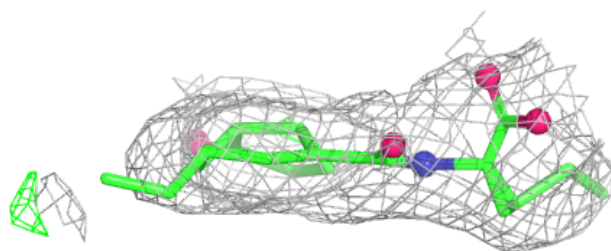
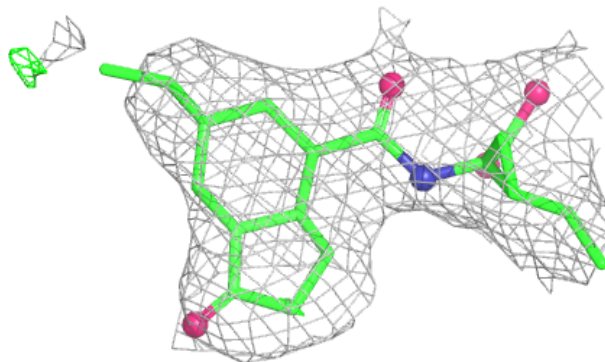
**Electron density around OGK B 1100:**

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

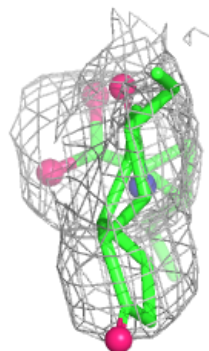
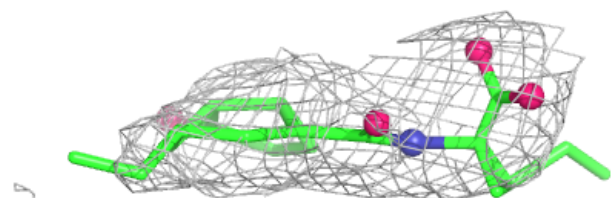
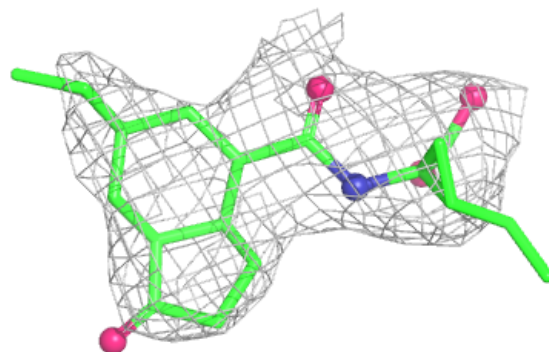


Electron density around OGK J 5100:

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

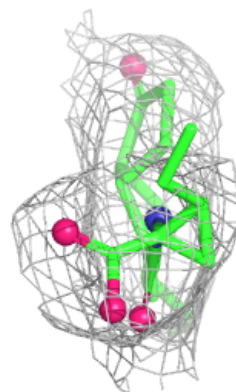
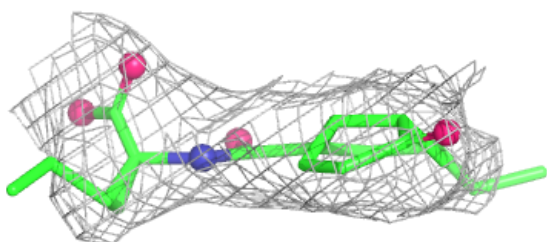
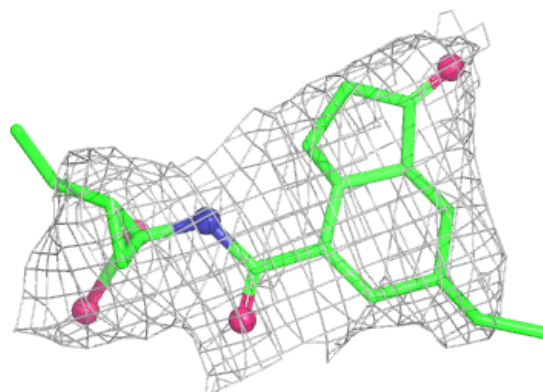
**Electron density around OGK P 8100:**

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

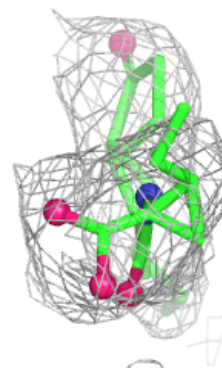
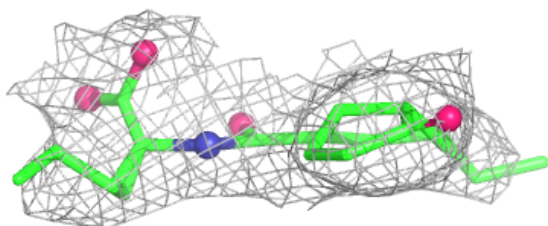
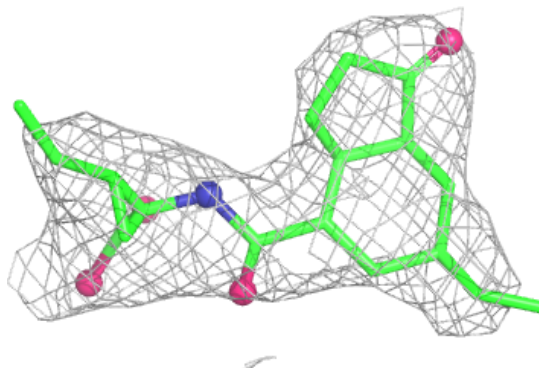


Electron density around OGK F 3100:

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

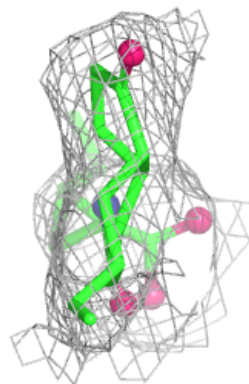
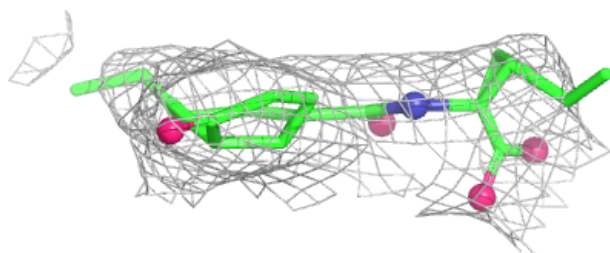
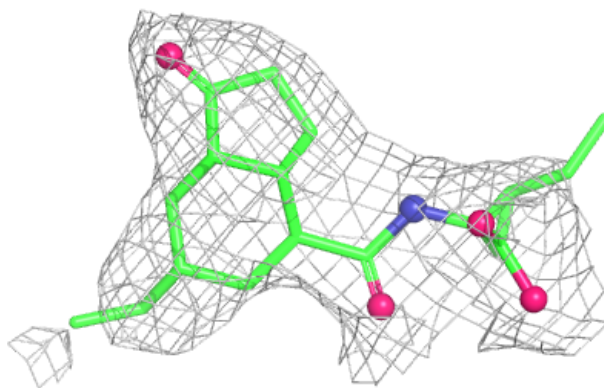
**Electron density around OGK D 2100:**

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



Electron density around OGK L 6100:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.