



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:16 PM UTC

PDB ID : 3OGK / pdb_00003ogk
Title : Structure of COI1-ASK1 in complex with coronatine and an incomplete 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 : 2010-08-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

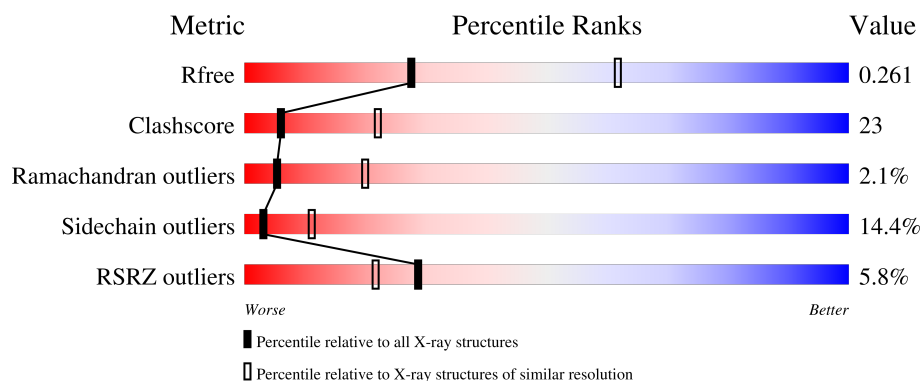
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	8% 54% 29% 8% 9%
1	C	160	8% 52% 29% 9% 9%
1	E	160	18% 56% 28% 7% 9%
1	G	160	6% 54% 29% 8% 9%

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Mol	Chain	Length	Quality of chain
1	I	160	
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	22	
3	R	22	
3	S	22	
3	U	22	
3	V	22	
3	W	22	
3	X	22	

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	B	1100	X	-	-	-
4	OGK	D	1100	X	-	-	-
4	OGK	H	1100	X	-	-	-
4	OGK	L	1100	X	-	X	-
5	PO4	B	1101	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	B	1102	-	X	-	-
5	PO4	B	1103	-	X	X	-
5	PO4	B	1104	-	X	-	-
5	PO4	D	1101	-	X	-	-
5	PO4	D	1102	-	X	-	-
5	PO4	D	1103	-	X	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	X	-
5	PO4	H	1102	-	X	-	-
5	PO4	H	1103	-	X	X	-
5	PO4	H	1104	-	X	-	-
5	PO4	J	1101	-	X	-	-
5	PO4	J	1102	-	X	-	-
5	PO4	J	1103	-	X	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	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 46526 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	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	C	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	E	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	G	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	I	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	K	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	M	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			
1	O	145	Total	C	N	O	S	0	0	0
			1152	723	186	237	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	D	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	F	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	H	562	Total	C	N	O	S	0	0	0
			4486	2840	779	831	36			
2	J	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	L	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			

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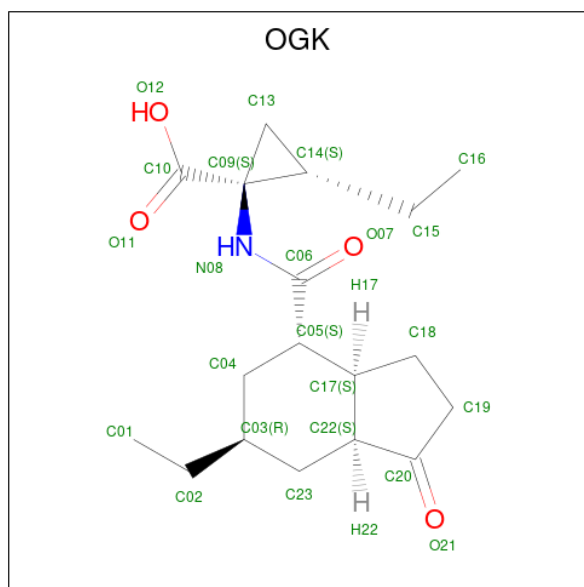
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			
2	P	566	Total	C	N	O	S	0	0	0
			4521	2862	785	838	36			

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

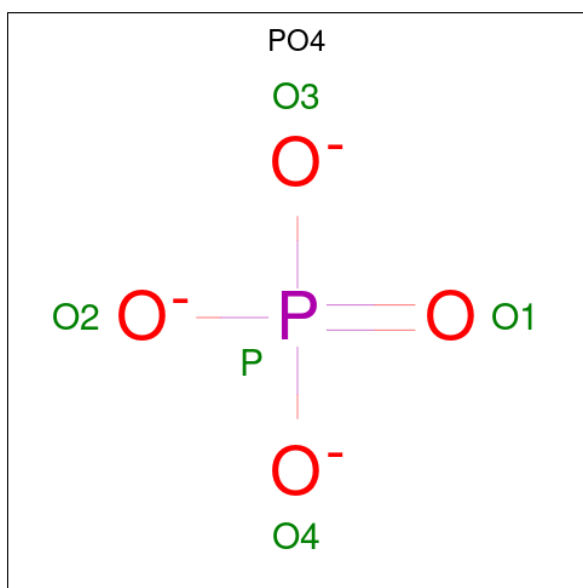
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	R	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	S	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	U	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	V	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	W	13	Total	C	N	O	0	0	0
			119	74	29	16			
3	X	13	Total	C	N	O	0	0	0
			119	74	29	16			

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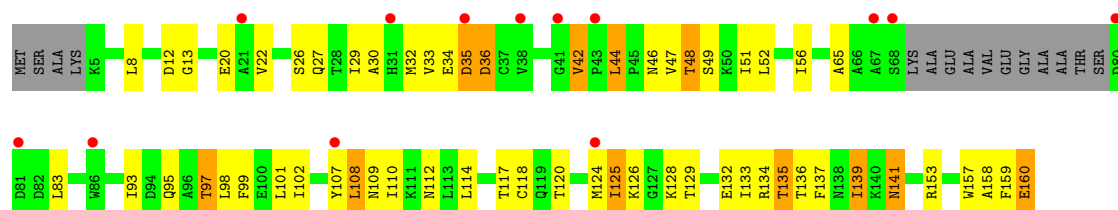
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0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

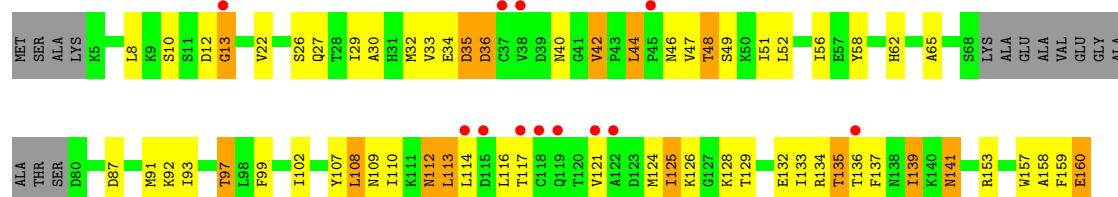
3 Residue-property plots [i](#)

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.

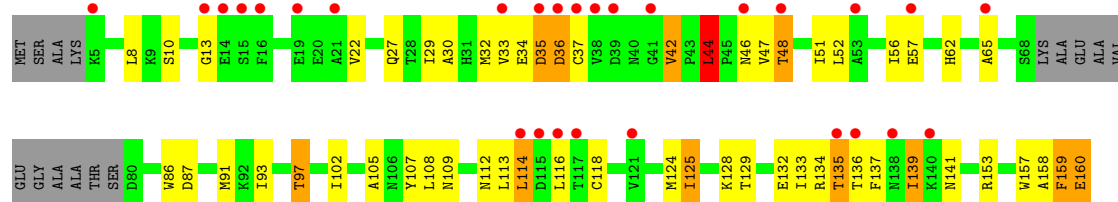
- Molecule 1: SKP1-like protein 1A



- Molecule 1: SKP1-like protein 1A

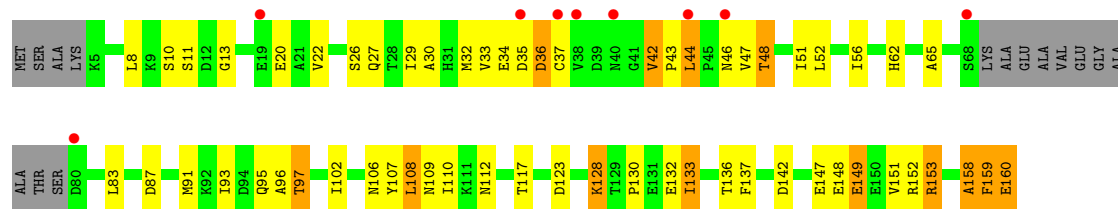


- Molecule 1: SKP1-like protein 1A

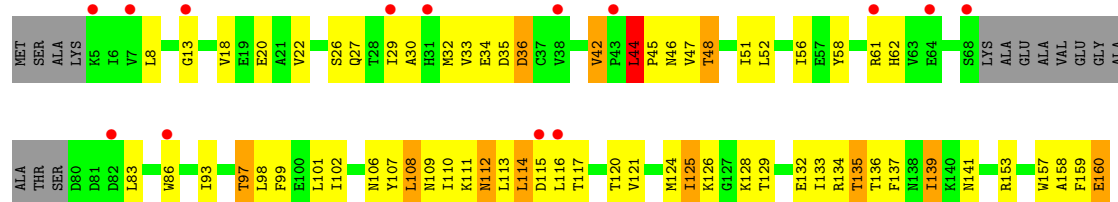


- Molecule 1: SKP1-like protein 1A

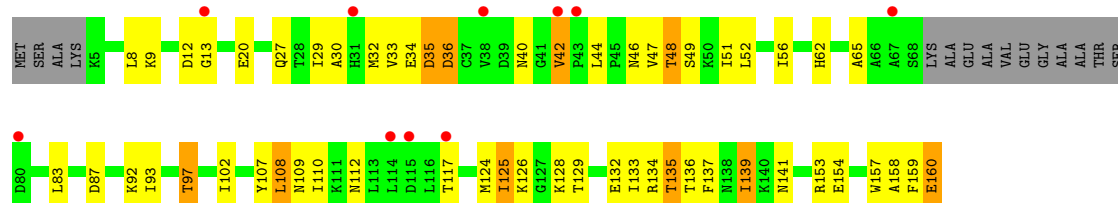




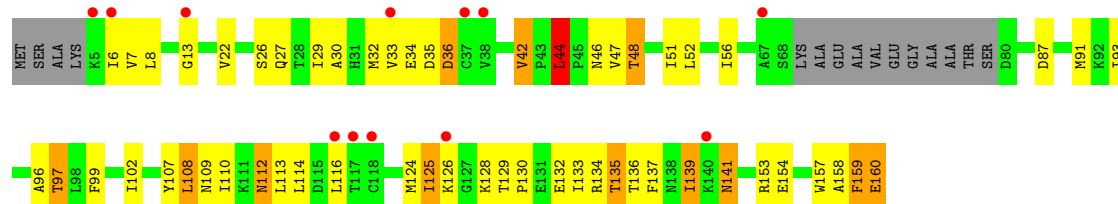
• Molecule 1: SKP1-like protein 1A



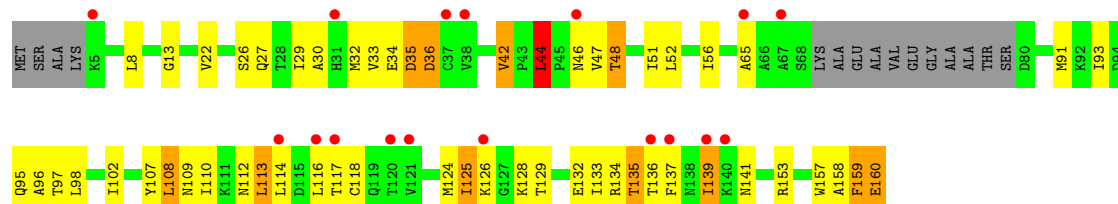
• Molecule 1: SKP1-like protein 1A



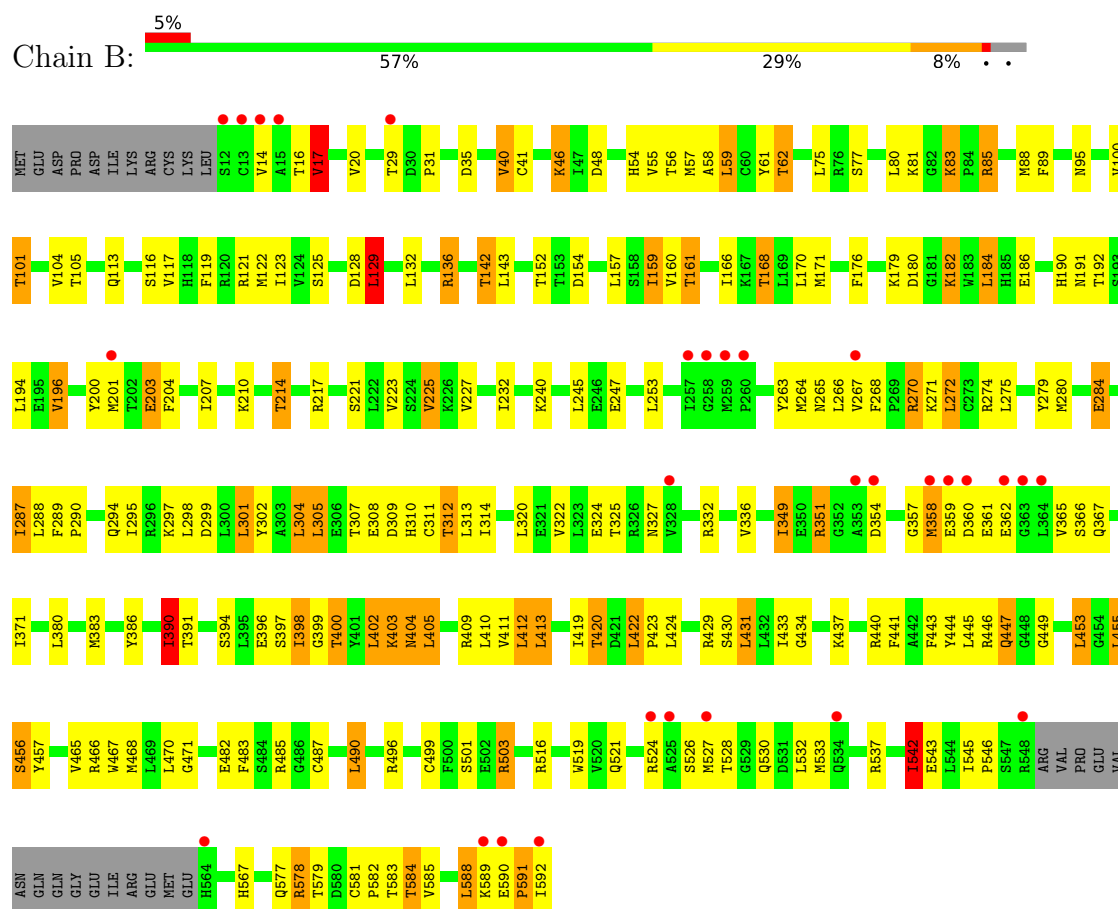
• Molecule 1: SKP1-like protein 1A



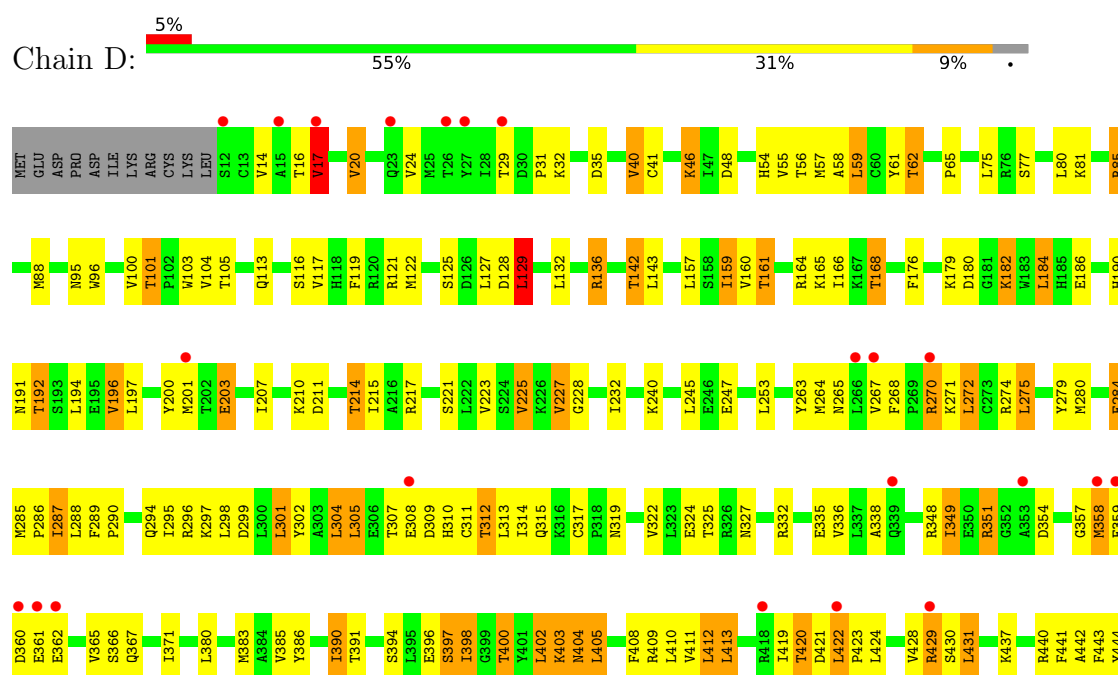
• Molecule 1: SKP1-like protein 1A

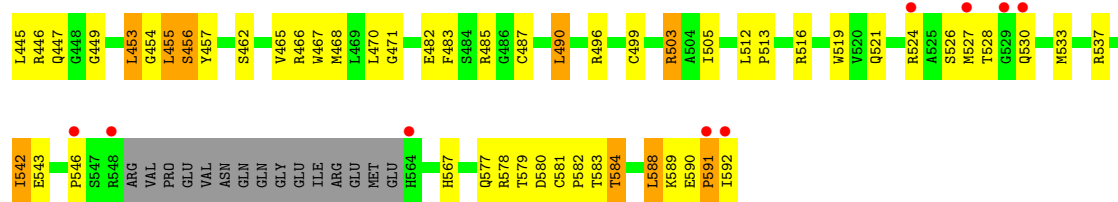


- Molecule 2: Coronatine-insensitive protein 1

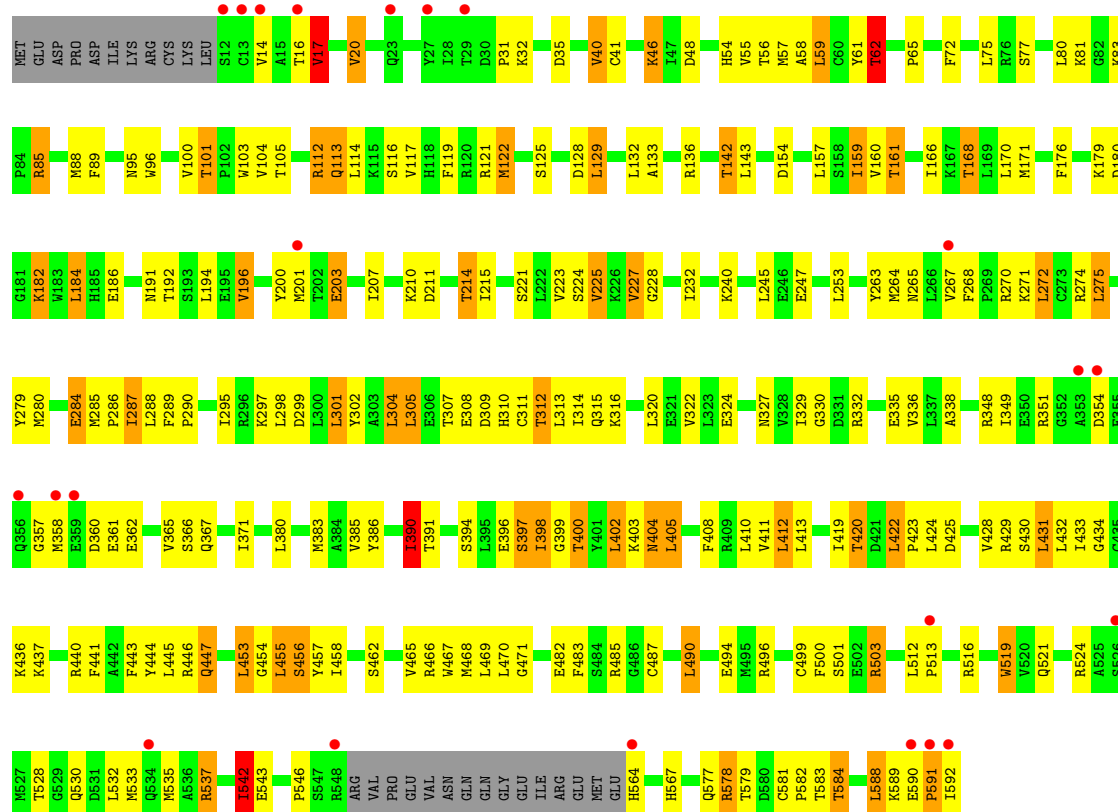


- Molecule 2: Coronatine-insensitive protein 1

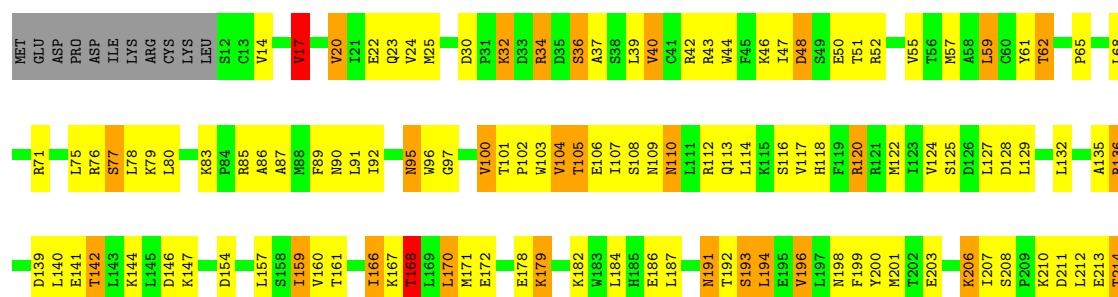


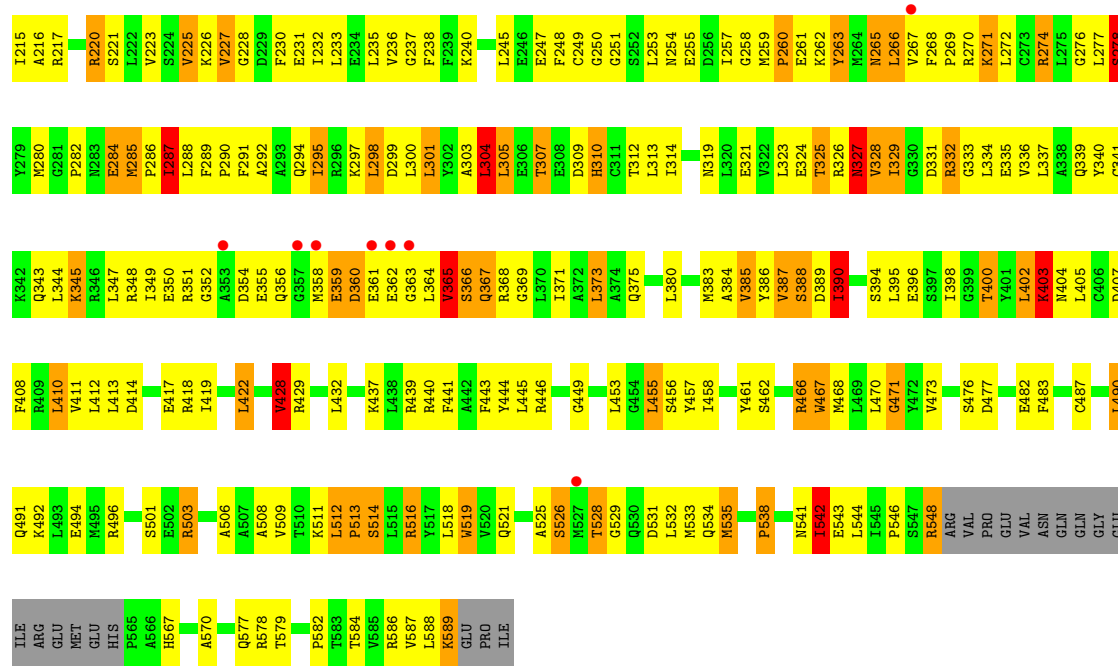


• Molecule 2: Coronatine-insensitive protein 1

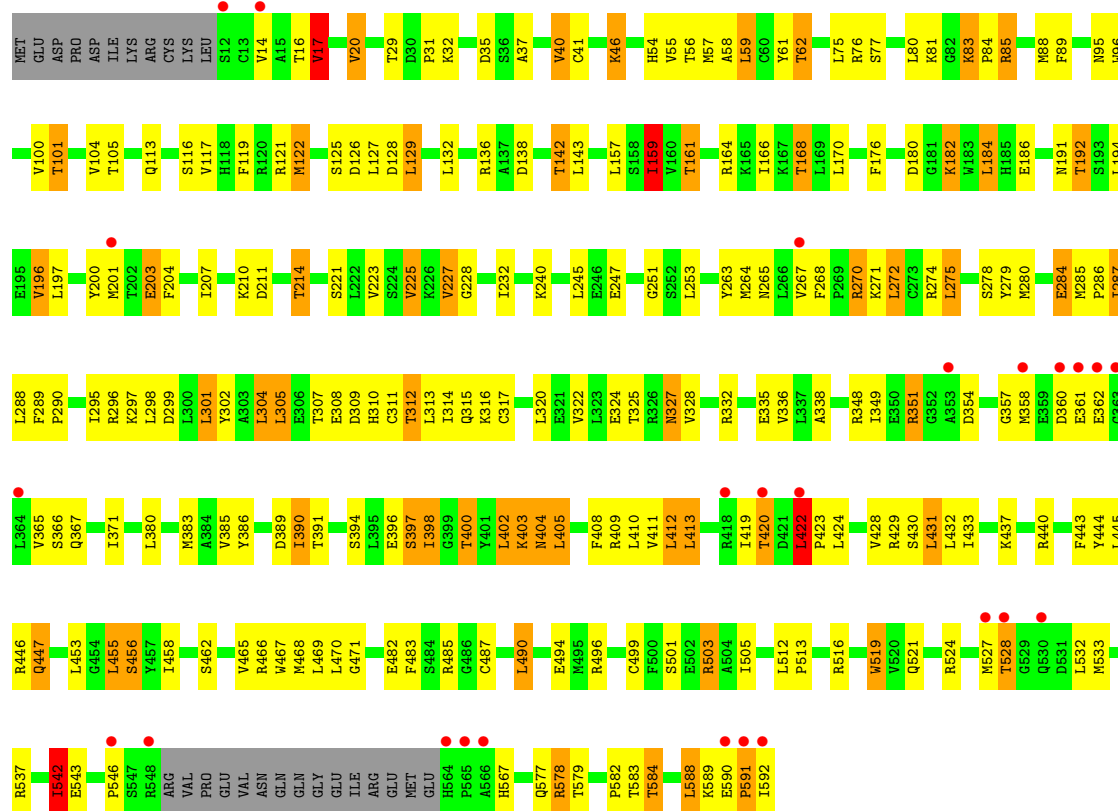


• Molecule 2: Coronatine-insensitive protein 1

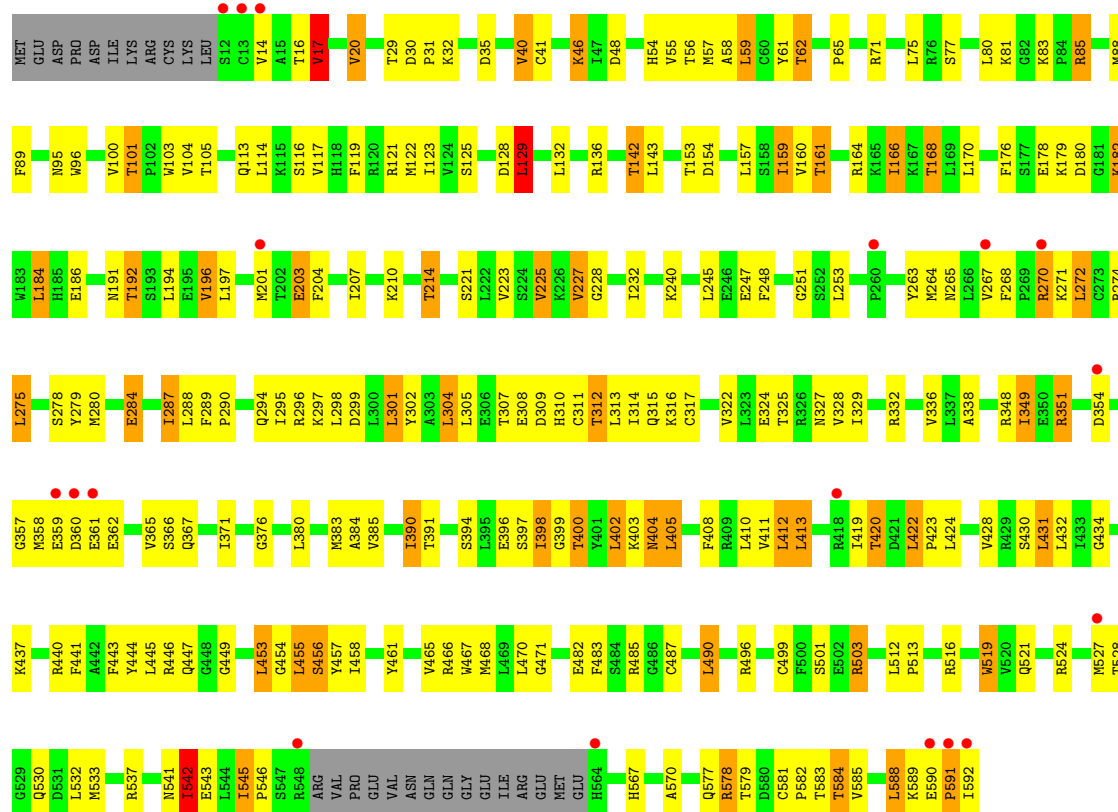


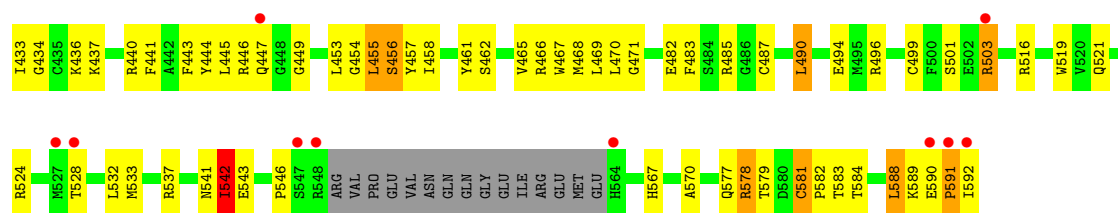


• Molecule 2: Coronatine-insensitive protein 1

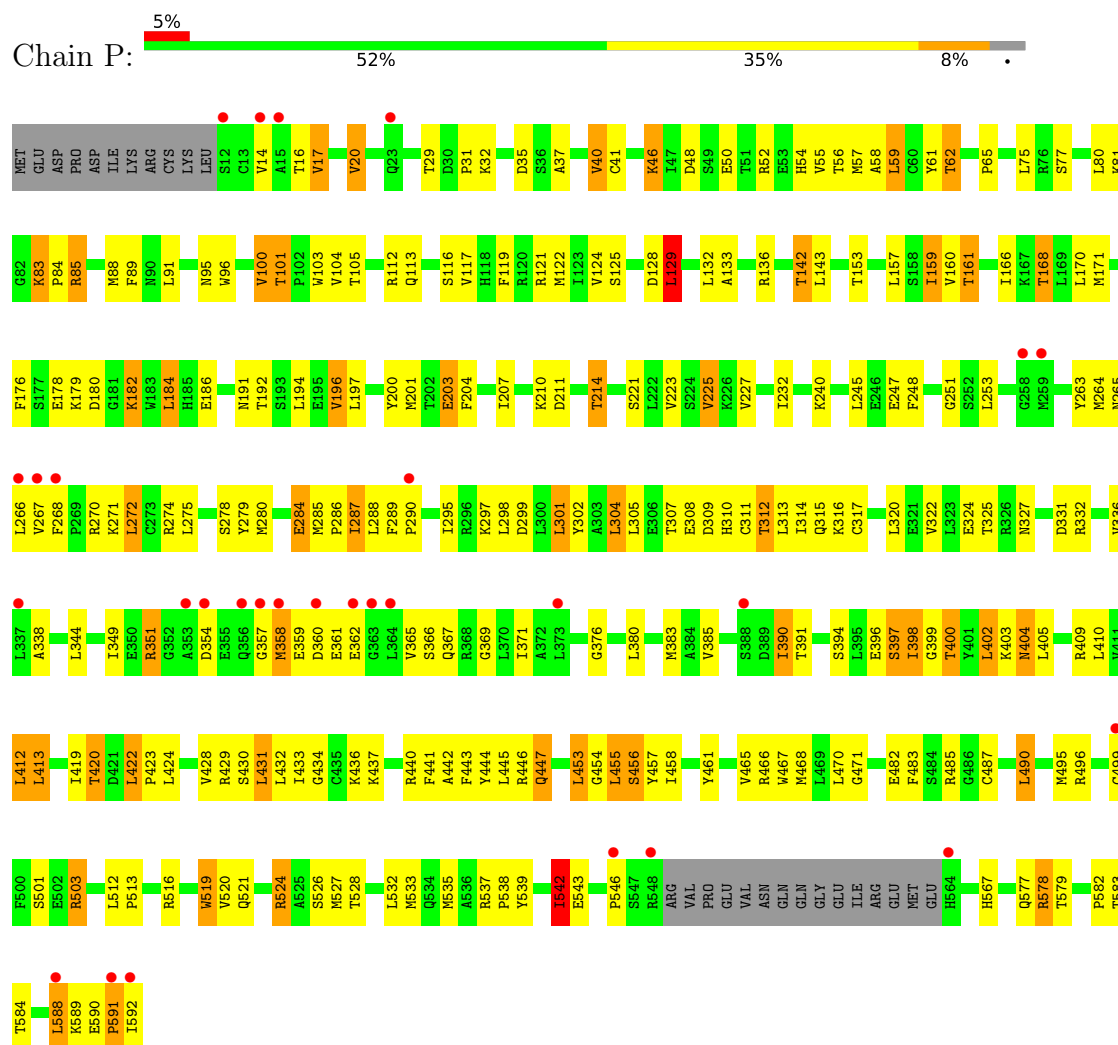


• Molecule 2: Coronatine-insensitive protein 1

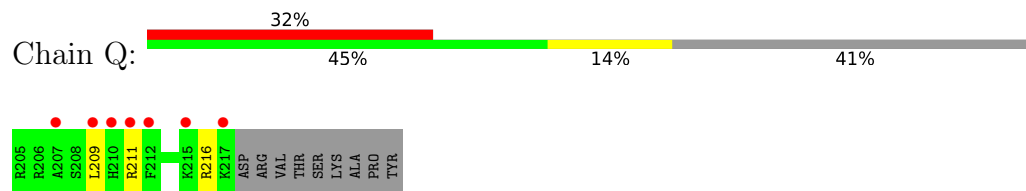




• Molecule 2: Coronatine-insensitive protein 1

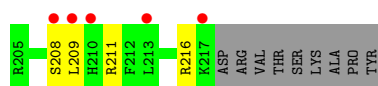


• Molecule 3: JAZ1 incomplete degron peptide

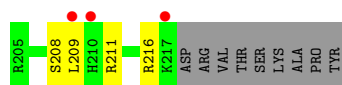


• Molecule 3: JAZ1 incomplete degron peptide

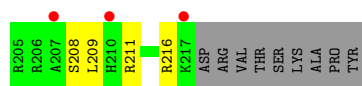




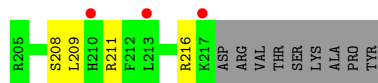
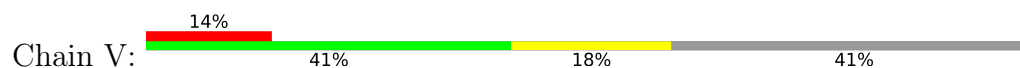
- Molecule 3: JAZ1 incomplete degron peptide



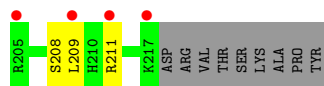
- Molecule 3: JAZ1 incomplete degron peptide



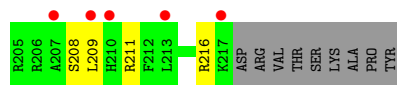
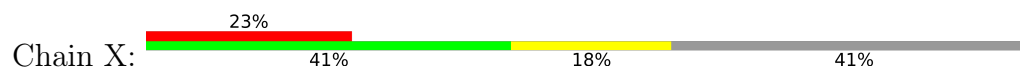
- Molecule 3: JAZ1 incomplete degron peptide



- Molecule 3: JAZ1 incomplete degron peptide



- Molecule 3: JAZ1 incomplete 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	121.85Å 221.46Å 148.47Å 90.00° 104.49° 90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.63-2.80) 93.7 (49.63-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.225 , 0.268 0.219 , 0.261	Depositor DCC
R_{free} test set	9332 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46526	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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	0.70	0/1168	0.91	1/1579 (0.1%)
1	C	0.81	3/1168 (0.3%)	0.96	5/1579 (0.3%)
1	E	0.85	2/1168 (0.2%)	1.01	7/1579 (0.4%)
1	G	0.81	0/1168	1.00	7/1579 (0.4%)
1	I	0.65	0/1168	0.94	3/1579 (0.2%)
1	K	0.65	0/1168	0.93	1/1579 (0.1%)
1	M	0.65	0/1168	0.93	3/1579 (0.2%)
1	O	0.72	0/1168	0.96	5/1579 (0.3%)
2	B	0.92	1/4603 (0.0%)	1.08	12/6212 (0.2%)
2	D	0.88	0/4603	1.07	15/6212 (0.2%)
2	F	0.80	1/4603 (0.0%)	1.08	14/6212 (0.2%)
2	H	0.94	2/4566 (0.0%)	1.31	39/6161 (0.6%)
2	J	0.79	1/4603 (0.0%)	1.09	16/6212 (0.3%)
2	L	0.75	1/4603 (0.0%)	1.05	13/6212 (0.2%)
2	N	0.81	1/4603 (0.0%)	1.10	17/6212 (0.3%)
2	P	0.77	1/4603 (0.0%)	1.07	7/6212 (0.1%)
3	Q	0.50	0/120	0.79	0/155
3	R	0.55	0/120	0.78	0/155
3	S	0.55	0/120	0.81	0/155
3	U	0.51	0/120	0.75	0/155
3	V	0.54	0/120	0.79	0/155
3	W	0.53	0/120	0.77	0/155
3	X	0.54	0/120	0.73	0/155
All	All	0.81	13/46971 (0.0%)	1.08	165/63362 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	LEU	C-N	9.53	1.45	1.33
1	C	114	LEU	N-CA	8.69	1.57	1.46
1	E	113	LEU	C-N	-7.15	1.23	1.33
1	C	113	LEU	CA-C	6.81	1.62	1.52
2	F	542	ILE	CA-CB	6.63	1.62	1.54
2	J	542	ILE	CA-CB	6.61	1.62	1.54
2	L	542	ILE	CA-CB	6.49	1.62	1.54
2	B	542	ILE	CA-CB	6.02	1.61	1.54
2	P	542	ILE	CA-CB	5.86	1.61	1.54
1	E	114	LEU	N-CA	-5.74	1.38	1.46
2	H	168	THR	CA-C	5.24	1.58	1.52
2	N	542	ILE	CA-CB	5.12	1.61	1.54
2	H	542	ILE	CA-CB	5.08	1.60	1.54

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	449	GLY	N-CA-C	11.33	128.34	113.27
2	H	366	SER	N-CA-C	-9.66	96.23	110.23
2	H	458	ILE	CB-CA-C	-8.73	100.80	111.97
2	H	512	LEU	CA-C-N	8.57	130.55	119.84
2	H	512	LEU	C-N-CA	8.57	130.55	119.84
1	E	114	LEU	N-CA-C	-8.31	103.65	113.88
2	H	17	VAL	CB-CA-C	-8.19	100.10	112.05
2	N	136	ARG	N-CA-C	-6.98	105.39	114.04
1	E	114	LEU	N-CA-CB	-6.75	101.61	110.59
2	H	390	ILE	CB-CA-C	-6.72	102.56	111.70
2	F	129	LEU	CA-CB-CG	6.71	139.79	116.30
2	F	200	TYR	CA-C-N	-6.67	113.85	122.79
2	F	200	TYR	C-N-CA	-6.67	113.85	122.79
1	G	158	ALA	N-CA-C	6.66	121.95	113.55
2	H	514	SER	N-CA-C	-6.58	98.52	109.24
1	G	159	PHE	N-CA-C	6.54	119.06	108.41
2	B	129	LEU	CA-CB-CG	6.45	138.86	116.30
2	H	365	VAL	CA-C-N	-6.41	111.61	120.71
2	H	365	VAL	C-N-CA	-6.41	111.61	120.71
2	D	462	SER	CA-C-N	6.41	126.03	119.56
2	D	462	SER	C-N-CA	6.41	126.03	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	462	SER	CA-C-N	6.35	125.97	119.56
2	J	462	SER	C-N-CA	6.35	125.97	119.56
2	H	428	VAL	CB-CA-C	-6.33	103.59	112.14
2	H	462	SER	CA-C-N	6.30	126.21	119.28
2	H	462	SER	C-N-CA	6.30	126.21	119.28
1	G	65	ALA	N-CA-C	-6.30	105.54	112.72
2	N	581	CYS	CA-C-N	6.24	126.20	120.21
2	N	581	CYS	C-N-CA	6.24	126.20	120.21
2	H	526	SER	N-CA-C	-6.15	99.72	109.07
2	L	449	GLY	N-CA-C	6.15	120.11	112.73
2	D	129	LEU	CA-CB-CG	6.10	137.66	116.30
1	K	65	ALA	N-CA-C	-6.10	105.76	112.72
2	J	505	ILE	CB-CA-C	-6.06	104.24	111.81
2	N	129	LEU	CA-CB-CG	6.04	137.46	116.30
2	H	535	MET	N-CA-C	-5.96	105.58	114.64
2	H	483	PHE	N-CA-C	-5.94	104.38	111.69
2	N	275	LEU	N-CA-C	5.94	117.81	108.96
1	I	114	LEU	N-CA-C	-5.93	104.82	111.28
2	D	275	LEU	N-CA-C	5.87	117.17	108.60
2	P	129	LEU	CA-CB-CG	5.86	136.81	116.30
2	J	17	VAL	CB-CA-C	-5.86	104.23	112.14
1	O	44	LEU	CA-C-N	5.83	127.12	119.84
1	O	44	LEU	C-N-CA	5.83	127.12	119.84
2	H	365	VAL	CB-CA-C	-5.81	101.76	111.29
2	B	83	LYS	CA-C-N	5.78	125.80	119.90
2	B	83	LYS	C-N-CA	5.78	125.80	119.90
2	H	110	ASN	N-CA-C	5.76	122.13	114.12
2	P	200	TYR	CA-C-N	-5.71	115.14	122.79
2	P	200	TYR	C-N-CA	-5.71	115.14	122.79
2	F	390	ILE	CB-CA-C	-5.70	103.38	111.19
1	C	113	LEU	CA-C-O	-5.70	111.64	119.05
2	P	83	LYS	CA-C-N	5.68	125.63	119.78
2	P	83	LYS	C-N-CA	5.68	125.63	119.78
2	J	200	TYR	CA-C-N	-5.65	115.22	122.79
2	J	200	TYR	C-N-CA	-5.65	115.22	122.79
2	N	411	VAL	CA-C-N	-5.63	115.28	122.77
2	N	411	VAL	C-N-CA	-5.63	115.28	122.77
2	J	76	ARG	N-CA-C	-5.63	106.95	113.88
2	J	127	LEU	N-CA-C	-5.63	105.06	111.14
1	E	65	ALA	N-CA-C	-5.63	106.31	112.72
2	H	91	LEU	N-CA-C	5.62	118.17	111.71
1	M	159	PHE	N-CA-C	5.58	117.87	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	TYR	N-CA-C	5.57	117.80	111.11
2	H	200	TYR	N-CA-C	5.56	118.41	110.24
2	H	71	ARG	CA-C-N	-5.55	116.67	122.89
2	H	71	ARG	C-N-CA	-5.55	116.67	122.89
2	H	304	LEU	N-CA-C	-5.55	106.34	114.39
2	L	275	LEU	N-CA-C	5.55	117.28	108.79
2	D	200	TYR	CA-C-N	-5.53	115.38	122.79
2	D	200	TYR	C-N-CA	-5.53	115.38	122.79
2	F	564	HIS	CA-C-N	5.53	125.47	119.78
2	F	564	HIS	C-N-CA	5.53	125.47	119.78
2	J	275	LEU	N-CA-C	5.52	116.66	108.60
2	L	545	ILE	CA-C-N	5.51	125.82	119.92
2	L	545	ILE	C-N-CA	5.51	125.82	119.92
1	M	44	LEU	CA-C-N	5.51	126.73	119.84
1	M	44	LEU	C-N-CA	5.51	126.73	119.84
2	J	317	CYS	CA-C-N	5.50	125.17	119.56
2	J	317	CYS	C-N-CA	5.50	125.17	119.56
2	F	462	SER	CA-C-N	5.49	125.16	119.56
2	F	462	SER	C-N-CA	5.49	125.16	119.56
1	E	44	LEU	CA-C-N	5.49	126.70	119.84
1	E	44	LEU	C-N-CA	5.49	126.70	119.84
2	L	123	ILE	CB-CA-C	-5.46	104.35	110.96
2	D	505	ILE	N-CA-C	-5.43	105.21	110.42
2	P	317	CYS	CA-C-N	5.43	125.25	119.28
2	P	317	CYS	C-N-CA	5.43	125.25	119.28
2	H	329	ILE	N-CA-C	-5.42	104.27	111.05
2	J	83	LYS	CA-C-N	5.41	125.41	119.89
2	J	83	LYS	C-N-CA	5.41	125.41	119.89
2	H	124	VAL	N-CA-CB	-5.40	105.33	112.34
1	E	113	LEU	CA-C-O	5.39	126.06	119.05
2	N	105	THR	N-CA-CB	5.39	118.14	110.16
2	B	581	CYS	CA-C-N	5.38	126.14	120.11
2	B	581	CYS	C-N-CA	5.38	126.14	120.11
2	L	83	LYS	CA-C-N	5.37	125.36	119.89
2	L	83	LYS	C-N-CA	5.37	125.36	119.89
1	G	133	ILE	CB-CA-C	-5.36	105.11	111.81
1	O	135	THR	N-CA-C	-5.36	105.13	110.97
2	L	129	LEU	CA-CB-CG	5.35	135.04	116.30
2	H	458	ILE	N-CA-CB	5.33	116.79	110.55
1	A	65	ALA	N-CA-C	-5.30	106.68	112.72
2	L	17	VAL	CB-CA-C	-5.29	103.96	112.16
2	F	129	LEU	N-CA-C	5.29	117.95	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	159	PHE	N-CA-C	5.28	117.12	108.52
2	B	200	TYR	CA-C-N	-5.27	115.73	122.79
2	B	200	TYR	C-N-CA	-5.27	115.73	122.79
1	O	65	ALA	N-CA-C	-5.27	106.71	112.72
2	N	462	SER	CA-C-N	5.26	124.93	119.56
2	N	462	SER	C-N-CA	5.26	124.93	119.56
1	I	44	LEU	CA-C-N	5.25	126.41	119.84
1	I	44	LEU	C-N-CA	5.25	126.41	119.84
1	G	44	LEU	CA-C-N	5.24	126.39	119.84
1	G	44	LEU	C-N-CA	5.24	126.39	119.84
2	H	83	LYS	CA-C-N	5.24	125.16	119.76
2	H	83	LYS	C-N-CA	5.24	125.16	119.76
1	C	137	PHE	N-CA-C	-5.24	106.41	114.16
2	N	449	GLY	N-CA-C	5.23	119.00	112.73
1	C	65	ALA	N-CA-C	-5.21	106.77	112.72
2	D	449	GLY	N-CA-C	5.21	118.98	112.73
1	G	123	ASP	N-CA-C	-5.20	106.78	113.23
2	H	30	ASP	CA-C-N	5.20	125.51	119.47
2	H	30	ASP	C-N-CA	5.20	125.51	119.47
1	C	113	LEU	CA-C-N	5.20	130.48	122.42
1	C	113	LEU	C-N-CA	5.20	130.48	122.42
2	B	17	VAL	CB-CA-C	-5.19	104.11	112.16
2	N	200	TYR	CA-C-N	-5.19	115.83	122.79
2	N	200	TYR	C-N-CA	-5.19	115.83	122.79
2	F	62	THR	N-CA-C	-5.15	106.84	113.23
2	F	83	LYS	CA-C-N	5.13	125.07	119.78
2	F	83	LYS	C-N-CA	5.13	125.07	119.78
2	D	200	TYR	N-CA-C	5.13	117.28	111.02
2	H	208	SER	CA-C-N	5.13	125.16	119.32
2	H	208	SER	C-N-CA	5.13	125.16	119.32
2	F	17	VAL	CB-CA-C	-5.12	104.22	112.16
2	H	310	HIS	N-CA-C	-5.12	105.70	111.28
2	N	200	TYR	N-CA-C	5.11	116.54	111.07
2	J	411	VAL	CA-C-N	-5.10	115.69	122.72
2	J	411	VAL	C-N-CA	-5.10	115.69	122.72
2	D	581	CYS	CA-C-N	5.09	125.81	120.11
2	D	581	CYS	C-N-CA	5.09	125.81	120.11
2	B	449	GLY	N-CA-C	5.08	118.83	112.73
2	N	109	ASN	N-CA-C	5.08	118.62	112.23
2	F	275	LEU	N-CA-C	5.07	116.55	108.79
2	D	24	VAL	N-CA-C	5.06	115.83	110.72
2	H	538	PRO	CA-C-N	-5.04	114.28	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	538	PRO	C-N-CA	-5.04	114.28	122.65
2	L	317	CYS	CA-C-N	5.04	124.70	119.56
2	L	317	CYS	C-N-CA	5.04	124.70	119.56
2	N	83	LYS	CA-C-N	5.04	124.97	119.78
2	N	83	LYS	C-N-CA	5.04	124.97	119.78
2	B	390	ILE	CB-CA-C	-5.04	104.29	111.19
2	J	159	ILE	N-CA-CB	5.04	118.13	110.58
1	E	159	PHE	N-CA-C	5.03	116.72	108.52
2	L	581	CYS	CA-C-N	5.03	125.04	120.21
2	L	581	CYS	C-N-CA	5.03	125.04	120.21
2	D	317	CYS	CA-C-N	5.03	124.81	119.28
2	D	317	CYS	C-N-CA	5.03	124.81	119.28
2	H	350	GLU	N-CA-C	5.03	117.57	107.41
2	H	182	LYS	N-CA-C	5.03	117.65	111.82
2	H	278	SER	CA-C-N	-5.03	112.34	122.55
2	H	278	SER	C-N-CA	-5.03	112.34	122.55
2	B	349	ILE	CB-CA-C	-5.02	105.01	111.53
2	D	17	VAL	CB-CA-C	-5.01	104.40	112.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	365	VAL	Peptide

5.2 Too-close contacts [i](#)

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	1152	0	1122	46	0
1	C	1152	0	1122	60	0
1	E	1152	0	1122	48	0
1	G	1152	0	1122	57	0
1	I	1152	0	1122	58	2
1	K	1152	0	1122	53	0
1	M	1152	0	1122	67	0
1	O	1152	0	1122	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4521	0	4564	182	0
2	D	4521	0	4564	215	2
2	F	4521	0	4564	204	0
2	H	4486	0	4534	373	0
2	J	4521	0	4564	202	0
2	L	4521	0	4564	204	0
2	N	4521	0	4564	230	0
2	P	4521	0	4564	205	0
3	Q	119	0	131	2	0
3	R	119	0	131	3	0
3	S	119	0	131	3	0
3	U	119	0	131	3	0
3	V	119	0	131	4	0
3	W	119	0	131	2	0
3	X	119	0	131	3	0
4	B	23	0	26	6	0
4	D	23	0	26	2	0
4	F	23	0	27	8	0
4	H	23	0	26	8	0
4	J	23	0	27	7	0
4	L	23	0	27	11	0
4	N	23	0	27	7	0
4	P	23	0	27	7	0
5	B	20	0	0	3	0
5	D	20	0	0	3	0
5	F	20	0	0	2	0
5	H	20	0	0	6	0
5	J	20	0	0	2	0
5	L	20	0	0	1	0
5	N	20	0	0	3	0
5	P	20	0	0	3	0
All	All	46526	0	46588	2115	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (2115) 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:168:THR:HB	2:H:196:VAL:HG13	1.34	1.08
2:H:305:LEU:HD23	2:H:305:LEU:H	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:102:ILE:HG21	2:N:20:VAL:HG22	1.43	1.00
2:H:364:LEU:HB3	2:H:365:VAL:HG22	1.41	1.00
2:B:444:TYR:HA	2:B:471:GLY:HA3	1.47	0.97
2:D:444:TYR:HA	2:D:471:GLY:HA3	1.43	0.96
2:J:444:TYR:HA	2:J:471:GLY:HA3	1.48	0.95
2:D:101:THR:HG22	2:D:128:ASP:OD1	1.65	0.95
2:N:444:TYR:HA	2:N:471:GLY:HA3	1.46	0.95
1:M:102:ILE:HG21	2:N:20:VAL:CG2	1.97	0.94
1:C:125:ILE:HG23	1:C:133:ILE:HD12	1.49	0.94
2:H:503:ARG:HE	2:H:503:ARG:H	1.15	0.94
2:H:533:MET:CE	2:H:588:LEU:HD13	1.98	0.93
2:L:444:TYR:HA	2:L:471:GLY:HA3	1.48	0.93
2:F:444:TYR:HA	2:F:471:GLY:HA3	1.50	0.93
2:H:323:LEU:HD12	2:H:324:GLU:N	1.83	0.93
2:J:164:ARG:HD2	2:N:112:ARG:HG2	1.50	0.91
2:H:161:THR:HG22	2:H:186:GLU:HG2	1.52	0.91
2:P:444:TYR:HA	2:P:471:GLY:HA3	1.52	0.91
2:N:203:GLU:OE1	3:W:211:ARG:HD3	1.71	0.90
2:J:101:THR:HG22	2:J:128:ASP:OD1	1.71	0.90
1:C:93:ILE:HD12	1:C:97:THR:HG22	1.53	0.89
2:H:364:LEU:HD13	2:H:388:SER:H	1.34	0.89
2:J:307:THR:HG21	2:J:362:GLU:HB2	1.54	0.89
1:K:125:ILE:HG23	1:K:133:ILE:HD12	1.55	0.88
2:N:307:THR:HG21	2:N:362:GLU:HB2	1.56	0.88
2:B:157:LEU:O	2:B:161:THR:HG23	1.73	0.88
2:H:390:ILE:CD1	2:H:412:LEU:HD21	2.05	0.87
2:L:307:THR:HG21	2:L:362:GLU:HB2	1.54	0.87
1:A:93:ILE:HD12	1:A:97:THR:HG22	1.56	0.87
2:F:307:THR:HG21	2:F:362:GLU:HB2	1.54	0.87
1:M:93:ILE:HD12	1:M:97:THR:HG22	1.56	0.87
2:H:390:ILE:HD12	2:H:410:LEU:HD21	1.55	0.86
1:K:93:ILE:HD12	1:K:97:THR:HG22	1.55	0.86
1:M:102:ILE:HD12	2:N:20:VAL:HG21	1.58	0.86
5:H:1101:PO4:O1	5:H:1103:PO4:O4	1.92	0.85
2:H:364:LEU:HD22	2:H:387:VAL:HA	1.57	0.85
2:F:157:LEU:O	2:F:161:THR:HG23	1.77	0.84
2:F:101:THR:HG22	2:F:128:ASP:OD1	1.77	0.84
2:D:307:THR:HG21	2:D:362:GLU:HB2	1.58	0.84
1:A:125:ILE:HG23	1:A:133:ILE:HD12	1.57	0.84
2:B:307:THR:HG21	2:B:362:GLU:HB2	1.60	0.84
2:N:398:ILE:HG23	2:N:402:LEU:HD11	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:444:TYR:HA	2:H:471:GLY:HA3	1.56	0.84
1:O:125:ILE:HG23	1:O:133:ILE:HD12	1.59	0.84
2:B:468:MET:HE3	2:B:470:LEU:HD21	1.57	0.84
1:C:40:ASN:HB3	1:K:13:GLY:O	1.77	0.84
1:M:112:ASN:C	1:M:114:LEU:H	1.84	0.83
2:N:101:THR:HG22	2:N:128:ASP:OD1	1.78	0.83
2:B:412:LEU:HD12	2:B:412:LEU:O	1.79	0.83
2:F:521:GLN:HG3	2:F:567:HIS:HD2	1.44	0.83
2:P:157:LEU:O	2:P:161:THR:HG23	1.79	0.83
2:J:412:LEU:HD12	2:J:412:LEU:O	1.78	0.82
2:L:412:LEU:HD12	2:L:412:LEU:O	1.79	0.82
2:B:592:ILE:H	2:B:592:ILE:HD12	1.44	0.82
2:N:468:MET:HE1	2:N:483:PHE:CE1	2.14	0.82
2:P:307:THR:HG21	2:P:362:GLU:HB2	1.61	0.82
1:I:125:ILE:HG23	1:I:133:ILE:HD12	1.62	0.82
2:L:157:LEU:O	2:L:161:THR:HG23	1.79	0.82
1:M:125:ILE:HG23	1:M:133:ILE:HD12	1.60	0.82
2:P:101:THR:HG22	2:P:128:ASP:OD1	1.78	0.82
2:F:89:PHE:CE2	4:F:1100:OGK:H04A	2.14	0.82
2:F:468:MET:HE3	2:F:470:LEU:HD21	1.61	0.82
1:C:113:LEU:O	1:C:117:THR:HG23	1.80	0.82
2:H:533:MET:HE1	2:H:588:LEU:HB3	1.60	0.82
2:D:590:GLU:HB3	2:D:591:PRO:HD2	1.61	0.81
2:P:412:LEU:HD12	2:P:412:LEU:O	1.81	0.81
2:P:468:MET:HE3	2:P:470:LEU:HD21	1.62	0.81
1:I:48:THR:HG22	1:I:51:ILE:H	1.46	0.81
2:N:412:LEU:HD12	2:N:412:LEU:O	1.80	0.81
2:J:80:LEU:HB2	2:J:122:MET:CE	2.11	0.81
2:L:101:THR:HG22	2:L:128:ASP:OD1	1.80	0.81
2:L:398:ILE:HG23	2:L:402:LEU:HD11	1.61	0.81
1:C:13:GLY:HA3	1:K:9:LYS:HZ2	1.46	0.81
2:F:592:ILE:H	2:F:592:ILE:HD12	1.46	0.81
2:H:37:ALA:O	2:H:40:VAL:HG13	1.81	0.81
2:L:468:MET:HE3	2:L:470:LEU:HD21	1.62	0.80
2:D:412:LEU:O	2:D:412:LEU:HD12	1.81	0.80
2:L:592:ILE:H	2:L:592:ILE:HD12	1.46	0.80
2:P:590:GLU:HB3	2:P:591:PRO:HD2	1.63	0.80
2:N:85:ARG:NH2	4:N:1100:OGK:O07	2.15	0.80
2:D:157:LEU:O	2:D:161:THR:HG23	1.81	0.80
2:H:364:LEU:CB	2:H:365:VAL:HG22	2.11	0.80
2:B:101:THR:HG22	2:B:128:ASP:OD1	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:158:ALA:HA	2:L:62:THR:HG21	1.64	0.80
1:M:102:ILE:CD1	2:N:20:VAL:HG21	2.13	0.80
1:C:160:GLU:HA	1:C:160:GLU:OE2	1.80	0.79
2:N:590:GLU:HB3	2:N:591:PRO:HD2	1.63	0.79
2:J:521:GLN:HG3	2:J:567:HIS:HD2	1.45	0.79
2:J:157:LEU:O	2:J:161:THR:HG23	1.81	0.79
2:P:398:ILE:HG23	2:P:402:LEU:HD11	1.64	0.79
2:B:590:GLU:HB3	2:B:591:PRO:HD2	1.63	0.79
2:P:592:ILE:H	2:P:592:ILE:HD12	1.47	0.79
2:F:412:LEU:HD12	2:F:412:LEU:O	1.81	0.79
2:H:444:TYR:HA	2:H:471:GLY:CA	2.13	0.79
2:J:468:MET:HE3	2:J:470:LEU:HD21	1.64	0.79
2:L:590:GLU:HB3	2:L:591:PRO:HD2	1.63	0.79
2:N:89:PHE:CE2	4:N:1100:OGK:H04A	2.18	0.79
2:N:521:GLN:HG3	2:N:567:HIS:HD2	1.48	0.79
2:J:590:GLU:HB3	2:J:591:PRO:HD2	1.65	0.79
2:P:116:SER:HB2	2:P:142:THR:HG23	1.65	0.79
1:C:48:THR:HG22	1:C:51:ILE:H	1.46	0.79
2:D:80:LEU:HB2	2:D:122:MET:CE	2.13	0.78
2:D:592:ILE:H	2:D:592:ILE:HD12	1.47	0.78
2:N:157:LEU:O	2:N:161:THR:HG23	1.83	0.78
2:F:521:GLN:HG3	2:F:567:HIS:CD2	2.18	0.78
2:J:592:ILE:H	2:J:592:ILE:HD12	1.48	0.78
1:K:48:THR:HG22	1:K:51:ILE:H	1.47	0.78
2:L:521:GLN:HG3	2:L:567:HIS:HD2	1.48	0.78
2:H:364:LEU:HD13	2:H:388:SER:N	1.99	0.78
2:B:396:GLU:O	2:B:400:THR:HG22	1.84	0.78
2:J:80:LEU:HB2	2:J:122:MET:HE1	1.65	0.78
1:E:125:ILE:HG23	1:E:133:ILE:HD12	1.65	0.78
2:F:142:THR:HB	2:F:168:THR:HG23	1.66	0.78
2:F:590:GLU:HB3	2:F:591:PRO:HD2	1.66	0.78
2:H:251:GLY:O	2:H:278:SER:HB2	1.83	0.78
2:H:274:ARG:HG2	2:H:297:LYS:HD2	1.66	0.78
1:E:48:THR:HG22	1:E:51:ILE:H	1.48	0.77
2:P:521:GLN:HG3	2:P:567:HIS:HD2	1.49	0.77
2:B:398:ILE:HG23	2:B:402:LEU:HD11	1.66	0.77
1:O:93:ILE:HD12	1:O:97:THR:HG22	1.66	0.77
2:B:521:GLN:HG3	2:B:567:HIS:HD2	1.49	0.77
2:H:331:ASP:OD2	2:H:366:SER:HB2	1.83	0.77
2:P:443:PHE:CE2	2:P:445:LEU:HD11	2.20	0.77
2:P:168:THR:HB	2:P:196:VAL:HG13	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:397:SER:HA	2:L:400:THR:CG2	2.15	0.77
2:J:521:GLN:HG3	2:J:567:HIS:CD2	2.19	0.77
1:O:158:ALA:HA	2:P:62:THR:HG21	1.66	0.77
2:N:592:ILE:HD12	2:N:592:ILE:H	1.49	0.76
2:J:533:MET:CE	2:J:588:LEU:HD13	2.15	0.76
1:E:93:ILE:HD12	1:E:97:THR:HG22	1.67	0.76
2:H:396:GLU:O	2:H:400:THR:HG23	1.84	0.76
2:H:533:MET:HE2	2:H:588:LEU:HD13	1.66	0.76
1:O:91:MET:SD	1:O:117:THR:HG22	2.25	0.76
2:J:398:ILE:HG23	2:J:402:LEU:HD11	1.66	0.76
2:P:55:VAL:HG23	2:P:75:LEU:HD21	1.65	0.76
1:G:93:ILE:HD12	1:G:97:THR:HG22	1.68	0.76
1:M:102:ILE:CG2	2:N:20:VAL:CG2	2.64	0.76
2:P:89:PHE:CE2	4:P:1100:OGK:H04A	2.20	0.76
1:A:98:LEU:HD21	1:A:120:THR:HG22	1.68	0.76
2:H:85:ARG:NH2	4:H:1100:OGK:O07	2.18	0.75
2:L:240:LYS:HG3	2:L:267:VAL:HG21	1.68	0.75
1:G:48:THR:HG22	1:G:51:ILE:H	1.51	0.75
2:L:80:LEU:HB2	2:L:122:MET:CE	2.17	0.75
2:H:428:VAL:HG13	2:H:443:PHE:CZ	2.22	0.75
1:I:158:ALA:HA	2:J:62:THR:HG21	1.69	0.75
2:H:282:PRO:HA	2:H:285:MET:HE2	1.69	0.75
2:H:501:SER:HB2	2:H:503:ARG:CZ	2.17	0.75
2:H:390:ILE:HD11	2:H:412:LEU:HD21	1.66	0.74
2:B:116:SER:HB2	2:B:142:THR:HG23	1.70	0.74
2:F:468:MET:HE1	2:F:483:PHE:CE1	2.21	0.74
2:H:65:PRO:HA	2:H:103:TRP:CZ3	2.21	0.74
1:I:160:GLU:HA	1:I:160:GLU:OE2	1.87	0.74
1:C:102:ILE:HG21	2:D:20:VAL:CG2	2.17	0.74
2:J:311:CYS:HB3	2:J:336:VAL:HG21	1.68	0.74
1:O:48:THR:HG22	1:O:51:ILE:H	1.51	0.74
2:D:533:MET:CE	2:D:588:LEU:HD13	2.18	0.74
2:N:240:LYS:HG3	2:N:267:VAL:HG21	1.69	0.74
2:L:203:GLU:OE1	3:V:211:ARG:HD3	1.87	0.74
2:D:240:LYS:HG3	2:D:267:VAL:HG21	1.70	0.74
1:I:93:ILE:HD12	1:I:97:THR:HG22	1.67	0.74
2:N:367:GLN:HG2	2:N:391:THR:HB	1.68	0.74
2:H:362:GLU:C	2:H:364:LEU:H	1.96	0.74
2:D:521:GLN:HG3	2:D:567:HIS:HD2	1.53	0.73
2:P:396:GLU:O	2:P:400:THR:HG22	1.88	0.73
2:D:294:GLN:NE2	1:G:107:TYR:OH	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:455:LEU:HD22	2:F:483:PHE:HB2	1.70	0.73
1:M:48:THR:HG22	1:M:51:ILE:H	1.52	0.73
1:E:158:ALA:HA	2:F:62:THR:HG21	1.69	0.73
2:D:80:LEU:HB2	2:D:122:MET:HE1	1.70	0.73
2:N:116:SER:HB2	2:N:142:THR:HG23	1.70	0.73
2:F:80:LEU:HB2	2:F:122:MET:CE	2.18	0.73
2:H:120:ARG:NH2	5:H:1103:PO4:P	2.62	0.73
2:P:240:LYS:HG3	2:P:267:VAL:HG21	1.70	0.73
2:H:118:HIS:HE1	2:H:146:ASP:OD2	1.72	0.73
2:H:327:ASN:C	2:H:329:ILE:H	1.96	0.73
2:D:367:GLN:HG2	2:D:391:THR:HB	1.70	0.73
2:N:521:GLN:HG3	2:N:567:HIS:CD2	2.23	0.73
2:J:468:MET:HE1	2:J:483:PHE:CE1	2.24	0.73
2:L:367:GLN:HG2	2:L:391:THR:HB	1.71	0.73
2:H:351:ARG:HG2	2:H:352:GLY:N	2.04	0.73
2:B:533:MET:CE	2:B:588:LEU:HD13	2.19	0.72
1:G:128:LYS:HB2	1:G:133:ILE:HD13	1.71	0.72
2:N:533:MET:HE3	2:N:588:LEU:HD13	1.71	0.72
2:F:398:ILE:HG23	2:F:402:LEU:HD11	1.69	0.72
2:F:397:SER:HA	2:F:400:THR:CG2	2.20	0.72
1:A:48:THR:HG22	1:A:51:ILE:H	1.53	0.72
2:H:528:THR:HG23	2:H:586:ARG:NH2	2.04	0.72
2:J:240:LYS:HG3	2:J:267:VAL:HG21	1.70	0.72
2:N:397:SER:HA	2:N:400:THR:CG2	2.20	0.72
2:P:468:MET:HE1	2:P:483:PHE:CE1	2.24	0.72
2:H:168:THR:CB	2:H:196:VAL:HG13	2.16	0.72
1:M:129:THR:O	1:M:133:ILE:HG12	1.89	0.72
2:P:367:GLN:HG2	2:P:391:THR:HB	1.71	0.72
2:H:332:ARG:HG2	2:H:332:ARG:HH11	1.55	0.72
2:L:533:MET:HE3	2:L:588:LEU:HD22	1.71	0.72
1:E:160:GLU:OE2	1:E:160:GLU:HA	1.90	0.72
2:F:240:LYS:HG3	2:F:267:VAL:HG21	1.70	0.72
2:J:533:MET:HE3	2:J:588:LEU:HD13	1.72	0.72
2:P:521:GLN:HG3	2:P:567:HIS:CD2	2.24	0.72
2:J:397:SER:HA	2:J:400:THR:CG2	2.20	0.71
2:N:468:MET:HE3	2:N:470:LEU:HD21	1.72	0.71
2:P:307:THR:HG22	2:P:360:ASP:OD2	1.90	0.71
2:D:443:PHE:CE2	2:D:445:LEU:HD11	2.25	0.71
2:N:443:PHE:CE2	2:N:445:LEU:HD11	2.24	0.71
2:P:367:GLN:O	2:P:371:ILE:HG22	1.89	0.71
2:B:397:SER:HA	2:B:400:THR:CG2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:455:LEU:HD22	2:L:483:PHE:HB2	1.71	0.71
2:H:519:TRP:CH2	2:H:567:HIS:ND1	2.59	0.71
2:J:161:THR:HG22	2:J:186:GLU:HG2	1.73	0.71
2:N:80:LEU:HB2	2:N:122:MET:HE1	1.72	0.71
2:D:533:MET:HE3	2:D:588:LEU:HD22	1.73	0.71
2:B:240:LYS:HG3	2:B:267:VAL:HG21	1.72	0.71
1:C:158:ALA:HA	2:D:62:THR:HG21	1.70	0.71
1:E:91:MET:HG2	1:E:116:LEU:HD21	1.73	0.71
2:L:89:PHE:CE2	4:L:1100:OGK:H04A	2.25	0.71
2:P:397:SER:HA	2:P:400:THR:CG2	2.21	0.71
1:A:160:GLU:HA	1:A:160:GLU:OE2	1.90	0.71
2:N:468:MET:HE1	2:N:483:PHE:HE1	1.55	0.71
2:B:533:MET:HE3	2:B:588:LEU:HD13	1.72	0.71
2:H:328:VAL:HG13	2:H:359:GLU:HG2	1.71	0.71
1:O:160:GLU:HA	1:O:160:GLU:OE2	1.88	0.71
2:N:168:THR:HB	2:N:196:VAL:HG13	1.72	0.70
2:D:397:SER:HA	2:D:400:THR:CG2	2.21	0.70
2:J:367:GLN:HG2	2:J:391:THR:HB	1.71	0.70
2:P:80:LEU:HB2	2:P:122:MET:CE	2.21	0.70
1:C:112:ASN:O	1:C:116:LEU:HB3	1.91	0.70
2:P:143:LEU:HD23	2:P:159:ILE:HD13	1.72	0.70
2:P:279:TYR:HA	2:P:304:LEU:HD22	1.72	0.70
2:P:310:HIS:O	2:P:314:ILE:HG12	1.90	0.70
2:B:521:GLN:HG3	2:B:567:HIS:CD2	2.25	0.70
2:H:386:TYR:HD2	2:H:413:LEU:HD21	1.55	0.70
2:J:397:SER:HA	2:J:400:THR:HG22	1.74	0.70
2:N:80:LEU:HB2	2:N:122:MET:CE	2.20	0.70
2:H:154:ASP:OD1	2:H:179:LYS:HE2	1.92	0.70
1:A:158:ALA:HA	2:B:62:THR:HG21	1.73	0.70
2:N:455:LEU:HD22	2:N:483:PHE:HB2	1.73	0.70
2:N:533:MET:CE	2:N:588:LEU:HD13	2.20	0.70
2:N:310:HIS:O	2:N:314:ILE:HG12	1.91	0.70
1:M:158:ALA:HA	2:N:62:THR:HG21	1.73	0.70
2:B:279:TYR:HA	2:B:304:LEU:HD22	1.74	0.70
2:B:404:ASN:HA	2:B:437:LYS:HD2	1.73	0.70
2:F:310:HIS:O	2:F:314:ILE:HG12	1.92	0.70
2:J:440:ARG:HB3	2:J:467:TRP:HE3	1.57	0.70
2:L:116:SER:HB2	2:L:142:THR:HG23	1.74	0.70
2:L:397:SER:HA	2:L:400:THR:HG22	1.73	0.70
2:N:404:ASN:HA	2:N:437:LYS:HD2	1.72	0.70
2:N:397:SER:HA	2:N:400:THR:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:337:LEU:HD11	2:H:344:LEU:HD22	1.72	0.69
1:G:160:GLU:HA	1:G:160:GLU:OE1	1.92	0.69
2:H:310:HIS:O	2:H:314:ILE:HG12	1.92	0.69
1:C:158:ALA:HA	2:D:62:THR:CG2	2.22	0.69
2:D:310:HIS:O	2:D:314:ILE:HG12	1.92	0.69
2:F:367:GLN:HG2	2:F:391:THR:HB	1.74	0.69
2:B:310:HIS:O	2:B:314:ILE:HG12	1.93	0.69
2:H:274:ARG:HG2	2:H:297:LYS:CD	2.23	0.69
2:L:521:GLN:HG3	2:L:567:HIS:CD2	2.26	0.69
2:B:440:ARG:HB3	2:B:467:TRP:HE3	1.57	0.69
1:E:48:THR:CG2	1:E:51:ILE:H	2.05	0.69
2:H:96:TRP:O	2:H:578:ARG:NH2	2.26	0.69
1:K:158:ALA:HA	2:L:62:THR:CG2	2.21	0.69
1:K:160:GLU:HG3	2:L:31:PRO:HB3	1.74	0.69
1:A:160:GLU:HG3	2:B:31:PRO:HB3	1.75	0.69
2:F:533:MET:CE	2:F:588:LEU:HD13	2.23	0.69
1:I:48:THR:CG2	1:I:51:ILE:H	2.06	0.69
2:L:533:MET:CE	2:L:588:LEU:HD13	2.23	0.69
1:E:160:GLU:HG3	2:F:31:PRO:HB3	1.75	0.69
2:B:161:THR:HG22	2:B:186:GLU:HG2	1.74	0.68
2:B:307:THR:HG22	2:B:360:ASP:OD2	1.93	0.68
2:H:528:THR:HG23	2:H:586:ARG:HH22	1.57	0.68
2:F:116:SER:HB2	2:F:142:THR:HG23	1.74	0.68
2:H:95:ASN:O	2:H:582:PRO:HG3	1.93	0.68
2:D:398:ILE:HG23	2:D:402:LEU:HD11	1.74	0.68
1:E:107:TYR:OH	2:L:294:GLN:NE2	2.26	0.68
2:F:443:PHE:CE2	2:F:445:LEU:HD11	2.27	0.68
2:L:80:LEU:HB2	2:L:122:MET:HE1	1.74	0.68
2:N:431:LEU:O	2:N:431:LEU:HD12	1.93	0.68
2:D:468:MET:HE3	2:D:470:LEU:HD21	1.76	0.68
2:H:141:GLU:HG2	2:H:167:LYS:HD3	1.75	0.68
1:M:124:MET:O	1:M:128:LYS:HE2	1.93	0.68
2:P:142:THR:HB	2:P:168:THR:HG23	1.74	0.68
1:C:48:THR:CG2	1:C:51:ILE:H	2.06	0.68
1:I:124:MET:O	1:I:128:LYS:HE2	1.94	0.68
2:L:542:ILE:HD11	2:L:588:LEU:HD12	1.75	0.68
1:O:153:ARG:HG2	1:O:157:TRP:CZ3	2.29	0.68
2:F:201:MET:HE3	3:S:208:SER:HB2	1.75	0.68
1:G:30:ALA:O	1:G:33:VAL:HG22	1.94	0.68
1:G:102:ILE:HG21	2:H:20:VAL:HG22	1.75	0.68
2:P:280:MET:HE1	2:P:288:LEU:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:455:LEU:HD22	2:D:483:PHE:HB2	1.75	0.68
2:B:455:LEU:HD22	2:B:483:PHE:HB2	1.75	0.68
2:D:161:THR:HG22	2:D:186:GLU:HG2	1.75	0.68
2:J:487:CYS:HB3	2:J:490:LEU:HB2	1.74	0.68
2:F:143:LEU:HD23	2:F:159:ILE:HD13	1.74	0.67
2:H:221:SER:O	2:H:223:VAL:HG13	1.95	0.67
2:N:487:CYS:HB3	2:N:490:LEU:HB2	1.76	0.67
2:J:164:ARG:CD	2:N:112:ARG:HG2	2.24	0.67
2:L:161:THR:HG22	2:L:186:GLU:HG2	1.75	0.67
2:D:521:GLN:HG3	2:D:567:HIS:CD2	2.30	0.67
2:B:367:GLN:HG2	2:B:391:THR:HB	1.74	0.67
2:J:307:THR:HG22	2:J:360:ASP:OD2	1.94	0.67
2:L:367:GLN:O	2:L:371:ILE:HG22	1.94	0.67
1:M:48:THR:CG2	1:M:51:ILE:H	2.07	0.67
1:O:160:GLU:HG3	2:P:31:PRO:HB3	1.76	0.67
2:P:455:LEU:HD22	2:P:483:PHE:HB2	1.76	0.67
2:F:275:LEU:HD11	2:F:288:LEU:HD21	1.77	0.67
2:F:533:MET:HE3	2:F:588:LEU:HD22	1.77	0.67
2:H:366:SER:HB3	2:H:368:ARG:HG2	1.76	0.67
2:N:161:THR:HG22	2:N:186:GLU:HG2	1.77	0.67
2:D:367:GLN:O	2:D:371:ILE:HG22	1.95	0.67
2:J:533:MET:HE3	2:J:588:LEU:HD22	1.76	0.67
2:B:143:LEU:HD23	2:B:159:ILE:HD13	1.77	0.67
1:I:101:LEU:HB3	1:I:117:THR:HG21	1.76	0.67
2:H:198:ASN:ND2	2:H:226:LYS:HD2	2.10	0.67
2:D:210:LYS:O	2:D:214:THR:HG22	1.96	0.66
2:F:85:ARG:NH2	4:F:1100:OGK:O07	2.25	0.66
2:P:533:MET:HE3	2:P:588:LEU:HD13	1.77	0.66
2:D:307:THR:HG22	2:D:360:ASP:OD2	1.96	0.66
2:H:307:THR:HB	2:H:328:VAL:O	1.95	0.66
2:J:168:THR:HB	2:J:196:VAL:HG13	1.78	0.66
2:J:263:TYR:O	2:J:265:ASN:N	2.29	0.66
2:J:310:HIS:O	2:J:314:ILE:HG12	1.94	0.66
2:N:58:ALA:HA	2:N:81:LYS:HD2	1.77	0.66
2:B:58:ALA:HA	2:B:81:LYS:HD2	1.77	0.66
2:D:58:ALA:HA	2:D:81:LYS:HD2	1.77	0.66
2:F:263:TYR:O	2:F:265:ASN:N	2.29	0.66
2:N:143:LEU:HD23	2:N:159:ILE:HD13	1.77	0.66
2:P:80:LEU:HB2	2:P:122:MET:HE1	1.76	0.66
1:C:113:LEU:O	1:C:117:THR:CG2	2.44	0.66
2:D:121:ARG:NH2	5:D:1103:PO4:O4	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:80:LEU:HB2	2:F:122:MET:HE1	1.76	0.66
2:D:533:MET:HE3	2:D:588:LEU:HD13	1.76	0.66
2:H:59:LEU:O	2:H:62:THR:HB	1.95	0.66
2:F:112:ARG:HG2	2:L:164:ARG:HD2	1.77	0.66
2:H:327:ASN:C	2:H:329:ILE:N	2.48	0.66
2:H:584:THR:O	2:H:584:THR:HG22	1.94	0.66
2:N:299:ASP:OD2	2:N:301:LEU:HB2	1.96	0.66
2:L:468:MET:HE1	2:L:483:PHE:CE1	2.30	0.66
1:G:128:LYS:HB2	1:G:133:ILE:CD1	2.26	0.66
2:H:544:LEU:O	2:H:546:PRO:HD3	1.96	0.66
1:I:111:LYS:O	1:I:115:ASP:HB2	1.96	0.66
1:I:160:GLU:HG3	2:J:31:PRO:HB3	1.77	0.66
1:M:160:GLU:HG3	2:N:31:PRO:HB3	1.78	0.66
2:N:221:SER:O	2:N:223:VAL:HG23	1.94	0.66
2:P:519:TRP:HE1	4:P:1100:OGK:H01	1.59	0.65
2:F:279:TYR:HA	2:F:304:LEU:HD22	1.78	0.65
2:P:221:SER:O	2:P:223:VAL:HG23	1.95	0.65
2:B:80:LEU:HB2	2:B:122:MET:CE	2.25	0.65
2:H:212:LEU:HD23	2:H:235:LEU:HD22	1.78	0.65
1:O:158:ALA:HA	2:P:62:THR:CG2	2.26	0.65
2:H:301:LEU:HD23	2:H:324:GLU:HB3	1.78	0.65
2:H:492:LYS:HZ3	2:H:516:ARG:HH11	1.42	0.65
2:J:367:GLN:O	2:J:371:ILE:HG22	1.96	0.65
2:N:431:LEU:HD12	2:N:431:LEU:C	2.20	0.65
2:D:279:TYR:HA	2:D:304:LEU:HD22	1.79	0.65
2:H:125:SER:HB3	2:H:127:LEU:N	2.11	0.65
1:I:30:ALA:O	1:I:33:VAL:HG22	1.94	0.65
2:J:164:ARG:HD2	2:N:112:ARG:CG	2.24	0.65
2:L:210:LYS:O	2:L:214:THR:HG22	1.96	0.65
2:N:307:THR:HG22	2:N:360:ASP:OD2	1.97	0.65
2:P:58:ALA:HA	2:P:81:LYS:HD2	1.78	0.65
2:P:443:PHE:HE2	2:P:445:LEU:HD11	1.62	0.65
2:D:397:SER:HA	2:D:400:THR:HG22	1.79	0.65
2:H:542:ILE:HD12	2:H:542:ILE:C	2.22	0.65
2:L:58:ALA:HA	2:L:81:LYS:HD2	1.79	0.65
2:L:431:LEU:HD12	2:L:431:LEU:O	1.96	0.65
2:B:367:GLN:O	2:B:371:ILE:HG22	1.96	0.65
1:C:160:GLU:HG3	2:D:31:PRO:HB3	1.79	0.65
2:H:533:MET:HE3	2:H:588:LEU:HD13	1.77	0.65
2:L:279:TYR:HA	2:L:304:LEU:HD22	1.77	0.65
2:N:57:MET:HE3	2:N:62:THR:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:LEU:O	1:O:113:LEU:HG	1.97	0.65
2:J:443:PHE:CE2	2:J:445:LEU:HD11	2.30	0.65
2:L:396:GLU:O	2:L:400:THR:HG22	1.97	0.65
1:M:158:ALA:HA	2:N:62:THR:CG2	2.27	0.65
1:E:158:ALA:HA	2:F:62:THR:CG2	2.27	0.65
2:F:397:SER:HA	2:F:400:THR:HG22	1.79	0.65
1:I:106:ASN:N	1:I:114:LEU:HD13	2.12	0.65
2:L:55:VAL:HG23	2:L:75:LEU:HD21	1.78	0.65
2:H:361:GLU:O	2:H:362:GLU:HG2	1.97	0.64
2:H:468:MET:CE	2:H:470:LEU:HD21	2.26	0.64
2:D:263:TYR:O	2:D:265:ASN:N	2.30	0.64
1:K:48:THR:CG2	1:K:51:ILE:H	2.10	0.64
2:L:168:THR:HB	2:L:196:VAL:HG13	1.79	0.64
2:N:279:TYR:HA	2:N:304:LEU:HD22	1.79	0.64
2:P:487:CYS:HB3	2:P:490:LEU:HB2	1.80	0.64
2:H:280:MET:HE1	2:H:288:LEU:CD1	2.27	0.64
2:H:503:ARG:H	2:H:503:ARG:NE	1.92	0.64
2:F:396:GLU:O	2:F:400:THR:HG22	1.98	0.64
2:H:337:LEU:O	2:H:341:CYS:HB2	1.97	0.64
2:N:55:VAL:HG23	2:N:75:LEU:HD21	1.78	0.64
2:B:89:PHE:CE2	4:B:1100:OGK:H04A	2.33	0.64
2:B:168:THR:HB	2:B:196:VAL:HG13	1.79	0.64
2:L:443:PHE:CE2	2:L:445:LEU:HD11	2.31	0.64
2:N:311:CYS:HB3	2:N:336:VAL:HG21	1.78	0.64
2:H:440:ARG:HB3	2:H:467:TRP:CD1	2.33	0.64
1:I:158:ALA:HA	2:J:62:THR:CG2	2.27	0.64
2:L:487:CYS:HB3	2:L:490:LEU:HB2	1.80	0.64
2:L:533:MET:HE3	2:L:588:LEU:HD13	1.79	0.64
2:N:275:LEU:HD11	2:N:288:LEU:HD21	1.80	0.64
1:M:30:ALA:O	1:M:33:VAL:HG22	1.97	0.64
2:D:440:ARG:HB3	2:D:467:TRP:HE3	1.63	0.64
2:P:89:PHE:CD2	4:P:1100:OGK:H04A	2.31	0.64
2:F:284:GLU:O	2:F:287:ILE:HD13	1.98	0.64
2:H:332:ARG:O	2:H:336:VAL:HG23	1.98	0.64
2:L:307:THR:HG22	2:L:360:ASP:OD2	1.97	0.64
1:O:124:MET:O	1:O:128:LYS:HE2	1.97	0.64
2:H:303:ALA:HB1	2:H:305:LEU:CD2	2.28	0.63
2:J:279:TYR:HA	2:J:304:LEU:HD22	1.80	0.63
2:N:268:PHE:HE1	2:N:287:ILE:HG13	1.61	0.63
2:B:468:MET:HE1	2:B:483:PHE:CE1	2.33	0.63
2:D:386:TYR:CE1	4:D:1100:OGK:H15A	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:PHE:HE1	2:F:287:ILE:HG13	1.62	0.63
2:J:542:ILE:HD11	2:J:588:LEU:HD12	1.80	0.63
4:P:1100:OGK:HN08	4:P:1100:OGK:H18A	1.63	0.63
2:D:468:MET:HE1	2:D:483:PHE:CE1	2.33	0.63
2:F:519:TRP:HE1	4:F:1100:OGK:H01	1.63	0.63
2:H:533:MET:CE	2:H:588:LEU:HB3	2.26	0.63
2:J:210:LYS:O	2:J:214:THR:HG22	1.98	0.63
2:P:210:LYS:O	2:P:214:THR:HG22	1.99	0.63
2:B:210:LYS:O	2:B:214:THR:HG22	1.97	0.63
2:F:55:VAL:HG23	2:F:75:LEU:HD21	1.80	0.63
2:H:366:SER:C	2:H:368:ARG:N	2.52	0.63
2:J:95:ASN:O	2:J:582:PRO:HG3	1.98	0.63
2:F:307:THR:HG22	2:F:360:ASP:OD2	1.97	0.63
2:H:211:ASP:O	2:H:215:ILE:HG13	1.99	0.63
2:H:34:ARG:NH1	2:H:48:ASP:OD1	2.32	0.63
2:H:329:ILE:HG12	2:H:333:GLY:HA3	1.81	0.63
2:H:542:ILE:HG13	2:H:588:LEU:HB2	1.80	0.63
2:N:396:GLU:O	2:N:400:THR:HG22	1.99	0.63
2:B:487:CYS:HB3	2:B:490:LEU:HB2	1.81	0.63
2:D:101:THR:HG21	2:N:179:LYS:NZ	2.14	0.63
1:E:30:ALA:O	1:E:33:VAL:HG22	1.98	0.63
1:E:153:ARG:HG2	1:E:157:TRP:CZ3	2.34	0.63
1:G:48:THR:CG2	1:G:51:ILE:H	2.10	0.63
2:H:191:ASN:HD21	2:H:194:LEU:H	1.45	0.63
2:H:390:ILE:HD11	2:H:410:LEU:HD11	1.81	0.63
2:J:55:VAL:HG23	2:J:75:LEU:HD21	1.81	0.63
1:M:153:ARG:HG2	1:M:157:TRP:CZ3	2.33	0.63
2:B:409:ARG:HB2	4:B:1100:OGK:H16B	1.81	0.63
2:B:533:MET:HE3	2:B:588:LEU:HD22	1.81	0.63
2:F:533:MET:HE3	2:F:588:LEU:HD13	1.79	0.63
2:D:116:SER:HB2	2:D:142:THR:HG23	1.80	0.63
2:F:542:ILE:HD11	2:F:588:LEU:HD12	1.81	0.62
2:J:116:SER:HB2	2:J:142:THR:HG23	1.80	0.62
2:N:201:MET:HE3	3:W:208:SER:HB2	1.80	0.62
2:H:125:SER:HB3	2:H:127:LEU:H	1.64	0.62
2:J:299:ASP:OD2	2:J:301:LEU:HB2	1.98	0.62
1:M:99:PHE:CD2	2:N:16:THR:C	2.78	0.62
1:G:149:GLU:OE1	1:G:153:ARG:NE	2.32	0.62
1:I:52:LEU:O	1:I:56:ILE:HG13	2.00	0.62
1:O:48:THR:CG2	1:O:51:ILE:H	2.12	0.62
2:P:431:LEU:HD12	2:P:431:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:MET:HE1	2:B:288:LEU:HD11	1.80	0.62
2:H:361:GLU:HA	2:H:364:LEU:HD12	1.80	0.62
2:H:366:SER:CB	2:H:368:ARG:HG2	2.29	0.62
2:D:40:VAL:O	2:D:41:CYS:HB3	2.00	0.62
2:H:57:MET:HE3	2:H:62:THR:HG22	1.81	0.62
2:J:456:SER:HB2	2:J:482:GLU:HB3	1.80	0.62
2:D:203:GLU:OE1	3:R:211:ARG:HD3	1.99	0.62
1:E:160:GLU:CG	2:F:31:PRO:HB3	2.29	0.62
2:F:267:VAL:HG23	2:F:267:VAL:O	2.00	0.62
2:H:305:LEU:H	2:H:305:LEU:CD2	2.06	0.62
1:K:160:GLU:HA	1:K:160:GLU:OE2	1.98	0.62
2:B:80:LEU:HB2	2:B:122:MET:HE1	1.81	0.62
2:H:428:VAL:CG1	2:H:443:PHE:CZ	2.82	0.62
2:J:40:VAL:O	2:J:41:CYS:HB3	2.00	0.62
2:J:468:MET:HE1	2:J:483:PHE:HE1	1.65	0.62
2:N:367:GLN:O	2:N:371:ILE:HG22	1.99	0.62
1:C:126:LYS:HZ1	2:D:29:THR:H	1.48	0.62
2:J:201:MET:HE3	3:U:208:SER:HB2	1.80	0.62
2:N:533:MET:HE3	2:N:588:LEU:HD22	1.82	0.62
2:P:299:ASP:OD2	2:P:301:LEU:HB2	2.00	0.62
2:F:404:ASN:HA	2:F:437:LYS:HD2	1.82	0.62
2:F:487:CYS:HB3	2:F:490:LEU:HB2	1.80	0.62
2:H:366:SER:C	2:H:368:ARG:H	2.07	0.62
2:L:57:MET:HE3	2:L:62:THR:HG22	1.82	0.62
2:H:327:ASN:HA	2:H:329:ILE:HG22	1.82	0.61
2:N:59:LEU:O	2:N:62:THR:HB	1.99	0.61
2:P:440:ARG:HB3	2:P:467:TRP:HE3	1.65	0.61
2:L:310:HIS:O	2:L:314:ILE:HG12	2.00	0.61
2:N:443:PHE:HE2	2:N:445:LEU:HD11	1.66	0.61
2:P:263:TYR:O	2:P:265:ASN:N	2.33	0.61
2:P:404:ASN:HA	2:P:437:LYS:HD2	1.82	0.61
2:P:519:TRP:NE1	4:P:1100:OGK:H01	2.15	0.61
2:D:456:SER:HB2	2:D:482:GLU:HB3	1.81	0.61
1:K:102:ILE:HG12	1:K:117:THR:HB	1.81	0.61
2:F:40:VAL:O	2:F:41:CYS:HB3	1.99	0.61
1:I:160:GLU:CG	2:J:31:PRO:HB3	2.31	0.61
1:K:30:ALA:O	1:K:33:VAL:HG22	1.99	0.61
2:N:465:VAL:HG11	2:N:468:MET:HG3	1.83	0.61
2:B:443:PHE:CE2	2:B:445:LEU:HD11	2.36	0.61
2:F:168:THR:HB	2:F:196:VAL:HG13	1.81	0.61
4:L:1100:OGK:H18A	4:L:1100:OGK:HN08	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:275:LEU:HD11	2:P:288:LEU:HD21	1.82	0.61
2:P:533:MET:CE	2:P:588:LEU:HD13	2.30	0.61
2:H:160:VAL:HG11	2:H:187:LEU:HG	1.82	0.61
1:M:99:PHE:HD2	2:N:15:ALA:O	1.84	0.61
1:O:129:THR:O	1:O:133:ILE:HG12	2.01	0.61
2:D:95:ASN:O	2:D:582:PRO:HG3	2.00	0.61
2:D:96:TRP:O	2:D:578:ARG:NH2	2.26	0.61
2:D:190:HIS:HB3	2:H:112:ARG:HD2	1.83	0.61
2:F:263:TYR:C	2:F:265:ASN:H	2.09	0.61
2:H:87:ALA:C	2:H:89:PHE:H	2.09	0.61
2:J:280:MET:HE1	2:J:288:LEU:HD11	1.83	0.61
1:G:159:PHE:O	1:G:160:GLU:HB2	1.99	0.61
2:H:285:MET:HE1	2:H:309:ASP:HB3	1.83	0.61
2:D:101:THR:CG2	2:D:128:ASP:OD1	2.46	0.61
2:D:164:ARG:HD2	2:H:112:ARG:HD3	1.83	0.61
1:M:48:THR:HG22	1:M:51:ILE:HB	1.83	0.61
1:M:102:ILE:CD1	2:N:20:VAL:CG2	2.78	0.61
2:N:95:ASN:O	2:N:582:PRO:HG3	2.01	0.61
2:P:390:ILE:HD13	2:P:424:LEU:HD11	1.83	0.61
2:D:54:HIS:HD2	2:D:77:SER:OG	1.83	0.61
2:H:492:LYS:NZ	2:H:516:ARG:HH11	1.98	0.61
1:I:126:LYS:HZ1	2:J:29:THR:H	1.48	0.61
2:J:58:ALA:HA	2:J:81:LYS:HD2	1.82	0.61
2:J:455:LEU:HD22	2:J:483:PHE:HB2	1.82	0.61
2:L:54:HIS:HE1	2:L:56:THR:OG1	1.83	0.61
2:N:456:SER:HB2	2:N:482:GLU:HB3	1.81	0.61
2:N:542:ILE:HD11	2:N:588:LEU:HD12	1.81	0.61
1:O:30:ALA:O	1:O:33:VAL:HG22	1.99	0.61
2:B:268:PHE:HE1	2:B:287:ILE:HG13	1.66	0.60
2:H:323:LEU:HD12	2:H:323:LEU:C	2.22	0.60
2:J:390:ILE:HD11	2:J:412:LEU:HD23	1.82	0.60
2:L:263:TYR:O	2:L:265:ASN:N	2.33	0.60
2:H:127:LEU:HD22	2:J:126:ASP:HB3	1.82	0.60
2:H:286:PRO:O	2:H:288:LEU:N	2.34	0.60
2:P:284:GLU:O	2:P:287:ILE:HD13	2.00	0.60
2:B:142:THR:HB	2:B:168:THR:HG23	1.82	0.60
2:H:144:LYS:HG2	2:H:170:LEU:HD13	1.83	0.60
2:B:311:CYS:HB3	2:B:336:VAL:HG21	1.82	0.60
1:G:151:VAL:HG12	2:H:39:LEU:HD21	1.83	0.60
2:H:161:THR:HG22	2:H:186:GLU:CG	2.28	0.60
2:H:327:ASN:HD22	2:H:364:LEU:HD21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:160:GLU:CG	2:N:31:PRO:HB3	2.32	0.60
2:N:89:PHE:CD2	4:N:1100:OGK:H04A	2.35	0.60
2:P:533:MET:HE3	2:P:588:LEU:HD22	1.82	0.60
1:C:30:ALA:O	1:C:33:VAL:HG22	2.02	0.60
2:H:100:VAL:HG23	2:H:122:MET:HE2	1.83	0.60
2:J:57:MET:HE3	2:J:62:THR:HG22	1.81	0.60
2:P:456:SER:HB2	2:P:482:GLU:HB3	1.82	0.60
2:D:80:LEU:HB2	2:D:122:MET:HE2	1.83	0.60
2:F:297:LYS:HG3	2:F:322:VAL:HB	1.83	0.60
2:H:386:TYR:CE1	4:H:1100:OGK:H15A	2.36	0.60
2:N:142:THR:HB	2:N:168:THR:HG23	1.83	0.60
2:P:263:TYR:C	2:P:265:ASN:H	2.10	0.60
2:B:297:LYS:HG3	2:B:322:VAL:HB	1.83	0.60
2:H:280:MET:HE1	2:H:288:LEU:HD12	1.84	0.60
1:K:129:THR:O	1:K:133:ILE:HG12	2.02	0.60
2:P:468:MET:HE1	2:P:483:PHE:HE1	1.67	0.60
1:A:48:THR:CG2	1:A:51:ILE:H	2.15	0.60
2:B:263:TYR:O	2:B:265:ASN:N	2.33	0.60
2:F:58:ALA:HA	2:F:81:LYS:HD2	1.82	0.60
2:F:85:ARG:HD2	5:F:1101:PO4:O2	2.02	0.60
2:H:367:GLN:CD	2:H:367:GLN:H	2.09	0.60
2:H:390:ILE:HD13	2:H:412:LEU:HD21	1.82	0.60
4:H:1100:OGK:H18A	4:H:1100:OGK:HN08	1.67	0.60
2:L:95:ASN:O	2:L:582:PRO:HG3	2.01	0.60
2:F:299:ASP:OD2	2:F:301:LEU:HB2	2.02	0.60
2:H:304:LEU:HD13	2:H:304:LEU:O	2.02	0.60
2:H:503:ARG:HE	2:H:503:ARG:N	1.94	0.60
2:L:268:PHE:HE1	2:L:287:ILE:HG13	1.66	0.60
2:L:359:GLU:HG2	3:V:216:ARG:HH22	1.67	0.60
1:A:95:GLN:HG2	1:A:124:MET:HE1	1.83	0.59
2:B:456:SER:HB2	2:B:482:GLU:HB3	1.83	0.59
2:D:168:THR:HB	2:D:196:VAL:HG13	1.82	0.59
2:D:396:GLU:O	2:D:400:THR:HG22	2.01	0.59
2:N:225:VAL:HG13	2:N:245:LEU:HD11	1.83	0.59
2:P:161:THR:HG22	2:P:186:GLU:HG2	1.84	0.59
2:B:267:VAL:HG23	2:B:267:VAL:O	2.02	0.59
2:B:85:ARG:HG2	2:B:88:MET:HE2	1.83	0.59
2:D:284:GLU:O	2:D:287:ILE:HD13	2.02	0.59
2:H:170:LEU:HD23	2:H:172:GLU:H	1.66	0.59
2:L:201:MET:HE1	2:L:302:TYR:CE2	2.37	0.59
2:L:456:SER:HB2	2:L:482:GLU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:MET:HG2	1:O:116:LEU:HD21	1.83	0.59
2:P:268:PHE:HE1	2:P:287:ILE:HG13	1.66	0.59
2:H:286:PRO:HA	2:H:289:PHE:CE2	2.37	0.59
2:D:201:MET:HE1	2:D:302:TYR:CE2	2.37	0.59
2:D:487:CYS:HB3	2:D:490:LEU:HB2	1.85	0.59
2:H:212:LEU:HD22	2:H:230:PHE:CE1	2.38	0.59
2:H:277:LEU:HD12	2:H:280:MET:HE3	1.84	0.59
2:D:267:VAL:HG23	2:D:267:VAL:O	2.02	0.59
2:P:311:CYS:HB3	2:P:336:VAL:HG21	1.84	0.59
1:C:13:GLY:HA3	1:K:9:LYS:NZ	2.17	0.59
2:D:263:TYR:C	2:D:265:ASN:H	2.10	0.59
2:D:390:ILE:HD11	2:D:412:LEU:HD23	1.85	0.59
2:H:225:VAL:O	2:H:248:PHE:HA	2.03	0.59
2:N:85:ARG:HG2	2:N:88:MET:HE2	1.85	0.59
2:P:397:SER:HA	2:P:400:THR:HG22	1.84	0.59
2:D:57:MET:HE3	2:D:62:THR:HG22	1.83	0.59
1:E:124:MET:O	1:E:128:LYS:HE2	2.02	0.59
2:H:284:GLU:O	2:H:287:ILE:HG23	2.03	0.59
2:H:292:ALA:C	2:H:294:GLN:H	2.09	0.59
1:K:160:GLU:CG	2:L:31:PRO:HB3	2.32	0.59
2:P:542:ILE:HD11	2:P:588:LEU:HD12	1.84	0.59
2:B:299:ASP:OD2	2:B:301:LEU:HB2	2.02	0.59
1:I:129:THR:O	1:I:133:ILE:HG12	2.03	0.59
2:J:267:VAL:HG23	2:J:267:VAL:O	2.03	0.59
1:M:160:GLU:OE2	1:M:160:GLU:HA	2.00	0.59
1:O:160:GLU:CG	2:P:31:PRO:HB3	2.32	0.59
2:B:275:LEU:HD11	2:B:288:LEU:HD21	1.85	0.59
1:C:102:ILE:HG21	2:D:20:VAL:HG21	1.84	0.59
2:J:221:SER:O	2:J:223:VAL:HG23	2.03	0.59
1:C:124:MET:O	1:C:128:LYS:HE2	2.02	0.58
2:D:85:ARG:HG2	2:D:88:MET:HE2	1.85	0.58
2:L:308:GLU:HG3	2:L:332:ARG:HH22	1.67	0.58
2:N:297:LYS:HG3	2:N:322:VAL:HB	1.85	0.58
2:B:40:VAL:O	2:B:41:CYS:HB3	2.03	0.58
2:B:101:THR:HG21	2:F:179:LYS:NZ	2.17	0.58
2:F:143:LEU:CD2	2:F:159:ILE:HD13	2.33	0.58
2:J:396:GLU:O	2:J:400:THR:HG22	2.03	0.58
2:N:210:LYS:O	2:N:214:THR:HG22	2.03	0.58
2:N:280:MET:HE1	2:N:288:LEU:HD11	1.85	0.58
2:N:398:ILE:CG2	2:N:402:LEU:HD11	2.31	0.58
4:N:1100:OGK:H18A	4:N:1100:OGK:HN08	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ALA:O	1:A:33:VAL:HG22	2.03	0.58
2:F:80:LEU:HD12	2:F:122:MET:HE1	1.86	0.58
2:H:171:MET:HE3	2:H:199:PHE:HB3	1.84	0.58
2:H:259:MET:C	2:H:261:GLU:H	2.11	0.58
2:L:40:VAL:O	2:L:41:CYS:HB3	2.02	0.58
2:B:190:HIS:CG	2:P:112:ARG:HH11	2.22	0.58
1:O:102:ILE:HD12	2:P:20:VAL:HG21	1.84	0.58
2:P:203:GLU:OE1	3:X:211:ARG:HD3	2.03	0.58
1:E:107:TYR:CD1	2:L:270:ARG:O	2.57	0.58
2:J:80:LEU:HB2	2:J:122:MET:HE2	1.83	0.58
2:P:85:ARG:HG2	2:P:88:MET:HE2	1.86	0.58
2:P:267:VAL:HG23	2:P:267:VAL:O	2.04	0.58
2:B:542:ILE:HD11	2:B:588:LEU:HD12	1.85	0.58
2:D:546:PRO:HD2	2:D:584:THR:O	2.03	0.58
2:H:349:ILE:HD12	2:H:385:VAL:CG2	2.33	0.58
2:L:267:VAL:O	2:L:267:VAL:HG23	2.03	0.58
1:A:158:ALA:HA	2:B:62:THR:CG2	2.32	0.58
2:D:297:LYS:HG3	2:D:322:VAL:HB	1.85	0.58
2:F:367:GLN:O	2:F:371:ILE:HG22	2.04	0.58
2:H:118:HIS:CE1	2:H:146:ASP:OD2	2.55	0.58
1:I:102:ILE:HG13	1:I:117:THR:HB	1.84	0.58
2:J:263:TYR:C	2:J:265:ASN:H	2.11	0.58
2:J:275:LEU:HD11	2:J:288:LEU:HD21	1.84	0.58
2:D:348:ARG:HH22	4:D:1100:OGK:C10	2.17	0.58
1:I:102:ILE:CG1	1:I:117:THR:HB	2.34	0.58
2:J:295:ILE:HG21	2:J:298:LEU:HD13	1.84	0.58
2:L:275:LEU:HD11	2:L:288:LEU:HD21	1.86	0.58
2:N:404:ASN:CB	2:N:437:LYS:HD2	2.34	0.58
2:H:386:TYR:CD2	2:H:413:LEU:HD21	2.38	0.58
2:F:456:SER:HB2	2:F:482:GLU:HB3	1.84	0.58
2:H:305:LEU:HD23	2:H:305:LEU:N	2.07	0.58
2:J:284:GLU:O	2:J:287:ILE:HD13	2.03	0.58
2:N:468:MET:HE1	2:N:483:PHE:CZ	2.39	0.58
2:D:580:ASP:HA	2:N:206:LYS:HE3	1.86	0.57
2:H:328:VAL:HG13	2:H:359:GLU:CG	2.34	0.57
2:J:440:ARG:HB3	2:J:467:TRP:CE3	2.38	0.57
2:L:431:LEU:HD12	2:L:431:LEU:C	2.28	0.57
2:B:440:ARG:HB3	2:B:467:TRP:CE3	2.39	0.57
1:E:48:THR:HG22	1:E:51:ILE:HB	1.86	0.57
2:H:213:GLU:CD	2:H:237:GLY:HA3	2.28	0.57
2:H:292:ALA:HA	2:H:295:ILE:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:263:TYR:O	2:N:265:ASN:N	2.37	0.57
2:F:308:GLU:HG3	2:F:332:ARG:HH22	1.69	0.57
2:H:390:ILE:CD1	2:H:410:LEU:HD11	2.34	0.57
1:I:26:SER:OG	1:I:108:LEU:HB3	2.04	0.57
2:L:143:LEU:HD23	2:L:159:ILE:HD13	1.86	0.57
2:L:384:ALA:HB1	4:L:1100:OGK:H16	1.87	0.57
2:N:85:ARG:HD2	5:N:1101:PO4:O2	2.04	0.57
1:I:153:ARG:HG2	1:I:157:TRP:CZ3	2.39	0.57
2:L:359:GLU:HG2	3:V:216:ARG:NH2	2.19	0.57
2:P:121:ARG:NH2	5:P:1103:PO4:O4	2.38	0.57
1:C:102:ILE:HG21	2:D:20:VAL:HG22	1.85	0.57
1:I:98:LEU:HD21	1:I:120:THR:HG22	1.87	0.57
2:N:267:VAL:HG23	2:N:267:VAL:O	2.05	0.57
2:J:54:HIS:HE1	2:J:56:THR:OG1	1.88	0.57
2:J:348:ARG:HH22	4:J:1100:OGK:C10	2.16	0.57
2:P:304:LEU:HD11	3:X:216:ARG:HG3	1.87	0.57
2:P:431:LEU:HD12	2:P:431:LEU:C	2.29	0.57
2:B:284:GLU:O	2:B:287:ILE:HD13	2.04	0.57
2:B:390:ILE:HD11	2:B:412:LEU:HD23	1.86	0.57
2:D:268:PHE:HE1	2:D:287:ILE:HG13	1.68	0.57
2:H:351:ARG:HG2	2:H:352:GLY:H	1.70	0.57
2:N:143:LEU:CD2	2:N:159:ILE:HD13	2.34	0.57
2:P:280:MET:HE1	2:P:288:LEU:CD1	2.34	0.57
1:E:37:CYS:SG	2:L:296:ARG:NH2	2.78	0.57
2:H:299:ASP:OD2	2:H:301:LEU:HB2	2.05	0.57
2:J:404:ASN:HA	2:J:437:LYS:HD2	1.87	0.57
2:L:201:MET:HE3	3:V:208:SER:HB2	1.86	0.57
1:E:30:ALA:C	1:E:32:MET:H	2.13	0.57
2:L:142:THR:HB	2:L:168:THR:HG23	1.85	0.57
1:G:130:PRO:HD3	2:H:36:SER:HB3	1.87	0.56
2:H:86:ALA:HA	4:H:1100:OGK:H27	1.87	0.56
2:B:263:TYR:C	2:B:265:ASN:H	2.13	0.56
2:D:142:THR:HB	2:D:168:THR:HG23	1.85	0.56
2:F:221:SER:O	2:F:223:VAL:HG23	2.04	0.56
2:F:390:ILE:HD13	2:F:424:LEU:HD11	1.87	0.56
2:J:201:MET:HE1	2:J:302:TYR:CE2	2.40	0.56
2:J:543:GLU:OE2	2:J:578:ARG:HD3	2.04	0.56
2:D:431:LEU:C	2:D:431:LEU:HD12	2.30	0.56
1:E:129:THR:O	1:E:133:ILE:HG12	2.04	0.56
2:F:468:MET:HE1	2:F:483:PHE:HE1	1.65	0.56
2:H:310:HIS:NE2	2:H:328:VAL:HG23	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:345:LYS:NZ	2:H:345:LYS:HB3	2.21	0.56
2:J:142:THR:HB	2:J:168:THR:HG23	1.86	0.56
2:H:286:PRO:C	2:H:288:LEU:H	2.12	0.56
2:L:263:TYR:C	2:L:265:ASN:H	2.12	0.56
2:L:297:LYS:HG3	2:L:322:VAL:HB	1.88	0.56
2:F:275:LEU:HD11	2:F:288:LEU:CD2	2.36	0.56
2:H:587:VAL:HG12	2:H:589:LYS:HD3	1.87	0.56
2:L:80:LEU:HB2	2:L:122:MET:HE2	1.86	0.56
2:L:299:ASP:OD2	2:L:301:LEU:HB2	2.06	0.56
2:H:178:GLU:CD	2:H:206:LYS:HB3	2.31	0.56
2:F:431:LEU:O	2:F:431:LEU:HD12	2.06	0.56
2:N:309:ASP:HA	2:N:312:THR:HG23	1.88	0.56
2:D:404:ASN:HA	2:D:437:LYS:HD2	1.88	0.56
1:G:142:ASP:OD2	2:H:42:ARG:HG3	2.06	0.56
2:J:268:PHE:HE1	2:J:287:ILE:HG13	1.70	0.56
1:K:52:LEU:O	1:K:56:ILE:HG13	2.06	0.56
2:P:57:MET:HE3	2:P:62:THR:HG22	1.86	0.56
2:B:221:SER:O	2:B:223:VAL:HG23	2.05	0.56
2:F:280:MET:HE1	2:F:288:LEU:HD11	1.87	0.56
2:H:362:GLU:C	2:H:364:LEU:N	2.62	0.56
1:K:124:MET:O	1:K:128:LYS:HE2	2.05	0.56
2:L:295:ILE:HG21	2:L:298:LEU:HD13	1.88	0.56
2:P:398:ILE:CG2	2:P:402:LEU:HD11	2.36	0.56
2:L:390:ILE:HD11	2:L:412:LEU:HD23	1.87	0.56
1:M:32:MET:HE3	1:M:42:VAL:HB	1.88	0.55
2:F:191:ASN:HD21	2:F:194:LEU:H	1.54	0.55
2:J:85:ARG:HG2	2:J:88:MET:HE2	1.87	0.55
2:H:332:ARG:HH11	2:H:332:ARG:CG	2.18	0.55
1:K:126:LYS:HZ1	2:L:29:THR:H	1.52	0.55
2:L:85:ARG:HG2	2:L:88:MET:HE2	1.88	0.55
1:M:102:ILE:HB	2:N:20:VAL:HG21	1.88	0.55
2:P:143:LEU:CD2	2:P:159:ILE:HD13	2.35	0.55
2:B:397:SER:HA	2:B:400:THR:HG22	1.87	0.55
2:H:298:LEU:CD2	2:H:300:LEU:HD21	2.36	0.55
2:H:541:ASN:O	2:H:570:ALA:HA	2.06	0.55
2:N:275:LEU:HD11	2:N:288:LEU:CD2	2.37	0.55
2:B:386:TYR:CE1	4:B:1100:OGK:H15A	2.42	0.55
2:N:170:LEU:C	2:N:170:LEU:HD23	2.30	0.55
2:B:59:LEU:O	2:B:62:THR:HB	2.07	0.55
2:L:311:CYS:HB3	2:L:336:VAL:HG21	1.89	0.55
2:L:440:ARG:HB3	2:L:467:TRP:HE3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:95:ASN:O	2:P:582:PRO:HG3	2.07	0.55
2:B:54:HIS:HE1	2:B:56:THR:OG1	1.89	0.55
2:F:80:LEU:HB2	2:F:122:MET:HE2	1.87	0.55
2:F:161:THR:HG22	2:F:186:GLU:HG2	1.88	0.55
2:H:471:GLY:O	2:H:496:ARG:O	2.25	0.55
2:D:275:LEU:HD11	2:D:288:LEU:HD21	1.89	0.55
2:F:431:LEU:HD12	2:F:431:LEU:C	2.32	0.55
2:H:323:LEU:HD12	2:H:324:GLU:H	1.68	0.55
2:H:543:GLU:OE2	2:H:578:ARG:HD3	2.07	0.55
1:A:98:LEU:CD2	1:A:120:THR:HG22	2.34	0.55
2:B:191:ASN:HD21	2:B:194:LEU:H	1.54	0.55
2:D:440:ARG:HB3	2:D:467:TRP:CE3	2.42	0.55
2:L:80:LEU:HD12	2:L:122:MET:HE1	1.87	0.55
2:N:201:MET:HE1	2:N:302:TYR:CE2	2.41	0.55
1:A:160:GLU:CG	2:B:31:PRO:HB3	2.35	0.54
2:B:289:PHE:N	2:B:290:PRO:CD	2.71	0.54
2:D:431:LEU:HD12	2:D:431:LEU:O	2.08	0.54
2:F:210:LYS:O	2:F:214:THR:HG22	2.07	0.54
2:H:467:TRP:HZ3	2:H:494:GLU:OE1	1.91	0.54
1:M:159:PHE:O	1:M:160:GLU:CB	2.54	0.54
2:P:40:VAL:O	2:P:41:CYS:HB3	2.06	0.54
2:P:54:HIS:HE1	2:P:56:THR:OG1	1.90	0.54
2:H:402:LEU:HD13	2:H:405:LEU:HG	1.89	0.54
2:J:121:ARG:HH22	5:J:1103:PO4:P	2.30	0.54
2:J:465:VAL:HG11	2:J:468:MET:HG3	1.90	0.54
1:K:34:GLU:C	1:K:36:ASP:H	2.15	0.54
1:M:112:ASN:O	1:M:114:LEU:N	2.36	0.54
2:P:55:VAL:CG2	2:P:75:LEU:HD21	2.37	0.54
1:C:160:GLU:CG	2:D:31:PRO:HB3	2.37	0.54
2:H:120:ARG:HH22	5:H:1103:PO4:P	2.29	0.54
2:H:325:THR:OG1	2:H:326:ARG:N	2.36	0.54
4:J:1100:OGK:H18A	4:J:1100:OGK:HN08	1.72	0.54
1:M:34:GLU:C	1:M:36:ASP:H	2.16	0.54
2:N:390:ILE:HD13	2:N:424:LEU:HD11	1.88	0.54
1:O:91:MET:CG	1:O:116:LEU:HD21	2.37	0.54
1:C:13:GLY:CA	1:K:9:LYS:NZ	2.70	0.54
1:I:108:LEU:HD12	1:I:110:ILE:HD11	1.87	0.54
2:J:422:LEU:O	2:J:423:PRO:C	2.50	0.54
2:N:429:ARG:O	2:N:433:ILE:HG13	2.07	0.54
2:H:365:VAL:HG13	2:H:387:VAL:CG2	2.38	0.54
2:H:519:TRP:HH2	2:H:567:HIS:CE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:543:GLU:OE2	2:L:578:ARG:HD3	2.06	0.54
2:N:54:HIS:HE1	2:N:56:THR:OG1	1.90	0.54
1:E:107:TYR:HD1	2:L:270:ARG:O	1.90	0.54
1:I:99:PHE:HZ	1:I:137:PHE:HE1	1.53	0.54
2:N:386:TYR:CE1	4:N:1100:OGK:H15A	2.42	0.54
2:P:59:LEU:O	2:P:62:THR:HB	2.08	0.54
2:B:543:GLU:OE2	2:B:578:ARG:HD3	2.08	0.54
2:L:465:VAL:HG11	2:L:468:MET:HG3	1.90	0.54
2:L:546:PRO:HD2	2:L:584:THR:O	2.07	0.54
2:N:96:TRP:O	2:N:578:ARG:NH2	2.30	0.54
2:P:170:LEU:HD23	2:P:170:LEU:C	2.32	0.54
1:E:34:GLU:C	1:E:36:ASP:H	2.15	0.54
2:L:404:ASN:HA	2:L:437:LYS:HD2	1.89	0.54
2:N:338:ALA:O	2:N:376:GLY:HA3	2.08	0.54
2:B:143:LEU:CD2	2:B:159:ILE:HD13	2.38	0.54
2:D:443:PHE:HE2	2:D:445:LEU:HD11	1.72	0.54
2:L:590:GLU:CB	2:L:591:PRO:HD2	2.36	0.54
1:O:34:GLU:C	1:O:36:ASP:H	2.16	0.54
2:F:59:LEU:O	2:F:62:THR:HB	2.08	0.54
2:F:309:ASP:HA	2:F:312:THR:HG23	1.90	0.54
2:F:311:CYS:HB3	2:F:336:VAL:HG21	1.90	0.54
2:H:227:VAL:HG13	2:H:228:GLY:N	2.22	0.53
2:J:431:LEU:HD12	2:J:431:LEU:O	2.07	0.53
2:N:308:GLU:HG3	2:N:332:ARG:HH22	1.73	0.53
2:N:390:ILE:HD11	2:N:412:LEU:HD23	1.90	0.53
2:D:80:LEU:HD12	2:D:122:MET:HE1	1.90	0.53
2:H:245:LEU:HB3	2:H:269:PRO:HG2	1.89	0.53
2:J:546:PRO:HD2	2:J:584:THR:O	2.07	0.53
2:L:225:VAL:HG13	2:L:245:LEU:HD11	1.90	0.53
2:N:367:GLN:HG2	2:N:391:THR:CB	2.38	0.53
2:H:89:PHE:CE2	4:H:1100:OGK:H04A	2.43	0.53
2:H:351:ARG:HD2	2:H:359:GLU:O	2.08	0.53
1:K:30:ALA:C	1:K:32:MET:H	2.16	0.53
2:N:263:TYR:C	2:N:265:ASN:H	2.14	0.53
2:P:577:GLN:HE22	2:P:589:LYS:HG2	1.73	0.53
2:F:386:TYR:CE1	4:F:1100:OGK:H15A	2.43	0.53
2:F:543:GLU:OE2	2:F:578:ARG:HD3	2.08	0.53
2:N:469:LEU:HA	2:N:494:GLU:O	2.09	0.53
1:A:34:GLU:C	1:A:36:ASP:H	2.17	0.53
2:H:303:ALA:HB1	2:H:305:LEU:HD23	1.91	0.53
2:J:143:LEU:CD2	2:J:159:ILE:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:577:GLN:HE22	2:N:589:LYS:HG2	1.73	0.53
2:P:301:LEU:CD2	2:P:324:GLU:HB3	2.38	0.53
2:D:543:GLU:OE2	2:D:578:ARG:HD3	2.09	0.53
1:E:102:ILE:HG21	2:F:20:VAL:HG22	1.90	0.53
2:F:95:ASN:O	2:F:582:PRO:HG3	2.09	0.53
2:H:303:ALA:HB1	2:H:305:LEU:HD21	1.89	0.53
2:H:506:ALA:HB1	2:H:535:MET:HB2	1.90	0.53
2:J:170:LEU:HD23	2:J:170:LEU:C	2.33	0.53
2:J:308:GLU:HG3	2:J:332:ARG:HH22	1.74	0.53
2:D:590:GLU:CB	2:D:591:PRO:HD2	2.35	0.53
2:F:247:GLU:HA	2:F:274:ARG:O	2.08	0.53
2:H:101:THR:HB	2:H:102:PRO:HD3	1.89	0.53
2:H:249:CYS:HA	2:H:276:GLY:O	2.09	0.53
2:H:253:LEU:HD13	2:H:284:GLU:HG3	1.91	0.53
2:H:289:PHE:HB2	2:H:290:PRO:HD3	1.90	0.53
2:J:367:GLN:HG2	2:J:391:THR:CB	2.37	0.53
2:N:121:ARG:NH2	5:N:1103:PO4:O4	2.42	0.53
2:B:95:ASN:O	2:B:582:PRO:HG3	2.09	0.53
2:D:296:ARG:NH2	1:G:37:CYS:SG	2.82	0.53
1:G:34:GLU:C	1:G:36:ASP:H	2.17	0.53
2:J:117:VAL:HG11	2:J:119:PHE:CZ	2.43	0.53
2:L:348:ARG:HH22	4:L:1100:OGK:C10	2.21	0.53
2:N:280:MET:HE1	2:N:288:LEU:CD1	2.39	0.53
2:N:284:GLU:O	2:N:287:ILE:HD13	2.08	0.53
2:N:404:ASN:CA	2:N:437:LYS:HD2	2.37	0.53
2:P:184:LEU:HD12	2:P:207:ILE:HB	1.90	0.53
2:P:429:ARG:O	2:P:433:ILE:HG13	2.09	0.53
2:B:203:GLU:OE1	3:Q:211:ARG:HD3	2.08	0.53
2:F:390:ILE:HD11	2:F:412:LEU:HD23	1.91	0.53
2:F:577:GLN:HE22	2:F:589:LYS:HG2	1.74	0.53
1:G:52:LEU:O	1:G:56:ILE:HG13	2.09	0.53
2:H:327:ASN:C	2:H:327:ASN:OD1	2.51	0.53
1:M:48:THR:HG22	1:M:51:ILE:CB	2.39	0.53
1:M:102:ILE:CB	2:N:20:VAL:HG21	2.39	0.53
2:N:180:ASP:OD1	2:N:182:LYS:HG3	2.09	0.53
2:F:57:MET:HE3	2:F:62:THR:HG22	1.90	0.53
2:F:440:ARG:HB3	2:F:467:TRP:HE3	1.74	0.53
1:G:106:ASN:OD1	2:H:23:GLN:OE1	2.27	0.53
2:J:59:LEU:O	2:J:62:THR:HB	2.08	0.53
2:P:367:GLN:HG2	2:P:391:THR:CB	2.39	0.53
2:B:59:LEU:HD22	2:B:61:TYR:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:419:ILE:HD11	2:D:446:ARG:HH22	1.74	0.52
1:E:91:MET:CG	1:E:116:LEU:HD21	2.39	0.52
2:L:284:GLU:O	2:L:287:ILE:HD13	2.09	0.52
2:N:590:GLU:CB	2:N:591:PRO:HD2	2.36	0.52
2:P:121:ARG:HH22	5:P:1103:PO4:P	2.33	0.52
2:P:440:ARG:HB3	2:P:467:TRP:CE3	2.44	0.52
1:C:12:ASP:O	1:K:40:ASN:CB	2.57	0.52
1:C:32:MET:HE3	1:C:42:VAL:HB	1.90	0.52
1:O:159:PHE:O	1:O:160:GLU:CB	2.57	0.52
2:P:380:LEU:HD13	2:P:383:MET:HE2	1.90	0.52
2:D:270:ARG:O	1:G:107:TYR:CD1	2.63	0.52
2:F:101:THR:CG2	2:F:128:ASP:OD1	2.54	0.52
2:H:61:TYR:CD2	2:H:578:ARG:HG2	2.44	0.52
2:H:178:GLU:OE1	2:H:206:LYS:HB3	2.10	0.52
2:J:471:GLY:O	2:J:496:ARG:O	2.27	0.52
2:F:125:SER:N	2:F:128:ASP:OD2	2.43	0.52
2:F:295:ILE:HG21	2:F:298:LEU:HD13	1.90	0.52
2:J:143:LEU:HD23	2:J:159:ILE:HD13	1.91	0.52
2:J:443:PHE:HE2	2:J:445:LEU:HD11	1.73	0.52
1:K:32:MET:HE3	1:K:42:VAL:HB	1.92	0.52
2:L:59:LEU:O	2:L:62:THR:HB	2.09	0.52
2:L:253:LEU:HD12	2:L:280:MET:HB2	1.92	0.52
1:M:27:GLN:HB2	1:M:109:ASN:HB3	1.90	0.52
2:N:440:ARG:HB3	2:N:467:TRP:HE3	1.73	0.52
2:D:221:SER:O	2:D:223:VAL:HG23	2.10	0.52
2:H:109:ASN:C	2:H:110:ASN:HD22	2.17	0.52
2:H:207:ILE:HD12	2:H:230:PHE:HZ	1.74	0.52
1:G:102:ILE:HG12	1:G:117:THR:OG1	2.10	0.52
2:H:286:PRO:C	2:H:288:LEU:N	2.68	0.52
2:N:301:LEU:CD2	2:N:324:GLU:HB3	2.40	0.52
2:B:431:LEU:C	2:B:431:LEU:HD12	2.35	0.52
2:N:125:SER:N	2:N:128:ASP:OD2	2.43	0.52
2:N:284:GLU:O	2:N:287:ILE:HG23	2.10	0.52
2:B:275:LEU:HD11	2:B:288:LEU:CD2	2.39	0.52
1:C:99:PHE:CE2	2:D:17:VAL:HG22	2.44	0.52
1:C:102:ILE:HD11	1:C:121:VAL:HG21	1.92	0.52
2:D:143:LEU:HD23	2:D:159:ILE:HD13	1.91	0.52
2:F:443:PHE:HE2	2:F:445:LEU:HD11	1.73	0.52
1:G:30:ALA:C	1:G:32:MET:H	2.16	0.52
2:J:431:LEU:HD12	2:J:431:LEU:C	2.35	0.52
2:N:311:CYS:O	2:N:315:GLN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:180:ASP:OD1	2:P:182:LYS:HG3	2.10	0.52
2:B:101:THR:CG2	2:F:179:LYS:HZ1	2.23	0.52
1:C:34:GLU:C	1:C:36:ASP:H	2.17	0.52
1:E:134:ARG:HB2	1:E:139:ILE:O	2.09	0.52
2:P:159:ILE:HG13	2:P:160:VAL:N	2.25	0.52
2:P:253:LEU:HD12	2:P:280:MET:HB2	1.92	0.52
2:B:225:VAL:HG13	2:B:245:LEU:HD11	1.91	0.52
2:D:296:ARG:CZ	1:G:37:CYS:SG	2.98	0.52
2:P:309:ASP:HA	2:P:312:THR:HG23	1.91	0.52
1:C:129:THR:O	1:C:133:ILE:HG12	2.10	0.51
2:F:419:ILE:HG21	2:F:422:LEU:HD13	1.92	0.51
2:H:157:LEU:O	2:H:161:THR:HG23	2.10	0.51
2:H:533:MET:C	2:H:535:MET:H	2.17	0.51
1:K:46:ASN:HB2	1:K:107:TYR:CZ	2.45	0.51
2:L:380:LEU:HD13	2:L:383:MET:HE2	1.93	0.51
2:L:390:ILE:HD13	2:L:424:LEU:HD11	1.92	0.51
2:N:422:LEU:O	2:N:423:PRO:C	2.53	0.51
1:C:30:ALA:C	1:C:32:MET:H	2.17	0.51
2:D:201:MET:HE2	2:D:302:TYR:OH	2.09	0.51
2:H:136:ARG:HB3	2:H:140:LEU:HB2	1.93	0.51
2:H:267:VAL:HG23	2:H:267:VAL:O	2.10	0.51
2:H:390:ILE:HD13	2:H:390:ILE:N	2.26	0.51
2:L:367:GLN:HG2	2:L:391:THR:CB	2.39	0.51
2:L:419:ILE:O	2:L:420:THR:C	2.53	0.51
2:B:289:PHE:N	2:B:290:PRO:HD2	2.25	0.51
1:C:102:ILE:CG2	2:D:20:VAL:CG2	2.86	0.51
2:D:59:LEU:O	2:D:62:THR:HB	2.09	0.51
2:D:143:LEU:CD2	2:D:159:ILE:HD13	2.41	0.51
2:D:299:ASP:OD2	2:D:301:LEU:HB2	2.09	0.51
1:G:137:PHE:HB3	2:H:17:VAL:HG21	1.92	0.51
2:N:289:PHE:N	2:N:290:PRO:HD2	2.26	0.51
2:P:311:CYS:O	2:P:315:GLN:HB2	2.10	0.51
1:C:135:THR:HG22	1:C:136:THR:N	2.24	0.51
2:D:191:ASN:HD21	2:D:194:LEU:H	1.58	0.51
2:H:371:ILE:HG22	2:H:375:GLN:HE21	1.74	0.51
1:M:26:SER:OG	1:M:108:LEU:HB3	2.10	0.51
2:P:308:GLU:HG3	2:P:332:ARG:HH22	1.75	0.51
1:A:46:ASN:HB2	1:A:107:TYR:CZ	2.46	0.51
2:D:296:ARG:NE	1:G:37:CYS:SG	2.84	0.51
2:H:212:LEU:HD22	2:H:230:PHE:HE1	1.75	0.51
2:J:386:TYR:CE1	4:J:1100:OGK:H15A	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:180:ASP:OD1	2:L:182:LYS:HG3	2.09	0.51
2:P:201:MET:HE1	2:P:302:TYR:CE2	2.45	0.51
2:B:295:ILE:HG21	2:B:298:LEU:HD13	1.91	0.51
2:B:468:MET:HE1	2:B:483:PHE:HE1	1.74	0.51
2:F:468:MET:HE1	2:F:483:PHE:CZ	2.45	0.51
2:J:519:TRP:HE1	4:J:1100:OGK:H01	1.76	0.51
2:L:308:GLU:HG3	2:L:332:ARG:NH2	2.26	0.51
1:M:112:ASN:C	1:M:114:LEU:N	2.52	0.51
2:B:294:GLN:NE2	1:O:107:TYR:OH	2.44	0.51
2:B:577:GLN:HE22	2:B:589:LYS:HG2	1.75	0.51
2:D:308:GLU:HG3	2:D:332:ARG:HH22	1.75	0.51
2:H:470:LEU:HD13	2:H:473:VAL:HG21	1.93	0.51
2:L:191:ASN:HD21	2:L:194:LEU:H	1.57	0.51
4:N:1100:OGK:HN08	4:N:1100:OGK:C18	2.23	0.51
2:P:295:ILE:HG21	2:P:298:LEU:HD13	1.93	0.51
2:B:55:VAL:HG23	2:B:75:LEU:HD21	1.92	0.51
2:B:404:ASN:CB	2:B:437:LYS:HD2	2.40	0.51
1:C:48:THR:HG22	1:C:51:ILE:N	2.21	0.51
2:D:361:GLU:HG3	2:D:361:GLU:O	2.09	0.51
2:F:85:ARG:HG2	2:F:88:MET:HE2	1.92	0.51
2:H:365:VAL:CG1	2:H:387:VAL:HG21	2.40	0.51
2:J:444:TYR:HA	2:J:471:GLY:CA	2.33	0.51
2:L:59:LEU:HD22	2:L:61:TYR:H	1.76	0.51
2:L:453:LEU:HD11	2:L:457:TYR:OH	2.11	0.51
2:D:180:ASP:OD1	2:D:182:LYS:HG3	2.11	0.51
2:J:390:ILE:HD13	2:J:424:LEU:HD11	1.92	0.51
2:L:184:LEU:HD12	2:L:207:ILE:HB	1.92	0.51
2:P:275:LEU:HD11	2:P:288:LEU:CD2	2.41	0.51
2:D:367:GLN:HG2	2:D:391:THR:CB	2.37	0.51
2:D:465:VAL:HG11	2:D:468:MET:HG3	1.93	0.51
1:I:34:GLU:C	1:I:36:ASP:H	2.19	0.51
1:I:159:PHE:O	1:I:160:GLU:CB	2.59	0.51
2:L:398:ILE:CG2	2:L:402:LEU:HD11	2.37	0.51
1:M:134:ARG:HB2	1:M:139:ILE:O	2.10	0.51
2:P:124:VAL:HG11	2:P:129:LEU:HD13	1.93	0.51
2:P:590:GLU:CB	2:P:591:PRO:HD2	2.38	0.51
1:A:32:MET:HE3	1:A:42:VAL:HB	1.91	0.50
1:A:99:PHE:HZ	1:A:137:PHE:HE1	1.60	0.50
1:C:12:ASP:O	1:K:40:ASN:ND2	2.43	0.50
1:E:48:THR:HG22	1:E:51:ILE:CB	2.41	0.50
2:F:59:LEU:HD22	2:F:61:TYR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:301:LEU:CD2	2:F:324:GLU:HB3	2.41	0.50
2:F:546:PRO:HD2	2:F:584:THR:O	2.11	0.50
2:H:335:GLU:OE2	2:H:368:ARG:NH1	2.44	0.50
2:J:309:ASP:HA	2:J:312:THR:HG23	1.92	0.50
2:P:390:ILE:HD11	2:P:412:LEU:HD23	1.93	0.50
2:P:465:VAL:HG11	2:P:468:MET:HG3	1.92	0.50
1:C:52:LEU:O	1:C:56:ILE:HG13	2.11	0.50
1:C:141:ASN:OD1	1:C:141:ASN:C	2.54	0.50
2:D:577:GLN:HE22	2:D:589:LYS:HG2	1.75	0.50
2:F:482:GLU:O	2:F:485:ARG:HG2	2.10	0.50
2:H:366:SER:CB	2:H:368:ARG:H	2.24	0.50
1:M:30:ALA:C	1:M:32:MET:H	2.18	0.50
2:B:170:LEU:HD23	2:B:170:LEU:C	2.36	0.50
2:B:380:LEU:HD13	2:B:383:MET:HE2	1.92	0.50
2:B:404:ASN:CA	2:B:437:LYS:HD2	2.40	0.50
2:D:225:VAL:HG13	2:D:245:LEU:HD11	1.92	0.50
1:E:37:CYS:SG	2:L:296:ARG:CZ	3.00	0.50
2:J:311:CYS:CB	2:J:336:VAL:HG21	2.41	0.50
2:P:274:ARG:HG2	2:P:297:LYS:HE3	1.93	0.50
1:E:52:LEU:O	1:E:56:ILE:HG13	2.11	0.50
2:F:380:LEU:HD13	2:F:383:MET:HE2	1.93	0.50
2:H:233:LEU:O	2:H:236:VAL:HG23	2.12	0.50
2:H:348:ARG:HG3	2:H:384:ALA:HB3	1.93	0.50
2:J:280:MET:HE1	2:J:288:LEU:CD1	2.41	0.50
2:N:399:GLY:O	2:N:434:GLY:HA3	2.11	0.50
1:O:27:GLN:HB2	1:O:109:ASN:HB3	1.93	0.50
1:O:32:MET:HE3	1:O:42:VAL:HB	1.94	0.50
2:D:295:ILE:HG21	2:D:298:LEU:HD13	1.94	0.50
1:M:44:LEU:HD12	1:M:44:LEU:O	2.11	0.50
2:B:419:ILE:O	2:B:420:THR:C	2.53	0.50
2:B:546:PRO:HD2	2:B:584:THR:O	2.12	0.50
1:C:153:ARG:HG2	1:C:157:TRP:CZ3	2.47	0.50
2:D:101:THR:CG2	2:N:179:LYS:HZ1	2.23	0.50
2:F:113:GLN:HE22	2:L:192:THR:CB	2.24	0.50
2:H:274:ARG:CG	2:H:297:LYS:HB3	2.41	0.50
2:H:402:LEU:CD1	2:H:405:LEU:HG	2.41	0.50
2:J:301:LEU:CD2	2:J:324:GLU:HB3	2.42	0.50
1:O:52:LEU:O	1:O:56:ILE:HG13	2.11	0.50
2:P:297:LYS:HG3	2:P:322:VAL:HB	1.94	0.50
1:A:124:MET:O	1:A:128:LYS:HE2	2.11	0.50
2:D:304:LEU:HD11	3:R:216:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:PHE:CD2	4:F:1100:OGK:H04A	2.47	0.50
2:F:419:ILE:O	2:F:420:THR:C	2.53	0.50
2:H:168:THR:HA	2:H:196:VAL:O	2.12	0.50
2:H:280:MET:HE2	2:H:285:MET:HA	1.93	0.50
2:J:192:THR:HG21	2:N:113:GLN:HE22	1.76	0.50
2:B:101:THR:HG21	2:F:179:LYS:HZ1	1.76	0.50
2:D:55:VAL:HG23	2:D:75:LEU:HD21	1.93	0.50
2:D:101:THR:CG2	2:N:179:LYS:NZ	2.75	0.50
2:F:201:MET:HE1	2:F:302:TYR:CE2	2.46	0.50
1:G:32:MET:HE3	1:G:42:VAL:HB	1.94	0.50
2:H:96:TRP:HA	2:H:582:PRO:HG2	1.93	0.50
2:J:367:GLN:HG2	2:J:391:THR:CG2	2.42	0.50
2:P:101:THR:CG2	2:P:128:ASP:OD1	2.56	0.50
2:D:349:ILE:HG13	2:D:385:VAL:HG22	1.94	0.50
2:F:154:ASP:OD2	2:F:179:LYS:NZ	2.39	0.50
2:F:404:ASN:CB	2:F:437:LYS:HD2	2.42	0.50
1:O:91:MET:SD	1:O:117:THR:CG2	2.99	0.50
2:P:125:SER:O	2:P:129:LEU:HD22	2.12	0.50
2:B:80:LEU:HB2	2:B:122:MET:HE2	1.93	0.49
2:D:247:GLU:HA	2:D:274:ARG:O	2.11	0.49
1:E:44:LEU:HD12	1:E:44:LEU:O	2.12	0.49
2:H:95:ASN:HD22	2:H:95:ASN:N	2.08	0.49
2:H:144:LYS:HE3	5:H:1104:PO4:O4	2.12	0.49
2:H:365:VAL:HG13	2:H:387:VAL:HG21	1.95	0.49
2:H:492:LYS:NZ	2:H:516:ARG:NH1	2.59	0.49
1:A:129:THR:O	1:A:133:ILE:HG12	2.12	0.49
2:H:61:TYR:CE2	2:H:578:ARG:HG2	2.47	0.49
2:H:443:PHE:CE2	2:H:445:LEU:HD11	2.47	0.49
2:J:240:LYS:CG	2:J:267:VAL:HG21	2.40	0.49
2:L:170:LEU:HD23	2:L:170:LEU:C	2.38	0.49
2:L:289:PHE:N	2:L:290:PRO:CD	2.75	0.49
1:O:30:ALA:C	1:O:32:MET:H	2.21	0.49
1:A:134:ARG:HB2	1:A:139:ILE:O	2.12	0.49
2:D:309:ASP:HA	2:D:312:THR:HG23	1.94	0.49
2:H:326:ARG:O	2:H:327:ASN:CB	2.60	0.49
2:H:363:GLY:O	2:H:364:LEU:C	2.55	0.49
2:H:476:SER:O	2:H:477:ASP:C	2.55	0.49
1:I:141:ASN:C	1:I:141:ASN:OD1	2.55	0.49
2:J:59:LEU:HD22	2:J:61:TYR:H	1.77	0.49
2:P:80:LEU:HB2	2:P:122:MET:HE2	1.93	0.49
2:H:327:ASN:ND2	2:H:364:LEU:HD21	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:GLN:HB2	1:K:109:ASN:HB3	1.94	0.49
1:K:108:LEU:HD12	1:K:110:ILE:HD11	1.94	0.49
1:M:102:ILE:CB	2:N:20:VAL:CG2	2.90	0.49
2:N:211:ASP:O	2:N:215:ILE:HG13	2.13	0.49
2:P:404:ASN:CB	2:P:437:LYS:HD2	2.43	0.49
2:B:431:LEU:HD12	2:B:431:LEU:O	2.12	0.49
2:P:248:PHE:C	2:P:248:PHE:CD2	2.90	0.49
2:B:465:VAL:HG11	2:B:468:MET:HG3	1.94	0.49
2:D:419:ILE:O	2:D:420:THR:C	2.56	0.49
2:H:108:SER:OG	2:H:135:ALA:HB2	2.13	0.49
2:H:265:ASN:OD1	2:H:265:ASN:N	2.45	0.49
2:J:275:LEU:HD11	2:J:288:LEU:CD2	2.42	0.49
2:J:419:ILE:O	2:J:420:THR:C	2.56	0.49
2:L:349:ILE:HG13	2:L:385:VAL:HG22	1.95	0.49
2:N:419:ILE:O	2:N:420:THR:C	2.55	0.49
1:C:48:THR:HG22	1:C:51:ILE:HB	1.94	0.49
2:D:422:LEU:O	2:D:423:PRO:C	2.54	0.49
2:F:180:ASP:OD1	2:F:182:LYS:HG3	2.13	0.49
2:F:304:LEU:HD11	3:S:216:ARG:HG3	1.94	0.49
2:H:494:GLU:HB3	2:H:519:TRP:HD1	1.76	0.49
2:L:275:LEU:HD11	2:L:288:LEU:CD2	2.43	0.49
1:O:134:ARG:HB2	1:O:139:ILE:O	2.13	0.49
2:P:225:VAL:HG13	2:P:245:LEU:HD11	1.95	0.49
2:B:154:ASP:OD2	2:B:179:LYS:NZ	2.40	0.49
2:B:190:HIS:CG	2:P:112:ARG:NH1	2.80	0.49
2:B:280:MET:HE1	2:B:288:LEU:CD1	2.42	0.49
2:D:121:ARG:HH22	5:D:1103:PO4:P	2.36	0.49
2:H:232:ILE:CG2	2:H:266:LEU:HD21	2.43	0.49
1:I:46:ASN:HB2	1:I:107:TYR:CZ	2.47	0.49
2:N:432:LEU:CD1	2:N:458:ILE:HA	2.43	0.49
1:A:46:ASN:HB2	1:A:107:TYR:CE2	2.48	0.49
2:H:404:ASN:HB2	2:H:437:LYS:HZ3	1.78	0.49
2:L:444:TYR:HA	2:L:471:GLY:CA	2.33	0.49
2:N:454:GLY:O	2:N:457:TYR:HB2	2.13	0.49
2:D:444:TYR:HA	2:D:471:GLY:CA	2.30	0.49
2:F:253:LEU:HD12	2:F:280:MET:HB2	1.95	0.49
2:H:404:ASN:HA	2:H:437:LYS:HD3	1.93	0.49
2:J:89:PHE:CE1	4:J:1100:OGK:H17	2.47	0.49
2:J:419:ILE:HD11	2:J:446:ARG:HH22	1.78	0.49
2:L:221:SER:O	2:L:223:VAL:HG23	2.12	0.49
2:L:471:GLY:O	2:L:496:ARG:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:LEU:HD11	2:D:288:LEU:CD2	2.43	0.48
2:J:164:ARG:HD2	2:N:112:ARG:NE	2.28	0.48
2:J:533:MET:HE3	2:J:588:LEU:CD1	2.43	0.48
1:K:134:ARG:HB2	1:K:139:ILE:O	2.12	0.48
2:N:253:LEU:HD12	2:N:280:MET:HB2	1.94	0.48
2:N:533:MET:HE3	2:N:588:LEU:CD1	2.42	0.48
2:P:311:CYS:CB	2:P:336:VAL:HG21	2.43	0.48
1:A:52:LEU:O	1:A:56:ILE:HG13	2.12	0.48
2:F:46:LYS:HE3	2:F:46:LYS:HB2	1.49	0.48
2:F:211:ASP:O	2:F:215:ILE:HG13	2.12	0.48
2:F:590:GLU:O	2:F:591:PRO:C	2.56	0.48
2:H:519:TRP:HZ3	2:H:567:HIS:HD1	1.51	0.48
2:L:468:MET:HE1	2:L:483:PHE:HE1	1.75	0.48
2:N:159:ILE:HG13	2:N:160:VAL:N	2.28	0.48
1:E:105:ALA:HB3	1:E:114:LEU:HD13	1.95	0.48
1:E:135:THR:HG22	1:E:136:THR:N	2.27	0.48
2:F:419:ILE:CG2	2:F:422:LEU:HD13	2.43	0.48
1:G:27:GLN:HB2	1:G:109:ASN:HB3	1.94	0.48
2:H:367:GLN:CD	2:H:367:GLN:N	2.72	0.48
2:H:432:LEU:HB3	2:H:461:TYR:O	2.13	0.48
2:J:203:GLU:OE1	3:U:211:ARG:HD3	2.14	0.48
2:J:289:PHE:N	2:J:290:PRO:HD2	2.28	0.48
2:J:311:CYS:O	2:J:315:GLN:HB2	2.14	0.48
2:J:349:ILE:HG13	2:J:385:VAL:HG22	1.95	0.48
2:J:391:THR:HG23	2:J:394:SER:H	1.78	0.48
2:L:391:THR:HG23	2:L:394:SER:H	1.76	0.48
2:L:443:PHE:HE2	2:L:445:LEU:HD11	1.75	0.48
2:L:590:GLU:O	2:L:591:PRO:C	2.56	0.48
2:N:295:ILE:HG21	2:N:298:LEU:HD13	1.95	0.48
2:N:501:SER:HA	2:N:524:ARG:HB2	1.94	0.48
2:B:304:LEU:HD11	3:Q:216:ARG:HG3	1.93	0.48
2:F:453:LEU:HD11	2:F:457:TYR:OH	2.13	0.48
2:J:101:THR:CG2	2:J:128:ASP:OD1	2.53	0.48
1:A:125:ILE:HG23	1:A:133:ILE:CD1	2.36	0.48
1:E:141:ASN:C	1:E:141:ASN:OD1	2.55	0.48
2:F:240:LYS:CG	2:F:267:VAL:HG21	2.40	0.48
2:H:89:PHE:CE1	4:H:1100:OGK:H17	2.49	0.48
2:H:298:LEU:HD21	2:H:300:LEU:HD21	1.94	0.48
1:I:8:LEU:HD22	1:I:29:ILE:HD13	1.95	0.48
2:J:191:ASN:HD21	2:J:194:LEU:H	1.60	0.48
2:N:55:VAL:CG2	2:N:75:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:419:ILE:O	2:P:420:THR:C	2.56	0.48
1:A:159:PHE:O	1:A:160:GLU:CB	2.60	0.48
2:B:125:SER:N	2:B:128:ASP:OD2	2.47	0.48
2:B:367:GLN:HG2	2:B:391:THR:CB	2.43	0.48
1:C:48:THR:HG22	1:C:51:ILE:CB	2.44	0.48
1:C:102:ILE:CG2	2:D:20:VAL:HG21	2.43	0.48
2:H:125:SER:HB2	2:H:128:ASP:H	1.78	0.48
2:H:490:LEU:O	2:H:514:SER:O	2.30	0.48
1:I:27:GLN:HB2	1:I:109:ASN:HB3	1.94	0.48
2:J:247:GLU:HA	2:J:274:ARG:O	2.13	0.48
1:K:46:ASN:HB2	1:K:107:TYR:CE2	2.49	0.48
2:N:391:THR:HG23	2:N:394:SER:H	1.76	0.48
2:P:453:LEU:HD11	2:P:457:TYR:OH	2.13	0.48
1:A:30:ALA:C	1:A:32:MET:H	2.22	0.48
2:B:180:ASP:OD1	2:B:182:LYS:HG3	2.12	0.48
1:C:8:LEU:HD22	1:C:29:ILE:HD13	1.96	0.48
2:D:54:HIS:HE1	2:D:56:THR:OG1	1.96	0.48
2:D:411:VAL:HG22	2:D:444:TYR:HB3	1.95	0.48
2:D:590:GLU:O	2:D:591:PRO:C	2.56	0.48
2:H:191:ASN:ND2	2:H:194:LEU:H	2.11	0.48
2:H:212:LEU:HD23	2:H:235:LEU:CD2	2.43	0.48
2:J:398:ILE:CG2	2:J:402:LEU:HD11	2.38	0.48
2:L:125:SER:N	2:L:128:ASP:OD2	2.47	0.48
2:L:247:GLU:HA	2:L:274:ARG:O	2.14	0.48
2:L:274:ARG:HG2	2:L:297:LYS:HE3	1.95	0.48
2:B:191:ASN:ND2	2:B:194:LEU:H	2.11	0.48
2:D:380:LEU:HD13	2:D:383:MET:HE2	1.95	0.48
2:L:280:MET:HE1	2:L:288:LEU:HD11	1.95	0.48
1:M:99:PHE:HB2	2:N:15:ALA:HB3	1.94	0.48
2:B:121:ARG:NH2	5:B:1103:PO4:O4	2.47	0.48
2:B:412:LEU:HD12	2:B:412:LEU:C	2.37	0.48
2:B:590:GLU:O	2:B:591:PRO:C	2.55	0.48
1:E:32:MET:HE3	1:E:42:VAL:HB	1.96	0.48
1:E:48:THR:HG22	1:E:51:ILE:N	2.24	0.48
2:H:394:SER:O	2:H:398:ILE:HD13	2.13	0.48
2:J:429:ARG:O	2:J:433:ILE:HG13	2.14	0.48
2:J:577:GLN:HE22	2:J:589:LYS:HG2	1.79	0.48
2:L:309:ASP:HA	2:L:312:THR:HG23	1.95	0.48
2:L:577:GLN:HE22	2:L:589:LYS:HG2	1.78	0.48
1:M:108:LEU:HD12	1:M:110:ILE:HD11	1.96	0.48
2:P:391:THR:HG23	2:P:394:SER:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ILE:CG2	2:B:402:LEU:HD11	2.40	0.48
2:D:419:ILE:HD11	2:D:446:ARG:NH2	2.29	0.48
2:F:367:GLN:HG2	2:F:391:THR:CB	2.43	0.48
2:F:590:GLU:CB	2:F:591:PRO:HD2	2.40	0.48
2:H:373:LEU:HD11	2:H:380:LEU:HD11	1.96	0.48
2:H:487:CYS:HB3	2:H:490:LEU:HB2	1.94	0.48
1:I:35:ASP:HB3	2:N:243:ALA:HB1	1.95	0.48
1:K:102:ILE:HG12	1:K:117:THR:CB	2.44	0.48
2:N:247:GLU:HA	2:N:274:ARG:O	2.14	0.48
2:P:454:GLY:O	2:P:457:TYR:HB2	2.13	0.48
1:A:132:GLU:O	1:A:136:THR:HG23	2.14	0.47
2:B:422:LEU:O	2:B:423:PRO:C	2.55	0.47
1:C:27:GLN:HB2	1:C:109:ASN:HB3	1.96	0.47
1:C:91:MET:HE2	1:C:91:MET:HA	1.95	0.47
1:C:159:PHE:O	1:C:160:GLU:CB	2.61	0.47
2:D:542:ILE:HD11	2:D:588:LEU:HD12	1.95	0.47
2:F:170:LEU:C	2:F:170:LEU:HD23	2.38	0.47
2:F:280:MET:HE1	2:F:288:LEU:CD1	2.44	0.47
2:H:170:LEU:HD23	2:H:170:LEU:C	2.38	0.47
2:H:526:SER:HB2	2:H:529:GLY:HA3	1.96	0.47
2:J:46:LYS:HB2	2:J:46:LYS:HE3	1.46	0.47
1:M:99:PHE:CE2	2:N:17:VAL:N	2.82	0.47
2:N:153:THR:HG23	2:N:178:GLU:HA	1.96	0.47
1:O:48:THR:HG22	1:O:51:ILE:HB	1.96	0.47
2:B:471:GLY:O	2:B:496:ARG:O	2.32	0.47
2:F:54:HIS:HD2	2:F:77:SER:OG	1.96	0.47
2:H:166:ILE:O	2:H:193:SER:HB2	2.14	0.47
2:H:303:ALA:O	2:H:326:ARG:NH1	2.46	0.47
2:L:96:TRP:O	2:L:578:ARG:NH2	2.36	0.47
4:P:1100:OGK:H18A	4:P:1100:OGK:N08	2.29	0.47
2:B:391:THR:HG23	2:B:394:SER:H	1.79	0.47
2:F:225:VAL:HG13	2:F:245:LEU:HD11	1.96	0.47
2:F:227:VAL:CG1	2:F:228:GLY:N	2.78	0.47
2:L:541:ASN:O	2:L:570:ALA:HA	2.13	0.47
2:D:125:SER:N	2:D:128:ASP:OD2	2.46	0.47
2:D:201:MET:CE	2:D:302:TYR:CZ	2.98	0.47
2:D:270:ARG:O	1:G:107:TYR:HD1	1.97	0.47
2:D:332:ARG:O	2:D:336:VAL:HG23	2.14	0.47
2:H:96:TRP:HA	2:H:582:PRO:CG	2.45	0.47
2:H:214:THR:HA	2:H:217:ARG:HG2	1.97	0.47
2:H:268:PHE:O	2:H:269:PRO:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:153:THR:HG23	2:P:178:GLU:HA	1.97	0.47
1:A:102:ILE:HG12	1:A:117:THR:OG1	2.14	0.47
2:F:176:PHE:C	2:F:176:PHE:CD2	2.93	0.47
1:G:83:LEU:HD23	1:G:83:LEU:HA	1.78	0.47
2:H:104:VAL:HG11	2:H:128:ASP:HB2	1.96	0.47
2:H:168:THR:HB	2:H:196:VAL:CG1	2.24	0.47
2:J:81:LYS:NZ	5:J:1103:PO4:O3	2.48	0.47
2:J:164:ARG:HE	2:N:112:ARG:HG3	1.80	0.47
2:J:389:ASP:OD2	2:J:419:ILE:HG23	2.14	0.47
2:J:469:LEU:HA	2:J:494:GLU:O	2.14	0.47
1:K:102:ILE:CG1	1:K:117:THR:HB	2.44	0.47
2:L:201:MET:CE	2:L:302:TYR:CZ	2.98	0.47
2:N:440:ARG:HB3	2:N:467:TRP:CE3	2.49	0.47
2:N:482:GLU:O	2:N:485:ARG:HG2	2.14	0.47
1:A:153:ARG:HG2	1:A:157:TRP:CZ3	2.49	0.47
2:B:270:ARG:O	1:O:107:TYR:CD1	2.68	0.47
2:B:351:ARG:HD3	2:B:413:LEU:HD11	1.96	0.47
2:D:311:CYS:HB3	2:D:336:VAL:HG21	1.95	0.47
2:H:108:SER:OG	2:H:135:ALA:CB	2.62	0.47
2:H:512:LEU:HA	2:H:513:PRO:HD3	1.52	0.47
2:B:179:LYS:NZ	2:F:101:THR:HG21	2.29	0.47
2:B:590:GLU:CB	2:B:591:PRO:HD2	2.37	0.47
1:C:99:PHE:CZ	2:D:17:VAL:HG22	2.49	0.47
2:F:201:MET:HE2	2:F:302:TYR:OH	2.15	0.47
2:F:446:ARG:HG2	2:F:447:GLN:H	1.79	0.47
2:H:347:LEU:CD2	2:H:373:LEU:HD21	2.45	0.47
2:H:468:MET:HE2	2:H:470:LEU:HD21	1.96	0.47
2:J:80:LEU:HD12	2:J:122:MET:HE1	1.96	0.47
2:J:96:TRP:O	2:J:578:ARG:NH2	2.38	0.47
2:J:468:MET:HE1	2:J:483:PHE:CZ	2.49	0.47
1:M:132:GLU:O	1:M:136:THR:HG23	2.14	0.47
2:N:311:CYS:CB	2:N:336:VAL:HG21	2.44	0.47
2:P:46:LYS:HE3	2:P:46:LYS:HB2	1.47	0.47
2:P:366:SER:HB2	2:P:367:GLN:OE1	2.14	0.47
2:B:54:HIS:HD2	2:B:77:SER:OG	1.98	0.47
2:B:201:MET:HE1	2:B:302:TYR:CE2	2.49	0.47
2:B:412:LEU:C	2:B:412:LEU:CD1	2.88	0.47
2:B:429:ARG:O	2:B:433:ILE:HG13	2.15	0.47
1:E:27:GLN:HB2	1:E:109:ASN:HB3	1.96	0.47
1:G:158:ALA:HA	2:H:62:THR:HG21	1.96	0.47
2:H:403:LYS:O	2:H:404:ASN:OD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:191:ASN:ND2	2:J:194:LEU:H	2.13	0.47
2:J:297:LYS:HG3	2:J:322:VAL:HB	1.96	0.47
2:J:404:ASN:CB	2:J:437:LYS:HD2	2.45	0.47
1:K:159:PHE:O	1:K:160:GLU:CB	2.63	0.47
2:L:201:MET:HE2	2:L:302:TYR:OH	2.14	0.47
2:L:440:ARG:HB3	2:L:467:TRP:CE3	2.48	0.47
2:H:142:THR:HB	2:H:168:THR:OG1	2.15	0.47
2:H:199:PHE:CE1	2:H:227:VAL:HG22	2.49	0.47
1:I:32:MET:HE3	1:I:42:VAL:HB	1.97	0.47
1:I:135:THR:HG22	1:I:136:THR:N	2.30	0.47
2:N:411:VAL:HG22	2:N:444:TYR:HB3	1.96	0.47
2:N:590:GLU:O	2:N:591:PRO:C	2.58	0.47
2:B:85:ARG:HD2	5:B:1101:PO4:O2	2.15	0.47
2:B:217:ARG:NH1	2:P:50:GLU:OE2	2.47	0.47
2:F:113:GLN:NE2	2:L:192:THR:HG21	2.30	0.47
2:F:191:ASN:ND2	2:F:194:LEU:H	2.12	0.47
2:F:227:VAL:HG13	2:F:228:GLY:N	2.30	0.47
2:F:274:ARG:HG2	2:F:297:LYS:HE3	1.97	0.47
2:H:120:ARG:NH2	5:H:1103:PO4:O2	2.48	0.47
2:H:170:LEU:HA	2:H:198:ASN:O	2.14	0.47
2:H:286:PRO:HA	2:H:289:PHE:CD2	2.50	0.47
2:H:548:ARG:HE	2:H:548:ARG:HB3	1.50	0.47
2:L:46:LYS:HB2	2:L:46:LYS:HE3	1.53	0.47
2:N:40:VAL:O	2:N:41:CYS:HB3	2.14	0.47
2:N:101:THR:CG2	2:N:128:ASP:OD1	2.58	0.47
2:P:482:GLU:O	2:P:485:ARG:HG2	2.15	0.47
1:A:48:THR:HG22	1:A:51:ILE:HB	1.96	0.46
2:D:211:ASP:O	2:D:215:ILE:HG13	2.15	0.46
2:H:285:MET:N	2:H:286:PRO:CD	2.78	0.46
2:J:54:HIS:HD2	2:J:77:SER:OG	1.98	0.46
2:D:165:LYS:NZ	2:H:139:ASP:OD1	2.38	0.46
2:D:192:THR:HB	2:H:113:GLN:NE2	2.30	0.46
2:F:96:TRP:O	2:F:578:ARG:NH2	2.34	0.46
2:F:366:SER:HB2	2:F:367:GLN:OE1	2.15	0.46
2:L:101:THR:CG2	2:L:128:ASP:OD1	2.58	0.46
2:N:201:MET:HE2	2:N:302:TYR:OH	2.16	0.46
2:N:543:GLU:OE2	2:N:578:ARG:HD3	2.15	0.46
2:P:191:ASN:HD21	2:P:194:LEU:H	1.63	0.46
2:P:289:PHE:N	2:P:290:PRO:HD2	2.30	0.46
1:A:101:LEU:HB3	1:A:117:THR:HG21	1.95	0.46
2:F:284:GLU:O	2:F:287:ILE:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:308:GLU:HG3	2:F:332:ARG:NH2	2.30	0.46
2:H:262:LYS:HD3	2:H:263:TYR:CZ	2.51	0.46
2:H:327:ASN:HD22	2:H:364:LEU:CD2	2.28	0.46
2:H:429:ARG:HD2	2:H:457:TYR:CD2	2.50	0.46
2:H:440:ARG:CB	2:H:467:TRP:HD1	2.28	0.46
2:J:184:LEU:HD12	2:J:207:ILE:HB	1.97	0.46
2:J:225:VAL:HG13	2:J:245:LEU:HD11	1.96	0.46
2:J:590:GLU:O	2:J:591:PRO:C	2.59	0.46
2:L:289:PHE:N	2:L:290:PRO:HD2	2.29	0.46
2:N:310:HIS:HE1	2:N:325:THR:OG1	1.99	0.46
2:P:468:MET:HE1	2:P:483:PHE:CZ	2.51	0.46
2:B:419:ILE:HD11	2:B:446:ARG:HH22	1.78	0.46
2:H:55:VAL:HG23	2:H:75:LEU:HD21	1.97	0.46
2:H:390:ILE:HD12	2:H:410:LEU:CD2	2.38	0.46
2:H:414:ASP:HB3	2:H:446:ARG:HH21	1.81	0.46
2:H:455:LEU:HD23	2:H:455:LEU:HA	1.65	0.46
1:I:111:LYS:O	1:I:115:ASP:CB	2.62	0.46
2:J:176:PHE:C	2:J:176:PHE:CD2	2.94	0.46
2:J:289:PHE:CD1	2:J:316:LYS:HD2	2.50	0.46
2:J:335:GLU:O	2:J:338:ALA:HB3	2.15	0.46
2:L:121:ARG:HH22	5:L:1103:PO4:P	2.39	0.46
2:L:311:CYS:O	2:L:315:GLN:HB2	2.16	0.46
2:N:46:LYS:HB2	2:N:46:LYS:HE3	1.47	0.46
1:O:132:GLU:O	1:O:136:THR:HG23	2.15	0.46
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.85	0.46
1:A:141:ASN:C	1:A:141:ASN:OD1	2.58	0.46
2:B:503:ARG:NH1	2:B:503:ARG:HB3	2.31	0.46
2:D:311:CYS:O	2:D:315:GLN:HB2	2.15	0.46
2:F:289:PHE:CD1	2:F:316:LYS:HD2	2.50	0.46
2:F:465:VAL:HG11	2:F:468:MET:HG3	1.98	0.46
2:H:220:ARG:HD2	2:H:220:ARG:HA	1.67	0.46
2:L:310:HIS:HE1	2:L:325:THR:OG1	1.98	0.46
2:P:289:PHE:CD1	2:P:316:LYS:HD2	2.51	0.46
2:P:409:ARG:HB3	2:P:442:ALA:HB3	1.97	0.46
2:P:432:LEU:CD1	2:P:458:ILE:HA	2.46	0.46
2:B:446:ARG:HG2	2:B:447:GLN:H	1.79	0.46
2:D:468:MET:HE1	2:D:483:PHE:CZ	2.50	0.46
2:F:289:PHE:N	2:F:290:PRO:HD2	2.31	0.46
2:H:32:LYS:HD3	2:H:32:LYS:HA	1.47	0.46
2:H:532:LEU:O	2:H:535:MET:HB3	2.15	0.46
1:I:30:ALA:C	1:I:32:MET:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:272:LEU:HD23	2:L:272:LEU:HA	1.71	0.46
1:M:35:ASP:O	1:M:36:ASP:C	2.59	0.46
2:P:176:PHE:C	2:P:176:PHE:CD2	2.94	0.46
2:D:274:ARG:HG2	2:D:297:LYS:HE3	1.97	0.46
2:D:402:LEU:HD12	2:D:402:LEU:O	2.16	0.46
2:F:429:ARG:O	2:F:433:ILE:HG13	2.16	0.46
1:G:48:THR:HG22	1:G:51:ILE:HB	1.98	0.46
2:H:109:ASN:C	2:H:110:ASN:ND2	2.74	0.46
2:H:216:ALA:HB2	2:H:238:PHE:CD1	2.50	0.46
2:J:409:ARG:HB2	4:J:1100:OGK:H16B	1.96	0.46
2:L:85:ARG:NH2	4:L:1100:OGK:O07	2.40	0.46
2:L:176:PHE:CZ	2:L:204:PHE:CZ	3.04	0.46
2:L:248:PHE:C	2:L:248:PHE:CD2	2.94	0.46
2:L:272:LEU:HD13	2:L:275:LEU:HD13	1.97	0.46
2:P:201:MET:HE2	2:P:302:TYR:OH	2.16	0.46
2:P:331:ASP:OD1	2:P:369:GLY:N	2.47	0.46
2:B:453:LEU:HD11	2:B:457:TYR:OH	2.16	0.46
2:D:176:PHE:C	2:D:176:PHE:CD2	2.94	0.46
2:J:180:ASP:OD1	2:J:182:LYS:HG3	2.15	0.46
2:J:284:GLU:O	2:J:287:ILE:HG23	2.15	0.46
2:L:412:LEU:HD12	2:L:412:LEU:C	2.39	0.46
2:L:441:PHE:O	2:L:468:MET:HA	2.15	0.46
2:N:289:PHE:CD1	2:N:316:LYS:HD2	2.51	0.46
1:O:26:SER:OG	1:O:108:LEU:HB3	2.15	0.46
2:B:101:THR:CG2	2:B:128:ASP:OD1	2.58	0.46
2:F:203:GLU:OE1	3:S:211:ARG:HD3	2.16	0.46
2:F:454:GLY:O	2:F:457:TYR:HB2	2.16	0.46
2:H:362:GLU:O	2:H:364:LEU:N	2.49	0.46
1:K:153:ARG:HG2	1:K:157:TRP:CZ3	2.51	0.46
2:L:117:VAL:HG11	2:L:119:PHE:CZ	2.51	0.46
2:L:197:LEU:O	2:L:225:VAL:HA	2.15	0.46
2:L:530:GLN:HE21	2:L:592:ILE:HD11	1.81	0.46
2:N:65:PRO:HA	2:N:103:TRP:CZ3	2.50	0.46
2:N:541:ASN:O	2:N:570:ALA:HA	2.16	0.46
2:P:191:ASN:ND2	2:P:194:LEU:H	2.14	0.46
2:B:270:ARG:O	1:O:107:TYR:HD1	1.98	0.46
2:D:253:LEU:HD12	2:D:280:MET:HB2	1.97	0.46
2:H:105:THR:HG22	2:H:106:GLU:N	2.31	0.46
2:H:258:GLY:O	2:H:260:PRO:HD2	2.16	0.46
1:I:46:ASN:HB2	1:I:107:TYR:CE2	2.51	0.46
2:J:590:GLU:CB	2:J:591:PRO:HD2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:65:PRO:HA	2:L:103:TRP:CZ3	2.51	0.46
2:N:503:ARG:HB3	2:N:503:ARG:NH1	2.30	0.46
2:D:305:LEU:O	2:D:305:LEU:HD23	2.16	0.45
1:E:46:ASN:HB2	1:E:107:TYR:CZ	2.51	0.45
2:F:311:CYS:O	2:F:315:GLN:HB2	2.16	0.45
1:G:35:ASP:O	1:G:36:ASP:C	2.59	0.45
2:H:440:ARG:HB3	2:H:467:TRP:HD1	1.81	0.45
2:H:441:PHE:O	2:H:468:MET:HA	2.15	0.45
2:H:509:VAL:HG21	2:H:535:MET:SD	2.56	0.45
2:H:546:PRO:HD2	2:H:584:THR:O	2.16	0.45
2:J:380:LEU:HD13	2:J:383:MET:HE2	1.97	0.45
2:N:16:THR:HG22	2:N:17:VAL:H	1.81	0.45
2:P:117:VAL:HG11	2:P:119:PHE:CZ	2.50	0.45
2:B:543:GLU:OE2	2:B:578:ARG:CD	2.65	0.45
2:F:391:THR:HG23	2:F:394:SER:H	1.81	0.45
2:H:253:LEU:HD12	2:H:280:MET:HA	1.98	0.45
2:H:291:PHE:O	2:H:294:GLN:HB3	2.16	0.45
2:H:334:LEU:HD22	2:H:373:LEU:HD22	1.99	0.45
2:J:405:LEU:HD13	2:J:408:PHE:HB2	1.96	0.45
2:J:501:SER:HA	2:J:524:ARG:HB2	1.99	0.45
2:N:532:LEU:HD23	2:N:532:LEU:HA	1.72	0.45
1:O:8:LEU:HD22	1:O:29:ILE:HD13	1.98	0.45
1:O:98:LEU:HD11	1:O:117:THR:HB	1.98	0.45
2:P:197:LEU:O	2:P:225:VAL:HA	2.16	0.45
2:P:338:ALA:O	2:P:376:GLY:HA3	2.16	0.45
2:B:247:GLU:HA	2:B:274:ARG:O	2.16	0.45
2:B:532:LEU:HD23	2:B:532:LEU:HA	1.76	0.45
1:C:108:LEU:HD12	1:C:110:ILE:HD11	1.98	0.45
2:D:59:LEU:HD22	2:D:61:TYR:H	1.80	0.45
2:D:65:PRO:HA	2:D:103:TRP:CZ3	2.51	0.45
1:E:8:LEU:HD22	1:E:29:ILE:HD13	1.98	0.45
2:H:519:TRP:CZ3	2:H:567:HIS:ND1	2.71	0.45
1:I:48:THR:HG22	1:I:51:ILE:N	2.23	0.45
1:I:102:ILE:HG12	1:I:117:THR:CB	2.47	0.45
1:K:132:GLU:O	1:K:136:THR:HG23	2.15	0.45
2:L:366:SER:HB2	2:L:367:GLN:OE1	2.16	0.45
2:N:274:ARG:HG2	2:N:297:LYS:HE3	1.99	0.45
1:A:27:GLN:HB2	1:A:109:ASN:HB3	1.97	0.45
1:G:158:ALA:HB2	2:H:62:THR:HG23	1.98	0.45
2:H:255:GLU:HB3	2:H:263:TYR:HE1	1.81	0.45
2:L:191:ASN:ND2	2:L:194:LEU:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:468:MET:HE1	2:L:483:PHE:CZ	2.51	0.45
1:M:102:ILE:HD13	2:N:20:VAL:CG2	2.46	0.45
2:N:441:PHE:O	2:N:468:MET:HA	2.17	0.45
2:N:444:TYR:HA	2:N:471:GLY:CA	2.32	0.45
2:P:361:GLU:HG3	2:P:361:GLU:O	2.15	0.45
2:P:399:GLY:O	2:P:434:GLY:HA3	2.16	0.45
2:P:419:ILE:HG21	2:P:422:LEU:HD13	1.97	0.45
2:P:590:GLU:O	2:P:591:PRO:C	2.59	0.45
1:A:8:LEU:HD22	1:A:29:ILE:HD13	1.98	0.45
1:E:35:ASP:O	1:E:36:ASP:C	2.59	0.45
1:G:48:THR:HG22	1:G:51:ILE:CB	2.46	0.45
1:G:108:LEU:HD12	1:G:110:ILE:HD11	1.98	0.45
2:H:259:MET:HB2	2:H:262:LYS:HB2	1.99	0.45
2:J:305:LEU:HD23	2:J:305:LEU:O	2.17	0.45
2:P:289:PHE:N	2:P:290:PRO:CD	2.78	0.45
1:A:26:SER:OG	1:A:108:LEU:HB3	2.16	0.45
1:A:98:LEU:HD21	1:A:120:THR:CG2	2.43	0.45
2:B:419:ILE:HG21	2:B:422:LEU:HD13	1.98	0.45
2:D:46:LYS:HB2	2:D:46:LYS:HE3	1.49	0.45
2:J:270:ARG:HB3	1:M:46:ASN:OD1	2.16	0.45
1:K:135:THR:HG22	1:K:136:THR:N	2.30	0.45
2:L:533:MET:HE3	2:L:588:LEU:CD2	2.44	0.45
2:N:308:GLU:HG3	2:N:332:ARG:NH2	2.32	0.45
2:N:366:SER:HB2	2:N:367:GLN:OE1	2.17	0.45
1:O:48:THR:HG22	1:O:51:ILE:CB	2.47	0.45
1:A:44:LEU:HD12	1:A:44:LEU:O	2.17	0.45
2:B:57:MET:HE3	2:B:62:THR:HG22	1.98	0.45
2:B:176:PHE:CZ	2:B:204:PHE:CZ	3.04	0.45
2:D:482:GLU:O	2:D:485:ARG:HG2	2.17	0.45
2:D:533:MET:HE3	2:D:588:LEU:CD2	2.45	0.45
2:H:120:ARG:HH11	2:H:147:LYS:HZ3	1.63	0.45
2:H:291:PHE:N	2:H:291:PHE:CD2	2.84	0.45
1:M:134:ARG:CZ	1:M:141:ASN:HB2	2.47	0.45
2:N:81:LYS:NZ	5:N:1103:PO4:O3	2.35	0.45
2:N:117:VAL:HG11	2:N:119:PHE:CZ	2.52	0.45
2:N:197:LEU:O	2:N:225:VAL:HA	2.16	0.45
2:N:432:LEU:HB3	2:N:461:TYR:O	2.17	0.45
2:P:80:LEU:HD12	2:P:122:MET:HE1	1.99	0.45
2:P:344:LEU:HD12	2:P:344:LEU:HA	1.83	0.45
2:P:441:PHE:O	2:P:468:MET:HA	2.17	0.45
2:D:136:ARG:HH11	2:D:136:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:MET:HE2	2:D:302:TYR:CZ	2.52	0.45
2:H:259:MET:O	2:H:261:GLU:N	2.49	0.45
2:H:508:ALA:O	2:H:509:VAL:C	2.60	0.45
1:I:134:ARG:HB2	1:I:139:ILE:O	2.17	0.45
2:J:412:LEU:HD12	2:J:412:LEU:C	2.41	0.45
1:M:87:ASP:CG	1:M:116:LEU:HD22	2.41	0.45
2:N:32:LYS:HD2	2:N:32:LYS:HA	1.89	0.45
1:O:137:PHE:CD1	2:P:17:VAL:HG21	2.52	0.45
2:D:296:ARG:NH1	1:G:35:ASP:OD1	2.45	0.45
2:D:301:LEU:CD2	2:D:324:GLU:HB3	2.47	0.45
2:H:280:MET:HE1	2:H:288:LEU:HD11	1.98	0.45
2:H:304:LEU:HD22	2:H:304:LEU:HA	1.79	0.45
2:H:326:ARG:O	2:H:327:ASN:HB3	2.17	0.45
2:H:494:GLU:HB3	2:H:519:TRP:CD1	2.51	0.45
1:K:8:LEU:HD22	1:K:29:ILE:HD13	1.98	0.45
2:L:301:LEU:CD2	2:L:324:GLU:HB3	2.47	0.45
2:L:432:LEU:HB3	2:L:461:TYR:O	2.17	0.45
2:P:245:LEU:HD12	2:P:245:LEU:HA	1.86	0.45
1:C:134:ARG:HB2	1:C:139:ILE:O	2.17	0.45
2:D:272:LEU:HD23	2:D:272:LEU:HA	1.72	0.45
2:D:404:ASN:CB	2:D:437:LYS:HD2	2.46	0.45
2:D:441:PHE:O	2:D:468:MET:HA	2.17	0.45
1:E:114:LEU:O	1:E:118:CYS:HB2	2.17	0.45
1:E:132:GLU:O	1:E:136:THR:HG23	2.16	0.45
2:H:269:PRO:C	2:H:271:LYS:H	2.25	0.45
2:H:339:GLN:HG3	2:H:340:TYR:CD1	2.52	0.45
2:H:349:ILE:HD12	2:H:385:VAL:HG23	1.98	0.45
2:H:373:LEU:HD12	2:H:373:LEU:C	2.42	0.45
2:H:414:ASP:OD2	2:H:418:ARG:NH2	2.50	0.45
1:I:112:ASN:OD1	1:I:112:ASN:N	2.50	0.45
2:L:367:GLN:HG2	2:L:391:THR:CG2	2.47	0.45
2:L:384:ALA:HB1	4:L:1100:OGK:C16	2.46	0.45
2:L:422:LEU:O	2:L:423:PRO:C	2.58	0.45
1:M:126:LYS:HZ3	2:N:29:THR:H	1.65	0.45
2:N:63:ALA:HB1	2:N:67:ARG:HD2	1.99	0.45
2:N:349:ILE:HG13	2:N:385:VAL:HG22	1.98	0.45
1:O:102:ILE:HD12	2:P:20:VAL:CG2	2.47	0.45
1:O:108:LEU:HD12	1:O:110:ILE:HD11	1.99	0.45
2:P:272:LEU:HD13	2:P:275:LEU:HD13	1.97	0.45
2:P:503:ARG:HB3	2:P:503:ARG:NH1	2.31	0.45
2:B:117:VAL:HG11	2:B:119:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:VAL:CG2	4:B:1100:OGK:H14	2.47	0.44
2:B:441:PHE:O	2:B:468:MET:HA	2.17	0.44
1:C:158:ALA:HA	2:D:62:THR:HG23	1.99	0.44
2:D:390:ILE:HD13	2:D:424:LEU:HD11	1.99	0.44
2:H:85:ARG:NH1	5:H:1101:PO4:O2	2.50	0.44
2:H:259:MET:C	2:H:261:GLU:N	2.74	0.44
4:J:1100:OGK:HN08	4:J:1100:OGK:C18	2.30	0.44
2:L:432:LEU:CD1	2:L:458:ILE:HA	2.47	0.44
1:M:8:LEU:HD22	1:M:29:ILE:HD13	1.98	0.44
2:P:546:PRO:HD2	2:P:584:THR:O	2.17	0.44
2:D:367:GLN:HG2	2:D:391:THR:CG2	2.46	0.44
2:D:454:GLY:O	2:D:457:TYR:HB2	2.17	0.44
1:G:48:THR:HG22	1:G:51:ILE:HG12	2.00	0.44
1:G:137:PHE:HB3	2:H:17:VAL:CG2	2.47	0.44
2:H:159:ILE:C	2:H:159:ILE:HD12	2.42	0.44
2:H:236:VAL:HG12	2:H:240:LYS:HE3	1.99	0.44
2:H:348:ARG:HA	2:H:384:ALA:O	2.17	0.44
2:H:383:MET:HE1	2:H:398:ILE:HG13	2.00	0.44
2:H:402:LEU:C	2:H:403:LYS:O	2.55	0.44
1:K:48:THR:HG22	1:K:51:ILE:N	2.24	0.44
2:L:501:SER:HA	2:L:524:ARG:HB2	2.00	0.44
2:L:503:ARG:NH1	2:L:503:ARG:HB3	2.32	0.44
2:P:298:LEU:HB2	2:P:320:LEU:HD11	1.99	0.44
2:B:85:ARG:NH2	4:B:1100:OGK:O07	2.39	0.44
2:B:361:GLU:O	2:B:361:GLU:HG3	2.18	0.44
2:F:501:SER:HA	2:F:524:ARG:HB2	2.00	0.44
2:H:366:SER:HB3	2:H:369:GLY:H	1.81	0.44
2:H:443:PHE:O	2:H:471:GLY:N	2.50	0.44
2:H:531:ASP:O	2:H:534:GLN:HG2	2.17	0.44
2:L:154:ASP:OD2	2:L:179:LYS:NZ	2.41	0.44
2:L:419:ILE:HD11	2:L:446:ARG:HH22	1.81	0.44
2:N:201:MET:CE	2:N:302:TYR:CZ	3.00	0.44
1:O:91:MET:HE2	1:O:91:MET:HA	2.00	0.44
2:P:211:ASP:HA	2:P:214:THR:HG23	2.00	0.44
2:P:284:GLU:O	2:P:287:ILE:HG23	2.16	0.44
1:A:108:LEU:HD12	1:A:110:ILE:HD11	1.99	0.44
2:B:121:ARG:HH22	5:B:1103:PO4:P	2.40	0.44
2:D:310:HIS:HE1	2:D:325:THR:OG1	2.00	0.44
2:D:391:THR:HG23	2:D:394:SER:H	1.82	0.44
2:F:444:TYR:HA	2:F:471:GLY:CA	2.36	0.44
1:G:26:SER:OG	1:G:108:LEU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:ILE:O	2:H:51:THR:HG23	2.17	0.44
1:I:132:GLU:O	1:I:136:THR:HG23	2.17	0.44
2:L:351:ARG:HD3	2:L:413:LEU:HD11	1.98	0.44
1:M:48:THR:HG22	1:M:51:ILE:N	2.28	0.44
2:B:253:LEU:HD12	2:B:280:MET:HB2	1.99	0.44
2:B:274:ARG:HG2	2:B:297:LYS:HE3	1.98	0.44
1:C:132:GLU:O	1:C:136:THR:HG23	2.17	0.44
2:F:503:ARG:HB3	2:F:503:ARG:NH1	2.33	0.44
2:H:467:TRP:CZ3	2:H:494:GLU:OE1	2.68	0.44
2:J:428:VAL:HG22	2:J:443:PHE:CZ	2.52	0.44
2:L:143:LEU:CD2	2:L:159:ILE:HD13	2.47	0.44
2:N:59:LEU:HD22	2:N:61:TYR:H	1.82	0.44
2:N:289:PHE:N	2:N:290:PRO:CD	2.81	0.44
2:N:546:PRO:HD2	2:N:584:THR:O	2.18	0.44
2:P:310:HIS:HE1	2:P:325:THR:OG1	2.01	0.44
2:B:159:ILE:HG13	2:B:160:VAL:N	2.32	0.44
2:B:309:ASP:HA	2:B:312:THR:HG23	1.99	0.44
2:B:533:MET:HE3	2:B:588:LEU:CD1	2.45	0.44
2:D:85:ARG:HD2	5:D:1101:PO4:O2	2.18	0.44
2:D:191:ASN:ND2	2:D:194:LEU:HB2	2.32	0.44
2:D:428:VAL:HG22	2:D:443:PHE:CZ	2.52	0.44
1:E:30:ALA:C	1:E:32:MET:N	2.75	0.44
1:G:128:LYS:HE3	1:G:136:THR:HG21	1.99	0.44
2:H:277:LEU:O	2:H:278:SER:C	2.60	0.44
2:L:496:ARG:HB2	2:L:521:GLN:HB3	2.00	0.44
1:O:113:LEU:O	1:O:113:LEU:CG	2.65	0.44
1:O:114:LEU:O	1:O:118:CYS:HB2	2.17	0.44
2:P:512:LEU:HA	2:P:513:PRO:HD2	1.83	0.44
2:B:419:ILE:HD11	2:B:446:ARG:NH2	2.33	0.44
1:C:102:ILE:HG12	1:C:117:THR:HB	1.98	0.44
2:D:284:GLU:O	2:D:287:ILE:HG23	2.18	0.44
2:H:194:LEU:HA	2:H:194:LEU:HD12	1.61	0.44
2:J:201:MET:HE2	2:J:302:TYR:OH	2.17	0.44
2:J:227:VAL:HG13	2:J:228:GLY:N	2.32	0.44
1:M:99:PHE:HB2	2:N:15:ALA:CB	2.48	0.44
2:N:154:ASP:OD2	2:N:179:LYS:NZ	2.46	0.44
2:B:545:ILE:HG12	2:B:585:VAL:HG22	2.00	0.44
1:C:125:ILE:HG23	1:C:133:ILE:CD1	2.33	0.44
2:D:125:SER:O	2:D:129:LEU:HD22	2.18	0.44
2:D:201:MET:HE3	3:R:208:SER:HB2	1.99	0.44
2:D:203:GLU:H	2:D:203:GLU:HG2	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:405:LEU:HD13	2:F:408:PHE:HB2	1.99	0.44
2:F:543:GLU:OE2	2:F:578:ARG:CD	2.66	0.44
2:J:308:GLU:HG3	2:J:332:ARG:NH2	2.32	0.44
1:K:83:LEU:HA	1:K:83:LEU:HD23	1.84	0.44
1:K:125:ILE:HG23	1:K:133:ILE:CD1	2.38	0.44
2:L:311:CYS:CB	2:L:336:VAL:HG21	2.48	0.44
1:M:102:ILE:HD13	2:N:20:VAL:HG22	2.00	0.44
2:N:80:LEU:HD12	2:N:122:MET:HE1	2.00	0.44
2:N:248:PHE:C	2:N:248:PHE:CD2	2.96	0.44
1:O:46:ASN:HB2	1:O:107:TYR:CZ	2.53	0.44
1:O:141:ASN:C	1:O:141:ASN:OD1	2.59	0.44
2:P:201:MET:CE	2:P:302:TYR:CZ	3.00	0.44
2:P:251:GLY:O	2:P:278:SER:HB2	2.18	0.44
2:P:419:ILE:CG2	2:P:422:LEU:HD13	2.48	0.44
2:D:227:VAL:CG1	2:D:228:GLY:N	2.80	0.44
2:D:512:LEU:HA	2:D:513:PRO:HD2	1.88	0.44
2:F:32:LYS:HD2	2:F:32:LYS:HA	1.85	0.44
2:F:133:ALA:HB2	2:F:159:ILE:HG22	2.00	0.44
2:F:194:LEU:HD12	2:F:194:LEU:HA	1.84	0.44
2:F:412:LEU:HD12	2:F:412:LEU:C	2.40	0.44
2:F:428:VAL:HG22	2:F:443:PHE:CZ	2.53	0.44
1:G:10:SER:OG	1:G:11:SER:N	2.49	0.44
2:J:138:ASP:OD2	2:J:164:ARG:HG3	2.18	0.44
2:J:192:THR:HG21	2:N:113:GLN:NE2	2.33	0.44
2:J:285:MET:HB3	2:J:286:PRO:HD3	2.00	0.44
2:J:327:ASN:HD22	2:J:328:VAL:N	2.16	0.44
1:K:48:THR:HG22	1:K:51:ILE:HB	1.99	0.44
1:M:91:MET:HE2	1:M:91:MET:HA	2.00	0.44
1:M:128:LYS:HB2	1:M:133:ILE:CD1	2.47	0.44
2:B:390:ILE:HD13	2:B:424:LEU:HD11	1.99	0.43
2:D:184:LEU:HD12	2:D:207:ILE:HB	2.00	0.43
2:D:453:LEU:HD11	2:D:457:TYR:OH	2.18	0.43
2:D:503:ARG:NH1	2:D:503:ARG:HB3	2.33	0.43
2:F:159:ILE:HG13	2:F:160:VAL:N	2.32	0.43
2:H:125:SER:CB	2:H:128:ASP:H	2.31	0.43
2:J:402:LEU:HD13	2:J:405:LEU:HG	2.00	0.43
2:J:402:LEU:C	2:J:403:LYS:O	2.58	0.43
2:N:272:LEU:HD23	2:N:272:LEU:HA	1.77	0.43
1:O:35:ASP:O	1:O:36:ASP:C	2.61	0.43
1:C:58:TYR:CE1	1:C:62:HIS:CE1	3.06	0.43
2:F:201:MET:CE	2:F:302:TYR:CZ	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:404:ASN:CA	2:F:437:LYS:HD2	2.48	0.43
2:F:412:LEU:C	2:F:412:LEU:CD1	2.91	0.43
2:F:422:LEU:O	2:F:424:LEU:HG	2.18	0.43
1:G:46:ASN:HB2	1:G:107:TYR:CZ	2.53	0.43
2:H:92:ILE:HD12	2:H:92:ILE:HG23	1.65	0.43
2:H:365:VAL:CG1	2:H:387:VAL:CG2	2.96	0.43
1:I:44:LEU:HD12	1:I:44:LEU:O	2.19	0.43
1:I:83:LEU:HD23	1:I:83:LEU:HA	1.80	0.43
2:J:272:LEU:HD13	2:J:275:LEU:HD13	2.00	0.43
2:L:101:THR:HG21	2:P:179:LYS:NZ	2.34	0.43
2:N:210:LYS:O	2:N:214:THR:CG2	2.66	0.43
2:N:301:LEU:HD13	2:N:301:LEU:HA	1.76	0.43
2:P:247:GLU:HA	2:P:274:ARG:O	2.17	0.43
2:B:402:LEU:O	2:B:402:LEU:HD12	2.19	0.43
2:D:191:ASN:ND2	2:D:194:LEU:H	2.16	0.43
2:D:351:ARG:HD3	2:D:413:LEU:HD11	2.00	0.43
2:D:419:ILE:HG21	2:D:422:LEU:HD13	2.01	0.43
2:D:422:LEU:O	2:D:424:LEU:HG	2.18	0.43
2:F:245:LEU:HD12	2:F:245:LEU:HA	1.83	0.43
2:F:441:PHE:O	2:F:468:MET:HA	2.18	0.43
2:J:227:VAL:CG1	2:J:228:GLY:N	2.81	0.43
2:L:32:LYS:HD2	2:L:32:LYS:HA	1.85	0.43
2:L:80:LEU:CD1	2:L:122:MET:HE1	2.48	0.43
2:L:338:ALA:O	2:L:376:GLY:HA3	2.17	0.43
2:L:519:TRP:HE1	4:L:1100:OGK:H01	1.82	0.43
2:N:289:PHE:HB2	2:N:290:PRO:HD3	1.99	0.43
1:O:91:MET:HE1	1:O:117:THR:HG22	2.00	0.43
2:P:96:TRP:O	2:P:578:ARG:NH2	2.35	0.43
2:P:422:LEU:O	2:P:423:PRO:C	2.59	0.43
2:P:428:VAL:HG22	2:P:443:PHE:CZ	2.53	0.43
2:D:240:LYS:CG	2:D:267:VAL:HG21	2.45	0.43
2:F:272:LEU:HD13	2:F:275:LEU:HD13	2.01	0.43
2:F:285:MET:HB3	2:F:286:PRO:HD3	2.00	0.43
2:H:57:MET:HB2	2:H:80:LEU:HD23	2.00	0.43
2:H:77:SER:HB3	2:H:116:SER:HB3	1.99	0.43
2:H:79:LYS:HG3	2:H:118:HIS:CD2	2.54	0.43
2:H:107:ILE:HG12	2:H:114:LEU:CD2	2.48	0.43
2:H:298:LEU:HD22	2:H:300:LEU:HD21	2.00	0.43
2:H:404:ASN:HB2	2:H:437:LYS:NZ	2.33	0.43
2:J:327:ASN:HD22	2:J:327:ASN:C	2.25	0.43
2:J:419:ILE:HD11	2:J:446:ARG:NH2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:432:LEU:CD1	2:J:458:ILE:HA	2.48	0.43
2:J:482:GLU:O	2:J:485:ARG:HG2	2.18	0.43
2:J:527:MET:O	2:J:528:THR:C	2.61	0.43
2:L:527:MET:O	2:L:528:THR:C	2.61	0.43
2:N:389:ASP:OD2	2:N:419:ILE:HG23	2.17	0.43
2:B:136:ARG:HG3	2:B:136:ARG:HH11	1.82	0.43
2:B:184:LEU:HD12	2:B:207:ILE:HB	1.99	0.43
2:D:80:LEU:CD1	2:D:122:MET:HE1	2.48	0.43
2:D:405:LEU:HD13	2:D:408:PHE:HB2	2.01	0.43
2:D:496:ARG:HB2	2:D:521:GLN:HB3	1.99	0.43
1:E:159:PHE:O	1:E:160:GLU:CB	2.66	0.43
2:F:65:PRO:HA	2:F:103:TRP:CZ3	2.53	0.43
2:F:114:LEU:HD12	2:F:114:LEU:HA	1.80	0.43
2:F:405:LEU:HD23	2:F:405:LEU:HA	1.88	0.43
2:F:436:LYS:HE2	2:F:436:LYS:HB3	1.84	0.43
2:F:440:ARG:HB3	2:F:467:TRP:CE3	2.53	0.43
1:G:158:ALA:CB	2:H:62:THR:HG23	2.49	0.43
2:J:272:LEU:HD23	2:J:272:LEU:HA	1.78	0.43
2:L:482:GLU:O	2:L:485:ARG:HG2	2.18	0.43
2:N:436:LYS:HE2	2:N:436:LYS:HB3	1.87	0.43
2:P:240:LYS:CG	2:P:267:VAL:HG21	2.44	0.43
2:B:119:PHE:CD1	2:B:122:MET:HE3	2.54	0.43
2:B:399:GLY:O	2:B:434:GLY:HA3	2.18	0.43
2:D:159:ILE:HG13	2:D:160:VAL:N	2.32	0.43
2:D:179:LYS:NZ	2:N:101:THR:HG21	2.34	0.43
1:E:128:LYS:HB2	1:E:133:ILE:CD1	2.49	0.43
2:F:54:HIS:HE1	2:F:56:THR:OG1	2.00	0.43
2:F:80:LEU:O	2:F:122:MET:HE2	2.18	0.43
2:F:121:ARG:HH22	5:F:1103:PO4:P	2.41	0.43
2:F:361:GLU:HG3	2:F:361:GLU:O	2.18	0.43
2:H:136:ARG:HG3	2:H:136:ARG:NH1	2.34	0.43
2:H:274:ARG:HG3	2:H:297:LYS:HB3	2.00	0.43
2:H:422:LEU:CD1	2:H:422:LEU:H	2.28	0.43
1:I:35:ASP:O	1:I:36:ASP:C	2.61	0.43
2:L:227:VAL:HG13	2:L:228:GLY:N	2.33	0.43
2:L:404:ASN:CB	2:L:437:LYS:HD2	2.49	0.43
2:L:419:ILE:CG2	2:L:422:LEU:HD13	2.48	0.43
2:L:532:LEU:HA	2:L:532:LEU:HD23	1.74	0.43
1:M:141:ASN:OD1	1:M:141:ASN:C	2.62	0.43
2:N:80:LEU:HB2	2:N:122:MET:HE2	1.97	0.43
2:N:419:ILE:HD11	2:N:446:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:532:LEU:HD22	2:P:535:MET:HE2	2.00	0.43
1:A:135:THR:HG22	1:A:136:THR:N	2.33	0.43
2:B:272:LEU:HA	2:B:272:LEU:HD23	1.72	0.43
1:G:160:GLU:CG	2:H:52:ARG:HH21	2.32	0.43
2:H:284:GLU:O	2:H:287:ILE:HD13	2.18	0.43
2:H:361:GLU:C	2:H:362:GLU:HG2	2.43	0.43
2:J:592:ILE:H	2:J:592:ILE:CD1	2.24	0.43
1:K:141:ASN:C	1:K:141:ASN:OD1	2.61	0.43
2:L:114:LEU:HD12	2:L:114:LEU:HA	1.78	0.43
2:L:454:GLY:O	2:L:457:TYR:HB2	2.19	0.43
1:M:102:ILE:HB	2:N:20:VAL:CG2	2.49	0.43
2:P:332:ARG:O	2:P:336:VAL:HG23	2.18	0.43
2:P:446:ARG:HG2	2:P:447:GLN:H	1.82	0.43
2:P:538:PRO:O	2:P:539:TYR:HB2	2.18	0.43
1:C:13:GLY:CA	1:K:9:LYS:HZ2	2.19	0.43
1:C:46:ASN:HB2	1:C:107:TYR:CZ	2.53	0.43
2:F:446:ARG:HG2	2:F:447:GLN:N	2.34	0.43
2:H:233:LEU:HD11	2:H:262:LYS:HG2	2.00	0.43
2:H:247:GLU:HA	2:H:274:ARG:O	2.18	0.43
2:H:298:LEU:HD22	2:H:300:LEU:CD2	2.49	0.43
1:K:133:ILE:HG21	2:L:40:VAL:HG11	2.00	0.43
2:L:251:GLY:O	2:L:278:SER:HB2	2.19	0.43
2:L:405:LEU:HD13	2:L:408:PHE:HB2	2.01	0.43
1:M:159:PHE:O	1:M:160:GLU:HB2	2.17	0.43
2:N:201:MET:HE2	2:N:302:TYR:CZ	2.53	0.43
4:N:1100:OGK:C18	4:N:1100:OGK:N08	2.80	0.43
1:O:98:LEU:HD11	1:O:117:THR:CB	2.48	0.43
2:P:32:LYS:HD2	2:P:32:LYS:HA	1.86	0.43
2:P:65:PRO:HA	2:P:103:TRP:CZ3	2.54	0.43
2:P:436:LYS:HE2	2:P:436:LYS:HB3	1.81	0.43
1:A:12:ASP:OD2	1:A:49:SER:HB2	2.19	0.43
2:D:227:VAL:HG13	2:D:228:GLY:N	2.33	0.43
2:F:119:PHE:CD1	2:F:122:MET:HE3	2.54	0.43
2:H:213:GLU:OE1	2:H:237:GLY:HA3	2.19	0.43
1:I:113:LEU:C	1:I:116:LEU:H	2.26	0.43
2:L:54:HIS:HD2	2:L:77:SER:OG	2.02	0.43
2:L:412:LEU:C	2:L:412:LEU:CD1	2.92	0.43
1:M:46:ASN:HB2	1:M:107:TYR:CZ	2.54	0.43
2:N:176:PHE:CZ	2:N:204:PHE:CZ	3.07	0.43
1:A:35:ASP:O	1:A:36:ASP:C	2.61	0.43
1:A:48:THR:HG22	1:A:51:ILE:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:GLN:HE21	2:B:592:ILE:HD11	1.83	0.43
2:D:117:VAL:HG11	2:D:119:PHE:CZ	2.53	0.43
2:D:211:ASP:HA	2:D:214:THR:HG23	2.01	0.43
2:D:590:GLU:HB3	2:D:591:PRO:CD	2.41	0.43
2:F:398:ILE:CG2	2:F:402:LEU:HD11	2.44	0.43
1:G:8:LEU:HD22	1:G:29:ILE:HD13	2.00	0.43
2:H:289:PHE:HB2	2:H:290:PRO:CD	2.49	0.43
2:H:292:ALA:C	2:H:294:GLN:N	2.73	0.43
2:H:327:ASN:ND2	2:H:364:LEU:CD2	2.81	0.43
2:H:439:ARG:HE	2:H:466:ARG:HH11	1.66	0.43
2:H:519:TRP:CH2	2:H:567:HIS:CE1	3.05	0.43
1:I:44:LEU:HA	1:I:45:PRO:HD3	1.79	0.43
1:I:111:LYS:HG2	1:I:115:ASP:OD2	2.19	0.43
2:J:83:LYS:HA	2:J:84:PRO:HD3	1.88	0.43
2:N:402:LEU:HD12	2:N:402:LEU:O	2.19	0.43
2:P:85:ARG:HD2	5:P:1101:PO4:O2	2.19	0.43
1:A:102:ILE:CG1	1:A:117:THR:HB	2.49	0.42
2:B:403:LYS:O	2:B:405:LEU:N	2.52	0.42
2:D:296:ARG:HH12	1:G:35:ASP:CG	2.26	0.42
2:D:308:GLU:HG3	2:D:332:ARG:NH2	2.34	0.42
2:D:412:LEU:CD1	2:D:412:LEU:C	2.92	0.42
2:F:311:CYS:CB	2:F:336:VAL:HG21	2.49	0.42
2:F:422:LEU:O	2:F:423:PRO:C	2.62	0.42
2:F:535:MET:O	2:F:537:ARG:HG3	2.19	0.42
2:H:274:ARG:HG2	2:H:297:LYS:HB3	2.01	0.42
2:H:367:GLN:O	2:H:371:ILE:HB	2.18	0.42
1:I:48:THR:HG22	1:I:51:ILE:HB	2.01	0.42
2:J:412:LEU:C	2:J:412:LEU:CD1	2.92	0.42
2:L:159:ILE:HG13	2:L:160:VAL:N	2.32	0.42
2:L:201:MET:HE2	2:L:302:TYR:CZ	2.54	0.42
4:L:1100:OGK:C18	4:L:1100:OGK:N08	2.81	0.42
2:P:125:SER:N	2:P:128:ASP:OD2	2.52	0.42
2:P:527:MET:O	2:P:528:THR:C	2.61	0.42
2:H:89:PHE:CD2	4:H:1100:OGK:H04A	2.54	0.42
2:H:332:ARG:CG	2:H:332:ARG:NH1	2.81	0.42
2:H:407:ASP:OD1	2:H:440:ARG:HD2	2.19	0.42
2:H:422:LEU:HD12	2:H:422:LEU:N	2.33	0.42
1:I:58:TYR:CE1	1:I:62:HIS:CE1	3.07	0.42
2:J:543:GLU:OE2	2:J:578:ARG:CD	2.67	0.42
1:K:62:HIS:HE1	1:K:87:ASP:OD1	2.03	0.42
2:P:201:MET:HE3	3:X:208:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:422:LEU:O	2:P:424:LEU:HG	2.18	0.42
2:P:501:SER:HA	2:P:524:ARG:HB2	2.00	0.42
2:P:543:GLU:OE2	2:P:578:ARG:HD3	2.19	0.42
2:B:136:ARG:HG3	2:B:136:ARG:NH1	2.35	0.42
1:C:46:ASN:HB2	1:C:107:TYR:CE2	2.55	0.42
2:D:280:MET:HE1	2:D:288:LEU:HD11	2.01	0.42
2:H:366:SER:OG	2:H:368:ARG:HB3	2.19	0.42
2:H:411:VAL:CG2	4:H:1100:OGK:H14	2.49	0.42
2:J:251:GLY:O	2:J:278:SER:HB2	2.18	0.42
1:K:35:ASP:O	1:K:36:ASP:C	2.62	0.42
1:K:48:THR:HG22	1:K:51:ILE:CB	2.49	0.42
1:M:137:PHE:CD1	2:N:17:VAL:HG21	2.54	0.42
2:B:358:MET:O	2:B:359:GLU:HB2	2.19	0.42
2:B:409:ARG:CB	4:B:1100:OGK:H16B	2.47	0.42
2:D:289:PHE:N	2:D:290:PRO:CD	2.82	0.42
2:D:296:ARG:HH22	1:G:35:ASP:HB2	1.83	0.42
2:D:366:SER:HB2	2:D:367:GLN:OE1	2.20	0.42
2:F:432:LEU:CD1	2:F:458:ILE:HA	2.50	0.42
1:G:91:MET:HE2	1:G:91:MET:HA	2.01	0.42
2:H:75:LEU:HD23	2:H:75:LEU:HA	1.91	0.42
2:H:301:LEU:CD2	2:H:324:GLU:HB3	2.47	0.42
2:H:314:ILE:HG21	2:H:337:LEU:HA	2.02	0.42
2:H:360:ASP:HB2	2:H:361:GLU:H	1.43	0.42
2:H:542:ILE:CG1	2:H:588:LEU:HB2	2.48	0.42
2:J:125:SER:N	2:J:128:ASP:OD2	2.52	0.42
2:L:428:VAL:HG22	2:L:443:PHE:CZ	2.54	0.42
1:M:6:ILE:HG22	1:M:7:VAL:N	2.34	0.42
2:P:503:ARG:HH11	2:P:503:ARG:H	1.66	0.42
2:B:176:PHE:C	2:B:176:PHE:CD2	2.97	0.42
2:B:191:ASN:ND2	2:B:194:LEU:HB2	2.35	0.42
2:D:217:ARG:NH1	2:H:50:GLU:OE2	2.53	0.42
2:D:285:MET:N	2:D:286:PRO:CD	2.82	0.42
2:F:297:LYS:HE3	2:F:297:LYS:HB2	1.90	0.42
2:F:399:GLY:O	2:F:434:GLY:HA3	2.20	0.42
1:G:128:LYS:HB3	1:G:132:GLU:HB2	2.01	0.42
2:H:24:VAL:O	2:H:25:MET:C	2.63	0.42
2:H:227:VAL:O	2:H:250:GLY:HA3	2.20	0.42
2:J:503:ARG:NH1	2:J:503:ARG:HB3	2.34	0.42
2:L:419:ILE:HD11	2:L:446:ARG:NH2	2.34	0.42
2:N:211:ASP:HA	2:N:214:THR:HG23	2.01	0.42
1:C:35:ASP:O	1:C:36:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:LYS:HA	2:D:32:LYS:HD2	1.83	0.42
2:D:471:GLY:O	2:D:496:ARG:O	2.37	0.42
2:F:305:LEU:O	2:F:305:LEU:HD23	2.19	0.42
2:L:328:VAL:O	2:L:329:ILE:C	2.62	0.42
1:M:99:PHE:CZ	2:N:17:VAL:HG22	2.55	0.42
1:M:154:GLU:OE2	2:N:71:ARG:HD3	2.20	0.42
2:P:367:GLN:HG2	2:P:391:THR:CG2	2.50	0.42
2:B:422:LEU:HD12	2:B:422:LEU:HA	1.70	0.42
1:C:44:LEU:O	1:C:44:LEU:HD12	2.20	0.42
2:D:289:PHE:N	2:D:290:PRO:HD2	2.34	0.42
1:E:62:HIS:HE1	1:E:87:ASP:OD1	2.02	0.42
1:G:149:GLU:OE1	1:G:153:ARG:CD	2.67	0.42
2:H:351:ARG:NH1	2:H:360:ASP:HA	2.33	0.42
2:H:533:MET:CE	2:H:588:LEU:CD1	2.86	0.42
1:I:113:LEU:HA	1:I:116:LEU:HB3	2.01	0.42
2:J:289:PHE:N	2:J:290:PRO:CD	2.82	0.42
2:L:75:LEU:HD23	2:L:75:LEU:HA	1.82	0.42
2:N:75:LEU:HD23	2:N:75:LEU:HA	1.89	0.42
2:N:405:LEU:HD13	2:N:408:PHE:HB2	2.02	0.42
2:N:412:LEU:HD12	2:N:412:LEU:C	2.42	0.42
1:O:44:LEU:HD12	1:O:44:LEU:O	2.19	0.42
2:B:501:SER:HA	2:B:524:ARG:HB2	2.02	0.42
2:D:402:LEU:C	2:D:403:LYS:O	2.62	0.42
1:E:158:ALA:CB	2:F:62:THR:HG23	2.50	0.42
1:G:133:ILE:HG21	2:H:44:TRP:CZ3	2.55	0.42
2:H:587:VAL:HG12	2:H:589:LYS:CD	2.49	0.42
2:J:298:LEU:HB2	2:J:320:LEU:HD11	2.01	0.42
2:J:361:GLU:HG3	2:J:361:GLU:O	2.20	0.42
2:L:519:TRP:NE1	4:L:1100:OGK:H01	2.35	0.42
2:N:402:LEU:HD13	2:N:405:LEU:HG	2.00	0.42
2:P:351:ARG:HD3	2:P:413:LEU:HD11	2.01	0.42
1:C:12:ASP:OD2	1:C:49:SER:HB2	2.19	0.42
2:D:127:LEU:HD22	2:N:126:ASP:HB3	2.01	0.42
2:F:298:LEU:HB2	2:F:320:LEU:HD11	2.02	0.42
2:F:411:VAL:CG2	4:F:1100:OGK:H14	2.50	0.42
2:F:469:LEU:HA	2:F:494:GLU:O	2.19	0.42
1:I:102:ILE:HG12	1:I:117:THR:HB	2.02	0.42
2:J:125:SER:O	2:J:129:LEU:HD22	2.20	0.42
2:J:253:LEU:HD12	2:J:280:MET:HB2	2.01	0.42
2:J:274:ARG:HG2	2:J:297:LYS:HE3	2.01	0.42
2:N:125:SER:O	2:N:129:LEU:HD22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:251:GLY:O	2:N:278:SER:HB2	2.20	0.42
2:P:52:ARG:HH11	2:P:52:ARG:HD3	1.73	0.42
2:P:432:LEU:HB3	2:P:461:TYR:O	2.19	0.42
2:P:495:MET:O	2:P:520:VAL:HA	2.19	0.42
2:B:80:LEU:HD12	2:B:122:MET:HE1	2.00	0.42
2:D:319:ASN:ND2	1:G:43:PRO:HG3	2.35	0.42
1:E:51:ILE:HD12	1:E:51:ILE:HG23	1.84	0.42
2:F:196:VAL:HB	2:F:224:SER:HB3	2.01	0.42
2:F:211:ASP:HA	2:F:214:THR:HG23	2.01	0.42
2:H:567:HIS:CD2	2:H:567:HIS:N	2.88	0.42
1:I:18:VAL:HG11	1:I:56:ILE:HD13	2.01	0.42
2:J:164:ARG:NE	2:N:112:ARG:CG	2.83	0.42
2:J:201:MET:CE	2:J:302:TYR:CZ	3.03	0.42
2:J:310:HIS:HE1	2:J:325:THR:OG1	2.01	0.42
2:L:153:THR:HG23	2:L:178:GLU:HA	2.02	0.42
1:M:96:ALA:HB2	2:N:14:VAL:HG12	2.02	0.42
2:N:184:LEU:HD12	2:N:207:ILE:HB	2.01	0.42
2:N:305:LEU:O	2:N:305:LEU:HD23	2.20	0.42
2:N:419:ILE:HD11	2:N:446:ARG:NH2	2.35	0.42
2:B:468:MET:HE3	2:B:470:LEU:CD2	2.41	0.41
2:D:75:LEU:HD23	2:D:75:LEU:HA	1.82	0.41
2:F:117:VAL:HG11	2:F:119:PHE:CZ	2.55	0.41
2:F:519:TRP:NE1	4:F:1100:OGK:H01	2.32	0.41
1:G:147:GLU:O	1:G:148:GLU:C	2.61	0.41
2:H:170:LEU:C	2:H:171:MET:HG3	2.45	0.41
2:H:274:ARG:HG2	2:H:297:LYS:HE3	2.02	0.41
2:H:405:LEU:HD13	2:H:408:PHE:HB2	2.02	0.41
2:H:456:SER:HB2	2:H:482:GLU:CB	2.50	0.41
2:J:37:ALA:O	2:J:40:VAL:HG13	2.20	0.41
2:J:57:MET:CE	2:J:62:THR:HG22	2.48	0.41
2:J:96:TRP:HA	2:J:582:PRO:HG2	2.02	0.41
2:J:164:ARG:CD	2:N:112:ARG:NE	2.83	0.41
2:J:211:ASP:HA	2:J:214:THR:HG23	2.02	0.41
2:J:422:LEU:O	2:J:424:LEU:HG	2.20	0.41
2:J:532:LEU:HA	2:J:532:LEU:HD23	1.77	0.41
2:N:412:LEU:C	2:N:412:LEU:CD1	2.93	0.41
2:P:285:MET:HB3	2:P:286:PRO:HD3	2.01	0.41
2:B:263:TYR:HB3	2:B:266:LEU:CD2	2.50	0.41
2:B:301:LEU:CD2	2:B:324:GLU:HB3	2.50	0.41
2:B:305:LEU:HD23	2:B:305:LEU:O	2.20	0.41
1:G:148:GLU:HG2	1:G:152:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:ARG:HD2	2:H:34:ARG:HA	1.79	0.41
2:H:288:LEU:HD23	2:H:291:PHE:CZ	2.55	0.41
2:H:319:ASN:HD22	2:H:319:ASN:N	2.18	0.41
1:I:102:ILE:HG12	1:I:117:THR:OG1	2.20	0.41
2:J:296:ARG:HH22	1:M:35:ASP:HB2	1.85	0.41
2:L:289:PHE:CD1	2:L:316:LYS:HD2	2.55	0.41
2:N:351:ARG:HD3	2:N:413:LEU:HD11	2.02	0.41
2:P:37:ALA:O	2:P:40:VAL:HG13	2.21	0.41
2:P:308:GLU:HG3	2:P:332:ARG:NH2	2.35	0.41
2:P:471:GLY:O	2:P:496:ARG:O	2.38	0.41
2:B:366:SER:HB2	2:B:367:GLN:OE1	2.20	0.41
2:D:398:ILE:CG2	2:D:402:LEU:HD11	2.45	0.41
2:F:184:LEU:HD12	2:F:207:ILE:HB	2.03	0.41
2:H:533:MET:HE3	2:H:588:LEU:HD22	2.02	0.41
1:I:48:THR:HG22	1:I:51:ILE:CB	2.50	0.41
1:K:30:ALA:C	1:K:32:MET:N	2.78	0.41
2:N:361:GLU:HG3	2:N:361:GLU:O	2.19	0.41
2:B:444:TYR:HA	2:B:471:GLY:CA	2.33	0.41
2:B:446:ARG:HG2	2:B:447:GLN:N	2.36	0.41
2:D:402:LEU:HD13	2:D:405:LEU:HG	2.01	0.41
1:E:51:ILE:HD13	1:E:51:ILE:HA	1.84	0.41
2:H:314:ILE:HG22	2:H:341:CYS:SG	2.59	0.41
2:H:321:GLU:HA	2:H:344:LEU:HA	2.03	0.41
2:H:364:LEU:CD1	2:H:388:SER:HB2	2.50	0.41
2:H:419:ILE:HD12	2:H:419:ILE:O	2.21	0.41
1:I:102:ILE:HD11	1:I:121:VAL:CG2	2.51	0.41
2:J:305:LEU:HD23	2:J:305:LEU:C	2.46	0.41
1:K:102:ILE:HG21	2:L:20:VAL:HG22	2.02	0.41
2:L:227:VAL:CG1	2:L:228:GLY:N	2.83	0.41
2:L:361:GLU:HG3	2:L:361:GLU:O	2.20	0.41
2:N:404:ASN:HB3	2:N:437:LYS:HD2	2.03	0.41
2:N:428:VAL:HG22	2:N:443:PHE:CZ	2.55	0.41
1:O:91:MET:CE	1:O:117:THR:HG22	2.50	0.41
2:P:349:ILE:HG13	2:P:385:VAL:HG22	2.01	0.41
2:B:308:GLU:HG3	2:B:332:ARG:HH22	1.85	0.41
1:E:57:GLU:OE1	1:E:86:TRP:HH2	2.03	0.41
2:F:581:CYS:HA	2:F:582:PRO:HD3	1.90	0.41
2:H:365:VAL:HG13	2:H:387:VAL:HG22	2.02	0.41
2:L:166:ILE:HG23	2:L:166:ILE:HD13	1.85	0.41
2:P:404:ASN:CA	2:P:437:LYS:HD2	2.49	0.41
2:B:453:LEU:HD13	2:B:457:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:THR:HG21	2:N:179:LYS:HZ3	1.83	0.41
2:D:197:LEU:O	2:D:225:VAL:HA	2.20	0.41
1:E:137:PHE:CD1	2:F:17:VAL:HG21	2.55	0.41
2:F:530:GLN:HE21	2:F:592:ILE:HD11	1.86	0.41
2:H:136:ARG:HG3	2:H:136:ARG:HH11	1.85	0.41
2:H:355:GLU:HB3	2:H:356:GLN:H	1.76	0.41
2:J:351:ARG:HD3	2:J:413:LEU:HD11	2.02	0.41
2:J:419:ILE:HD13	2:J:446:ARG:NH1	2.36	0.41
1:K:107:TYR:C	1:K:108:LEU:O	2.63	0.41
2:L:125:SER:O	2:L:129:LEU:HD22	2.20	0.41
2:L:419:ILE:HG21	2:L:422:LEU:HD13	2.01	0.41
1:M:52:LEU:O	1:M:56:ILE:HG13	2.21	0.41
2:N:176:PHE:CD2	2:N:176:PHE:C	2.99	0.41
2:B:46:LYS:HB2	2:B:46:LYS:HE3	1.44	0.41
2:B:310:HIS:HE1	2:B:325:THR:OG1	2.04	0.41
1:C:26:SER:OG	1:C:108:LEU:HB3	2.20	0.41
2:D:412:LEU:HD12	2:D:412:LEU:C	2.44	0.41
2:D:468:MET:HE1	2:D:483:PHE:HE1	1.81	0.41
2:D:503:ARG:HH11	2:D:503:ARG:H	1.68	0.41
2:D:527:MET:O	2:D:528:THR:C	2.63	0.41
2:F:348:ARG:HH22	4:F:1100:OGK:C10	2.33	0.41
2:F:512:LEU:HA	2:F:513:PRO:HD2	1.87	0.41
1:G:95:GLN:O	1:G:96:ALA:C	2.63	0.41
2:H:298:LEU:CD2	2:H:300:LEU:CD2	2.99	0.41
2:J:304:LEU:HD11	3:U:216:ARG:HG3	2.02	0.41
2:L:30:ASP:OD1	2:L:31:PRO:HD2	2.21	0.41
1:M:135:THR:HG22	1:M:136:THR:N	2.35	0.41
2:N:159:ILE:HD11	2:N:169:LEU:HD13	2.03	0.41
2:N:422:LEU:O	2:N:424:LEU:HG	2.21	0.41
2:N:496:ARG:HB2	2:N:521:GLN:HB3	2.01	0.41
2:P:85:ARG:NH2	4:P:1100:OGK:O07	2.45	0.41
2:P:91:LEU:O	2:P:567:HIS:HE1	2.03	0.41
2:P:100:VAL:HG23	2:P:122:MET:HE3	2.01	0.41
2:P:358:MET:O	2:P:359:GLU:HB2	2.20	0.41
2:P:412:LEU:HD12	2:P:412:LEU:C	2.43	0.41
2:P:412:LEU:CD1	2:P:412:LEU:C	2.93	0.41
1:A:126:LYS:HZ3	2:B:29:THR:H	1.67	0.41
1:C:62:HIS:HE1	1:C:87:ASP:OD1	2.04	0.41
2:D:57:MET:CE	2:D:62:THR:HG22	2.51	0.41
2:F:80:LEU:CD1	2:F:122:MET:HE1	2.50	0.41
2:J:197:LEU:O	2:J:225:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:57:MET:CE	2:L:62:THR:HG22	2.49	0.41
2:L:411:VAL:HG22	2:L:444:TYR:HB3	2.03	0.41
2:N:133:ALA:HB2	2:N:159:ILE:HG22	2.02	0.41
2:P:54:HIS:HD2	2:P:77:SER:OG	2.04	0.41
2:P:201:MET:HE2	2:P:302:TYR:CZ	2.55	0.41
2:B:83:LYS:O	2:B:121:ARG:HD2	2.20	0.41
1:C:102:ILE:HD11	1:C:121:VAL:CG2	2.50	0.41
2:D:136:ARG:HG3	2:D:136:ARG:NH1	2.35	0.41
2:D:335:GLU:O	2:D:338:ALA:HB3	2.20	0.41
2:H:78:LEU:HA	2:H:78:LEU:HD12	1.66	0.41
2:H:274:ARG:HD2	2:H:297:LYS:HE3	2.02	0.41
2:H:352:GLY:C	2:H:354:ASP:N	2.78	0.41
2:H:496:ARG:HG3	2:H:521:GLN:HB3	2.02	0.41
2:J:176:PHE:CZ	2:J:204:PHE:CZ	3.09	0.41
2:J:298:LEU:HD12	2:J:298:LEU:HA	1.83	0.41
2:J:366:SER:HB2	2:J:367:GLN:OE1	2.21	0.41
1:K:154:GLU:OE2	2:L:71:ARG:HD3	2.21	0.41
1:K:158:ALA:CB	2:L:62:THR:HG23	2.51	0.41
4:L:1100:OGK:HN08	4:L:1100:OGK:C18	2.30	0.41
1:M:96:ALA:CB	2:N:14:VAL:HG12	2.50	0.41
2:D:358:MET:O	2:D:359:GLU:HB2	2.20	0.41
2:F:289:PHE:N	2:F:290:PRO:CD	2.83	0.41
2:F:532:LEU:HA	2:F:532:LEU:HD23	1.71	0.41
1:G:160:GLU:HG3	2:H:52:ARG:HH21	1.86	0.41
2:H:80:LEU:HD23	2:H:80:LEU:HA	1.68	0.41
2:H:114:LEU:HA	2:H:114:LEU:HD12	1.77	0.41
1:I:26:SER:OG	1:I:29:ILE:HG13	2.21	0.41
1:I:137:PHE:CD1	2:J:17:VAL:HG21	2.55	0.41
2:J:512:LEU:HA	2:J:513:PRO:HD2	1.92	0.41
2:L:176:PHE:CD2	2:L:176:PHE:C	2.98	0.41
2:L:590:GLU:HB3	2:L:591:PRO:CD	2.43	0.41
2:P:263:TYR:HB3	2:P:266:LEU:CD2	2.51	0.41
1:A:114:LEU:O	1:A:118:CYS:HB2	2.22	0.40
2:B:125:SER:O	2:B:129:LEU:HD22	2.21	0.40
2:B:482:GLU:O	2:B:485:ARG:HG2	2.20	0.40
2:D:533:MET:HE3	2:D:588:LEU:CD1	2.46	0.40
2:F:201:MET:HE2	2:F:302:TYR:CZ	2.55	0.40
2:F:329:ILE:HG23	2:F:330:GLY:N	2.35	0.40
2:F:422:LEU:HD12	2:F:422:LEU:HA	1.72	0.40
2:H:230:PHE:CD1	2:H:235:LEU:HD21	2.56	0.40
2:H:428:VAL:HG23	2:H:429:ARG:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:289:PHE:HB2	2:J:290:PRO:HD3	2.02	0.40
2:J:503:ARG:HH11	2:J:503:ARG:H	1.69	0.40
2:L:89:PHE:CE1	4:L:1100:OGK:H17	2.56	0.40
2:L:329:ILE:HG21	2:L:349:ILE:HD12	2.02	0.40
2:N:590:GLU:HB3	2:N:591:PRO:CD	2.43	0.40
2:P:83:LYS:HA	2:P:84:PRO:HD3	1.87	0.40
2:P:533:MET:HE3	2:P:588:LEU:CD1	2.50	0.40
2:B:527:MET:O	2:B:528:THR:C	2.63	0.40
2:B:533:MET:HE3	2:B:588:LEU:CD2	2.51	0.40
2:D:96:TRP:HA	2:D:582:PRO:HG2	2.02	0.40
2:D:409:ARG:HB3	2:D:442:ALA:HB3	2.02	0.40
2:F:55:VAL:HG21	2:F:72:PHE:CD1	2.56	0.40
2:F:335:GLU:O	2:F:338:ALA:HB3	2.21	0.40
1:G:62:HIS:HE1	1:G:87:ASP:OD1	2.04	0.40
2:H:34:ARG:HB3	2:H:34:ARG:HH11	1.86	0.40
2:H:210:LYS:HD3	2:H:210:LYS:HA	1.87	0.40
2:H:467:TRP:CD1	2:H:467:TRP:O	2.74	0.40
2:J:446:ARG:HG2	2:J:447:GLN:H	1.87	0.40
1:K:12:ASP:OD2	1:K:49:SER:HB2	2.21	0.40
2:N:91:LEU:O	2:N:567:HIS:HE1	2.04	0.40
1:O:126:LYS:HZ3	2:P:29:THR:H	1.68	0.40
2:P:59:LEU:HD22	2:P:61:TYR:H	1.86	0.40
2:P:133:ALA:HB2	2:P:159:ILE:HG22	2.03	0.40
2:P:176:PHE:CZ	2:P:204:PHE:CZ	3.09	0.40
2:P:390:ILE:CD1	2:P:424:LEU:HD11	2.50	0.40
2:B:267:VAL:O	2:B:267:VAL:CG2	2.70	0.40
2:B:298:LEU:HB2	2:B:320:LEU:HD11	2.03	0.40
2:B:308:GLU:HG3	2:B:332:ARG:NH2	2.36	0.40
2:D:530:GLN:HE21	2:D:592:ILE:HD11	1.86	0.40
2:H:159:ILE:HD13	2:H:166:ILE:HD11	2.03	0.40
2:H:274:ARG:HG2	2:H:297:LYS:CE	2.51	0.40
2:H:354:ASP:OD2	2:H:355:GLU:N	2.54	0.40
1:I:128:LYS:HB2	1:I:133:ILE:CD1	2.50	0.40
2:D:578:ARG:H	2:D:578:ARG:HG3	1.78	0.40
2:F:349:ILE:HG13	2:F:385:VAL:HG22	2.03	0.40
2:F:496:ARG:HB2	2:F:521:GLN:HB3	2.02	0.40
1:G:30:ALA:C	1:G:32:MET:N	2.79	0.40
2:H:22:GLU:HG2	2:H:47:ILE:HD11	2.03	0.40
2:H:136:ARG:HA	2:H:136:ARG:NE	2.37	0.40
2:H:282:PRO:HB3	2:H:309:ASP:OD2	2.22	0.40
2:H:349:ILE:HD13	2:H:349:ILE:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:383:MET:O	2:H:408:PHE:HA	2.21	0.40
2:J:32:LYS:HA	2:J:32:LYS:HD2	1.82	0.40
1:K:137:PHE:CD1	2:L:17:VAL:HG21	2.56	0.40
2:L:512:LEU:HA	2:L:513:PRO:HD2	1.93	0.40
1:M:130:PRO:O	1:M:134:ARG:HG2	2.22	0.40
2:N:301:LEU:HD23	2:N:324:GLU:HB3	2.02	0.40
2:N:503:ARG:HH11	2:N:503:ARG:H	1.70	0.40
1:O:95:GLN:O	1:O:96:ALA:C	2.65	0.40
1:A:137:PHE:CD1	2:B:17:VAL:HG21	2.57	0.40
2:B:301:LEU:HD13	2:B:301:LEU:HA	1.83	0.40
2:D:119:PHE:CD1	2:D:122:MET:HE3	2.56	0.40
2:F:112:ARG:HH11	2:F:112:ARG:HD3	1.76	0.40
2:F:402:LEU:HD13	2:F:405:LEU:HG	2.03	0.40
2:H:440:ARG:CB	2:H:467:TRP:CD1	3.02	0.40
2:J:285:MET:N	2:J:286:PRO:CD	2.85	0.40
2:L:399:GLY:O	2:L:434:GLY:HA3	2.21	0.40
2:L:545:ILE:HG12	2:L:585:VAL:HG22	2.04	0.40
2:N:240:LYS:CG	2:N:267:VAL:HG21	2.45	0.40
2:N:344:LEU:HD12	2:N:344:LEU:HA	1.85	0.40
2:N:581:CYS:HA	2:N:582:PRO:HD3	1.94	0.40
1:O:137:PHE:CD1	2:P:17:VAL:CG2	3.04	0.40
2:P:446:ARG:HG2	2:P:447:GLN:N	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:ARG:NH2	1:I:61:ARG:NH1[2_555]	2.03	0.17
2:D:429:ARG:NH1	1:I:86:TRP:CE3[2_555]	2.06	0.14

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	141/160 (88%)	115 (82%)	21 (15%)	5 (4%)	3	10
1	C	141/160 (88%)	115 (82%)	21 (15%)	5 (4%)	3	10
1	E	141/160 (88%)	117 (83%)	21 (15%)	3 (2%)	5	20
1	G	141/160 (88%)	119 (84%)	18 (13%)	4 (3%)	4	14
1	I	141/160 (88%)	116 (82%)	21 (15%)	4 (3%)	4	14
1	K	141/160 (88%)	118 (84%)	19 (14%)	4 (3%)	4	14
1	M	141/160 (88%)	114 (81%)	22 (16%)	5 (4%)	3	10
1	O	141/160 (88%)	114 (81%)	23 (16%)	4 (3%)	4	14
2	B	562/592 (95%)	509 (91%)	44 (8%)	9 (2%)	7	27
2	D	562/592 (95%)	508 (90%)	44 (8%)	10 (2%)	6	23
2	F	562/592 (95%)	509 (91%)	44 (8%)	9 (2%)	7	27
2	H	558/592 (94%)	475 (85%)	63 (11%)	20 (4%)	2	10
2	J	562/592 (95%)	508 (90%)	44 (8%)	10 (2%)	6	23
2	L	562/592 (95%)	508 (90%)	46 (8%)	8 (1%)	9	30
2	N	562/592 (95%)	505 (90%)	49 (9%)	8 (1%)	9	30
2	P	562/592 (95%)	503 (90%)	49 (9%)	10 (2%)	6	23
3	Q	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	R	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	S	11/22 (50%)	9 (82%)	2 (18%)	0	100	100
3	U	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	V	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	W	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
3	X	11/22 (50%)	10 (91%)	1 (9%)	0	100	100
All	All	5697/6170 (92%)	5022 (88%)	557 (10%)	118 (2%)	5	20

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	LYS
2	B	404	ASN
2	B	420	THR
2	D	271	LYS
2	D	420	THR
2	D	591	PRO
2	F	271	LYS

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Mol	Chain	Res	Type
2	F	420	THR
2	F	591	PRO
2	H	254	ASN
2	H	278	SER
2	H	287	ILE
2	H	365	VAL
2	J	271	LYS
2	J	404	ASN
2	J	420	THR
2	L	271	LYS
2	L	420	THR
2	L	591	PRO
2	N	271	LYS
2	N	420	THR
2	P	271	LYS
2	P	420	THR
2	P	591	PRO
1	A	36	ASP
2	B	357	GLY
2	B	358	MET
2	B	591	PRO
1	C	36	ASP
2	D	357	GLY
2	D	358	MET
2	D	404	ASN
1	E	36	ASP
1	E	108	LEU
2	F	264	MET
2	F	357	GLY
2	F	404	ASN
1	G	36	ASP
1	G	108	LEU
2	H	201	MET
2	H	295	ILE
2	H	367	GLN
2	H	528	THR
1	I	36	ASP
2	J	264	MET
2	J	403	LYS
2	J	591	PRO
1	K	36	ASP
1	K	108	LEU

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Mol	Chain	Res	Type
2	L	357	GLY
2	L	358	MET
2	L	404	ASN
1	M	36	ASP
1	M	108	LEU
2	N	357	GLY
2	N	358	MET
2	N	404	ASN
2	N	591	PRO
1	O	36	ASP
1	O	108	LEU
2	P	357	GLY
2	P	358	MET
2	P	404	ASN
1	A	108	LEU
1	A	141	ASN
2	B	264	MET
2	B	403	LYS
1	C	92	LYS
1	C	108	LEU
2	D	264	MET
2	D	403	LYS
2	F	358	MET
2	H	206	LYS
2	H	260	PRO
2	H	270	ARG
2	H	328	VAL
2	H	525	ALA
1	I	108	LEU
2	J	357	GLY
2	J	358	MET
2	L	264	MET
2	L	403	LYS
1	M	141	ASN
2	N	264	MET
2	N	403	LYS
2	P	264	MET
2	D	524	ARG
2	H	327	ASN
2	H	403	LYS
2	H	471	GLY
1	I	20	GLU

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Mol	Chain	Res	Type
2	P	403	LYS
2	F	403	LYS
2	F	500	PHE
1	G	20	GLU
1	K	20	GLU
1	M	113	LEU
1	O	113	LEU
2	P	524	ARG
1	A	20	GLU
2	B	526	SER
1	C	141	ASN
2	D	526	SER
2	H	14	VAL
1	K	92	LYS
2	P	526	SER
1	E	13	GLY
1	G	13	GLY
2	H	538	PRO
1	I	13	GLY
1	M	13	GLY
2	J	20	VAL
1	A	13	GLY
1	C	13	GLY
2	H	513	PRO
1	O	13	GLY
2	H	97	GLY
2	J	422	LEU

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	128/137 (93%)	116 (91%)	12 (9%)	8	27
1	C	128/137 (93%)	115 (90%)	13 (10%)	7	23
1	E	128/137 (93%)	115 (90%)	13 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	128/137 (93%)	117 (91%)	11 (9%)	10	31
1	I	128/137 (93%)	117 (91%)	11 (9%)	10	31
1	K	128/137 (93%)	117 (91%)	11 (9%)	10	31
1	M	128/137 (93%)	117 (91%)	11 (9%)	10	31
1	O	128/137 (93%)	117 (91%)	11 (9%)	10	31
2	B	498/523 (95%)	420 (84%)	78 (16%)	2	9
2	D	498/523 (95%)	421 (84%)	77 (16%)	2	9
2	F	498/523 (95%)	418 (84%)	80 (16%)	2	8
2	H	494/523 (94%)	396 (80%)	98 (20%)	1	5
2	J	498/523 (95%)	422 (85%)	76 (15%)	3	10
2	L	498/523 (95%)	423 (85%)	75 (15%)	3	10
2	N	498/523 (95%)	425 (85%)	73 (15%)	3	10
2	P	498/523 (95%)	423 (85%)	75 (15%)	3	10
3	Q	12/20 (60%)	11 (92%)	1 (8%)	10	32
3	R	12/20 (60%)	11 (92%)	1 (8%)	10	32
3	S	12/20 (60%)	11 (92%)	1 (8%)	10	32
3	U	12/20 (60%)	11 (92%)	1 (8%)	10	32
3	V	12/20 (60%)	11 (92%)	1 (8%)	10	32
3	W	12/20 (60%)	11 (92%)	1 (8%)	10	32
3	X	12/20 (60%)	11 (92%)	1 (8%)	10	32
All	All	5088/5420 (94%)	4356 (86%)	732 (14%)	3	11

All (732) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	35	ASP
1	A	42	VAL
1	A	44	LEU
1	A	47	VAL
1	A	48	THR
1	A	97	THR
1	A	112	ASN
1	A	125	ILE
1	A	135	THR

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Mol	Chain	Res	Type
1	A	139	ILE
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	59	LEU
2	B	62	THR
2	B	85	ARG
2	B	100	VAL
2	B	101	THR
2	B	104	VAL
2	B	105	THR
2	B	113	GLN
2	B	123	ILE
2	B	129	LEU
2	B	132	LEU
2	B	136	ARG
2	B	142	THR
2	B	152	THR
2	B	159	ILE
2	B	161	THR
2	B	166	ILE
2	B	168	THR
2	B	171	MET
2	B	182	LYS
2	B	184	LEU
2	B	192	THR
2	B	196	VAL
2	B	203	GLU
2	B	214	THR
2	B	225	VAL
2	B	227	VAL
2	B	232	ILE
2	B	270	ARG
2	B	272	LEU
2	B	284	GLU
2	B	287	ILE

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Mol	Chain	Res	Type
2	B	301	LEU
2	B	304	LEU
2	B	305	LEU
2	B	312	THR
2	B	313	LEU
2	B	327	ASN
2	B	349	ILE
2	B	351	ARG
2	B	354	ASP
2	B	365	VAL
2	B	390	ILE
2	B	398	ILE
2	B	400	THR
2	B	402	LEU
2	B	405	LEU
2	B	410	LEU
2	B	412	LEU
2	B	413	LEU
2	B	422	LEU
2	B	430	SER
2	B	431	LEU
2	B	447	GLN
2	B	453	LEU
2	B	455	LEU
2	B	456	SER
2	B	466	ARG
2	B	490	LEU
2	B	499	CYS
2	B	503	ARG
2	B	516	ARG
2	B	519	TRP
2	B	537	ARG
2	B	542	ILE
2	B	578	ARG
2	B	579	THR
2	B	583	THR
2	B	584	THR
2	B	588	LEU
3	Q	209	LEU
1	C	10	SER
1	C	22	VAL
1	C	35	ASP

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Mol	Chain	Res	Type
1	C	42	VAL
1	C	44	LEU
1	C	47	VAL
1	C	48	THR
1	C	97	THR
1	C	112	ASN
1	C	125	ILE
1	C	135	THR
1	C	139	ILE
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	59	LEU
2	D	62	THR
2	D	85	ARG
2	D	100	VAL
2	D	101	THR
2	D	104	VAL
2	D	105	THR
2	D	113	GLN
2	D	129	LEU
2	D	132	LEU
2	D	136	ARG
2	D	142	THR
2	D	159	ILE
2	D	161	THR
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	203	GLU
2	D	214	THR
2	D	225	VAL
2	D	227	VAL

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Mol	Chain	Res	Type
2	D	232	ILE
2	D	270	ARG
2	D	272	LEU
2	D	284	GLU
2	D	287	ILE
2	D	301	LEU
2	D	304	LEU
2	D	305	LEU
2	D	312	THR
2	D	313	LEU
2	D	327	ASN
2	D	349	ILE
2	D	351	ARG
2	D	354	ASP
2	D	365	VAL
2	D	390	ILE
2	D	397	SER
2	D	398	ILE
2	D	400	THR
2	D	402	LEU
2	D	405	LEU
2	D	410	LEU
2	D	412	LEU
2	D	413	LEU
2	D	421	ASP
2	D	422	LEU
2	D	429	ARG
2	D	430	SER
2	D	431	LEU
2	D	447	GLN
2	D	453	LEU
2	D	455	LEU
2	D	456	SER
2	D	466	ARG
2	D	490	LEU
2	D	499	CYS
2	D	503	ARG
2	D	516	ARG
2	D	519	TRP
2	D	537	ARG
2	D	542	ILE
2	D	579	THR

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Mol	Chain	Res	Type
2	D	583	THR
2	D	584	THR
2	D	588	LEU
3	R	209	LEU
1	E	10	SER
1	E	22	VAL
1	E	35	ASP
1	E	42	VAL
1	E	44	LEU
1	E	47	VAL
1	E	48	THR
1	E	97	THR
1	E	112	ASN
1	E	125	ILE
1	E	135	THR
1	E	139	ILE
1	E	160	GLU
2	F	14	VAL
2	F	16	THR
2	F	17	VAL
2	F	20	VAL
2	F	35	ASP
2	F	40	VAL
2	F	46	LYS
2	F	48	ASP
2	F	59	LEU
2	F	62	THR
2	F	85	ARG
2	F	100	VAL
2	F	101	THR
2	F	104	VAL
2	F	105	THR
2	F	112	ARG
2	F	113	GLN
2	F	122	MET
2	F	129	LEU
2	F	132	LEU
2	F	136	ARG
2	F	142	THR
2	F	159	ILE
2	F	161	THR
2	F	166	ILE

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Mol	Chain	Res	Type
2	F	168	THR
2	F	171	MET
2	F	182	LYS
2	F	184	LEU
2	F	192	THR
2	F	196	VAL
2	F	203	GLU
2	F	214	THR
2	F	225	VAL
2	F	227	VAL
2	F	232	ILE
2	F	270	ARG
2	F	272	LEU
2	F	284	GLU
2	F	287	ILE
2	F	301	LEU
2	F	304	LEU
2	F	305	LEU
2	F	312	THR
2	F	313	LEU
2	F	327	ASN
2	F	351	ARG
2	F	354	ASP
2	F	365	VAL
2	F	390	ILE
2	F	397	SER
2	F	398	ILE
2	F	400	THR
2	F	402	LEU
2	F	405	LEU
2	F	410	LEU
2	F	412	LEU
2	F	413	LEU
2	F	422	LEU
2	F	425	ASP
2	F	430	SER
2	F	431	LEU
2	F	447	GLN
2	F	453	LEU
2	F	455	LEU
2	F	456	SER
2	F	466	ARG

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Mol	Chain	Res	Type
2	F	490	LEU
2	F	499	CYS
2	F	503	ARG
2	F	516	ARG
2	F	519	TRP
2	F	528	THR
2	F	537	ARG
2	F	542	ILE
2	F	578	ARG
2	F	579	THR
2	F	583	THR
2	F	584	THR
2	F	588	LEU
3	S	209	LEU
1	G	22	VAL
1	G	42	VAL
1	G	44	LEU
1	G	47	VAL
1	G	48	THR
1	G	97	THR
1	G	112	ASN
1	G	128	LYS
1	G	149	GLU
1	G	153	ARG
1	G	160	GLU
2	H	17	VAL
2	H	20	VAL
2	H	32	LYS
2	H	34	ARG
2	H	36	SER
2	H	40	VAL
2	H	43	ARG
2	H	46	LYS
2	H	48	ASP
2	H	59	LEU
2	H	62	THR
2	H	68	LEU
2	H	76	ARG
2	H	77	SER
2	H	90	ASN
2	H	95	ASN
2	H	100	VAL

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Mol	Chain	Res	Type
2	H	104	VAL
2	H	105	THR
2	H	117	VAL
2	H	120	ARG
2	H	129	LEU
2	H	132	LEU
2	H	136	ARG
2	H	142	THR
2	H	159	ILE
2	H	166	ILE
2	H	168	THR
2	H	170	LEU
2	H	179	LYS
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	220	ARG
2	H	225	VAL
2	H	227	VAL
2	H	231	GLU
2	H	257	ILE
2	H	263	TYR
2	H	265	ASN
2	H	266	LEU
2	H	271	LYS
2	H	272	LEU
2	H	274	ARG
2	H	284	GLU
2	H	285	MET
2	H	287	ILE
2	H	298	LEU
2	H	301	LEU
2	H	304	LEU
2	H	305	LEU
2	H	307	THR
2	H	312	THR
2	H	313	LEU

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Mol	Chain	Res	Type
2	H	325	THR
2	H	327	ASN
2	H	332	ARG
2	H	343	GLN
2	H	345	LYS
2	H	358	MET
2	H	359	GLU
2	H	360	ASP
2	H	365	VAL
2	H	373	LEU
2	H	385	VAL
2	H	387	VAL
2	H	388	SER
2	H	389	ASP
2	H	390	ILE
2	H	395	LEU
2	H	400	THR
2	H	402	LEU
2	H	403	LYS
2	H	410	LEU
2	H	417	GLU
2	H	422	LEU
2	H	428	VAL
2	H	453	LEU
2	H	455	LEU
2	H	466	ARG
2	H	467	TRP
2	H	490	LEU
2	H	491	GLN
2	H	503	ARG
2	H	511	LYS
2	H	516	ARG
2	H	518	LEU
2	H	519	TRP
2	H	542	ILE
2	H	548	ARG
2	H	577	GLN
2	H	579	THR
2	H	589	LYS
1	I	22	VAL
1	I	42	VAL
1	I	44	LEU

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Mol	Chain	Res	Type
1	I	47	VAL
1	I	48	THR
1	I	97	THR
1	I	112	ASN
1	I	125	ILE
1	I	135	THR
1	I	139	ILE
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	59	LEU
2	J	62	THR
2	J	85	ARG
2	J	100	VAL
2	J	101	THR
2	J	104	VAL
2	J	105	THR
2	J	113	GLN
2	J	122	MET
2	J	129	LEU
2	J	132	LEU
2	J	136	ARG
2	J	142	THR
2	J	159	ILE
2	J	161	THR
2	J	166	ILE
2	J	168	THR
2	J	182	LYS
2	J	184	LEU
2	J	192	THR
2	J	196	VAL
2	J	203	GLU
2	J	214	THR
2	J	225	VAL
2	J	227	VAL
2	J	232	ILE
2	J	270	ARG

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Mol	Chain	Res	Type
2	J	272	LEU
2	J	284	GLU
2	J	287	ILE
2	J	301	LEU
2	J	304	LEU
2	J	305	LEU
2	J	312	THR
2	J	313	LEU
2	J	327	ASN
2	J	351	ARG
2	J	354	ASP
2	J	365	VAL
2	J	390	ILE
2	J	397	SER
2	J	398	ILE
2	J	400	THR
2	J	402	LEU
2	J	405	LEU
2	J	410	LEU
2	J	412	LEU
2	J	413	LEU
2	J	422	LEU
2	J	430	SER
2	J	431	LEU
2	J	447	GLN
2	J	453	LEU
2	J	455	LEU
2	J	456	SER
2	J	466	ARG
2	J	490	LEU
2	J	499	CYS
2	J	503	ARG
2	J	516	ARG
2	J	519	TRP
2	J	528	THR
2	J	537	ARG
2	J	542	ILE
2	J	578	ARG
2	J	579	THR
2	J	583	THR
2	J	584	THR
2	J	588	LEU

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Mol	Chain	Res	Type
3	U	209	LEU
1	K	35	ASP
1	K	42	VAL
1	K	44	LEU
1	K	47	VAL
1	K	48	THR
1	K	97	THR
1	K	112	ASN
1	K	125	ILE
1	K	135	THR
1	K	139	ILE
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	59	LEU
2	L	62	THR
2	L	85	ARG
2	L	100	VAL
2	L	101	THR
2	L	104	VAL
2	L	105	THR
2	L	113	GLN
2	L	129	LEU
2	L	132	LEU
2	L	136	ARG
2	L	142	THR
2	L	159	ILE
2	L	161	THR
2	L	166	ILE
2	L	168	THR
2	L	182	LYS
2	L	184	LEU
2	L	192	THR
2	L	196	VAL
2	L	203	GLU
2	L	214	THR

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Mol	Chain	Res	Type
2	L	225	VAL
2	L	227	VAL
2	L	232	ILE
2	L	270	ARG
2	L	272	LEU
2	L	284	GLU
2	L	287	ILE
2	L	301	LEU
2	L	304	LEU
2	L	305	LEU
2	L	312	THR
2	L	313	LEU
2	L	327	ASN
2	L	349	ILE
2	L	351	ARG
2	L	354	ASP
2	L	365	VAL
2	L	390	ILE
2	L	398	ILE
2	L	400	THR
2	L	402	LEU
2	L	405	LEU
2	L	410	LEU
2	L	412	LEU
2	L	413	LEU
2	L	422	LEU
2	L	430	SER
2	L	431	LEU
2	L	447	GLN
2	L	453	LEU
2	L	455	LEU
2	L	456	SER
2	L	466	ARG
2	L	490	LEU
2	L	499	CYS
2	L	503	ARG
2	L	516	ARG
2	L	519	TRP
2	L	537	ARG
2	L	542	ILE
2	L	578	ARG
2	L	579	THR

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Mol	Chain	Res	Type
2	L	583	THR
2	L	584	THR
2	L	588	LEU
3	V	209	LEU
1	M	22	VAL
1	M	42	VAL
1	M	44	LEU
1	M	47	VAL
1	M	48	THR
1	M	97	THR
1	M	112	ASN
1	M	125	ILE
1	M	135	THR
1	M	139	ILE
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	85	ARG
2	N	100	VAL
2	N	101	THR
2	N	104	VAL
2	N	105	THR
2	N	113	GLN
2	N	129	LEU
2	N	132	LEU
2	N	136	ARG
2	N	142	THR
2	N	159	ILE
2	N	166	ILE
2	N	168	THR
2	N	182	LYS
2	N	184	LEU
2	N	192	THR
2	N	196	VAL

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Mol	Chain	Res	Type
2	N	203	GLU
2	N	214	THR
2	N	225	VAL
2	N	227	VAL
2	N	232	ILE
2	N	270	ARG
2	N	272	LEU
2	N	284	GLU
2	N	287	ILE
2	N	301	LEU
2	N	304	LEU
2	N	305	LEU
2	N	312	THR
2	N	313	LEU
2	N	327	ASN
2	N	351	ARG
2	N	354	ASP
2	N	365	VAL
2	N	390	ILE
2	N	397	SER
2	N	398	ILE
2	N	400	THR
2	N	402	LEU
2	N	405	LEU
2	N	410	LEU
2	N	412	LEU
2	N	413	LEU
2	N	422	LEU
2	N	431	LEU
2	N	447	GLN
2	N	453	LEU
2	N	455	LEU
2	N	456	SER
2	N	466	ARG
2	N	490	LEU
2	N	499	CYS
2	N	503	ARG
2	N	516	ARG
2	N	519	TRP
2	N	528	THR
2	N	537	ARG
2	N	542	ILE

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Mol	Chain	Res	Type
2	N	578	ARG
2	N	579	THR
2	N	583	THR
2	N	588	LEU
3	W	209	LEU
1	O	22	VAL
1	O	35	ASP
1	O	42	VAL
1	O	44	LEU
1	O	47	VAL
1	O	48	THR
1	O	112	ASN
1	O	125	ILE
1	O	135	THR
1	O	139	ILE
1	O	160	GLU
2	P	14	VAL
2	P	16	THR
2	P	17	VAL
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	85	ARG
2	P	100	VAL
2	P	101	THR
2	P	104	VAL
2	P	105	THR
2	P	113	GLN
2	P	129	LEU
2	P	132	LEU
2	P	136	ARG
2	P	142	THR
2	P	159	ILE
2	P	161	THR
2	P	166	ILE
2	P	168	THR
2	P	171	MET
2	P	182	LYS

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Mol	Chain	Res	Type
2	P	184	LEU
2	P	192	THR
2	P	196	VAL
2	P	203	GLU
2	P	214	THR
2	P	225	VAL
2	P	227	VAL
2	P	232	ILE
2	P	270	ARG
2	P	272	LEU
2	P	284	GLU
2	P	287	ILE
2	P	301	LEU
2	P	304	LEU
2	P	305	LEU
2	P	312	THR
2	P	313	LEU
2	P	327	ASN
2	P	351	ARG
2	P	354	ASP
2	P	365	VAL
2	P	390	ILE
2	P	397	SER
2	P	398	ILE
2	P	400	THR
2	P	402	LEU
2	P	405	LEU
2	P	410	LEU
2	P	412	LEU
2	P	413	LEU
2	P	422	LEU
2	P	430	SER
2	P	431	LEU
2	P	447	GLN
2	P	453	LEU
2	P	455	LEU
2	P	456	SER
2	P	466	ARG
2	P	490	LEU
2	P	499	CYS
2	P	503	ARG
2	P	516	ARG

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Mol	Chain	Res	Type
2	P	519	TRP
2	P	537	ARG
2	P	542	ILE
2	P	578	ARG
2	P	579	THR
2	P	583	THR
2	P	588	LEU
3	X	209	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	62	HIS
2	B	54	HIS
2	B	74	ASN
2	B	191	ASN
2	B	294	GLN
2	B	310	HIS
2	B	327	ASN
2	B	343	GLN
2	B	460	GLN
2	B	489	ASN
2	B	530	GLN
1	C	31	HIS
1	C	62	HIS
1	C	106	ASN
1	C	119	GLN
2	D	54	HIS
2	D	74	ASN
2	D	109	ASN
2	D	110	ASN
2	D	190	HIS
2	D	191	ASN
2	D	294	GLN
2	D	310	HIS
2	D	327	ASN
2	D	343	GLN
2	D	426	ASN
2	D	460	GLN
2	D	489	ASN
2	D	530	GLN

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Mol	Chain	Res	Type
1	E	31	HIS
1	E	62	HIS
2	F	54	HIS
2	F	74	ASN
2	F	113	GLN
2	F	191	ASN
2	F	310	HIS
2	F	327	ASN
2	F	343	GLN
2	F	426	ASN
2	F	460	GLN
2	F	489	ASN
2	F	530	GLN
1	G	31	HIS
1	G	62	HIS
2	H	23	GLN
2	H	54	HIS
2	H	74	ASN
2	H	95	ASN
2	H	110	ASN
2	H	118	HIS
2	H	191	ASN
2	H	315	GLN
2	H	319	ASN
2	H	343	GLN
2	H	375	GLN
2	H	447	GLN
2	H	460	GLN
2	H	530	GLN
1	I	31	HIS
1	I	62	HIS
1	I	109	ASN
1	I	119	GLN
2	J	23	GLN
2	J	54	HIS
2	J	109	ASN
2	J	191	ASN
2	J	294	GLN
2	J	310	HIS
2	J	327	ASN
2	J	343	GLN
2	J	426	ASN

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Mol	Chain	Res	Type
2	J	460	GLN
2	J	489	ASN
2	J	530	GLN
1	K	31	HIS
1	K	62	HIS
1	K	106	ASN
1	K	119	GLN
2	L	54	HIS
2	L	109	ASN
2	L	191	ASN
2	L	294	GLN
2	L	310	HIS
2	L	327	ASN
2	L	343	GLN
2	L	426	ASN
2	L	460	GLN
2	L	489	ASN
2	L	530	GLN
1	M	31	HIS
1	M	62	HIS
1	M	109	ASN
2	N	54	HIS
2	N	109	ASN
2	N	113	GLN
2	N	191	ASN
2	N	310	HIS
2	N	327	ASN
2	N	343	GLN
2	N	426	ASN
2	N	460	GLN
2	N	489	ASN
2	N	530	GLN
1	O	31	HIS
1	O	62	HIS
1	O	109	ASN
2	P	54	HIS
2	P	109	ASN
2	P	191	ASN
2	P	310	HIS
2	P	327	ASN
2	P	343	GLN
2	P	426	ASN

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Mol	Chain	Res	Type
2	P	460	GLN
2	P	489	ASN
2	P	530	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	4.42	4 (100%)	6,6,6	1.25	1 (16%)
5	PO4	D	1102	-	4,4,4	4.55	4 (100%)	6,6,6	0.60	0
5	PO4	L	1101	-	4,4,4	4.27	4 (100%)	6,6,6	1.58	1 (16%)
5	PO4	L	1103	-	4,4,4	4.52	4 (100%)	6,6,6	0.86	0
5	PO4	J	1103	-	4,4,4	4.19	4 (100%)	6,6,6	1.03	0
5	PO4	B	1103	-	4,4,4	4.25	3 (75%)	6,6,6	1.58	2 (33%)
5	PO4	J	1101	-	4,4,4	4.52	4 (100%)	6,6,6	0.83	0
5	PO4	N	1104	-	4,4,4	4.51	4 (100%)	6,6,6	0.87	0
5	PO4	D	1101	-	4,4,4	4.29	4 (100%)	6,6,6	1.21	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	N	1102	-	4,4,4	4.43	4 (100%)	6,6,6	0.54	0
5	PO4	D	1103	-	4,4,4	4.09	4 (100%)	6,6,6	0.99	0
5	PO4	L	1104	-	4,4,4	4.42	4 (100%)	6,6,6	0.61	0
5	PO4	P	1103	-	4,4,4	4.42	4 (100%)	6,6,6	1.10	0
5	PO4	F	1102	-	4,4,4	4.58	4 (100%)	6,6,6	0.60	0
5	PO4	N	1103	-	4,4,4	4.34	4 (100%)	6,6,6	1.04	0
4	OGK	L	1100	-	25,25,25	6.93	12 (48%)	31,38,38	3.02	16 (51%)
5	PO4	H	1104	-	4,4,4	4.38	3 (75%)	6,6,6	2.27	3 (50%)
4	OGK	J	1100	-	25,25,25	6.65	10 (40%)	31,38,38	2.73	14 (45%)
5	PO4	L	1102	-	4,4,4	4.47	4 (100%)	6,6,6	0.63	0
5	PO4	F	1101	-	4,4,4	4.38	4 (100%)	6,6,6	1.63	1 (16%)
5	PO4	H	1103	-	4,4,4	4.52	4 (100%)	6,6,6	0.54	0
5	PO4	N	1101	-	4,4,4	4.37	4 (100%)	6,6,6	1.26	1 (16%)
5	PO4	F	1103	-	4,4,4	4.33	4 (100%)	6,6,6	1.00	0
5	PO4	J	1104	-	4,4,4	4.29	4 (100%)	6,6,6	0.85	0
4	OGK	F	1100	-	25,25,25	6.91	10 (40%)	31,38,38	2.53	16 (51%)
5	PO4	P	1104	-	4,4,4	4.95	3 (75%)	6,6,6	1.37	1 (16%)
5	PO4	B	1104	-	4,4,4	4.17	4 (100%)	6,6,6	1.26	1 (16%)
4	OGK	B	1100	-	25,25,25	6.83	11 (44%)	31,38,38	2.78	12 (38%)
5	PO4	F	1104	-	4,4,4	4.61	4 (100%)	6,6,6	1.40	1 (16%)
5	PO4	P	1101	-	4,4,4	4.30	4 (100%)	6,6,6	0.88	0
4	OGK	H	1100	-	25,25,25	6.82	11 (44%)	31,38,38	2.54	15 (48%)
5	PO4	H	1102	-	4,4,4	4.75	4 (100%)	6,6,6	0.70	0
4	OGK	N	1100	-	25,25,25	6.87	11 (44%)	31,38,38	2.51	10 (32%)
5	PO4	B	1102	-	4,4,4	4.53	4 (100%)	6,6,6	0.48	0
5	PO4	D	1104	-	4,4,4	4.29	4 (100%)	6,6,6	1.43	1 (16%)
4	OGK	P	1100	-	25,25,25	7.01	11 (44%)	31,38,38	2.84	13 (41%)
4	OGK	D	1100	-	25,25,25	6.78	10 (40%)	31,38,38	3.12	13 (41%)
5	PO4	P	1102	-	4,4,4	4.52	4 (100%)	6,6,6	0.66	0
5	PO4	B	1101	-	4,4,4	4.32	4 (100%)	6,6,6	0.89	0
5	PO4	J	1102	-	4,4,4	4.59	4 (100%)	6,6,6	0.77	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	H	1100	-	1/1/9/10	9/19/52/52	0/3/3/3
4	OGK	F	1100	-	-	12/19/52/52	0/3/3/3
4	OGK	N	1100	-	-	7/19/52/52	0/3/3/3
4	OGK	P	1100	-	-	12/19/52/52	0/3/3/3
4	OGK	D	1100	-	1/1/9/10	7/19/52/52	0/3/3/3
4	OGK	L	1100	-	1/1/9/10	11/19/52/52	0/3/3/3
4	OGK	J	1100	-	-	5/19/52/52	0/3/3/3
4	OGK	B	1100	-	1/1/9/10	8/19/52/52	0/3/3/3

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1100	OGK	C13-C09	-22.91	1.27	1.51
4	P	1100	OGK	C13-C09	-22.58	1.27	1.51
4	L	1100	OGK	C13-C09	-22.33	1.28	1.51
4	F	1100	OGK	C13-C09	-22.09	1.28	1.51
4	H	1100	OGK	C13-C09	-22.01	1.28	1.51
4	B	1100	OGK	C13-C09	-21.91	1.28	1.51
4	J	1100	OGK	C13-C09	-21.69	1.28	1.51
4	N	1100	OGK	C13-C09	-21.67	1.28	1.51
4	P	1100	OGK	C09-C14	-17.52	1.34	1.52
4	B	1100	OGK	C09-C14	-17.52	1.34	1.52
4	F	1100	OGK	C09-C14	-17.43	1.34	1.52
4	N	1100	OGK	C09-C14	-17.25	1.34	1.52
4	L	1100	OGK	C09-C14	-16.61	1.35	1.52
4	H	1100	OGK	C09-C14	-16.54	1.35	1.52
4	J	1100	OGK	C09-C14	-16.27	1.35	1.52
4	D	1100	OGK	C09-C14	-16.21	1.35	1.52
4	L	1100	OGK	C09-C10	-15.56	1.15	1.52
4	H	1100	OGK	C09-C10	-15.56	1.15	1.52
4	N	1100	OGK	C09-C10	-15.55	1.15	1.52
4	P	1100	OGK	C09-C10	-15.36	1.15	1.52
4	F	1100	OGK	C09-C10	-15.16	1.16	1.52
4	B	1100	OGK	C09-C10	-14.97	1.16	1.52
4	D	1100	OGK	C09-C10	-14.74	1.17	1.52
4	J	1100	OGK	C09-C10	-14.63	1.17	1.52
5	P	1104	PO4	P-O1	8.30	1.69	1.50
4	F	1100	OGK	C13-C14	-7.72	1.32	1.50
4	B	1100	OGK	C13-C14	-7.63	1.32	1.50
4	L	1100	OGK	C13-C14	-7.50	1.32	1.50
4	J	1100	OGK	C13-C14	-7.43	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1100	OGK	C13-C14	-7.40	1.32	1.50
4	H	1100	OGK	C13-C14	-7.37	1.32	1.50
4	P	1100	OGK	C13-C14	-7.34	1.33	1.50
4	N	1100	OGK	C13-C14	-7.25	1.33	1.50
4	N	1100	OGK	C06-N08	7.17	1.49	1.34
5	F	1103	PO4	P-O1	7.10	1.67	1.50
5	F	1104	PO4	P-O1	7.01	1.66	1.50
5	H	1102	PO4	P-O1	6.96	1.66	1.50
4	P	1100	OGK	C06-N08	6.95	1.48	1.34
5	L	1104	PO4	P-O1	6.95	1.66	1.50
5	L	1103	PO4	P-O1	6.93	1.66	1.50
4	L	1100	OGK	C06-N08	6.92	1.48	1.34
4	F	1100	OGK	C06-N08	6.88	1.48	1.34
5	B	1103	PO4	P-O1	6.86	1.66	1.50
5	P	1103	PO4	P-O1	6.80	1.66	1.50
5	H	1103	PO4	P-O1	6.77	1.66	1.50
5	J	1102	PO4	P-O1	6.75	1.66	1.50
5	N	1104	PO4	P-O1	6.74	1.66	1.50
5	F	1102	PO4	P-O1	6.73	1.66	1.50
5	B	1102	PO4	P-O1	6.69	1.66	1.50
5	J	1104	PO4	P-O1	6.67	1.66	1.50
5	H	1104	PO4	P-O1	6.65	1.66	1.50
5	L	1102	PO4	P-O1	6.64	1.66	1.50
5	N	1102	PO4	P-O1	6.64	1.66	1.50
5	N	1103	PO4	P-O1	6.58	1.65	1.50
5	P	1102	PO4	P-O1	6.57	1.65	1.50
5	D	1102	PO4	P-O1	6.55	1.65	1.50
5	J	1101	PO4	P-O1	6.55	1.65	1.50
5	D	1103	PO4	P-O1	6.53	1.65	1.50
4	B	1100	OGK	C06-N08	6.52	1.47	1.34
5	J	1103	PO4	P-O1	6.49	1.65	1.50
5	L	1101	PO4	P-O1	6.26	1.65	1.50
5	D	1104	PO4	P-O1	6.25	1.65	1.50
5	B	1101	PO4	P-O1	6.25	1.65	1.50
5	P	1101	PO4	P-O1	6.11	1.64	1.50
5	F	1101	PO4	P-O1	6.09	1.64	1.50
4	J	1100	OGK	C06-N08	6.07	1.46	1.34
5	B	1104	PO4	P-O1	6.06	1.64	1.50
5	N	1101	PO4	P-O1	6.05	1.64	1.50
5	H	1101	PO4	P-O1	6.04	1.64	1.50
5	D	1101	PO4	P-O1	6.03	1.64	1.50
4	H	1100	OGK	C06-N08	5.77	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1100	OGK	C06-N08	5.66	1.45	1.34
5	H	1102	PO4	P-O3	4.45	1.67	1.54
5	B	1101	PO4	P-O3	4.35	1.67	1.54
5	F	1104	PO4	P-O3	4.32	1.67	1.54
5	F	1101	PO4	P-O3	4.32	1.67	1.54
5	H	1101	PO4	P-O3	4.31	1.67	1.54
5	D	1102	PO4	P-O3	4.27	1.67	1.54
5	D	1101	PO4	P-O3	4.27	1.67	1.54
5	J	1102	PO4	P-O3	4.27	1.67	1.54
5	J	1101	PO4	P-O3	4.27	1.67	1.54
4	F	1100	OGK	C18-C17	-4.23	1.43	1.54
5	N	1104	PO4	P-O4	4.21	1.66	1.54
5	H	1102	PO4	P-O4	4.21	1.66	1.54
5	P	1101	PO4	P-O4	4.20	1.66	1.54
4	L	1100	OGK	C23-C22	4.18	1.60	1.53
4	H	1100	OGK	C23-C22	4.18	1.60	1.53
5	N	1101	PO4	P-O3	4.16	1.66	1.54
5	P	1102	PO4	P-O3	4.13	1.66	1.54
5	F	1102	PO4	P-O3	4.12	1.66	1.54
5	D	1104	PO4	P-O4	4.07	1.66	1.54
5	N	1101	PO4	P-O4	4.03	1.66	1.54
5	H	1104	PO4	P-O4	4.01	1.66	1.54
5	L	1102	PO4	P-O3	4.00	1.66	1.54
4	P	1100	OGK	C23-C22	3.97	1.59	1.53
5	L	1101	PO4	P-O3	3.96	1.66	1.54
5	L	1103	PO4	P-O3	3.96	1.66	1.54
5	H	1103	PO4	P-O3	3.95	1.66	1.54
5	B	1104	PO4	P-O3	3.90	1.66	1.54
5	B	1102	PO4	P-O3	3.90	1.66	1.54
5	F	1102	PO4	P-O4	3.89	1.66	1.54
4	N	1100	OGK	C23-C22	3.89	1.59	1.53
5	D	1102	PO4	P-O4	3.88	1.65	1.54
5	P	1102	PO4	P-O4	3.88	1.65	1.54
5	H	1104	PO4	P-O3	3.87	1.65	1.54
5	H	1101	PO4	P-O4	3.86	1.65	1.54
5	N	1103	PO4	P-O3	3.85	1.65	1.54
5	N	1102	PO4	P-O4	3.84	1.65	1.54
5	D	1101	PO4	P-O4	3.84	1.65	1.54
5	J	1102	PO4	P-O4	3.77	1.65	1.54
4	P	1100	OGK	C18-C17	-3.76	1.44	1.54
5	B	1103	PO4	P-O3	3.73	1.65	1.54
5	L	1102	PO4	P-O4	3.73	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1100	OGK	O12-C10	3.73	1.43	1.30
5	J	1101	PO4	P-O4	3.73	1.65	1.54
5	P	1103	PO4	P-O4	3.71	1.65	1.54
5	P	1103	PO4	P-O3	3.71	1.65	1.54
5	N	1102	PO4	P-O3	3.69	1.65	1.54
5	B	1102	PO4	P-O4	3.68	1.65	1.54
4	N	1100	OGK	O12-C10	3.67	1.43	1.30
5	B	1104	PO4	P-O4	3.65	1.65	1.54
5	N	1104	PO4	P-O3	3.65	1.65	1.54
4	J	1100	OGK	C18-C17	-3.64	1.44	1.54
5	D	1104	PO4	P-O3	3.63	1.65	1.54
5	P	1104	PO4	P-O4	3.63	1.65	1.54
5	L	1104	PO4	P-O4	3.61	1.65	1.54
4	F	1100	OGK	O12-C10	3.57	1.43	1.30
5	P	1101	PO4	P-O3	3.55	1.65	1.54
4	H	1100	OGK	O12-C10	3.54	1.43	1.30
5	J	1103	PO4	P-O3	3.54	1.64	1.54
5	J	1104	PO4	P-O3	3.53	1.64	1.54
5	F	1103	PO4	P-O4	3.52	1.64	1.54
5	L	1104	PO4	P-O3	3.51	1.64	1.54
5	P	1104	PO4	P-O3	3.49	1.64	1.54
4	N	1100	OGK	C18-C17	-3.47	1.45	1.54
4	L	1100	OGK	C09-N08	3.45	1.51	1.45
4	L	1100	OGK	O12-C10	3.45	1.42	1.30
4	B	1100	OGK	C18-C17	-3.45	1.45	1.54
4	J	1100	OGK	C05-C06	3.44	1.57	1.51
5	N	1103	PO4	P-O4	3.40	1.64	1.54
5	F	1101	PO4	P-O4	3.38	1.64	1.54
4	P	1100	OGK	O12-C10	3.38	1.42	1.30
4	D	1100	OGK	C18-C17	-3.37	1.45	1.54
5	J	1104	PO4	P-O4	3.36	1.64	1.54
4	L	1100	OGK	C05-C06	3.33	1.57	1.51
5	L	1103	PO4	P-O4	3.32	1.64	1.54
5	H	1103	PO4	P-O4	3.31	1.64	1.54
4	L	1100	OGK	C18-C17	-3.27	1.45	1.54
5	F	1104	PO4	P-O4	3.25	1.64	1.54
4	H	1100	OGK	C18-C17	-3.21	1.46	1.54
5	L	1101	PO4	P-O4	3.20	1.64	1.54
4	D	1100	OGK	O07-C06	-3.17	1.17	1.23
4	B	1100	OGK	O12-C10	3.16	1.41	1.30
5	F	1101	PO4	P-O2	-3.12	1.45	1.54
4	H	1100	OGK	C09-N08	3.10	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1101	PO4	P-O4	3.10	1.63	1.54
4	D	1100	OGK	O12-C10	3.07	1.41	1.30
5	D	1103	PO4	P-O4	3.06	1.63	1.54
4	H	1100	OGK	O07-C06	-3.05	1.17	1.23
5	H	1103	PO4	P-O2	-3.02	1.45	1.54
5	J	1103	PO4	P-O4	3.01	1.63	1.54
5	D	1103	PO4	P-O3	2.99	1.63	1.54
4	P	1100	OGK	O07-C06	-2.98	1.17	1.23
5	B	1102	PO4	P-O2	-2.93	1.46	1.54
5	H	1101	PO4	P-O2	-2.91	1.46	1.54
4	B	1100	OGK	C23-C22	2.90	1.58	1.53
4	F	1100	OGK	C09-N08	2.89	1.50	1.45
5	B	1103	PO4	P-O4	2.88	1.63	1.54
5	L	1101	PO4	P-O2	-2.81	1.46	1.54
5	F	1103	PO4	P-O3	2.76	1.62	1.54
4	D	1100	OGK	C05-C06	2.75	1.56	1.51
4	P	1100	OGK	C09-N08	2.75	1.50	1.45
5	B	1101	PO4	P-O2	-2.70	1.46	1.54
5	L	1103	PO4	P-O2	-2.63	1.47	1.54
5	J	1101	PO4	P-O2	-2.61	1.47	1.54
5	F	1104	PO4	P-O2	-2.59	1.47	1.54
5	D	1102	PO4	P-O2	-2.56	1.47	1.54
4	J	1100	OGK	C09-N08	2.56	1.49	1.45
5	F	1102	PO4	P-O2	-2.55	1.47	1.54
5	J	1103	PO4	P-O2	-2.55	1.47	1.54
4	D	1100	OGK	C23-C22	2.53	1.57	1.53
5	P	1101	PO4	P-O2	-2.53	1.47	1.54
5	P	1102	PO4	P-O2	-2.53	1.47	1.54
4	J	1100	OGK	C23-C22	2.49	1.57	1.53
5	N	1102	PO4	P-O2	-2.48	1.47	1.54
5	J	1102	PO4	P-O2	-2.48	1.47	1.54
4	B	1100	OGK	O07-C06	-2.47	1.18	1.23
5	N	1101	PO4	P-O2	-2.47	1.47	1.54
4	F	1100	OGK	O07-C06	-2.42	1.18	1.23
5	L	1102	PO4	P-O2	-2.42	1.47	1.54
5	D	1103	PO4	P-O2	-2.40	1.47	1.54
4	L	1100	OGK	O07-C06	-2.37	1.18	1.23
4	B	1100	OGK	C04-C05	-2.37	1.50	1.53
5	N	1103	PO4	P-O2	-2.35	1.47	1.54
5	J	1104	PO4	P-O2	-2.34	1.47	1.54
4	P	1100	OGK	C05-C06	2.31	1.55	1.51
4	B	1100	OGK	C22-C17	-2.29	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	1100	OGK	C05-C06	2.29	1.55	1.51
4	F	1100	OGK	C04-C05	-2.28	1.50	1.53
4	N	1100	OGK	C04-C05	-2.25	1.50	1.53
5	N	1104	PO4	P-O2	-2.23	1.48	1.54
5	D	1104	PO4	P-O2	-2.16	1.48	1.54
5	F	1103	PO4	P-O2	-2.14	1.48	1.54
5	L	1104	PO4	P-O2	-2.12	1.48	1.54
5	B	1104	PO4	P-O2	-2.11	1.48	1.54
5	H	1102	PO4	P-O2	-2.10	1.48	1.54
5	P	1103	PO4	P-O2	-2.06	1.48	1.54
4	H	1100	OGK	C05-C06	2.05	1.55	1.51
5	D	1101	PO4	P-O2	-2.05	1.48	1.54
4	L	1100	OGK	C04-C05	-2.03	1.50	1.53
4	N	1100	OGK	C09-N08	2.02	1.49	1.45

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1100	OGK	C14-C09-C10	7.72	134.32	117.69
4	P	1100	OGK	C13-C09-N08	-7.40	108.01	117.77
4	B	1100	OGK	C04-C05-C17	7.22	123.99	110.06
4	D	1100	OGK	C13-C14-C09	-6.88	56.76	60.30
4	L	1100	OGK	C05-C04-C03	6.79	123.03	109.20
4	B	1100	OGK	C14-C09-C10	6.32	131.31	117.69
4	L	1100	OGK	C13-C14-C09	-6.02	57.21	60.30
4	N	1100	OGK	C18-C17-C22	5.99	110.93	103.97
4	P	1100	OGK	C13-C14-C09	-5.98	57.22	60.30
4	N	1100	OGK	C14-C09-C10	5.97	130.55	117.69
4	H	1100	OGK	C13-C14-C09	-5.87	57.28	60.30
4	J	1100	OGK	C14-C09-C10	5.79	130.16	117.69
4	J	1100	OGK	C13-C14-C09	-5.63	57.41	60.30
4	D	1100	OGK	C04-C05-C17	5.50	120.67	110.06
4	D	1100	OGK	C14-C09-N08	-5.42	102.80	117.62
4	N	1100	OGK	C13-C14-C09	-5.31	57.57	60.30
4	J	1100	OGK	C05-C04-C03	5.28	119.96	109.20
4	F	1100	OGK	C13-C14-C09	-5.13	57.66	60.30
4	D	1100	OGK	C05-C04-C03	5.04	119.47	109.20
4	B	1100	OGK	C14-C09-N08	-5.02	103.91	117.62
4	B	1100	OGK	C13-C14-C09	-5.02	57.72	60.30
4	L	1100	OGK	C15-C14-C13	-4.99	114.26	121.32
4	P	1100	OGK	O07-C06-C05	-4.82	115.90	121.67
4	L	1100	OGK	C04-C05-C17	4.79	119.29	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1100	OGK	C05-C04-C03	4.71	118.80	109.20
4	J	1100	OGK	C14-C09-N08	-4.67	104.87	117.62
4	H	1100	OGK	C18-C17-C22	4.61	109.33	103.97
4	P	1100	OGK	C04-C03-C02	-4.55	104.11	112.25
4	J	1100	OGK	C04-C05-C17	4.55	118.83	110.06
4	L	1100	OGK	C14-C09-C10	4.50	127.38	117.69
4	B	1100	OGK	C04-C03-C02	-4.48	104.24	112.25
4	B	1100	OGK	C05-C04-C03	4.41	118.19	109.20
4	P	1100	OGK	C05-C04-C03	4.39	118.14	109.20
4	L	1100	OGK	C13-C09-N08	-4.35	112.03	117.77
4	F	1100	OGK	C14-C09-C10	4.32	127.01	117.69
4	H	1100	OGK	C14-C09-C10	4.31	126.97	117.69
5	H	1104	PO4	O3-P-O2	4.30	121.30	107.91
4	N	1100	OGK	C14-C09-N08	-4.28	105.92	117.62
4	F	1100	OGK	C04-C05-C17	4.05	117.86	110.06
4	F	1100	OGK	C14-C09-N08	-4.02	106.64	117.62
4	D	1100	OGK	C04-C03-C02	-3.95	105.18	112.25
4	P	1100	OGK	C15-C14-C13	-3.93	115.75	121.32
4	J	1100	OGK	O12-C10-C09	3.88	123.96	113.66
4	H	1100	OGK	C14-C09-N08	-3.88	107.03	117.62
4	H	1100	OGK	C05-C04-C03	3.86	117.06	109.20
4	L	1100	OGK	C04-C03-C02	-3.85	105.37	112.25
4	D	1100	OGK	C13-C09-N08	-3.77	112.80	117.77
4	F	1100	OGK	O12-C10-C09	3.72	123.53	113.66
4	N	1100	OGK	C04-C03-C02	-3.63	105.76	112.25
4	D	1100	OGK	C09-C13-C14	3.62	62.64	60.84
4	P	1100	OGK	C14-C09-C10	3.61	125.46	117.69
4	P	1100	OGK	C13-C09-C14	3.60	60.97	59.12
4	N	1100	OGK	C22-C23-C03	3.59	116.51	109.20
4	H	1100	OGK	O07-C06-N08	-3.52	115.80	123.15
4	L	1100	OGK	O07-C06-N08	-3.52	115.81	123.15
4	D	1100	OGK	O12-C10-O11	-3.51	112.64	123.86
4	H	1100	OGK	C22-C23-C03	3.51	116.34	109.20
4	L	1100	OGK	C05-C06-N08	3.44	120.67	116.18
4	L	1100	OGK	C18-C17-C22	3.38	107.89	103.97
4	J	1100	OGK	C18-C17-C22	3.32	107.83	103.97
4	B	1100	OGK	O07-C06-C05	-3.29	117.74	121.67
4	L	1100	OGK	C22-C23-C03	3.24	115.81	109.20
4	N	1100	OGK	C13-C09-C14	3.21	60.77	59.12
4	N	1100	OGK	C05-C04-C03	3.19	115.70	109.20
4	J	1100	OGK	C04-C03-C02	-3.16	106.59	112.25
4	F	1100	OGK	C22-C23-C03	3.15	115.61	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1100	OGK	O12-C10-C09	3.13	121.97	113.66
4	L	1100	OGK	C09-C13-C14	3.03	62.34	60.84
4	F	1100	OGK	C18-C19-C20	-2.98	102.44	105.39
4	J	1100	OGK	C09-C13-C14	2.96	62.31	60.84
4	D	1100	OGK	O07-C06-N08	-2.90	117.09	123.15
4	B	1100	OGK	C13-C09-N08	-2.89	113.96	117.77
4	J	1100	OGK	C13-C09-C10	2.88	121.45	116.57
4	D	1100	OGK	C13-C09-C14	2.88	60.60	59.12
5	F	1101	PO4	O4-P-O3	2.86	116.82	107.91
4	P	1100	OGK	O07-C06-N08	-2.86	117.17	123.15
5	B	1103	PO4	O4-P-O3	-2.85	99.04	107.91
4	D	1100	OGK	O12-C10-C09	2.84	121.19	113.66
5	D	1104	PO4	O3-P-O1	-2.83	100.93	110.95
4	F	1100	OGK	C04-C03-C02	-2.80	107.24	112.25
4	H	1100	OGK	C04-C05-C17	2.77	115.41	110.06
4	H	1100	OGK	C09-C13-C14	2.76	62.21	60.84
5	L	1101	PO4	O4-P-O1	-2.75	101.21	110.95
4	H	1100	OGK	C05-C06-N08	2.75	119.77	116.18
4	P	1100	OGK	C04-C05-C17	2.71	115.28	110.06
4	H	1100	OGK	C13-C09-C14	2.70	60.51	59.12
4	F	1100	OGK	C13-C09-N08	-2.70	114.21	117.77
4	J	1100	OGK	O07-C06-N08	-2.69	117.54	123.15
4	H	1100	OGK	O07-C06-C05	-2.68	118.46	121.67
4	H	1100	OGK	C23-C03-C02	2.67	117.04	112.25
4	J	1100	OGK	C13-C09-N08	-2.61	114.33	117.77
4	L	1100	OGK	C14-C09-N08	-2.60	110.52	117.62
4	B	1100	OGK	C13-C09-C14	2.60	60.46	59.12
5	P	1104	PO4	O2-P-O1	2.59	120.12	110.95
4	L	1100	OGK	C13-C09-C14	2.59	60.45	59.12
4	F	1100	OGK	O07-C06-C05	-2.57	118.60	121.67
4	P	1100	OGK	C14-C09-N08	-2.54	110.67	117.62
4	B	1100	OGK	O12-C10-O11	-2.54	115.73	123.86
4	H	1100	OGK	C15-C14-C13	2.44	124.77	121.32
4	B	1100	OGK	C18-C19-C20	-2.43	102.98	105.39
4	D	1100	OGK	O07-C06-C05	2.42	124.57	121.67
4	F	1100	OGK	C13-C09-C14	2.40	60.36	59.12
5	H	1104	PO4	O3-P-O1	-2.40	102.46	110.95
5	N	1101	PO4	O4-P-O3	2.40	115.39	107.91
5	H	1104	PO4	O4-P-O3	-2.39	100.49	107.91
4	F	1100	OGK	O12-C10-O11	-2.38	116.24	123.86
5	B	1103	PO4	O3-P-O2	2.38	115.31	107.91
4	P	1100	OGK	O12-C10-C09	2.37	119.94	113.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1100	OGK	C13-C09-C10	2.36	120.57	116.57
4	J	1100	OGK	O12-C10-O11	-2.34	116.38	123.86
5	B	1104	PO4	O4-P-O1	-2.32	102.75	110.95
4	F	1100	OGK	C09-C13-C14	2.30	61.98	60.84
5	H	1101	PO4	O4-P-O3	2.29	115.04	107.91
4	J	1100	OGK	C13-C09-C14	2.27	60.29	59.12
5	F	1104	PO4	O2-P-O1	2.23	118.84	110.95
5	D	1101	PO4	O3-P-O1	-2.22	103.11	110.95
4	H	1100	OGK	O12-C10-C09	2.21	119.52	113.66
4	B	1100	OGK	C22-C23-C03	2.19	113.67	109.20
4	F	1100	OGK	C15-C14-C13	-2.14	118.28	121.32
4	N	1100	OGK	O12-C10-C09	2.12	119.29	113.66
4	P	1100	OGK	C18-C17-C22	2.11	106.42	103.97
4	L	1100	OGK	C23-C03-C04	2.05	113.60	109.69
4	N	1100	OGK	C13-C09-N08	-2.03	115.09	117.77

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1100	OGK	C05
4	D	1100	OGK	C05
4	H	1100	OGK	C03
4	L	1100	OGK	C05

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1100	OGK	C01-C02-C03-C04
4	B	1100	OGK	C01-C02-C03-C23
4	B	1100	OGK	C17-C05-C06-O07
4	B	1100	OGK	C17-C05-C06-N08
4	B	1100	OGK	N08-C09-C10-O12
4	B	1100	OGK	C14-C09-C10-O12
4	D	1100	OGK	C17-C05-C06-O07
4	D	1100	OGK	C17-C05-C06-N08
4	D	1100	OGK	N08-C09-C10-O12
4	D	1100	OGK	C14-C09-C10-O12
4	F	1100	OGK	C17-C05-C06-O07
4	F	1100	OGK	C17-C05-C06-N08
4	F	1100	OGK	N08-C09-C10-O11
4	F	1100	OGK	N08-C09-C10-O12
4	F	1100	OGK	C14-C09-C10-O11

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Mol	Chain	Res	Type	Atoms
4	F	1100	OGK	C14-C09-C10-O12
4	H	1100	OGK	C17-C05-C06-O07
4	H	1100	OGK	C17-C05-C06-N08
4	H	1100	OGK	N08-C09-C10-O12
4	H	1100	OGK	C14-C09-C10-O11
4	H	1100	OGK	C14-C09-C10-O12
4	J	1100	OGK	C17-C05-C06-O07
4	J	1100	OGK	C17-C05-C06-N08
4	J	1100	OGK	N08-C09-C10-O12
4	J	1100	OGK	C14-C09-C10-O11
4	J	1100	OGK	C14-C09-C10-O12
4	L	1100	OGK	C01-C02-C03-C04
4	L	1100	OGK	C01-C02-C03-C23
4	L	1100	OGK	C17-C05-C06-O07
4	L	1100	OGK	C17-C05-C06-N08
4	L	1100	OGK	N08-C09-C10-O12
4	L	1100	OGK	C14-C09-C10-O11
4	L	1100	OGK	C14-C09-C10-O12
4	N	1100	OGK	C01-C02-C03-C04
4	N	1100	OGK	C01-C02-C03-C23
4	N	1100	OGK	C17-C05-C06-O07
4	N	1100	OGK	C17-C05-C06-N08
4	N	1100	OGK	N08-C09-C10-O12
4	N	1100	OGK	C14-C09-C10-O12
4	P	1100	OGK	C01-C02-C03-C04
4	P	1100	OGK	C01-C02-C03-C23
4	P	1100	OGK	C17-C05-C06-O07
4	P	1100	OGK	C17-C05-C06-N08
4	P	1100	OGK	N08-C09-C10-O11
4	P	1100	OGK	N08-C09-C10-O12
4	P	1100	OGK	C14-C09-C10-O11
4	P	1100	OGK	C14-C09-C10-O12
4	P	1100	OGK	O07-C06-N08-C09
4	H	1100	OGK	O07-C06-N08-C09
4	F	1100	OGK	C01-C02-C03-C04
4	F	1100	OGK	C01-C02-C03-C23
4	F	1100	OGK	C13-C14-C15-C16
4	H	1100	OGK	C13-C14-C15-C16
4	L	1100	OGK	C13-C14-C15-C16
4	N	1100	OGK	C13-C14-C15-C16
4	P	1100	OGK	C13-C14-C15-C16
4	F	1100	OGK	O07-C06-N08-C09

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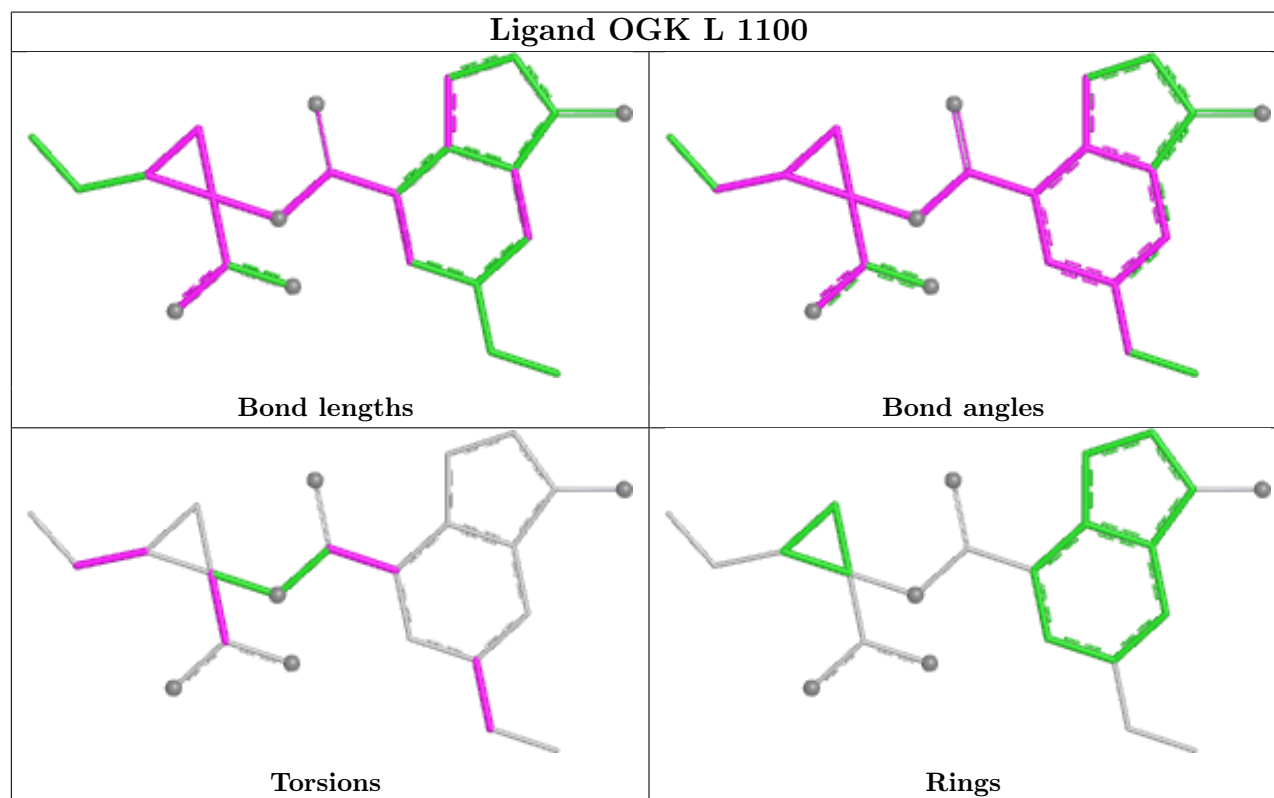
Mol	Chain	Res	Type	Atoms
4	D	1100	OGK	C04-C05-C06-N08
4	H	1100	OGK	C04-C05-C06-N08
4	L	1100	OGK	N08-C09-C10-O11
4	F	1100	OGK	C04-C05-C06-O07
4	B	1100	OGK	C13-C09-C10-O12
4	D	1100	OGK	C13-C09-C10-O12
4	H	1100	OGK	C13-C09-C10-O12
4	L	1100	OGK	C13-C09-C10-O12
4	D	1100	OGK	C04-C05-C06-O07
4	P	1100	OGK	C04-C05-C06-O07
4	B	1100	OGK	C04-C05-C06-N08
4	L	1100	OGK	C04-C05-C06-N08
4	F	1100	OGK	C13-C09-C10-O11
4	P	1100	OGK	C13-C09-C10-O11

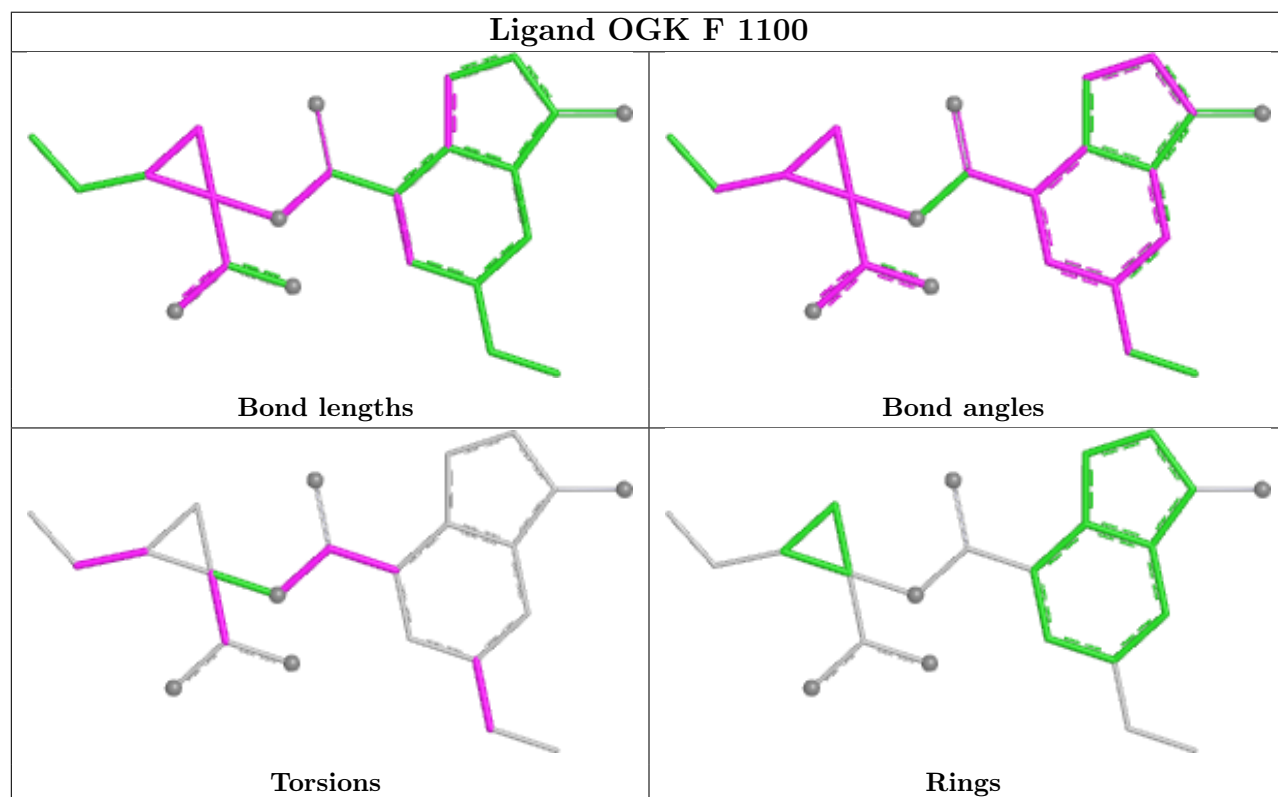
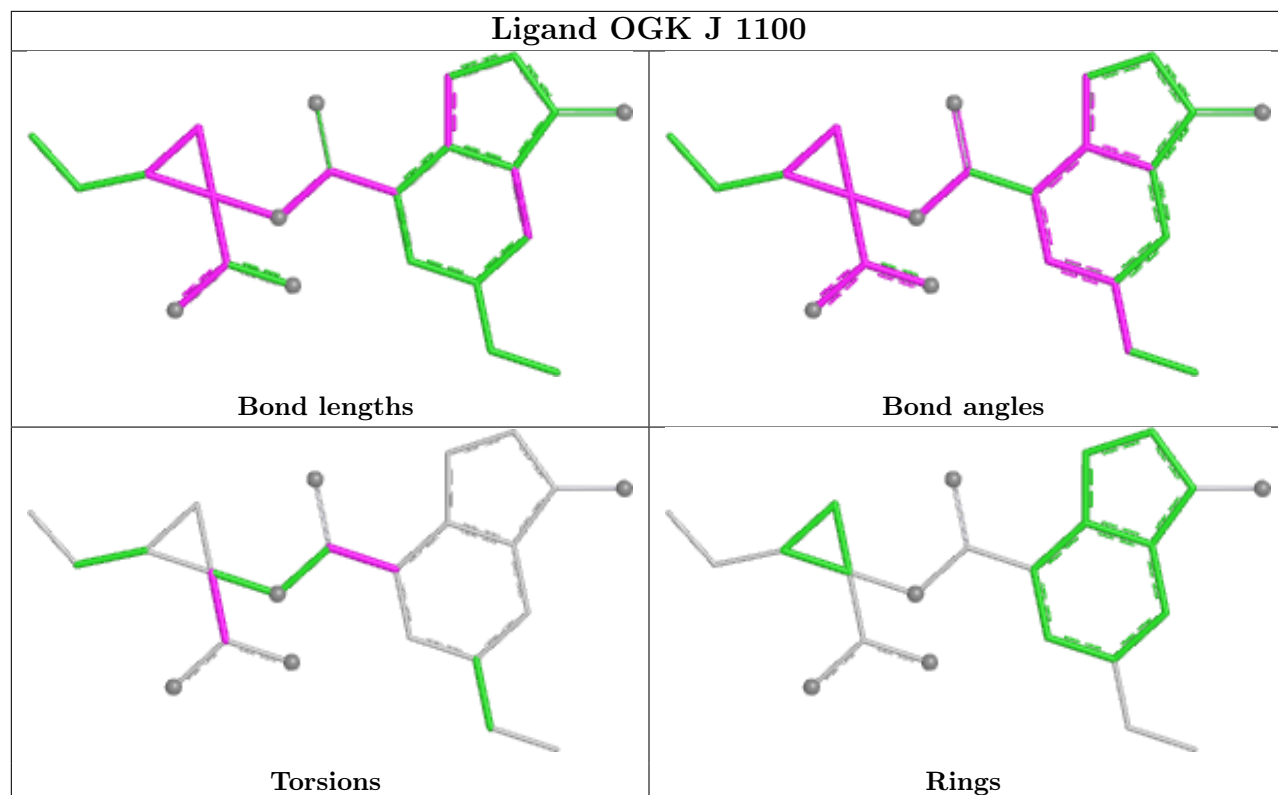
There are no ring outliers.

23 monomers are involved in 79 short contacts:

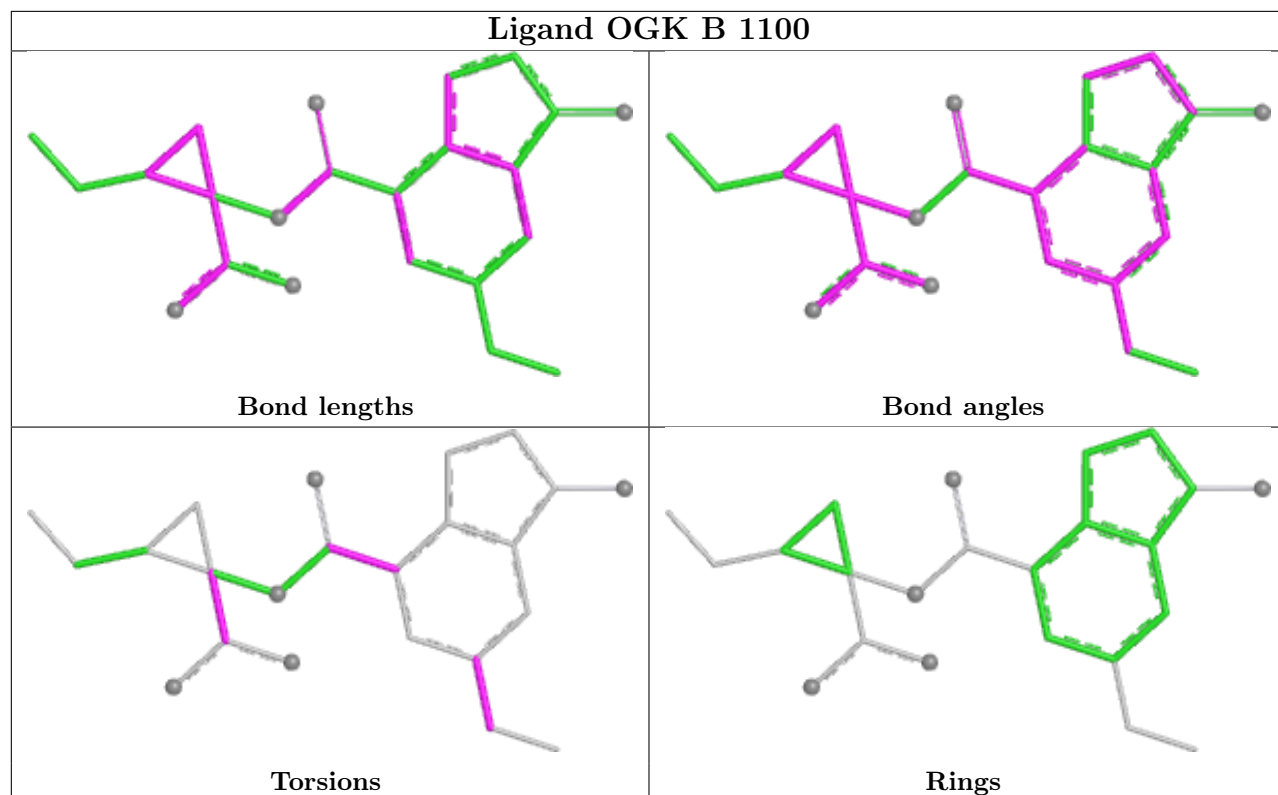
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1101	PO4	2	0
5	L	1103	PO4	1	0
5	J	1103	PO4	2	0
5	B	1103	PO4	2	0
5	D	1101	PO4	1	0
5	D	1103	PO4	2	0
5	P	1103	PO4	2	0
5	N	1103	PO4	2	0
4	L	1100	OGK	11	0
5	H	1104	PO4	1	0
4	J	1100	OGK	7	0
5	F	1101	PO4	1	0
5	H	1103	PO4	4	0
5	N	1101	PO4	1	0
5	F	1103	PO4	1	0
4	F	1100	OGK	8	0
4	B	1100	OGK	6	0
5	P	1101	PO4	1	0
4	H	1100	OGK	8	0
4	N	1100	OGK	7	0
4	P	1100	OGK	7	0
4	D	1100	OGK	2	0
5	B	1101	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.

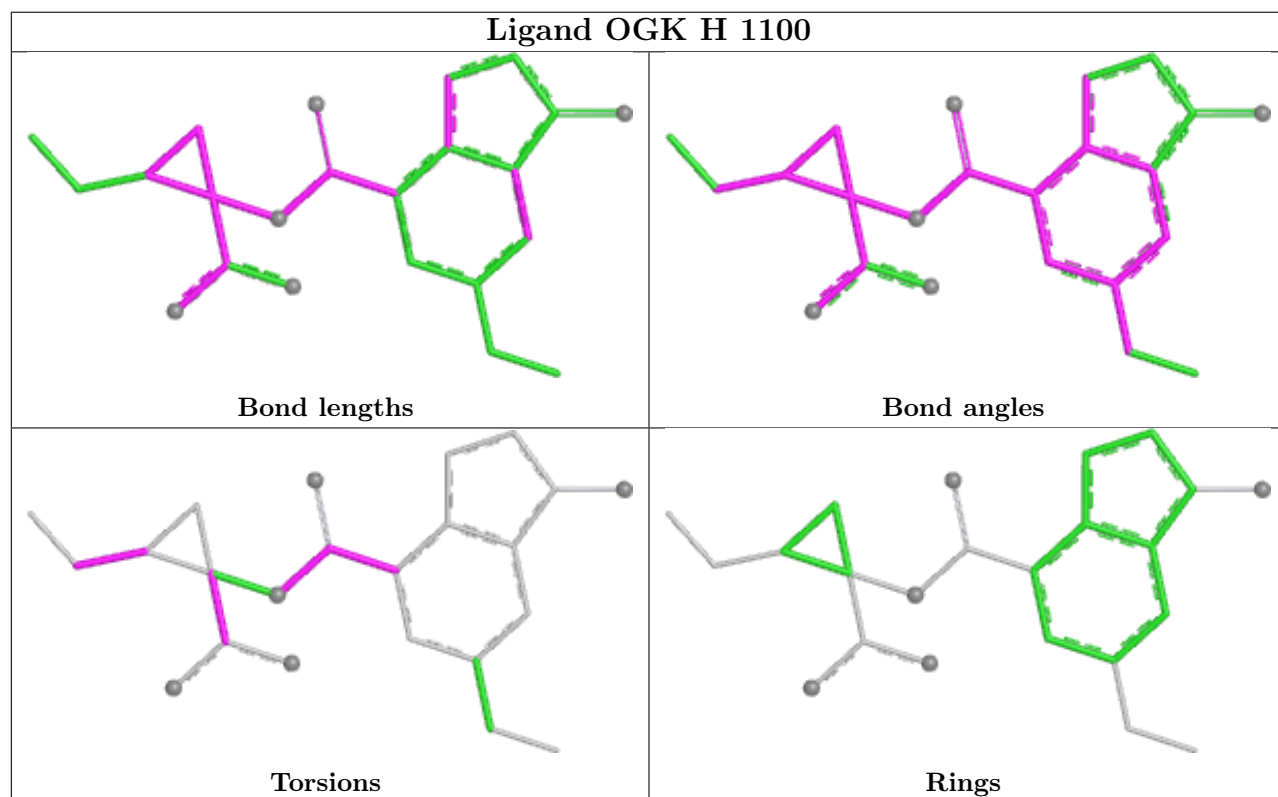




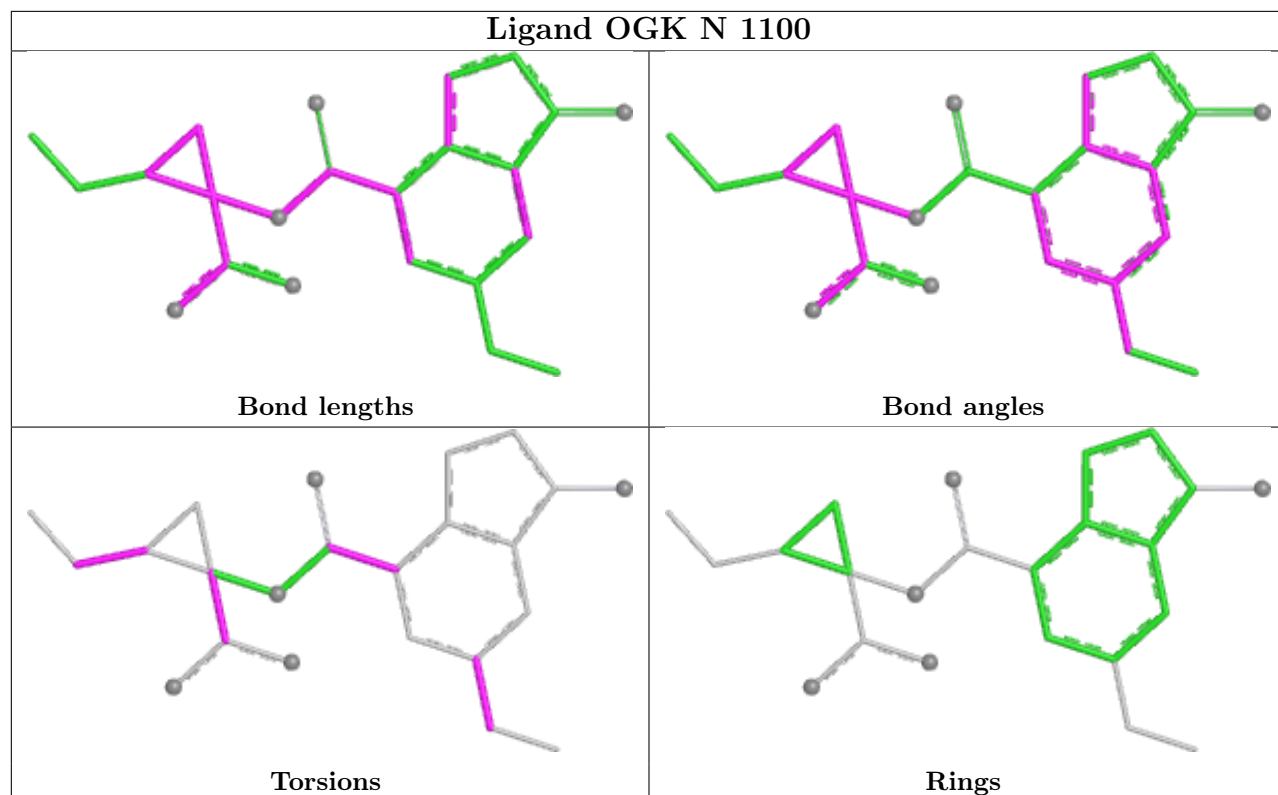
Ligand OGK B 1100



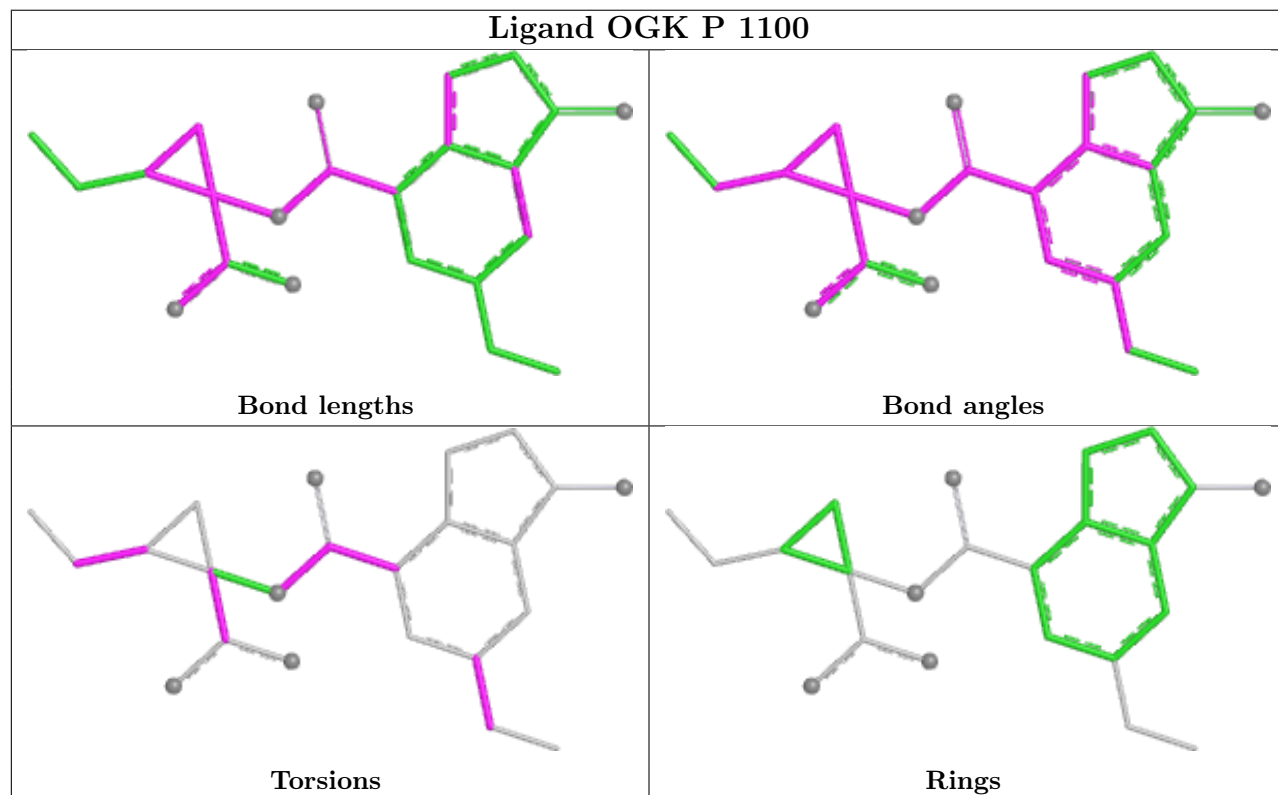
Ligand OGK H 1100

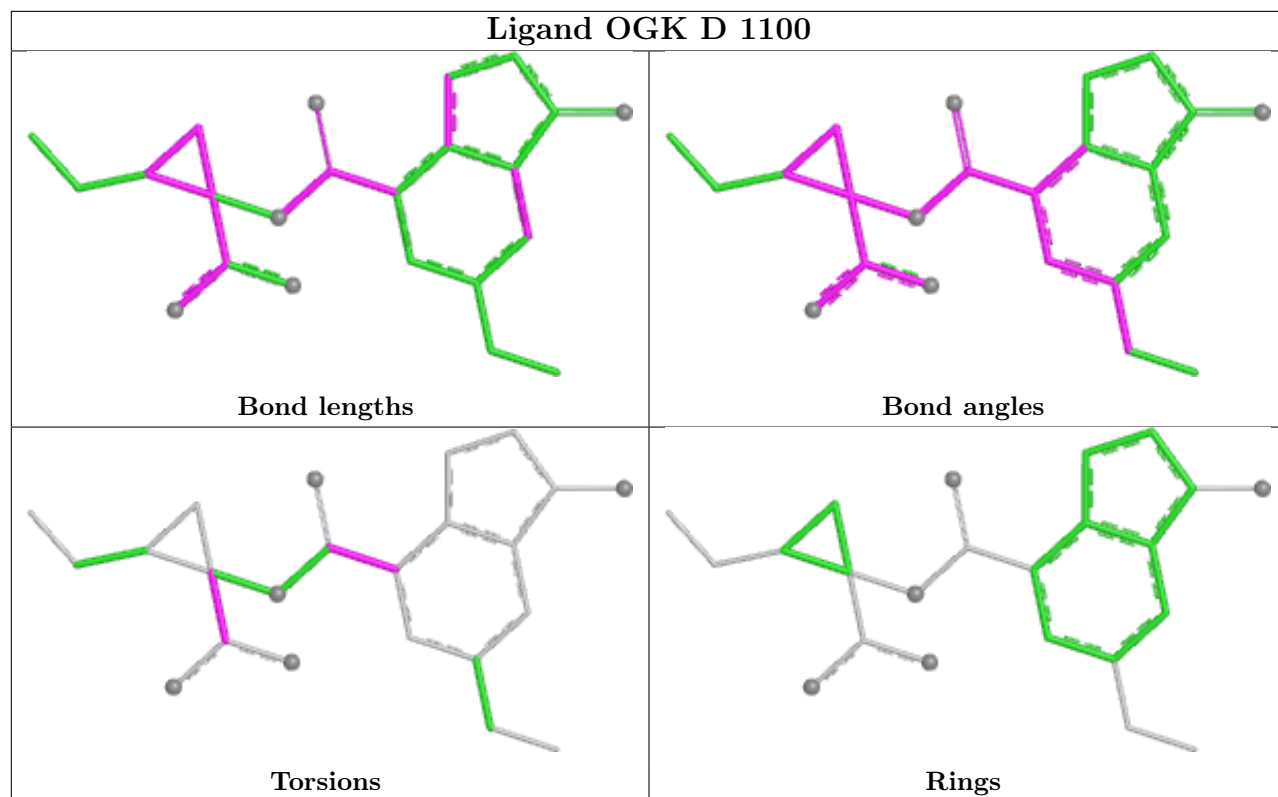


Ligand OGK N 1100



Ligand OGK P 1100





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(Å²)	Q<0.9
1	A	145/160 (90%)	0.79	13 (8%)	15	11	27, 72, 133, 163	0
1	C	145/160 (90%)	0.88	12 (8%)	17	12	26, 75, 134, 163	0
1	E	145/160 (90%)	1.10	28 (19%)	3	2	28, 70, 133, 161	0
1	G	145/160 (90%)	0.39	9 (6%)	26	20	27, 66, 134, 161	0
1	I	145/160 (90%)	0.89	14 (9%)	13	10	29, 73, 134, 163	0
1	K	145/160 (90%)	0.60	10 (6%)	23	16	28, 75, 134, 165	0
1	M	145/160 (90%)	0.80	12 (8%)	17	12	32, 75, 133, 162	0
1	O	145/160 (90%)	0.95	17 (11%)	9	7	32, 76, 134, 164	0
2	B	566/592 (95%)	0.18	29 (5%)	33	25	21, 45, 107, 175	0
2	D	566/592 (95%)	0.16	31 (5%)	30	23	21, 46, 110, 176	0
2	F	566/592 (95%)	0.05	22 (3%)	43	34	20, 49, 111, 177	0
2	H	562/592 (94%)	-0.51	8 (1%)	73	64	19, 38, 91, 171	0
2	J	566/592 (95%)	0.05	25 (4%)	39	31	22, 49, 110, 177	0
2	L	566/592 (95%)	-0.03	18 (3%)	50	40	21, 50, 111, 176	0
2	N	566/592 (95%)	0.55	30 (5%)	32	24	24, 53, 112, 178	0
2	P	566/592 (95%)	0.44	29 (5%)	33	25	23, 54, 114, 176	0
3	Q	13/22 (59%)	2.11	7 (53%)	0	0	79, 102, 125, 126	0
3	R	13/22 (59%)	1.97	5 (38%)	1	0	86, 109, 128, 129	0
3	S	13/22 (59%)	1.51	3 (23%)	2	1	89, 108, 129, 131	0
3	U	13/22 (59%)	1.71	3 (23%)	2	1	87, 111, 128, 130	0
3	V	13/22 (59%)	1.50	3 (23%)	2	1	88, 111, 128, 128	0
3	W	13/22 (59%)	1.53	4 (30%)	1	1	88, 111, 128, 129	0
3	X	13/22 (59%)	1.89	5 (38%)	1	0	89, 110, 128, 129	0
All	All	5775/6170 (93%)	0.27	337 (5%)	29	22	19, 53, 119, 178	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	CYS	6.7
2	D	429	ARG	5.0
2	P	267	VAL	4.8
2	F	14	VAL	4.8
2	L	14	VAL	4.6
2	F	592	ILE	4.4
2	D	267	VAL	4.3
2	D	361	GLU	4.2
2	J	267	VAL	4.1
2	B	14	VAL	4.1
1	E	46	ASN	4.1
2	D	360	ASP	4.0
2	B	267	VAL	4.0
1	C	117	THR	4.0
1	O	117	THR	4.0
2	P	353	ALA	3.9
2	P	14	VAL	3.9
2	D	27	TYR	3.9
2	F	267	VAL	3.9
2	N	592	ILE	3.8
1	O	38	VAL	3.6
1	C	122	ALA	3.6
2	J	548	ARG	3.6
1	E	13	GLY	3.6
1	C	114	LEU	3.6
1	E	116	LEU	3.6
1	A	43	PRO	3.6
2	D	362	GLU	3.5
1	O	114	LEU	3.5
2	P	23	GLN	3.5
1	E	138	ASN	3.5
2	J	592	ILE	3.4
1	E	37	CYS	3.4
2	P	358	MET	3.4
1	A	21	ALA	3.4
2	B	258	GLY	3.4
3	R	217	LYS	3.4
2	N	267	VAL	3.4
2	J	564	HIS	3.4
2	D	529	GLY	3.4
1	E	117	THR	3.4
2	L	267	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	528	THR	3.3
1	E	38	VAL	3.3
2	F	513	PRO	3.3
2	B	592	ILE	3.3
2	N	13	CYS	3.3
2	J	418	ARG	3.3
2	J	528	THR	3.3
1	O	116	LEU	3.2
3	S	217	LYS	3.2
2	J	363	GLY	3.2
1	C	121	VAL	3.1
2	J	591	PRO	3.1
2	P	564	HIS	3.1
3	Q	217	LYS	3.1
1	G	38	VAL	3.1
2	J	422	LEU	3.1
2	P	266	LEU	3.1
2	B	564	HIS	3.1
2	H	362	GLU	3.1
2	N	14	VAL	3.1
1	G	68	SER	3.1
2	D	12	SER	3.1
3	R	208	SER	3.1
2	H	363	GLY	3.1
2	F	564	HIS	3.0
1	K	115	ASP	3.0
1	E	135	THR	3.0
2	F	353	ALA	3.0
2	L	592	ILE	3.0
2	N	548	ARG	3.0
2	P	548	ARG	3.0
2	B	260	PRO	3.0
1	E	48	THR	3.0
1	G	37	CYS	3.0
2	F	16	THR	3.0
2	P	268	PHE	3.0
1	K	38	VAL	3.0
3	V	217	LYS	2.9
2	P	592	ILE	2.9
2	D	23	GLN	2.9
3	U	207	ALA	2.9
2	D	546	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	359	GLU	2.9
1	E	19	GLU	2.9
2	N	373	LEU	2.9
2	F	534	GLN	2.9
2	J	362	GLU	2.9
1	G	46	ASN	2.9
2	J	360	ASP	2.9
2	B	548	ARG	2.9
2	N	12	SER	2.9
2	B	363	GLY	2.8
2	F	591	PRO	2.8
1	I	115	ASP	2.8
1	M	37	CYS	2.8
2	F	548	ARG	2.8
1	A	80	ASP	2.8
2	B	360	ASP	2.8
1	I	43	PRO	2.8
2	D	564	HIS	2.8
2	F	354	ASP	2.8
1	I	116	LEU	2.8
2	D	422	LEU	2.8
3	W	217	LYS	2.8
3	Q	209	LEU	2.7
3	X	213	LEU	2.7
1	I	31	HIS	2.7
1	A	68	SER	2.7
1	C	119	GLN	2.7
1	O	37	CYS	2.7
2	B	259	MET	2.7
2	H	527	MET	2.7
1	G	40	ASN	2.7
2	H	267	VAL	2.7
2	D	15	ALA	2.7
1	M	118	CYS	2.7
3	R	210	HIS	2.7
1	A	35	ASP	2.7
2	N	591	PRO	2.7
1	E	33	VAL	2.7
1	E	121	VAL	2.7
3	X	217	LYS	2.7
1	K	13	GLY	2.7
1	E	15	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	68	SER	2.7
2	B	15	ALA	2.6
2	H	353	ALA	2.6
2	J	590	GLU	2.6
1	M	67	ALA	2.6
2	B	525	ALA	2.6
2	D	358	MET	2.6
2	H	358	MET	2.6
2	F	13	CYS	2.6
1	M	116	LEU	2.6
1	O	139	ILE	2.6
1	I	86	TRP	2.6
2	J	565	PRO	2.6
3	S	209	LEU	2.6
2	F	201	MET	2.6
1	E	114	LEU	2.6
2	L	527	MET	2.6
2	F	23	GLN	2.6
1	C	115	ASP	2.6
2	D	524	ARG	2.5
2	L	548	ARG	2.5
2	N	112	ARG	2.5
2	P	364	LEU	2.5
1	M	6	ILE	2.5
1	O	120	THR	2.5
3	X	207	ALA	2.5
1	E	35	ASP	2.5
1	G	35	ASP	2.5
2	D	418	ARG	2.5
2	B	12	SER	2.5
2	D	201	MET	2.5
1	I	38	VAL	2.5
2	B	29	THR	2.5
2	J	361	GLU	2.5
1	O	46	ASN	2.5
2	N	32	LYS	2.5
3	Q	215	LYS	2.5
2	D	592	ILE	2.5
2	N	590	GLU	2.5
1	I	61	ARG	2.5
2	B	524	ARG	2.5
2	D	548	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	5	LYS	2.5
2	N	313	LEU	2.5
2	P	591	PRO	2.5
1	M	13	GLY	2.5
3	W	205	ARG	2.5
2	L	260	PRO	2.4
1	A	38	VAL	2.4
1	M	38	VAL	2.4
2	F	526	SER	2.4
1	G	19	GLU	2.4
1	A	107	TYR	2.4
2	D	530	GLN	2.4
1	K	31	HIS	2.4
2	J	358	MET	2.4
1	K	80	ASP	2.4
2	N	257	ILE	2.4
2	J	14	VAL	2.4
2	N	376	GLY	2.4
2	N	428	VAL	2.4
2	B	589	LYS	2.4
2	D	353	ALA	2.4
2	J	353	ALA	2.4
2	D	26	THR	2.4
2	N	564	HIS	2.4
2	B	201	MET	2.4
2	L	13	CYS	2.4
2	B	354	ASP	2.4
1	O	137	PHE	2.4
2	L	201	MET	2.4
3	V	210	HIS	2.4
3	R	209	LEU	2.4
2	P	499	CYS	2.4
3	Q	211	ARG	2.4
2	F	590	GLU	2.4
2	B	527	MET	2.4
3	R	213	LEU	2.4
1	C	45	PRO	2.4
1	K	43	PRO	2.4
2	J	546	PRO	2.4
2	L	591	PRO	2.4
1	E	14	GLU	2.3
1	E	65	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	67	ALA	2.3
2	P	12	SER	2.3
1	C	136	THR	2.3
2	N	401	TYR	2.3
2	B	257	ILE	2.3
1	M	140	LYS	2.3
1	O	126	LYS	2.3
1	I	13	GLY	2.3
1	E	115	ASP	2.3
2	N	15	ALA	2.3
2	P	15	ALA	2.3
2	B	358	MET	2.3
2	J	527	MET	2.3
1	C	38	VAL	2.3
2	P	363	GLY	2.3
2	J	566	ALA	2.3
2	L	359	GLU	2.3
2	N	338	ALA	2.3
2	J	201	MET	2.3
2	N	266	LEU	2.3
1	M	126	LYS	2.3
2	F	12	SER	2.3
2	J	420	THR	2.3
2	N	503	ARG	2.3
2	D	591	PRO	2.3
2	P	357	GLY	2.3
1	A	67	ALA	2.3
2	B	359	GLU	2.3
2	L	590	GLU	2.3
1	O	140	LYS	2.3
1	O	136	THR	2.3
2	L	418	ARG	2.3
1	I	7	VAL	2.3
1	C	13	GLY	2.3
2	F	358	MET	2.2
1	I	64	GLU	2.2
2	P	337	LEU	2.2
3	W	209	LEU	2.2
1	G	80	ASP	2.2
2	L	354	ASP	2.2
1	O	31	HIS	2.2
2	L	12	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	547	SER	2.2
1	E	53	ALA	2.2
2	B	353	ALA	2.2
1	E	5	LYS	2.2
1	O	5	LYS	2.2
1	A	31	HIS	2.2
2	D	270	ARG	2.2
2	L	360	ASP	2.2
1	M	33	VAL	2.2
1	O	121	VAL	2.2
2	F	29	THR	2.2
2	P	258	GLY	2.2
1	M	5	LYS	2.2
1	E	57	GLU	2.2
2	B	362	GLU	2.2
2	J	530	GLN	2.2
1	A	81	ASP	2.2
1	K	117	THR	2.2
2	N	527	MET	2.2
2	J	12	SER	2.2
1	E	16	PHE	2.2
3	Q	212	PHE	2.2
1	K	67	ALA	2.2
2	D	308	GLU	2.2
2	B	328	VAL	2.2
2	P	290	PRO	2.2
1	G	44	LEU	2.2
1	K	114	LEU	2.2
1	E	21	ALA	2.2
2	D	339	GLN	2.1
2	N	447	GLN	2.1
3	Q	210	HIS	2.1
3	S	210	HIS	2.1
3	X	210	HIS	2.1
2	N	201	MET	2.1
2	P	360	ASP	2.1
3	U	217	LYS	2.1
2	P	373	LEU	2.1
2	B	13	CYS	2.1
2	B	590	GLU	2.1
2	D	17	VAL	2.1
1	E	36	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	GLY	2.1
1	E	41	GLY	2.1
2	D	29	THR	2.1
2	B	364	LEU	2.1
1	A	86	TRP	2.1
3	W	211	ARG	2.1
1	C	37	CYS	2.1
2	L	361	GLU	2.1
2	L	564	HIS	2.1
3	U	210	HIS	2.1
1	E	140	LYS	2.1
2	P	546	PRO	2.1
1	E	39	ASP	2.1
2	D	266	LEU	2.1
2	L	270	ARG	2.1
1	I	29	ILE	2.1
2	N	353	ALA	2.1
2	P	362	GLU	2.1
2	B	534	GLN	2.1
3	V	213	LEU	2.1
2	N	357	GLY	2.1
1	E	136	THR	2.1
1	I	82	ASP	2.1
1	M	117	THR	2.1
2	N	16	THR	2.1
2	P	354	ASP	2.1
3	Q	207	ALA	2.1
2	H	361	GLU	2.1
1	A	124	MET	2.0
2	N	430	SER	2.0
2	P	388	SER	2.0
2	F	356	GLN	2.0
2	P	588	LEU	2.0
1	O	65	ALA	2.0
2	F	27	TYR	2.0
2	D	527	MET	2.0
2	P	259	MET	2.0
1	K	42	VAL	2.0
2	P	356	GLN	2.0
2	J	364	LEU	2.0
3	X	209	LEU	2.0
2	H	357	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	359	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
5	PO4	P	1102	5/5	0.70	0.20	70,91,121,132	0
5	PO4	H	1102	5/5	0.73	0.17	58,70,91,138	0
5	PO4	F	1102	5/5	0.79	0.17	67,80,101,127	0
5	PO4	J	1102	5/5	0.82	0.16	54,71,85,106	0
5	PO4	N	1102	5/5	0.85	0.14	78,89,102,114	0
5	PO4	D	1102	5/5	0.87	0.13	48,60,103,128	0
5	PO4	H	1101	5/5	0.87	0.09	65,65,83,99	0
5	PO4	L	1102	5/5	0.88	0.11	56,67,112,139	0
5	PO4	P	1104	5/5	0.89	0.10	30,51,77,101	0
5	PO4	L	1104	5/5	0.90	0.09	54,54,85,104	0
5	PO4	N	1104	5/5	0.91	0.08	32,59,102,105	0
4	OGK	N	1100	23/23	0.91	0.11	33,54,73,77	0
5	PO4	B	1102	5/5	0.91	0.11	51,71,81,85	0
5	PO4	D	1104	5/5	0.92	0.09	32,38,82,83	0
5	PO4	N	1101	5/5	0.93	0.07	47,54,57,87	0
5	PO4	L	1101	5/5	0.93	0.09	34,39,58,68	0
5	PO4	N	1103	5/5	0.93	0.09	40,60,78,102	0
5	PO4	H	1104	5/5	0.94	0.06	23,27,62,87	0
5	PO4	J	1101	5/5	0.94	0.09	42,53,62,65	0
4	OGK	H	1100	23/23	0.94	0.08	23,41,56,62	0
5	PO4	P	1103	5/5	0.94	0.07	55,56,64,76	0
4	OGK	P	1100	23/23	0.94	0.09	40,52,64,68	0

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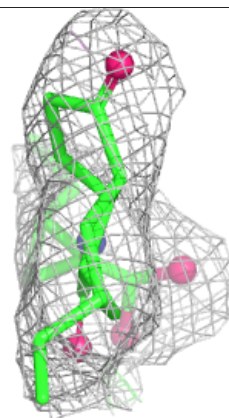
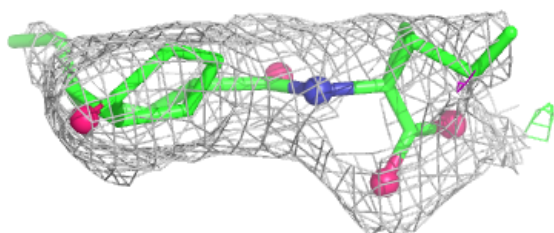
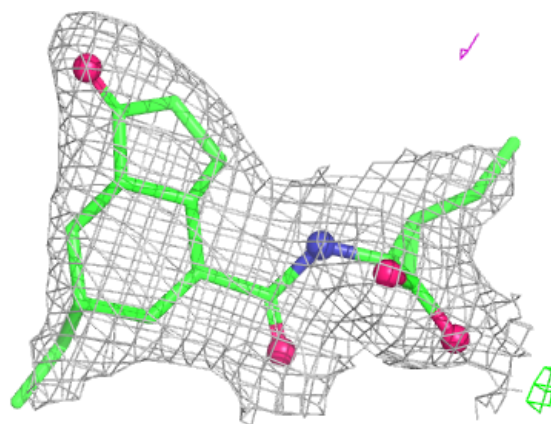
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	F	1104	5/5	0.95	0.08	28,33,60,69	0
5	PO4	H	1103	5/5	0.95	0.07	45,60,71,83	0
4	OGK	J	1100	23/23	0.95	0.09	24,36,51,65	0
4	OGK	F	1100	23/23	0.96	0.08	23,41,50,70	0
5	PO4	B	1104	5/5	0.96	0.08	23,44,66,67	0
5	PO4	P	1101	5/5	0.96	0.06	47,50,65,73	0
4	OGK	L	1100	23/23	0.96	0.08	31,43,62,67	0
5	PO4	B	1101	5/5	0.96	0.08	31,37,44,44	0
5	PO4	J	1104	5/5	0.96	0.07	44,46,72,76	0
5	PO4	L	1103	5/5	0.97	0.06	31,41,62,72	0
4	OGK	D	1100	23/23	0.97	0.06	24,32,41,45	0
5	PO4	F	1103	5/5	0.97	0.06	32,36,48,80	0
5	PO4	D	1101	5/5	0.97	0.07	29,32,43,57	0
5	PO4	F	1101	5/5	0.97	0.08	25,37,47,70	0
5	PO4	B	1103	5/5	0.98	0.05	23,25,30,45	0
4	OGK	B	1100	23/23	0.98	0.06	14,26,38,48	0
5	PO4	D	1103	5/5	0.98	0.06	28,30,38,79	0
5	PO4	J	1103	5/5	0.99	0.04	34,39,48,64	0

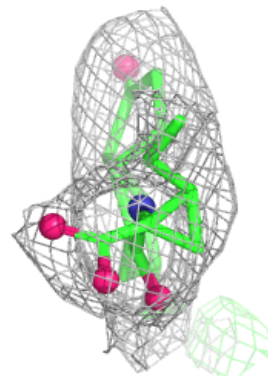
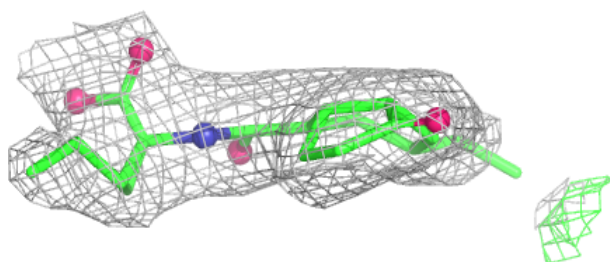
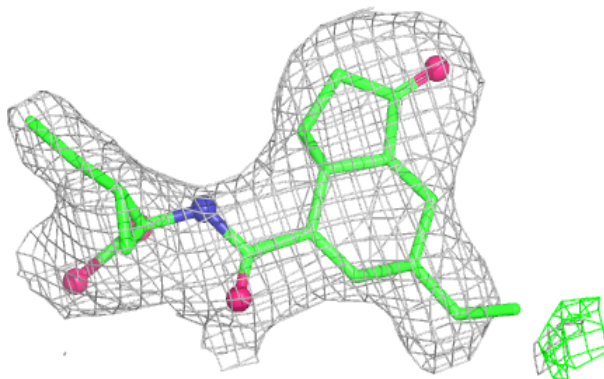
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OGK N 1100:

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

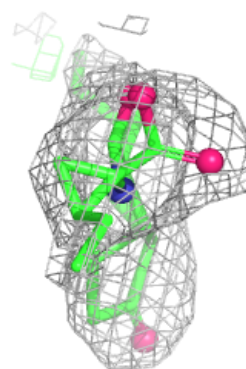
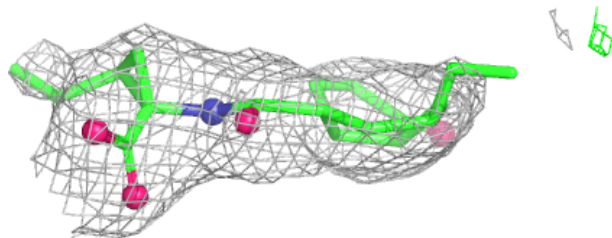
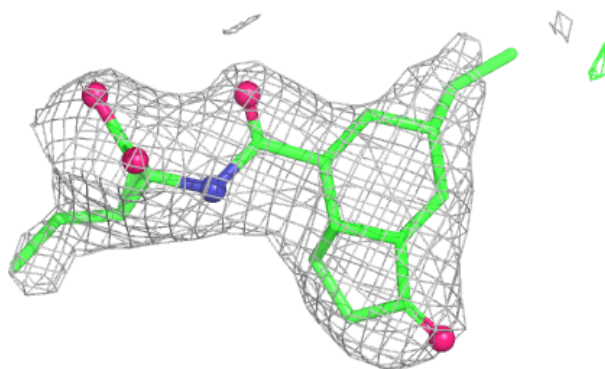
**Electron density around OGK H 1100:**

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

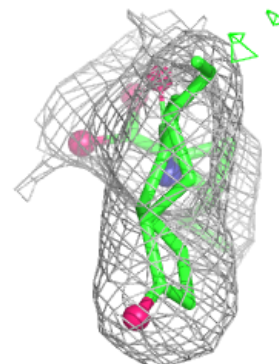
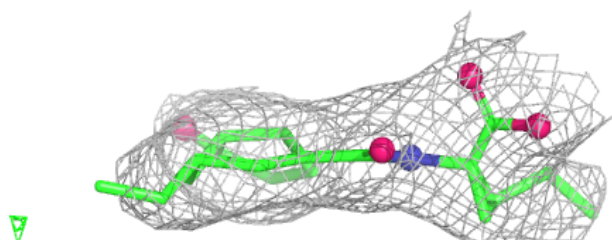
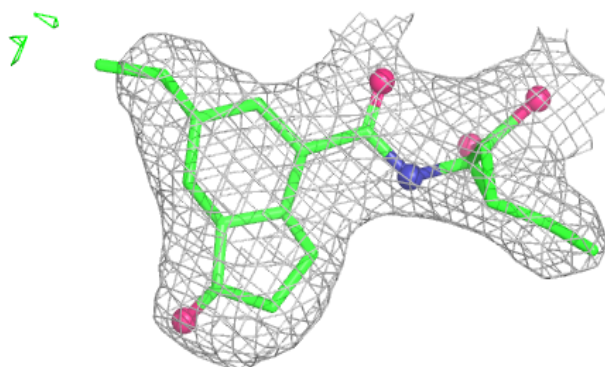


Electron density around OGK P 1100:

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

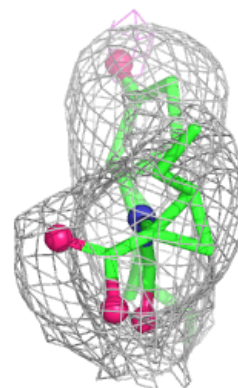
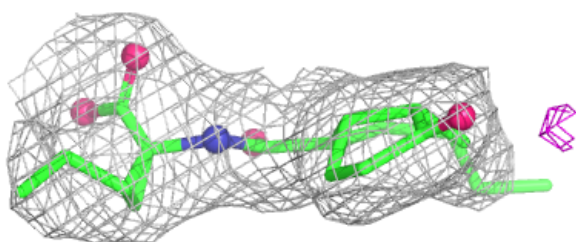
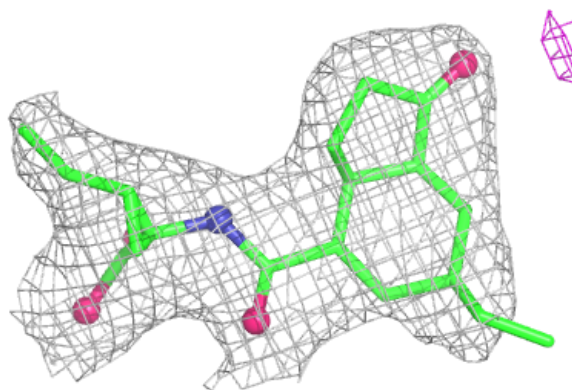
**Electron density around OGK J 1100:**

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

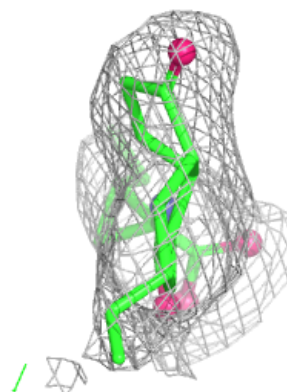
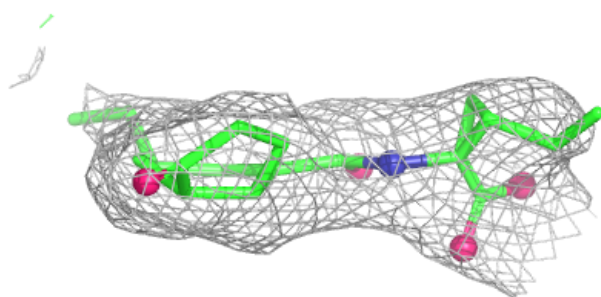
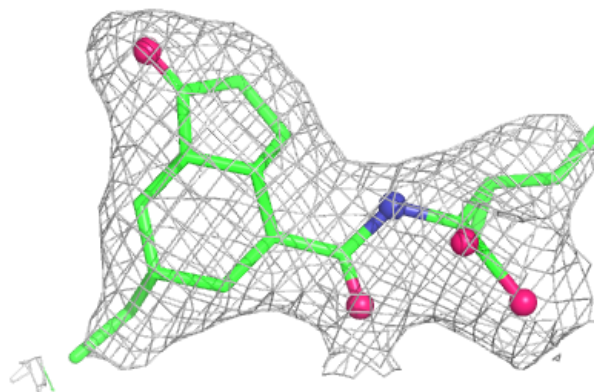


Electron density around OGK F 1100:

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

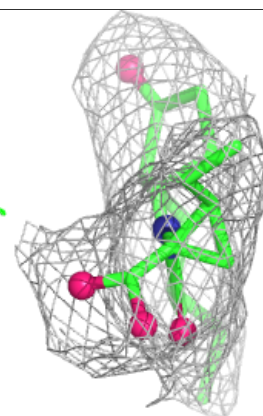
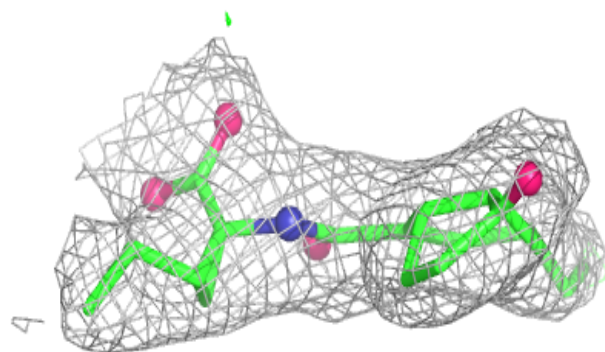
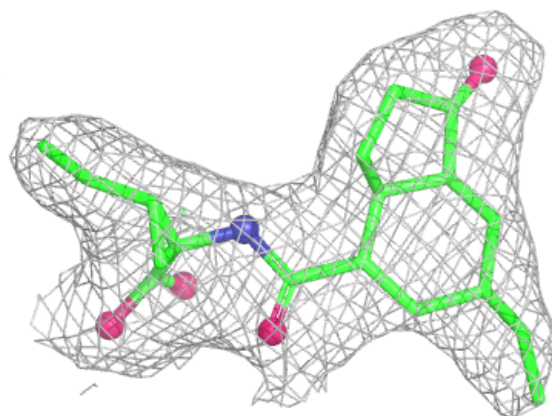
**Electron density around OGK L 1100:**

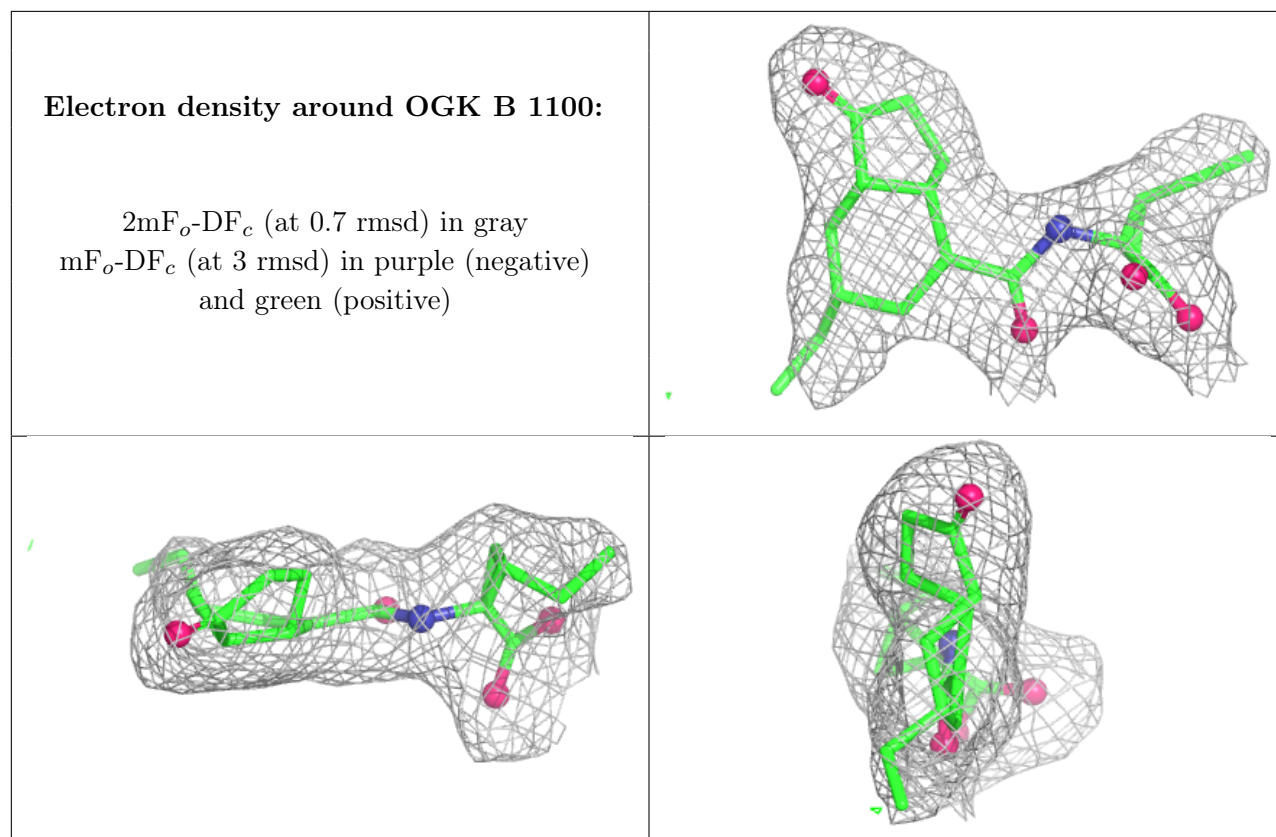
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OGK D 1100:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.