Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:23 pm BST

PDB ID	:	3OGM
Title	:	Structure of COI1-ASK1 in complex with coronatine and the JAZ1 degron
Authors	:	Sheard, L.B.; Tan, X.; Mao, H.; Withers, J.; Ben-Nissan, G.; Hinds, T.R.; Hsu, F.; Sharon, M.; Browse, J.; He, S.Y.; Rizo, J.; Howe, G.A.; Zheng, N.
Deposited on	:	2010-08-17
Resolution	:	3.34 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

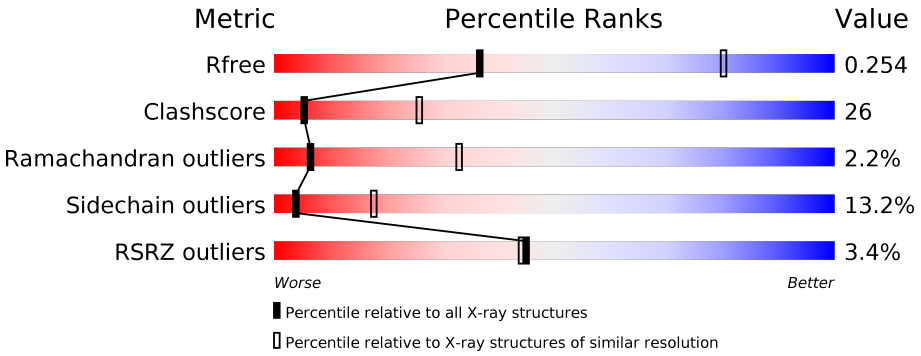
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 <=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	4% 49% 36% 6% 10%
1	C	160	6% 52% 33% 6% 10%
1	E	160	4% 51% 34% 5% 10%
1	G	160	% 48% 38% • • 10%
1	I	160	4% 46% 39% 6% 10%
1	K	160	11% 52% 32% 6% 10%

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Mol	Chain	Length	Quality of chain
1	M	160	9% 46% 39% 10%
1	O	160	11% 48% 37% 5% 10%
2	B	592	% 53% 35% 7%
2	D	592	% 53% 35% 8%
2	F	592	3% 50% 39% 7%
2	H	592	2% 33% 46% 15% 5%
2	J	592	2% 53% 35% 8%
2	L	592	2% 52% 36% 8%
2	N	592	7% 49% 39% 8%
2	P	592	2% 51% 38% 7%
3	Q	21	62% 24% 14%
3	R	21	71% 14% 14%
3	S	21	67% 19% 14%
3	U	21	67% 19% 14%
3	V	21	5% 67% 19% 14%
3	W	21	5% 67% 19% 14%
3	X	21	5% 67% 19% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OGK	H	4100	X	-	X	-
5	PO4	B	1101	-	X	-	-
5	PO4	B	1102	-	X	-	-
5	PO4	B	1103	-	X	-	-
5	PO4	B	1104	-	X	-	-
5	PO4	D	1101	-	X	-	-
5	PO4	D	1102	-	X	-	-
5	PO4	D	1103	-	X	-	-

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

2 Entry composition

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

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

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

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

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

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

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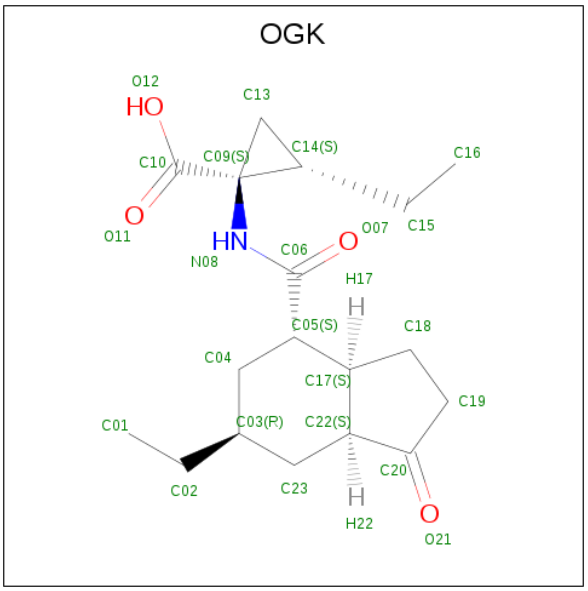
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	P	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

- Molecule 3 is a protein called JAZ1 degron peptide.

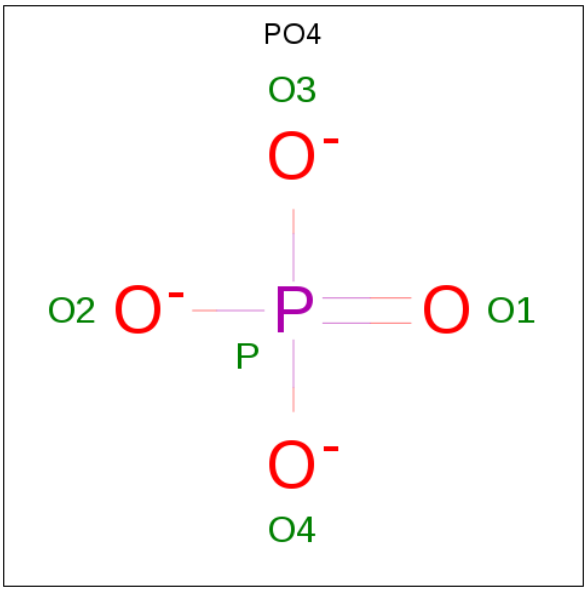
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156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

- Molecule 4 is (1S,2S)-2-ethyl-1-({[(3aS,4S,6R,7aS)-6-ethyl-1-oxooctahydro-1H-inden-4-yl]carbonyl}amino)cyclopropanecarboxylic acid (three-letter code: OGK) (formula: $C_{18}H_{27}NO_4$).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

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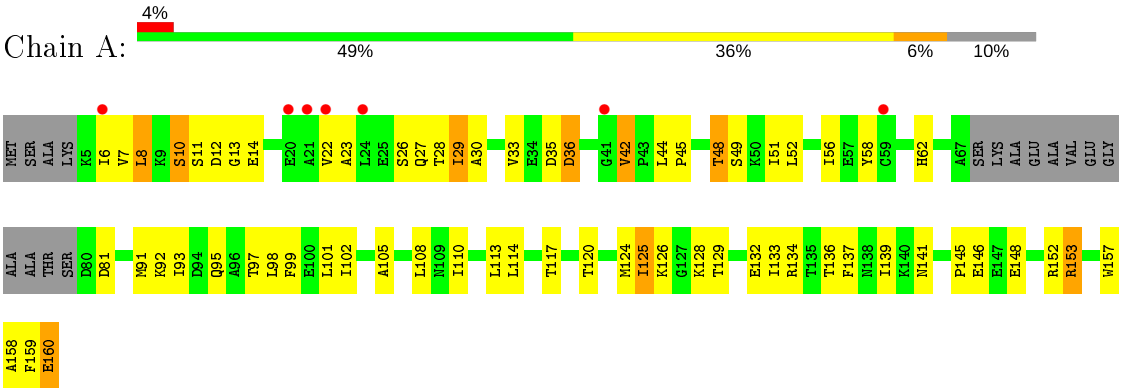
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	N	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

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

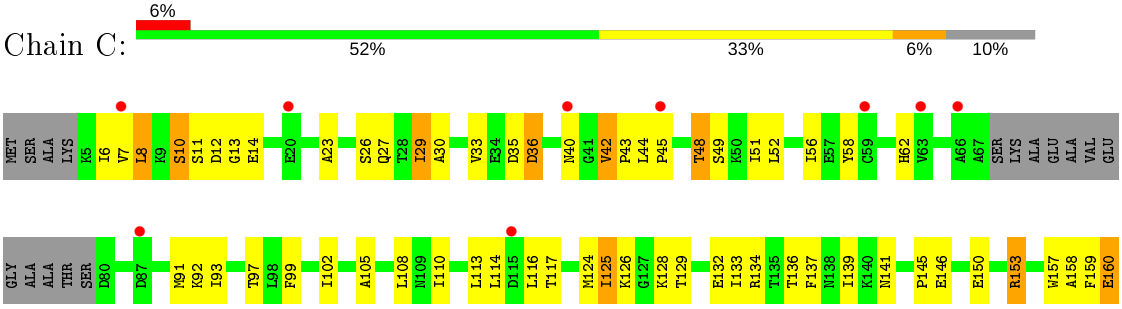
- Molecule 1: SKP1-like protein 1A

Chain A:



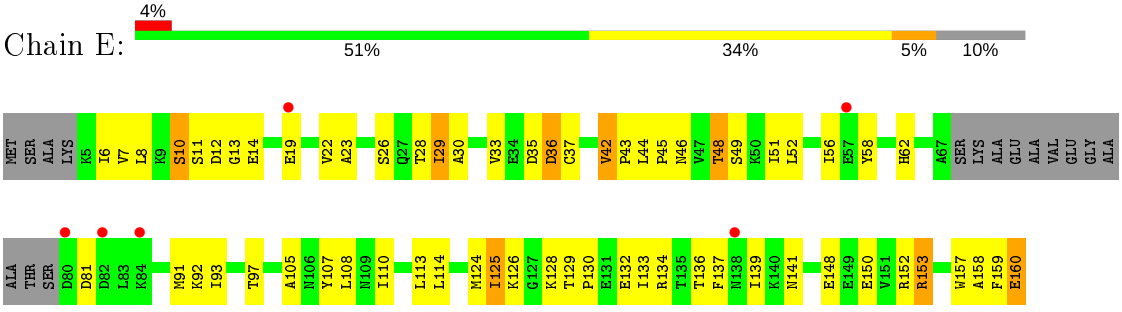
- Molecule 1: SKP1-like protein 1A

Chain C:



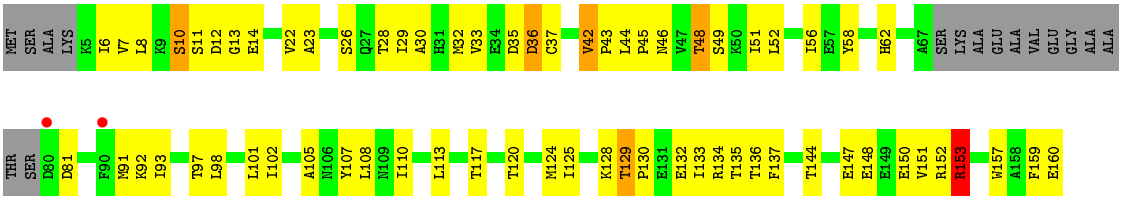
- Molecule 1: SKP1-like protein 1A

Chain E:



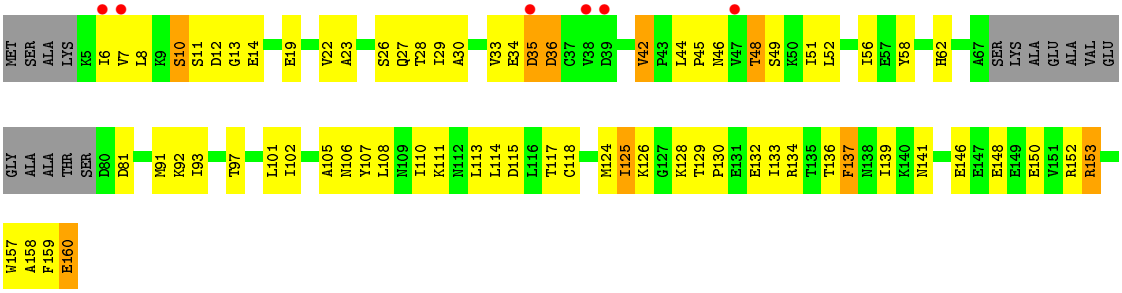
- Molecule 1: SKP1-like protein 1A

Chain G:



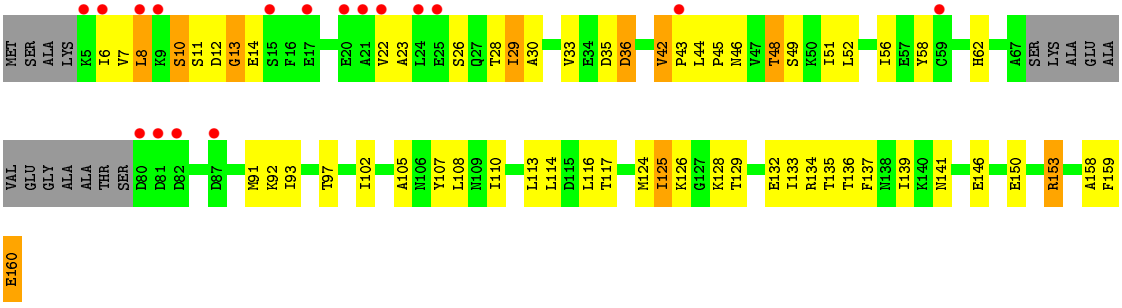
• Molecule 1: SKP1-like protein 1A

Chain I:



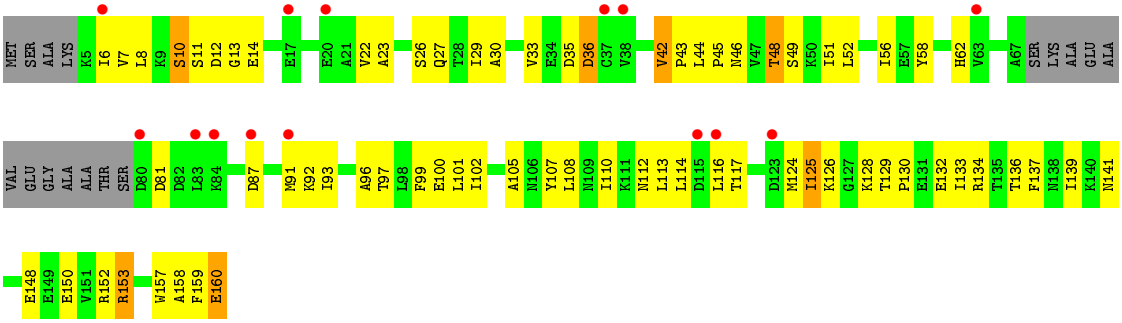
• Molecule 1: SKP1-like protein 1A

Chain K:



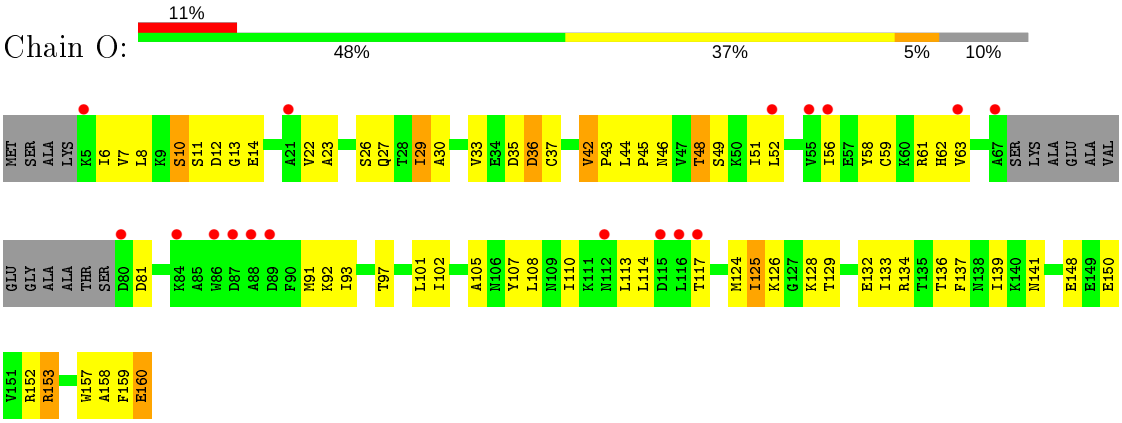
• Molecule 1: SKP1-like protein 1A

Chain M:



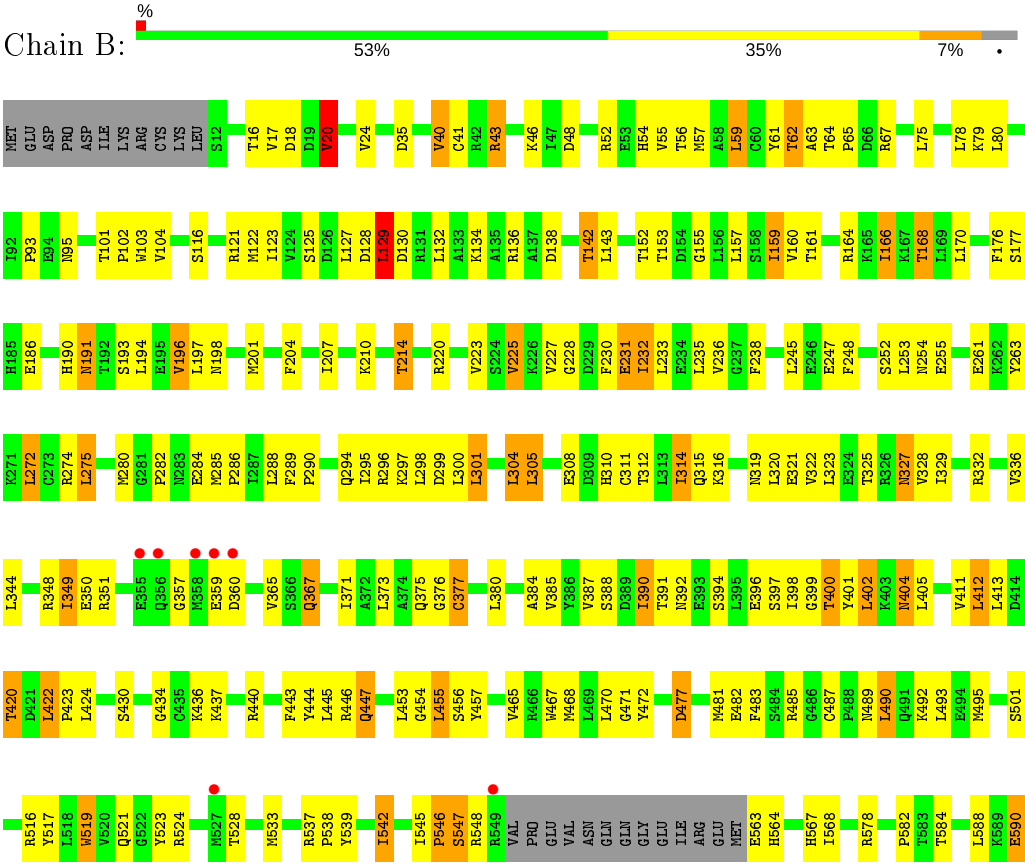
• Molecule 1: SKP1-like protein 1A

Chain O:



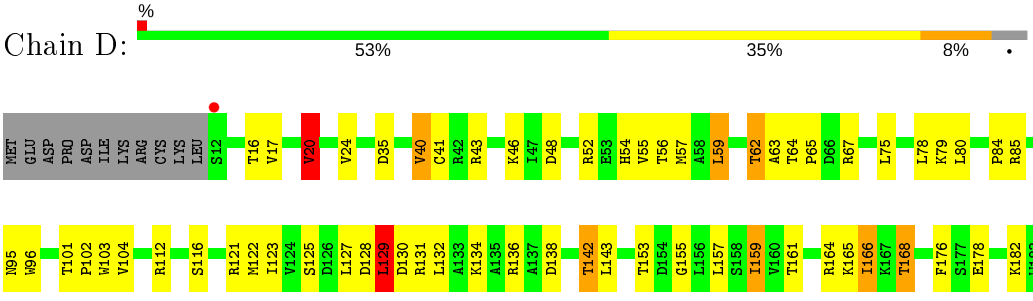
- Molecule 2: Coronatine-insensitive protein 1

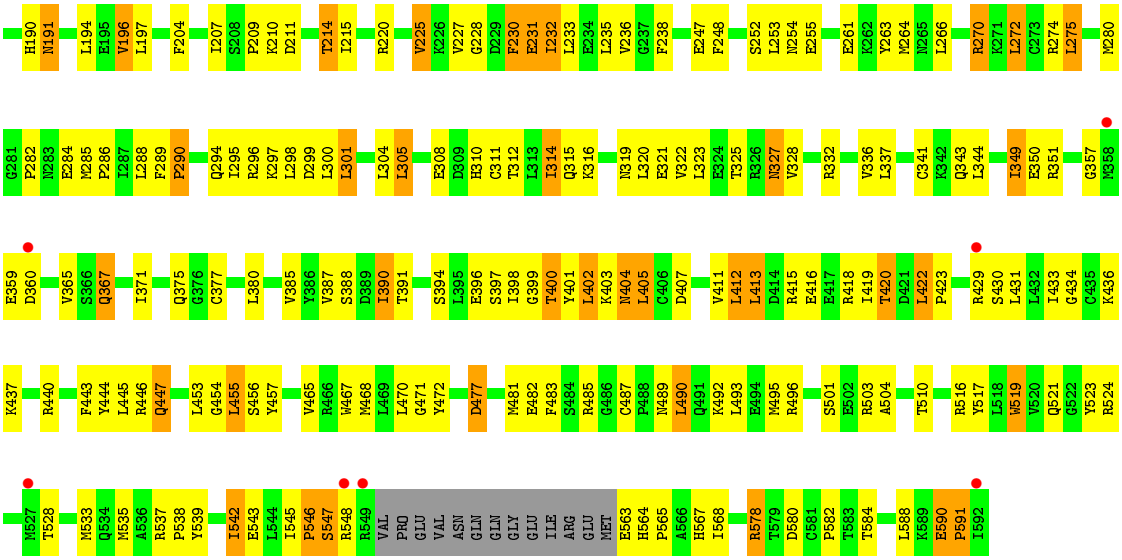
Chain B:



- Molecule 2: Coronatine-insensitive protein 1

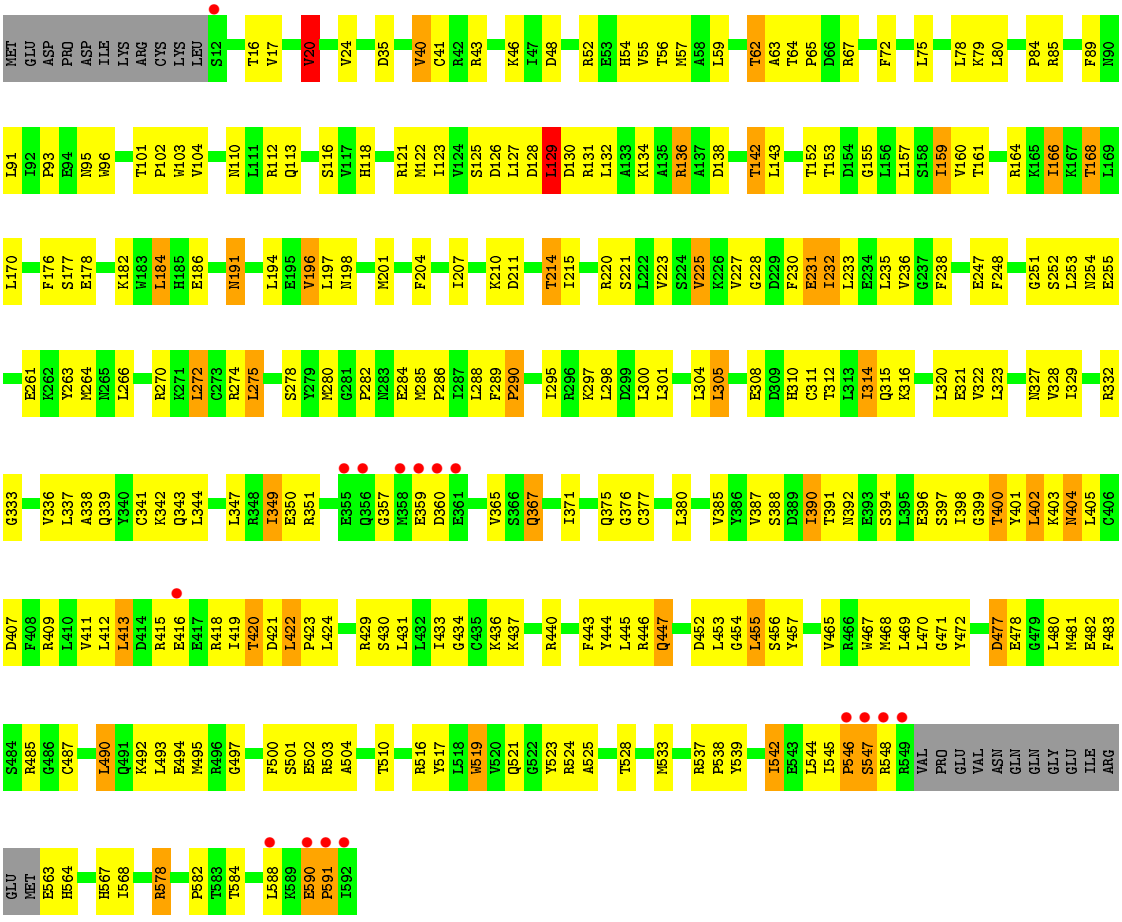
Chain D:





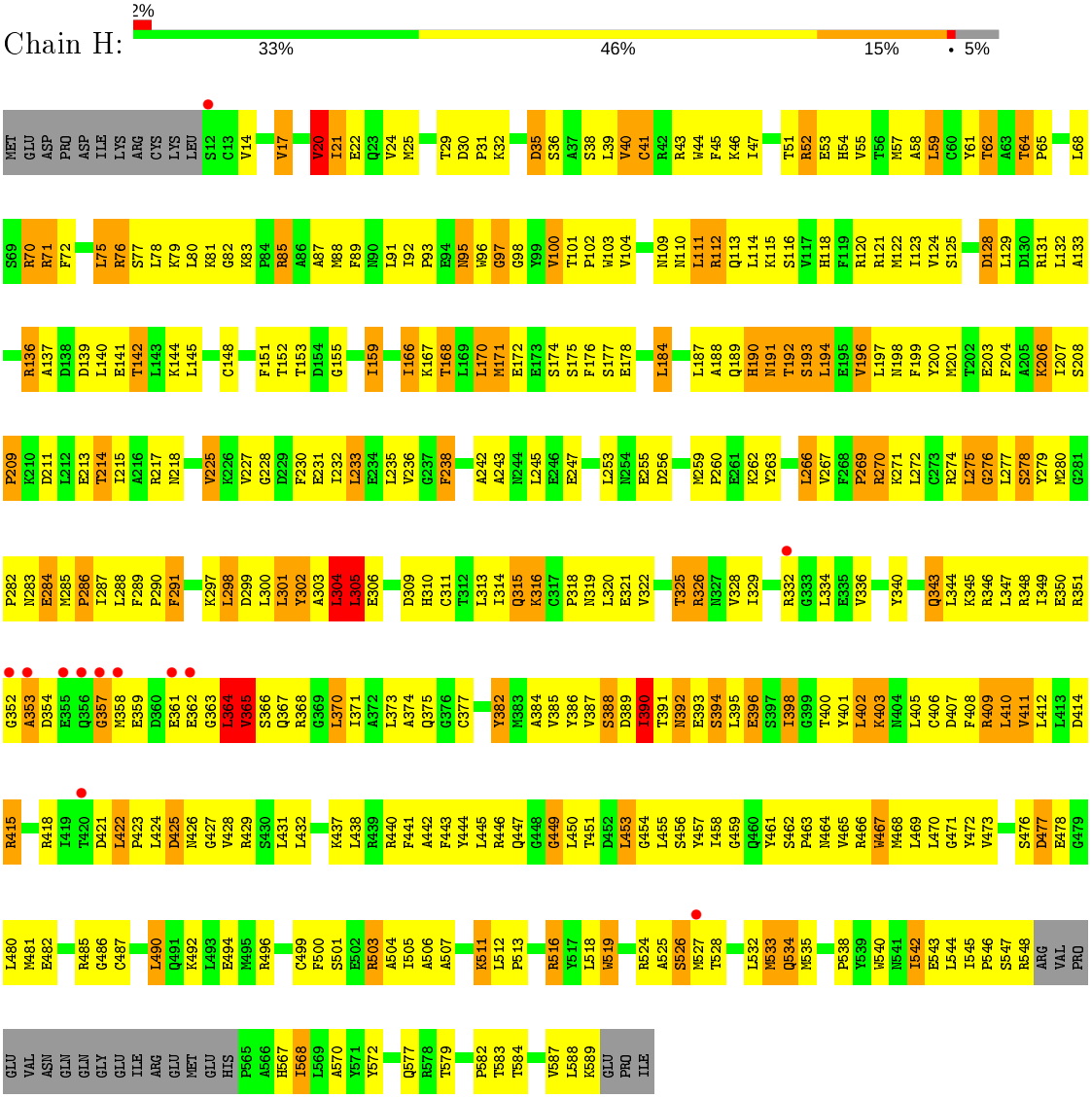
- Molecule 2: Coronatine-insensitive protein 1

Chain F:



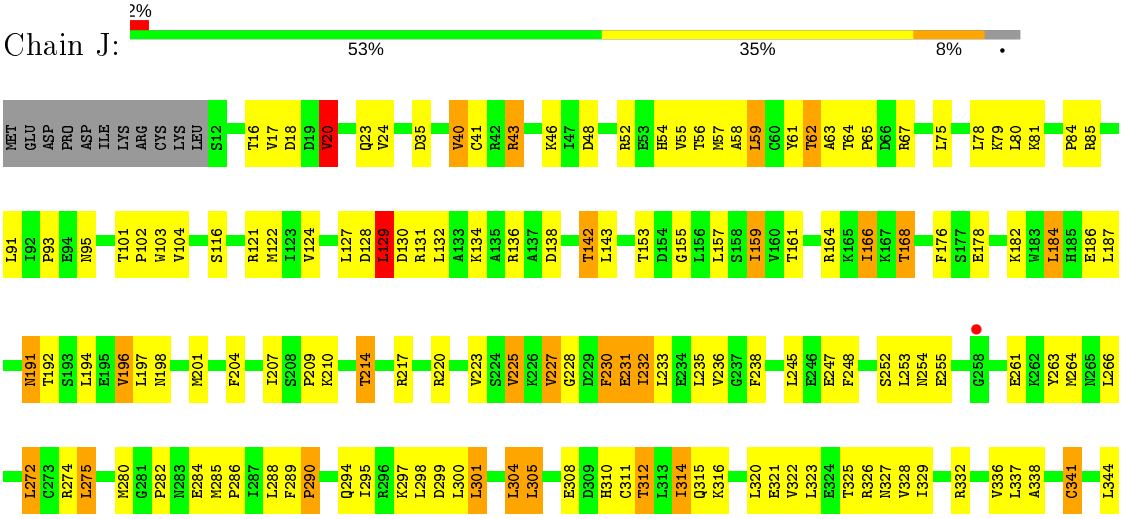
- Molecule 2: Coronatine-insensitive protein 1

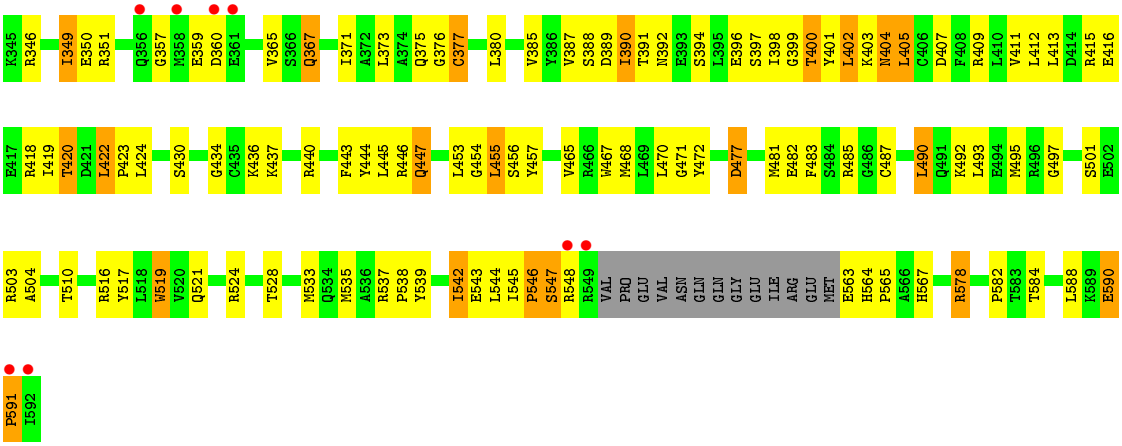
Chain H:

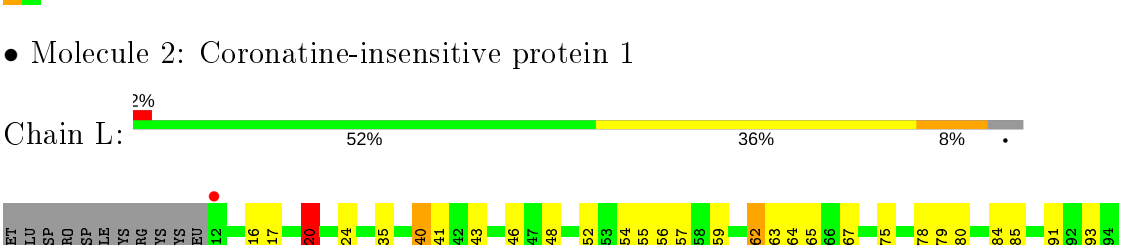


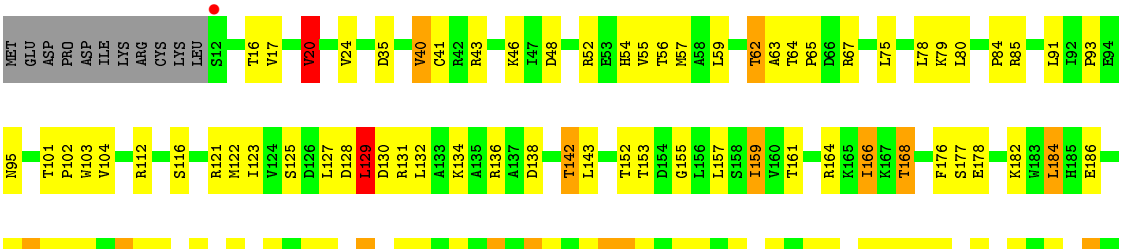
• Molecule 2: Coronatine-insensitive protein 1

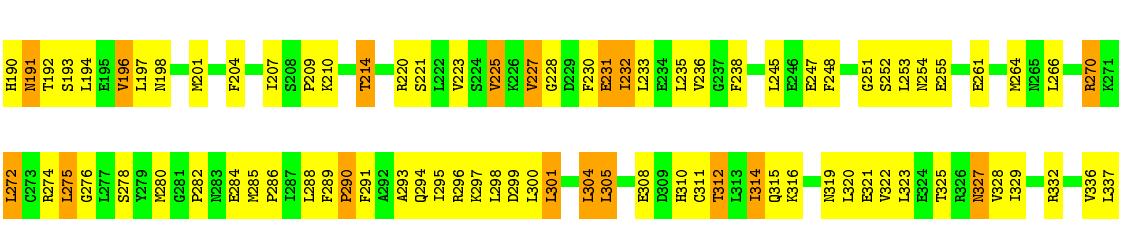
Chain J:

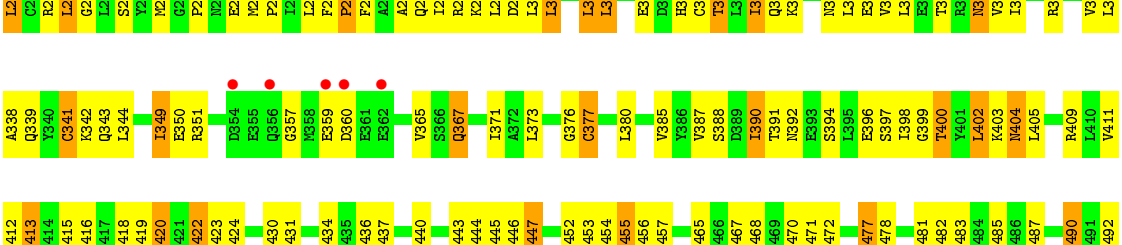


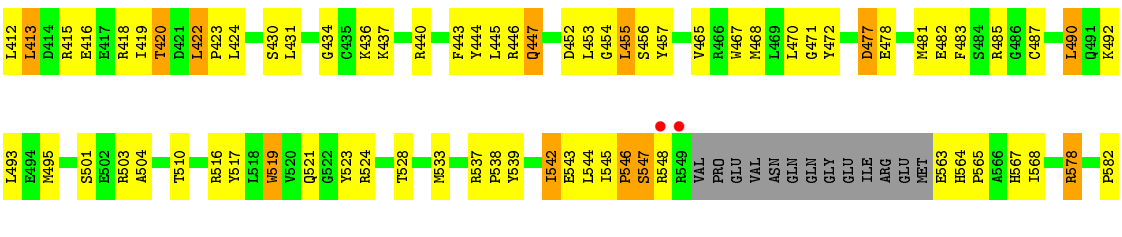


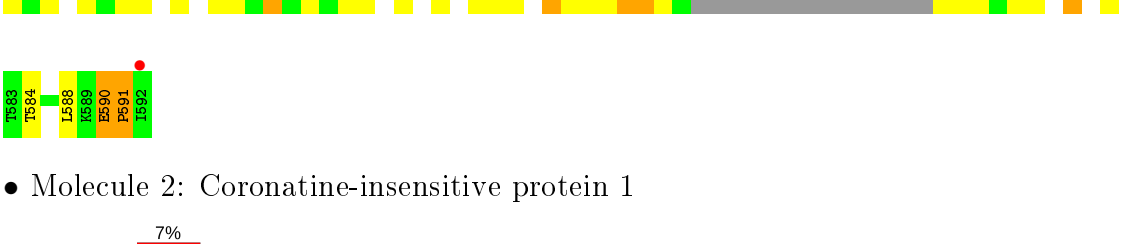


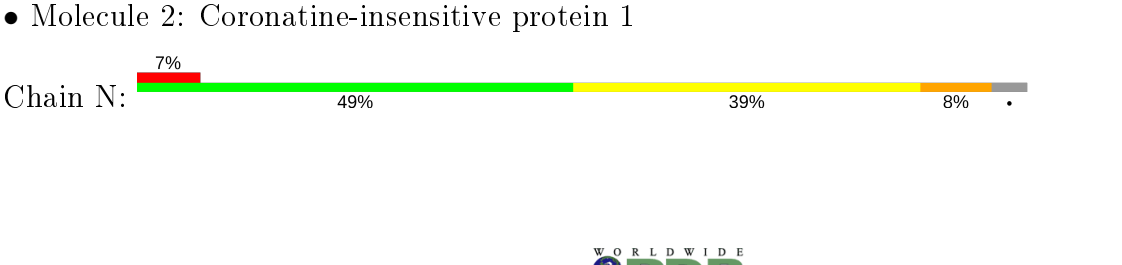










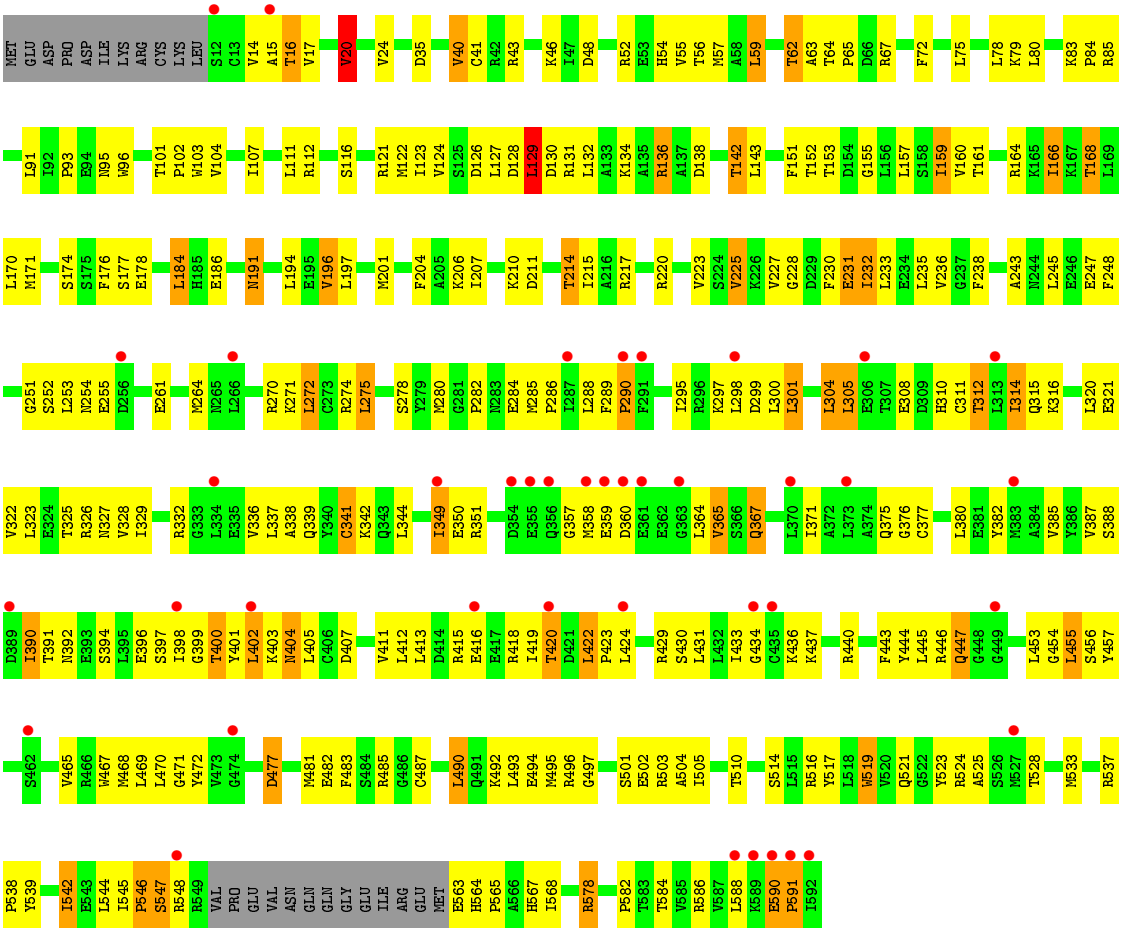


• Molecule 2: Coronatine-insensitive protein 1

Chain L:

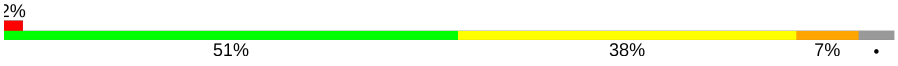
• Molecule 2: Coronatine-insensitive protein 1

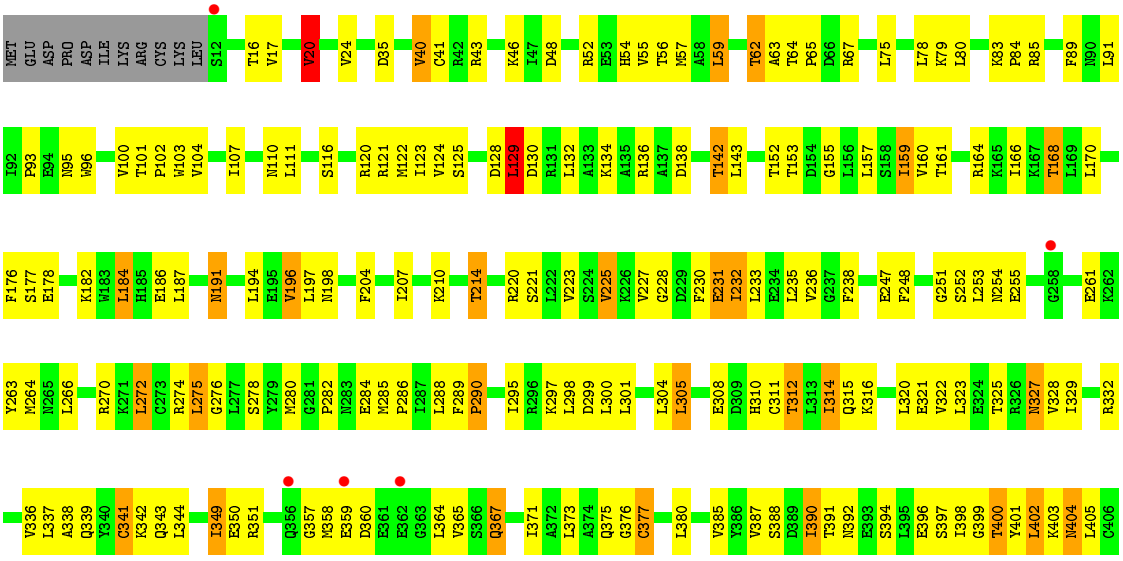
Chain N:

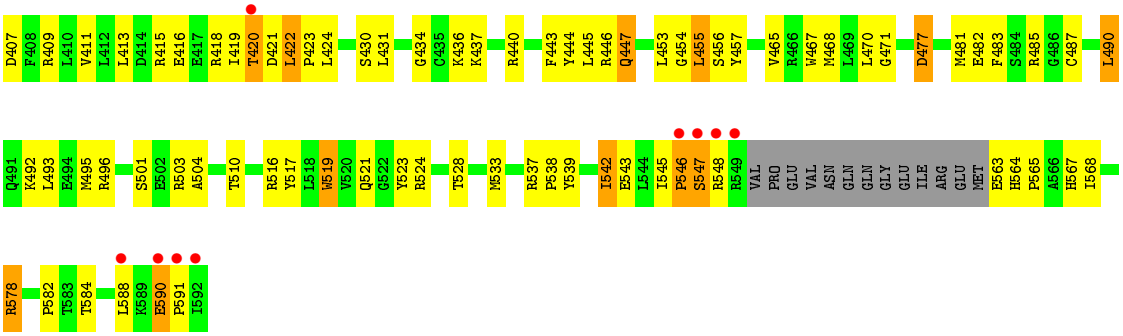


• Molecule 2: Coronatine-insensitive protein 1

Chain P:

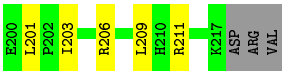






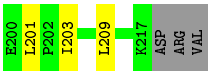
- Molecule 3: JAZ1 degron peptide

Chain Q:



- Molecule 3: JAZ1 degron peptide

Chain R:



- Molecule 3: JAZ1 degron peptide

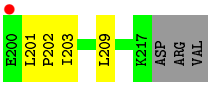
Chain S:

- Molecule 3: JAZ1 degron peptide

Chain U:

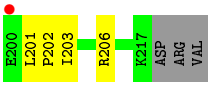
- Molecule 3: JAZ1 degron peptide

Chain V:



- Molecule 3: JAZ1 degron peptide

Chain W:



- Molecule 3: JAZ1 degron peptide

Chain X:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	123.17Å 220.76Å 149.54Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	49.94 – 3.34 49.94 – 3.34	Depositor EDS
% Data completeness (in resolution range)	85.8 (49.94-3.34) 85.8 (49.94-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.226 , 0.270 0.214 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	68.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	46877	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	0/1162	0.56	0/1571
1	C	0.45	0/1162	0.58	0/1571
1	E	0.45	0/1162	0.59	0/1571
1	G	0.52	0/1162	0.63	0/1571
1	I	0.44	0/1162	0.57	0/1571
1	K	0.43	0/1162	0.57	0/1571
1	M	0.50	0/1162	0.59	0/1571
1	O	0.45	0/1162	0.56	0/1571
2	B	0.49	0/4623	0.63	1/6238 (0.0%)
2	D	0.50	0/4623	0.64	1/6238 (0.0%)
2	F	0.46	0/4623	0.64	1/6238 (0.0%)
2	H	0.58	0/4566	0.83	2/6161 (0.0%)
2	J	0.49	0/4623	0.64	1/6238 (0.0%)
2	L	0.45	0/4623	0.63	1/6238 (0.0%)
2	N	0.58	0/4623	0.67	1/6238 (0.0%)
2	P	0.47	0/4623	0.63	1/6238 (0.0%)
3	Q	0.42	0/158	0.53	0/208
3	R	0.39	0/158	0.52	0/208
3	S	0.38	0/158	0.55	0/208
3	U	0.46	0/158	0.55	0/208
3	V	0.41	0/158	0.54	0/208
3	W	0.43	0/158	0.57	0/208
3	X	0.40	0/158	0.53	0/208
All	All	0.50	0/47329	0.65	9/63851 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	129	LEU	CA-CB-CG	7.63	132.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	129	LEU	CA-CB-CG	7.51	132.58	115.30
2	L	129	LEU	CA-CB-CG	7.50	132.54	115.30
2	B	129	LEU	CA-CB-CG	7.40	132.32	115.30
2	N	129	LEU	CA-CB-CG	7.21	131.87	115.30
2	D	129	LEU	CA-CB-CG	7.03	131.47	115.30
2	P	129	LEU	CA-CB-CG	6.39	130.00	115.30
2	H	304	LEU	CA-CB-CG	-5.41	102.86	115.30
2	H	390	ILE	CB-CA-C	-5.06	101.47	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1146	0	1117	63	0
1	C	1146	0	1117	57	0
1	E	1146	0	1117	69	0
1	G	1146	0	1117	65	0
1	I	1146	0	1117	69	0
1	K	1146	0	1117	55	0
1	M	1146	0	1117	86	0
1	O	1146	0	1117	69	0
2	B	4541	0	4583	222	0
2	D	4541	0	4583	225	0
2	F	4541	0	4583	219	0
2	H	4486	0	4534	431	0
2	J	4541	0	4583	226	0
2	L	4541	0	4583	233	0
2	N	4541	0	4583	271	0
2	P	4541	0	4583	224	0
3	Q	156	0	171	7	0
3	R	156	0	171	5	0
3	S	156	0	171	5	0
3	U	156	0	171	6	0
3	V	156	0	171	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	156	0	171	7	0
3	X	156	0	171	5	0
4	B	23	0	27	7	0
4	D	23	0	27	7	0
4	F	23	0	27	7	0
4	H	23	0	27	16	0
4	J	23	0	27	7	0
4	L	23	0	27	7	0
4	N	23	0	27	6	0
4	P	23	0	27	8	0
5	B	20	0	0	3	0
5	D	20	0	0	2	0
5	F	20	0	0	2	0
5	H	20	0	0	3	0
5	J	20	0	0	2	0
5	L	20	0	0	2	0
5	N	20	0	0	3	0
5	P	20	0	0	3	0
All	All	46877	0	46964	2465	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (2465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:116:SER:HB2	2:H:142:THR:HG23	1.35	1.09
2:P:168:THR:HB	2:P:196:VAL:HG13	1.35	1.08
2:D:168:THR:HB	2:D:196:VAL:HG13	1.35	1.08
2:J:168:THR:HB	2:J:196:VAL:HG13	1.35	1.06
2:L:168:THR:HB	2:L:196:VAL:HG13	1.35	1.06
2:L:542:ILE:HD11	2:L:588:LEU:HD12	1.35	1.06
2:B:168:THR:HB	2:B:196:VAL:HG13	1.37	1.05
2:N:168:THR:HB	2:N:196:VAL:HG13	1.38	1.05
2:N:142:THR:HB	2:N:168:THR:HG23	1.38	1.05
1:M:93:ILE:HD12	1:M:97:THR:HG22	1.40	1.04
2:H:311:CYS:HB3	2:H:336:VAL:HG21	1.34	1.04
2:H:78:LEU:HD12	2:H:79:LYS:H	1.22	1.04
2:F:142:THR:HB	2:F:168:THR:HG23	1.40	1.04
2:D:542:ILE:HD11	2:D:588:LEU:HD12	1.40	1.04
2:J:542:ILE:HD11	2:J:588:LEU:HD12	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD12	1:A:97:THR:HG22	1.40	1.02
2:F:168:THR:HB	2:F:196:VAL:HG13	1.39	1.01
2:F:542:ILE:HD11	2:F:588:LEU:HD12	1.43	1.01
2:H:310:HIS:O	2:H:314:ILE:HG12	1.61	1.00
2:P:142:THR:HB	2:P:168:THR:HG23	1.43	1.00
2:N:542:ILE:HD11	2:N:588:LEU:HD12	1.40	0.99
2:P:542:ILE:HD11	2:P:588:LEU:HD12	1.45	0.98
2:F:93:PRO:HA	2:F:548:ARG:HB2	1.44	0.98
2:L:142:THR:HB	2:L:168:THR:HG23	1.46	0.98
2:P:357:GLY:HA2	2:P:415:ARG:HH22	1.29	0.97
2:L:93:PRO:HA	2:L:548:ARG:HB2	1.42	0.97
2:P:93:PRO:HA	2:P:548:ARG:HB2	1.44	0.97
2:F:357:GLY:HA2	2:F:415:ARG:HH22	1.30	0.96
1:M:159:PHE:O	1:M:160:GLU:HB2	1.63	0.96
2:H:392:ASN:O	2:H:396:GLU:HG2	1.66	0.96
2:B:357:GLY:HA2	2:B:415:ARG:HH22	1.31	0.96
1:K:93:ILE:HD12	1:K:97:THR:HG22	1.45	0.95
2:D:93:PRO:HA	2:D:548:ARG:HB2	1.48	0.95
2:H:152:THR:HG22	2:H:177:SER:HB2	1.47	0.95
1:O:93:ILE:HD12	1:O:97:THR:HG22	1.49	0.95
2:B:93:PRO:HA	2:B:548:ARG:HB2	1.48	0.94
2:J:93:PRO:HA	2:J:548:ARG:HB2	1.48	0.94
2:L:357:GLY:HA2	2:L:415:ARG:HH22	1.29	0.94
1:K:159:PHE:O	1:K:160:GLU:HB2	1.66	0.94
2:N:93:PRO:HA	2:N:548:ARG:HB2	1.50	0.94
2:J:357:GLY:HA2	2:J:415:ARG:HH22	1.30	0.94
1:E:93:ILE:HD12	1:E:97:THR:HG22	1.46	0.94
2:H:95:ASN:H	2:H:95:ASN:HD22	1.09	0.93
2:J:142:THR:HB	2:J:168:THR:HG23	1.49	0.93
2:B:142:THR:HB	2:B:168:THR:HG23	1.51	0.93
1:C:93:ILE:HD12	1:C:97:THR:HG22	1.49	0.93
1:I:93:ILE:HD12	1:I:97:THR:HG22	1.47	0.93
2:B:542:ILE:HD11	2:B:588:LEU:HD12	1.50	0.93
1:A:159:PHE:O	1:A:160:GLU:HB2	1.69	0.93
1:E:159:PHE:O	1:E:160:GLU:HB2	1.67	0.92
1:O:159:PHE:O	1:O:160:GLU:HB2	1.67	0.92
2:D:357:GLY:HA2	2:D:415:ARG:HH22	1.32	0.92
1:G:160:GLU:HG3	2:H:52:ARG:HH21	1.35	0.92
1:I:159:PHE:O	1:I:160:GLU:HB2	1.67	0.91
2:N:357:GLY:HA2	2:N:415:ARG:HH22	1.32	0.91
1:G:93:ILE:HD12	1:G:97:THR:HG22	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:286:PRO:HA	2:H:289:PHE:CE2	2.06	0.91
2:H:415:ARG:HH12	2:H:472:TYR:HE1	1.08	0.91
1:C:159:PHE:O	1:C:160:GLU:HB2	1.69	0.90
2:J:590:GLU:HB3	2:J:591:PRO:HD2	1.54	0.90
2:B:444:TYR:HA	2:B:471:GLY:HA3	1.54	0.90
2:B:210:LYS:O	2:B:214:THR:HG22	1.72	0.90
2:D:444:TYR:HA	2:D:471:GLY:HA3	1.53	0.89
2:F:590:GLU:HB3	2:F:591:PRO:HD2	1.54	0.89
2:L:590:GLU:HB3	2:L:591:PRO:HD2	1.54	0.89
2:D:590:GLU:HB3	2:D:591:PRO:HD2	1.55	0.89
2:J:419:ILE:HD13	2:J:446:ARG:HH12	1.38	0.88
2:N:444:TYR:HA	2:N:471:GLY:HA3	1.55	0.88
2:H:322:VAL:HG22	2:H:346:ARG:HB2	1.54	0.88
1:E:107:TYR:OH	2:L:294:GLN:NE2	2.07	0.88
2:P:590:GLU:HB3	2:P:591:PRO:HD2	1.53	0.88
2:N:590:GLU:HB3	2:N:591:PRO:HD2	1.54	0.87
2:B:590:GLU:HB3	2:B:591:PRO:HD2	1.54	0.87
2:F:444:TYR:HA	2:F:471:GLY:HA3	1.55	0.87
2:J:367:GLN:HB3	2:J:391:THR:HG22	1.58	0.86
2:L:444:TYR:HA	2:L:471:GLY:HA3	1.57	0.86
1:E:105:ALA:HB3	1:E:114:LEU:HD13	1.56	0.86
2:B:419:ILE:HD13	2:B:446:ARG:HH12	1.40	0.86
1:K:108:LEU:HD12	1:K:110:ILE:HD11	1.58	0.86
2:H:365:VAL:HG11	2:H:387:VAL:HG22	1.55	0.85
2:H:519:TRP:NE1	4:H:4100:OGK:H01	1.90	0.85
1:M:125:ILE:HG23	1:M:133:ILE:HD12	1.58	0.85
2:N:367:GLN:HB3	2:N:391:THR:HG22	1.57	0.85
2:J:444:TYR:HA	2:J:471:GLY:HA3	1.56	0.85
2:J:210:LYS:O	2:J:214:THR:HG22	1.77	0.85
2:L:349:ILE:HG13	2:L:385:VAL:HG22	1.57	0.85
1:E:43:PRO:HG2	2:L:319:ASN:ND2	1.92	0.85
2:P:286:PRO:HA	2:P:289:PHE:CE2	2.12	0.85
2:H:152:THR:CG2	2:H:177:SER:HB2	2.07	0.85
1:M:102:ILE:HD12	2:N:20:VAL:HG21	1.58	0.84
2:H:40:VAL:O	2:H:41:CYS:HB3	1.78	0.84
2:H:285:MET:HG2	2:H:286:PRO:HD3	1.57	0.84
2:H:415:ARG:NH1	2:H:472:TYR:CE1	2.46	0.84
2:H:440:ARG:HB3	2:H:467:TRP:HD1	1.43	0.84
1:G:153:ARG:HG3	1:G:157:TRP:CZ3	2.13	0.84
2:H:95:ASN:H	2:H:95:ASN:ND2	1.75	0.83
2:B:116:SER:HB2	2:B:142:THR:HG23	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:THR:HB	2:D:168:THR:HG23	1.58	0.83
2:H:199:PHE:CZ	2:H:227:VAL:HG23	2.13	0.83
1:I:125:ILE:HG23	1:I:133:ILE:HD12	1.58	0.83
2:N:328:VAL:HG22	2:N:359:GLU:HB2	1.61	0.82
2:D:210:LYS:O	2:D:214:THR:HG22	1.77	0.82
2:F:210:LYS:O	2:F:214:THR:HG22	1.79	0.82
2:L:210:LYS:O	2:L:214:THR:HG22	1.80	0.82
2:F:367:GLN:HB3	2:F:391:THR:HG22	1.61	0.82
2:L:367:GLN:HB3	2:L:391:THR:HG22	1.60	0.82
2:P:444:TYR:HA	2:P:471:GLY:HA3	1.61	0.82
2:D:116:SER:HB2	2:D:142:THR:HG23	1.62	0.82
1:I:108:LEU:HD12	1:I:110:ILE:HD11	1.62	0.81
1:M:108:LEU:HD12	1:M:110:ILE:HD11	1.62	0.81
2:H:387:VAL:HG11	2:H:390:ILE:HD13	1.60	0.81
1:A:108:LEU:HD12	1:A:110:ILE:HD11	1.61	0.81
2:D:367:GLN:HB3	2:D:391:THR:HG22	1.60	0.81
2:P:419:ILE:HD13	2:P:446:ARG:HH12	1.44	0.81
2:H:256:ASP:OD2	2:H:259:MET:HG2	1.80	0.81
2:J:286:PRO:HA	2:J:289:PHE:CE2	2.16	0.81
2:N:419:ILE:HD13	2:N:446:ARG:HH12	1.44	0.81
2:H:253:LEU:HD11	2:H:277:LEU:HD13	1.62	0.81
2:J:164:ARG:HE	2:N:112:ARG:CG	1.94	0.81
1:M:102:ILE:HG21	2:N:20:VAL:HG22	1.62	0.81
2:N:116:SER:HB2	2:N:142:THR:HG23	1.60	0.81
4:N:7100:OGK:H18A	4:N:7100:OGK:HN08	1.45	0.81
2:P:328:VAL:HG22	2:P:359:GLU:HB2	1.62	0.81
2:D:419:ILE:HD13	2:D:446:ARG:HH12	1.44	0.80
2:N:210:LYS:O	2:N:214:THR:HG22	1.81	0.80
2:P:210:LYS:O	2:P:214:THR:HG22	1.79	0.80
2:H:286:PRO:HA	2:H:289:PHE:CD2	2.15	0.80
2:L:286:PRO:HA	2:L:289:PHE:CE2	2.15	0.80
2:P:367:GLN:HB3	2:P:391:THR:HG22	1.63	0.80
2:H:361:GLU:HA	2:H:388:SER:OG	1.81	0.80
2:B:328:VAL:HG22	2:B:359:GLU:HB2	1.64	0.80
2:F:419:ILE:HD13	2:F:446:ARG:HH12	1.47	0.79
2:N:349:ILE:HG13	2:N:385:VAL:HG22	1.62	0.79
1:A:125:ILE:HG23	1:A:133:ILE:HD12	1.65	0.79
2:H:441:PHE:O	2:H:468:MET:HA	1.82	0.79
1:O:125:ILE:HG23	1:O:133:ILE:HD12	1.63	0.79
2:L:289:PHE:CD1	2:L:316:LYS:HD2	2.18	0.79
2:D:328:VAL:HG22	2:D:359:GLU:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:VAL:HG22	2:F:359:GLU:HB2	1.63	0.79
2:F:112:ARG:HG2	2:L:164:ARG:HD2	1.65	0.79
2:B:367:GLN:HB3	2:B:391:THR:HG22	1.63	0.79
2:H:364:LEU:HD13	2:H:388:SER:OG	1.81	0.79
4:B:1100:OGK:HN08	4:B:1100:OGK:H18A	1.48	0.78
2:F:116:SER:HB2	2:F:142:THR:HG23	1.65	0.78
2:B:286:PRO:HA	2:B:289:PHE:CE2	2.18	0.78
2:B:289:PHE:CD1	2:B:316:LYS:HD2	2.18	0.78
2:J:328:VAL:HG22	2:J:359:GLU:HB2	1.66	0.78
2:L:161:THR:HG22	2:L:186:GLU:HG2	1.65	0.78
2:P:116:SER:HB2	2:P:142:THR:HG23	1.65	0.78
2:J:349:ILE:HG13	2:J:385:VAL:HG22	1.64	0.78
2:H:283:ASN:O	2:H:286:PRO:HD2	1.83	0.78
2:L:419:ILE:HD13	2:L:446:ARG:HH12	1.49	0.78
1:M:96:ALA:HB1	2:N:14:VAL:HG12	1.65	0.78
2:D:349:ILE:HG13	2:D:385:VAL:HG22	1.63	0.77
2:H:411:VAL:HG13	2:H:444:TYR:HB3	1.66	0.77
2:D:289:PHE:CD1	2:D:316:LYS:HD2	2.19	0.77
2:H:519:TRP:HE1	4:H:4100:OGK:H01	1.46	0.77
2:L:116:SER:HB2	2:L:142:THR:HG23	1.64	0.77
2:F:286:PRO:HA	2:F:289:PHE:CE2	2.19	0.77
2:H:533:MET:CE	2:H:588:LEU:HD13	2.14	0.77
2:H:387:VAL:CG1	2:H:390:ILE:HD13	2.14	0.77
1:M:102:ILE:HG21	2:N:20:VAL:CG2	2.14	0.77
4:H:4100:OGK:H18A	4:H:4100:OGK:HN08	1.50	0.77
1:K:125:ILE:HG23	1:K:133:ILE:HD12	1.67	0.77
4:P:8100:OGK:HN08	4:P:8100:OGK:H18A	1.49	0.77
2:H:459:GLY:O	2:H:486:GLY:HA3	1.84	0.77
1:I:105:ALA:HB3	1:I:114:LEU:HD13	1.66	0.77
2:L:328:VAL:HG22	2:L:359:GLU:HB2	1.65	0.77
2:D:286:PRO:HA	2:D:289:PHE:CE2	2.20	0.77
2:N:492:LYS:HE3	2:N:517:TYR:CE2	2.20	0.77
2:N:286:PRO:HA	2:N:289:PHE:CE2	2.19	0.77
2:H:450:LEU:HD11	2:H:454:GLY:HA3	1.65	0.76
2:N:289:PHE:CD1	2:N:316:LYS:HD2	2.19	0.76
1:C:125:ILE:HG23	1:C:133:ILE:HD12	1.65	0.76
2:H:542:ILE:HD11	2:H:588:LEU:HB2	1.67	0.76
4:D:2100:OGK:HN08	4:D:2100:OGK:H18A	1.49	0.76
2:P:286:PRO:HA	2:P:289:PHE:CD2	2.20	0.76
2:J:164:ARG:HE	2:N:112:ARG:HG3	1.51	0.76
4:F:3100:OGK:HN08	4:F:3100:OGK:H18A	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:168:THR:HB	2:P:196:VAL:CG1	2.13	0.75
2:P:289:PHE:CD1	2:P:316:LYS:HD2	2.20	0.75
2:J:116:SER:HB2	2:J:142:THR:HG23	1.65	0.75
2:J:308:GLU:HG3	2:J:332:ARG:HH22	1.52	0.75
2:N:168:THR:HB	2:N:196:VAL:CG1	2.16	0.75
1:C:108:LEU:HD12	1:C:110:ILE:HD11	1.69	0.75
1:E:125:ILE:HG23	1:E:133:ILE:HD12	1.69	0.75
1:E:108:LEU:HD12	1:E:110:ILE:HD11	1.68	0.75
2:H:321:GLU:HA	2:H:344:LEU:HA	1.69	0.75
2:H:365:VAL:HG21	2:H:387:VAL:HG13	1.68	0.75
2:H:467:TRP:HH2	2:H:494:GLU:OE1	1.70	0.75
2:N:391:THR:HG23	2:N:394:SER:H	1.52	0.75
2:F:289:PHE:CD1	2:F:316:LYS:HD2	2.22	0.74
2:H:170:LEU:HD23	2:H:170:LEU:O	1.86	0.74
2:L:308:GLU:HG3	2:L:332:ARG:HH22	1.51	0.74
2:H:415:ARG:NH1	2:H:472:TYR:HE1	1.84	0.74
1:K:124:MET:O	1:K:128:LYS:HE2	1.87	0.74
2:B:270:ARG:HB3	1:O:107:TYR:CD1	2.22	0.74
2:H:298:LEU:HD22	2:H:300:LEU:HG	1.70	0.74
1:O:108:LEU:HD12	1:O:110:ILE:HD11	1.70	0.74
2:J:289:PHE:CD1	2:J:316:LYS:HD2	2.22	0.74
1:M:124:MET:O	1:M:128:LYS:HE2	1.88	0.74
3:S:203:ILE:HD12	3:S:203:ILE:H	1.53	0.74
1:E:43:PRO:CG	2:L:319:ASN:ND2	2.50	0.74
1:M:129:THR:O	1:M:133:ILE:HG12	1.86	0.74
2:N:84:PRO:HB3	2:N:517:TYR:OH	1.87	0.73
2:F:472:TYR:OH	3:S:201:LEU:HB2	1.88	0.73
2:B:161:THR:HG22	2:B:186:GLU:HG2	1.68	0.73
2:J:286:PRO:HA	2:J:289:PHE:CD2	2.24	0.73
4:L:6100:OGK:H18A	4:L:6100:OGK:HN08	1.52	0.73
2:B:391:THR:HG23	2:B:394:SER:H	1.53	0.73
2:F:308:GLU:HG3	2:F:332:ARG:HH22	1.53	0.73
2:J:164:ARG:HD2	2:N:112:ARG:HG2	1.70	0.73
2:L:168:THR:HB	2:L:196:VAL:CG1	2.16	0.73
1:E:124:MET:O	1:E:128:LYS:HE2	1.89	0.73
2:H:136:ARG:NE	2:H:136:ARG:HA	2.04	0.73
2:H:120:ARG:NH2	5:H:1102:PO4:O3	2.20	0.73
2:P:391:THR:HG23	2:P:394:SER:H	1.54	0.73
2:H:412:LEU:HD11	2:H:445:LEU:HD22	1.69	0.72
2:J:391:THR:HG23	2:J:394:SER:H	1.54	0.72
4:J:5100:OGK:HN08	4:J:5100:OGK:H18A	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:308:GLU:HG3	2:N:332:ARG:HH22	1.54	0.72
2:B:253:LEU:HD12	2:B:280:MET:HB2	1.72	0.72
2:D:440:ARG:HB3	2:D:467:TRP:HE3	1.54	0.72
1:K:129:THR:O	1:K:133:ILE:HG12	1.89	0.72
2:H:467:TRP:CH2	2:H:494:GLU:OE1	2.42	0.72
2:H:76:ARG:HG2	2:H:76:ARG:HH11	1.55	0.72
2:J:168:THR:HB	2:J:196:VAL:CG1	2.17	0.72
2:L:286:PRO:HA	2:L:289:PHE:CD2	2.24	0.72
2:B:349:ILE:HG13	2:B:385:VAL:HG22	1.71	0.72
1:I:124:MET:O	1:I:128:LYS:HE2	1.89	0.72
2:D:319:ASN:ND2	1:G:43:PRO:HG2	2.03	0.72
2:H:391:THR:OG1	2:H:393:GLU:HB2	1.90	0.72
2:P:308:GLU:HG3	2:P:332:ARG:HH22	1.53	0.72
3:W:203:ILE:HD12	3:W:203:ILE:H	1.55	0.72
2:D:308:GLU:HG3	2:D:332:ARG:HH22	1.55	0.71
1:G:108:LEU:HD12	1:G:110:ILE:HD11	1.72	0.71
2:H:78:LEU:HD12	2:H:79:LYS:N	2.01	0.71
2:P:161:THR:HG22	2:P:186:GLU:HG2	1.71	0.71
2:D:391:THR:HG23	2:D:394:SER:H	1.54	0.71
1:M:99:PHE:HD2	2:N:15:ALA:O	1.73	0.71
2:B:157:LEU:O	2:B:161:THR:HG23	1.91	0.71
2:H:334:LEU:CD2	2:H:373:LEU:HD22	2.21	0.71
2:B:308:GLU:HG3	2:B:332:ARG:HH22	1.56	0.71
2:F:286:PRO:HA	2:F:289:PHE:CD2	2.25	0.71
1:E:129:THR:O	1:E:133:ILE:HG12	1.89	0.71
2:P:349:ILE:HG13	2:P:385:VAL:HG22	1.72	0.71
3:V:203:ILE:HD12	3:V:203:ILE:H	1.55	0.71
2:H:540:TRP:CZ2	2:H:570:ALA:HB1	2.25	0.71
2:D:492:LYS:HE3	2:D:517:TYR:CE2	2.26	0.70
2:H:211:ASP:O	2:H:215:ILE:HG13	1.91	0.70
1:E:105:ALA:CB	1:E:114:LEU:HD13	2.21	0.70
1:M:112:ASN:C	1:M:114:LEU:H	1.95	0.70
2:N:55:VAL:HG23	2:N:75:LEU:HD21	1.72	0.70
2:J:161:THR:HG22	2:J:186:GLU:HG2	1.73	0.70
3:U:203:ILE:H	3:U:203:ILE:HD12	1.56	0.70
2:F:161:THR:HG22	2:F:186:GLU:HG2	1.72	0.70
2:H:76:ARG:HH11	2:H:76:ARG:CG	2.04	0.70
2:L:391:THR:HG23	2:L:394:SER:H	1.56	0.70
2:F:85:ARG:NH2	4:F:3100:OGK:O07	2.23	0.70
2:B:492:LYS:HE3	2:B:517:TYR:CE2	2.25	0.70
2:H:116:SER:CB	2:H:142:THR:HG23	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:LEU:HD22	2:H:61:TYR:HB2	1.73	0.70
2:H:311:CYS:CB	2:H:336:VAL:HG21	2.19	0.70
2:H:370:LEU:N	2:H:370:LEU:HD23	2.06	0.70
2:P:55:VAL:HG23	2:P:75:LEU:HD21	1.73	0.70
2:H:191:ASN:HD21	2:H:194:LEU:H	1.37	0.70
2:H:364:LEU:HD22	2:H:388:SER:H	1.54	0.70
2:H:118:HIS:CD2	2:H:144:LYS:HD3	2.26	0.70
1:C:124:MET:O	1:C:128:LYS:HE2	1.92	0.70
2:F:101:THR:HG22	2:F:128:ASP:OD1	1.91	0.70
2:H:450:LEU:CD1	2:H:454:GLY:HA3	2.22	0.69
2:J:419:ILE:HD13	2:J:446:ARG:NH1	2.07	0.69
2:D:286:PRO:HA	2:D:289:PHE:CD2	2.28	0.69
2:H:325:THR:O	2:H:349:ILE:HA	1.91	0.69
1:I:35:ASP:HB3	2:N:243:ALA:HB1	1.73	0.69
2:P:191:ASN:HD21	2:P:194:LEU:H	1.40	0.69
2:L:143:LEU:HD23	2:L:159:ILE:HD13	1.75	0.69
1:M:10:SER:HB2	1:M:52:LEU:HD23	1.74	0.69
2:B:101:THR:HG22	2:B:128:ASP:OD1	1.92	0.69
2:B:350:GLU:HB3	3:Q:209:LEU:HD21	1.74	0.69
2:F:295:ILE:HG21	2:F:298:LEU:HD13	1.74	0.69
2:D:161:THR:HG22	2:D:186:GLU:HG2	1.75	0.69
2:N:521:GLN:HG3	2:N:567:HIS:HD2	1.55	0.69
2:B:419:ILE:HD13	2:B:446:ARG:NH1	2.08	0.69
2:F:168:THR:HB	2:F:196:VAL:CG1	2.18	0.69
2:F:349:ILE:HG13	2:F:385:VAL:HG22	1.73	0.69
2:H:176:PHE:CZ	2:H:204:PHE:CZ	2.80	0.69
2:H:367:GLN:O	2:H:371:ILE:HG13	1.93	0.69
2:F:297:LYS:HG3	2:F:322:VAL:HB	1.75	0.69
2:B:286:PRO:HA	2:B:289:PHE:CD2	2.27	0.69
2:F:157:LEU:O	2:F:161:THR:HG23	1.92	0.69
2:H:116:SER:HB2	2:H:142:THR:CG2	2.18	0.69
2:H:133:ALA:HB2	2:H:159:ILE:HG22	1.75	0.69
1:M:93:ILE:HD12	1:M:97:THR:CG2	2.21	0.69
2:P:492:LYS:HE3	2:P:517:TYR:CE2	2.28	0.69
3:R:203:ILE:HD12	3:R:203:ILE:H	1.56	0.69
3:X:203:ILE:HD12	3:X:203:ILE:H	1.58	0.69
2:F:391:THR:HG23	2:F:394:SER:H	1.55	0.68
2:N:161:THR:HG22	2:N:186:GLU:HG2	1.76	0.68
2:H:414:ASP:HB3	2:H:446:ARG:NH2	2.08	0.68
2:N:286:PRO:HA	2:N:289:PHE:CD2	2.28	0.68
2:H:278:SER:O	2:H:280:MET:N	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:ARG:NE	2:N:112:ARG:CG	2.55	0.68
1:K:10:SER:HB2	1:K:52:LEU:HD23	1.76	0.68
3:Q:203:ILE:HD12	3:Q:203:ILE:H	1.57	0.68
1:A:124:MET:O	1:A:128:LYS:HE2	1.94	0.68
2:H:519:TRP:HH2	2:H:567:HIS:CE1	2.10	0.68
2:L:253:LEU:HD12	2:L:280:MET:HB2	1.74	0.68
2:N:519:TRP:HE1	4:N:7100:OGK:H01	1.57	0.68
2:P:101:THR:HG22	2:P:128:ASP:OD1	1.93	0.68
2:B:168:THR:HB	2:B:196:VAL:CG1	2.18	0.68
2:L:468:MET:HE3	2:L:470:LEU:HD21	1.76	0.68
2:J:164:ARG:CD	2:N:112:ARG:HG2	2.24	0.68
4:N:7100:OGK:C18	4:N:7100:OGK:HN08	2.07	0.68
2:J:297:LYS:HG3	2:J:322:VAL:HB	1.75	0.68
1:M:100:GLU:HG2	2:N:15:ALA:HB2	1.76	0.68
2:D:57:MET:HE3	2:D:62:THR:HG22	1.76	0.68
1:O:129:THR:O	1:O:133:ILE:HG12	1.94	0.68
2:P:547:SER:HB3	2:P:564:HIS:CB	2.24	0.67
2:B:143:LEU:HD23	2:B:159:ILE:HD13	1.75	0.67
2:B:547:SER:HB3	2:B:564:HIS:CB	2.25	0.67
2:H:444:TYR:HA	2:H:471:GLY:HA3	1.76	0.67
1:I:129:THR:O	1:I:133:ILE:HG12	1.94	0.67
2:J:101:THR:HG22	2:J:128:ASP:OD1	1.94	0.67
2:J:295:ILE:HG21	2:J:298:LEU:HD13	1.76	0.67
2:L:492:LYS:HE3	2:L:517:TYR:CE2	2.29	0.67
2:B:84:PRO:HB3	2:B:517:TYR:OH	1.94	0.67
2:H:81:LYS:HG2	2:H:120:ARG:HD3	1.77	0.67
2:J:547:SER:HB3	2:J:564:HIS:CB	2.24	0.67
2:J:337:LEU:HD12	2:J:341:CYS:SG	2.34	0.67
1:C:40:ASN:HB3	1:K:13:GLY:O	1.94	0.67
2:N:282:PRO:HA	2:N:285:MET:HE2	1.77	0.67
2:P:295:ILE:HG21	2:P:298:LEU:HD13	1.75	0.67
2:L:487:CYS:HB3	2:L:490:LEU:HB2	1.76	0.67
2:P:157:LEU:O	2:P:161:THR:HG23	1.93	0.67
2:J:350:GLU:HB3	3:U:209:LEU:HD21	1.77	0.67
2:D:297:LYS:HG3	2:D:322:VAL:HB	1.77	0.67
2:N:388:SER:O	2:N:416:GLU:HG3	1.95	0.67
2:H:52:ARG:NH1	2:H:72:PHE:CZ	2.63	0.67
2:L:547:SER:HB3	2:L:564:HIS:CB	2.25	0.67
2:D:547:SER:HB3	2:D:564:HIS:CB	2.25	0.66
2:H:85:ARG:NH2	4:H:4100:OGK:O07	2.29	0.66
1:O:105:ALA:HB3	1:O:114:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:ILE:HG21	2:D:298:LEU:HD13	1.78	0.66
2:N:157:LEU:O	2:N:161:THR:HG23	1.96	0.66
2:N:297:LYS:HG3	2:N:322:VAL:HB	1.78	0.66
2:H:533:MET:HE1	2:H:588:LEU:HD13	1.77	0.66
2:H:59:LEU:CD2	2:H:61:TYR:HB2	2.25	0.66
2:J:440:ARG:HB3	2:J:467:TRP:HE3	1.59	0.66
1:M:52:LEU:O	1:M:56:ILE:HG13	1.96	0.66
2:H:398:ILE:HG23	2:H:402:LEU:HD11	1.76	0.66
2:P:253:LEU:HD12	2:P:280:MET:HB2	1.77	0.66
2:N:295:ILE:HG21	2:N:298:LEU:HD13	1.78	0.66
1:A:93:ILE:HD12	1:A:97:THR:CG2	2.22	0.66
2:F:455:LEU:HD22	2:F:483:PHE:HB2	1.78	0.66
2:J:492:LYS:HE3	2:J:517:TYR:CE2	2.30	0.66
2:N:101:THR:HG22	2:N:128:ASP:OD1	1.96	0.66
2:P:419:ILE:HD13	2:P:446:ARG:NH1	2.11	0.66
1:G:10:SER:HB2	1:G:52:LEU:HD23	1.77	0.66
2:J:157:LEU:O	2:J:161:THR:HG23	1.95	0.66
2:L:472:TYR:OH	3:V:201:LEU:HB2	1.96	0.66
2:H:546:PRO:HD2	2:H:584:THR:O	1.96	0.65
2:J:487:CYS:HB3	2:J:490:LEU:HB2	1.79	0.65
2:P:282:PRO:HA	2:P:285:MET:HE2	1.78	0.65
2:D:472:TYR:OH	3:R:201:LEU:HB2	1.96	0.65
2:B:487:CYS:HB3	2:B:490:LEU:HB2	1.77	0.65
2:D:282:PRO:HA	2:D:285:MET:HE2	1.79	0.65
2:H:492:LYS:NZ	2:H:516:ARG:HH11	1.93	0.65
1:I:105:ALA:HB3	1:I:114:LEU:CD1	2.26	0.65
2:B:85:ARG:NH2	4:B:1100:OGK:O07	2.28	0.65
2:B:590:GLU:HB3	2:B:591:PRO:CD	2.27	0.65
2:H:40:VAL:O	2:H:41:CYS:CB	2.43	0.65
2:J:138:ASP:OD2	2:J:164:ARG:HG3	1.96	0.65
2:N:547:SER:HB3	2:N:564:HIS:CB	2.26	0.65
2:N:57:MET:HE3	2:N:62:THR:HG22	1.79	0.65
2:H:304:LEU:HD13	2:H:304:LEU:O	1.96	0.65
2:H:375:GLN:HG2	2:H:401:TYR:CD1	2.31	0.65
2:N:129:LEU:HD21	2:N:155:GLY:HA3	1.78	0.65
2:P:487:CYS:HB3	2:P:490:LEU:HB2	1.77	0.65
1:E:37:CYS:SG	2:L:296:ARG:NH2	2.69	0.65
2:H:95:ASN:HD22	2:H:95:ASN:N	1.78	0.65
2:J:164:ARG:NE	2:N:112:ARG:HG2	2.11	0.65
2:N:143:LEU:HD23	2:N:159:ILE:HD13	1.78	0.65
1:C:10:SER:HB2	1:C:52:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:PRO:HB3	2:F:517:TYR:OH	1.96	0.65
2:J:191:ASN:HD21	2:J:194:LEU:H	1.45	0.65
2:F:350:GLU:HB3	3:S:209:LEU:HD21	1.77	0.65
2:H:533:MET:HE3	2:H:588:LEU:HD13	1.78	0.65
2:N:487:CYS:HB3	2:N:490:LEU:HB2	1.77	0.65
2:B:440:ARG:HB3	2:B:467:TRP:HE3	1.61	0.64
2:H:545:ILE:HB	2:H:567:HIS:HB2	1.79	0.64
2:H:492:LYS:NZ	2:H:516:ARG:NH1	2.45	0.64
2:L:297:LYS:HG3	2:L:322:VAL:HB	1.80	0.64
2:N:399:GLY:O	2:N:434:GLY:HA3	1.97	0.64
2:B:295:ILE:HG21	2:B:298:LEU:HD13	1.79	0.64
1:C:113:LEU:O	1:C:117:THR:HG23	1.96	0.64
2:H:442:ALA:HB1	2:H:469:LEU:HB3	1.78	0.64
2:H:52:ARG:NH1	2:H:72:PHE:CE2	2.66	0.64
2:P:440:ARG:HB3	2:P:467:TRP:HE3	1.62	0.64
2:D:101:THR:HG22	2:D:128:ASP:OD1	1.98	0.64
2:F:101:THR:OG1	2:F:102:PRO:HD3	1.96	0.64
1:I:26:SER:OG	1:I:108:LEU:HB3	1.98	0.64
2:D:191:ASN:HD21	2:D:194:LEU:H	1.44	0.64
2:H:371:ILE:O	2:H:375:GLN:HG3	1.97	0.64
2:F:143:LEU:HD23	2:F:159:ILE:HD13	1.78	0.64
2:H:286:PRO:C	2:H:288:LEU:H	2.00	0.64
2:L:440:ARG:HB3	2:L:467:TRP:HE3	1.61	0.64
2:J:253:LEU:HD12	2:J:280:MET:HB2	1.80	0.64
1:O:10:SER:HB2	1:O:52:LEU:HD23	1.79	0.64
2:D:487:CYS:HB3	2:D:490:LEU:HB2	1.80	0.64
1:M:102:ILE:CD1	2:N:20:VAL:HG21	2.26	0.64
2:F:253:LEU:HD12	2:F:280:MET:HB2	1.79	0.64
2:F:40:VAL:O	2:F:41:CYS:HB3	1.96	0.64
2:H:104:VAL:HG21	2:H:128:ASP:HB2	1.80	0.64
2:H:409:ARG:HB2	4:H:4100:OGK:H16B	1.79	0.64
2:H:384:ALA:HB2	2:H:409:ARG:HG3	1.79	0.64
2:P:85:ARG:NH2	4:P:8100:OGK:O07	2.29	0.64
2:H:364:LEU:O	2:H:365:VAL:HG13	1.97	0.64
2:L:157:LEU:O	2:L:161:THR:HG23	1.98	0.64
1:A:10:SER:HB2	1:A:52:LEU:HD23	1.78	0.63
1:I:10:SER:HB2	1:I:52:LEU:HD23	1.78	0.63
1:A:12:ASP:OD2	1:A:49:SER:HB2	1.98	0.63
2:B:521:GLN:HG3	2:B:567:HIS:HD2	1.63	0.63
2:D:388:SER:O	2:D:416:GLU:HG3	1.99	0.63
2:H:225:VAL:HG22	2:H:245:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:57:MET:HE3	2:P:62:THR:HG22	1.81	0.63
2:F:57:MET:HE3	2:F:62:THR:HG22	1.80	0.63
2:N:298:LEU:HD23	2:N:300:LEU:HD11	1.81	0.63
2:N:521:GLN:HG3	2:N:567:HIS:CD2	2.33	0.63
1:C:129:THR:O	1:C:133:ILE:HG12	1.99	0.63
2:L:191:ASN:HD21	2:L:194:LEU:H	1.46	0.63
1:O:124:MET:O	1:O:128:LYS:HE2	1.97	0.63
1:A:129:THR:O	1:A:133:ILE:HG12	1.98	0.63
1:M:96:ALA:HB1	2:N:14:VAL:CG1	2.28	0.63
2:J:55:VAL:HG23	2:J:75:LEU:HD21	1.79	0.63
1:M:102:ILE:CG2	2:N:20:VAL:CG2	2.76	0.63
2:D:168:THR:HB	2:D:196:VAL:CG1	2.21	0.63
2:F:521:GLN:HG3	2:F:567:HIS:HD2	1.64	0.63
2:H:357:GLY:C	2:H:359:GLU:H	2.02	0.63
1:K:102:ILE:HG12	1:K:117:THR:HB	1.80	0.63
1:M:12:ASP:OD2	1:M:49:SER:HB2	1.99	0.63
2:N:519:TRP:NE1	4:N:7100:OGK:H01	2.12	0.63
2:P:311:CYS:HB3	2:P:336:VAL:HG21	1.80	0.63
2:D:294:GLN:NE2	1:G:107:TYR:OH	2.32	0.63
1:I:102:ILE:HG23	1:I:118:CYS:SG	2.39	0.63
2:N:311:CYS:HB3	2:N:336:VAL:HG21	1.79	0.63
2:N:419:ILE:HD13	2:N:446:ARG:NH1	2.13	0.63
2:B:191:ASN:HD21	2:B:194:LEU:H	1.47	0.62
2:F:547:SER:HB3	2:F:564:HIS:CB	2.28	0.62
2:H:230:PHE:HB3	2:H:235:LEU:HD21	1.81	0.62
2:H:501:SER:HB3	2:H:524:ARG:NH1	2.14	0.62
2:J:590:GLU:HB3	2:J:591:PRO:CD	2.27	0.62
2:D:590:GLU:HB3	2:D:591:PRO:CD	2.28	0.62
1:E:10:SER:HB2	1:E:52:LEU:HD23	1.79	0.62
1:E:45:PRO:HB2	2:L:291:PHE:HA	1.81	0.62
2:F:282:PRO:HA	2:F:285:MET:HE2	1.81	0.62
2:F:492:LYS:HE3	2:F:517:TYR:CE2	2.34	0.62
2:H:366:SER:OG	2:H:368:ARG:HG2	1.99	0.62
2:N:85:ARG:NH2	4:N:7100:OGK:O07	2.28	0.62
2:D:190:HIS:CG	2:H:112:ARG:HH11	2.17	0.62
2:J:164:ARG:HE	2:N:112:ARG:HG2	1.64	0.62
2:N:310:HIS:O	2:N:314:ILE:HG12	2.00	0.62
2:F:590:GLU:HB3	2:F:591:PRO:CD	2.28	0.62
2:L:138:ASP:OD2	2:L:164:ARG:HG3	1.98	0.62
2:L:295:ILE:HG21	2:L:298:LEU:HD13	1.79	0.62
2:L:455:LEU:HD22	2:L:483:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:84:PRO:HB3	2:L:517:TYR:OH	1.99	0.62
2:L:55:VAL:HG23	2:L:75:LEU:HD21	1.81	0.62
2:N:253:LEU:HD12	2:N:280:MET:HB2	1.81	0.62
2:N:63:ALA:HB1	2:N:67:ARG:HD2	1.82	0.62
2:D:350:GLU:HB3	3:R:209:LEU:HD21	1.81	0.62
2:F:468:MET:HE3	2:F:470:LEU:HD21	1.82	0.62
2:H:544:LEU:O	2:H:546:PRO:HD3	2.00	0.62
2:J:521:GLN:HG3	2:J:567:HIS:HD2	1.65	0.62
2:F:440:ARG:HB3	2:F:467:TRP:HE3	1.65	0.62
2:B:388:SER:O	2:B:416:GLU:HG3	2.00	0.62
2:F:487:CYS:HB3	2:F:490:LEU:HB2	1.80	0.62
2:D:419:ILE:HD13	2:D:446:ARG:NH1	2.13	0.62
2:H:101:THR:HG23	2:H:131:ARG:HH12	1.65	0.61
2:P:129:LEU:HD21	2:P:155:GLY:HA3	1.82	0.61
2:H:442:ALA:CB	2:H:469:LEU:HB3	2.30	0.61
2:P:184:LEU:HD12	2:P:207:ILE:HB	1.81	0.61
2:F:365:VAL:HG23	2:F:387:VAL:HA	1.83	0.61
2:F:399:GLY:O	2:F:434:GLY:HA3	2.00	0.61
2:H:253:LEU:HD13	2:H:284:GLU:HG3	1.82	0.61
2:H:440:ARG:HB3	2:H:467:TRP:CD1	2.31	0.61
2:J:164:ARG:NE	2:N:112:ARG:HG3	2.15	0.61
2:N:455:LEU:HD22	2:N:483:PHE:HB2	1.82	0.61
1:A:99:PHE:HZ	1:A:137:PHE:HE1	1.46	0.61
2:B:282:PRO:HA	2:B:285:MET:HE2	1.82	0.61
2:D:253:LEU:HD12	2:D:280:MET:HB2	1.81	0.61
2:H:85:ARG:O	2:H:88:MET:HG2	2.01	0.61
1:K:52:LEU:O	1:K:56:ILE:HG13	2.01	0.61
2:N:101:THR:OG1	2:N:102:PRO:HD3	2.00	0.61
2:H:89:PHE:CE1	4:H:4100:OGK:H17	2.35	0.61
2:J:57:MET:HE3	2:J:62:THR:HG22	1.82	0.61
2:L:184:LEU:HD12	2:L:207:ILE:HB	1.82	0.61
2:L:419:ILE:HD13	2:L:446:ARG:NH1	2.15	0.61
1:M:137:PHE:CD1	2:N:17:VAL:HG21	2.36	0.61
1:E:48:THR:HG22	1:E:51:ILE:HB	1.82	0.61
2:H:461:TYR:C	2:H:463:PRO:HD3	2.20	0.61
1:O:137:PHE:CD1	2:P:17:VAL:HG21	2.35	0.61
2:P:310:HIS:O	2:P:314:ILE:HG12	2.00	0.61
4:P:8100:OGK:C18	4:P:8100:OGK:HN08	2.13	0.61
2:D:227:VAL:CG1	2:D:228:GLY:N	2.64	0.61
2:F:419:ILE:HD13	2:F:446:ARG:NH1	2.16	0.61
2:H:412:LEU:HD12	2:H:445:LEU:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:SER:OG	1:M:108:LEU:HB3	2.00	0.61
2:P:533:MET:HE3	2:P:588:LEU:HD13	1.83	0.61
2:H:40:VAL:O	2:H:40:VAL:HG23	1.99	0.61
2:L:85:ARG:NH2	4:L:6100:OGK:O07	2.30	0.61
1:E:12:ASP:OD2	1:E:49:SER:HB2	2.00	0.61
2:J:129:LEU:HD21	2:J:155:GLY:HA3	1.82	0.61
2:P:455:LEU:HD22	2:P:483:PHE:HB2	1.81	0.61
2:P:590:GLU:HB3	2:P:591:PRO:CD	2.26	0.61
1:A:137:PHE:CD1	2:B:17:VAL:HG21	2.36	0.60
2:L:388:SER:O	2:L:416:GLU:HG3	2.01	0.60
2:L:590:GLU:HB3	2:L:591:PRO:CD	2.27	0.60
2:N:311:CYS:O	2:N:315:GLN:HB2	2.00	0.60
2:H:428:VAL:HG11	2:H:443:PHE:CZ	2.36	0.60
2:J:101:THR:OG1	2:J:102:PRO:HD3	2.00	0.60
2:L:542:ILE:CD1	2:L:588:LEU:HD12	2.21	0.60
2:N:272:LEU:HD21	2:N:275:LEU:HB3	1.82	0.60
2:B:533:MET:HE3	2:B:588:LEU:HD13	1.82	0.60
1:E:6:ILE:HD12	1:E:23:ALA:HB3	1.82	0.60
1:E:52:LEU:O	1:E:56:ILE:HG13	2.01	0.60
2:H:124:VAL:O	2:H:151:PHE:HB3	2.02	0.60
2:H:392:ASN:HD22	2:H:422:LEU:HD13	1.66	0.60
2:L:227:VAL:CG1	2:L:228:GLY:N	2.64	0.60
2:H:109:ASN:C	2:H:110:ASN:HD22	2.05	0.60
2:H:233:LEU:HA	2:H:236:VAL:HG23	1.82	0.60
2:J:547:SER:HB3	2:J:564:HIS:HB3	1.83	0.60
2:N:367:GLN:O	2:N:371:ILE:HG22	2.01	0.60
2:P:388:SER:O	2:P:416:GLU:HG3	2.00	0.60
2:P:565:PRO:HG2	3:X:201:LEU:HD21	1.83	0.60
2:F:130:ASP:OD1	2:F:134:LYS:HE3	2.00	0.60
1:G:52:LEU:O	1:G:56:ILE:HG13	2.02	0.60
1:I:52:LEU:O	1:I:56:ILE:HG13	2.01	0.60
2:J:519:TRP:HE1	4:J:5100:OGK:H01	1.66	0.60
2:L:521:GLN:HG3	2:L:567:HIS:HD2	1.64	0.60
2:B:311:CYS:O	2:B:315:GLN:HB2	2.01	0.60
2:B:365:VAL:HG23	2:B:387:VAL:HA	1.84	0.60
2:D:91:LEU:O	2:D:567:HIS:HE1	1.83	0.60
1:G:137:PHE:HB3	2:H:17:VAL:HG21	1.82	0.60
2:H:396:GLU:O	2:H:400:THR:HG23	2.01	0.60
2:H:425:ASP:OD2	2:H:451:THR:HG23	2.02	0.60
2:L:101:THR:HG22	2:L:128:ASP:OD1	2.01	0.60
1:A:58:TYR:CD2	1:A:113:LEU:HD13	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:PRO:HB3	2:D:517:TYR:OH	2.02	0.60
4:F:3100:OGK:HN08	4:F:3100:OGK:C18	2.15	0.60
2:F:310:HIS:O	2:F:314:ILE:HG12	2.02	0.60
2:L:227:VAL:HG13	2:L:228:GLY:N	2.16	0.60
2:B:443:PHE:CE2	2:B:445:LEU:HD11	2.37	0.60
2:D:101:THR:HG22	2:D:128:ASP:HB3	1.83	0.60
2:H:87:ALA:HB2	2:H:92:ILE:HG13	1.83	0.60
1:M:100:GLU:HG2	2:N:15:ALA:CB	2.31	0.60
2:B:298:LEU:HD23	2:B:300:LEU:HD11	1.84	0.60
2:D:367:GLN:HB3	2:D:391:THR:CG2	2.31	0.60
2:H:445:LEU:HD12	2:H:473:VAL:HG12	1.83	0.60
2:H:469:LEU:HD12	2:H:494:GLU:O	2.01	0.60
2:H:47:ILE:O	2:H:51:THR:HG23	2.02	0.60
2:J:519:TRP:NE1	4:J:5100:OGK:H01	2.17	0.60
2:P:547:SER:HB3	2:P:564:HIS:HB3	1.84	0.60
2:B:101:THR:OG1	2:B:102:PRO:HD3	2.02	0.60
2:B:468:MET:HE3	2:B:470:LEU:HD21	1.82	0.60
1:G:30:ALA:O	1:G:33:VAL:HG22	2.01	0.60
2:H:76:ARG:NH1	2:H:76:ARG:CG	2.65	0.60
2:B:297:LYS:HG3	2:B:322:VAL:HB	1.83	0.59
2:D:157:LEU:O	2:D:161:THR:HG23	2.02	0.59
1:E:30:ALA:O	1:E:33:VAL:HG22	2.02	0.59
1:G:153:ARG:HG2	1:G:153:ARG:NH1	2.17	0.59
2:J:367:GLN:HB3	2:J:391:THR:CG2	2.31	0.59
2:L:365:VAL:HG23	2:L:387:VAL:HA	1.84	0.59
1:M:158:ALA:HA	2:N:62:THR:HG21	1.84	0.59
1:M:48:THR:HG22	1:M:51:ILE:HB	1.84	0.59
1:M:99:PHE:HB2	2:N:15:ALA:CB	2.32	0.59
2:B:121:ARG:NH2	5:B:1103:PO4:O4	2.34	0.59
2:H:22:GLU:HG2	2:H:47:ILE:CD1	2.32	0.59
2:N:65:PRO:HB3	2:N:103:TRP:CE3	2.37	0.59
2:N:275:LEU:HD11	2:N:288:LEU:HD21	1.83	0.59
2:N:91:LEU:O	2:N:567:HIS:HE1	1.85	0.59
2:H:230:PHE:CD1	2:H:235:LEU:HD21	2.37	0.59
2:J:388:SER:O	2:J:416:GLU:HG3	2.03	0.59
2:D:184:LEU:HD12	2:D:207:ILE:HB	1.84	0.59
2:D:40:VAL:O	2:D:41:CYS:HB3	2.02	0.59
2:P:298:LEU:HD23	2:P:300:LEU:HD11	1.84	0.59
2:D:101:THR:OG1	2:D:102:PRO:HD3	2.02	0.59
2:H:392:ASN:O	2:H:396:GLU:CG	2.45	0.59
1:O:93:ILE:HD12	1:O:97:THR:CG2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:SER:HB2	2:H:128:ASP:H	1.67	0.59
2:H:444:TYR:OH	2:H:496:ARG:HD3	2.01	0.59
2:L:129:LEU:HD21	2:L:155:GLY:HA3	1.85	0.59
2:N:367:GLN:HB3	2:N:391:THR:CG2	2.30	0.59
2:P:357:GLY:HA2	2:P:415:ARG:NH2	2.11	0.59
2:B:227:VAL:CG1	2:B:228:GLY:N	2.65	0.59
2:D:311:CYS:O	2:D:315:GLN:HB2	2.03	0.59
1:G:130:PRO:HD3	2:H:36:SER:HB2	1.84	0.59
2:H:22:GLU:HG2	2:H:47:ILE:HD11	1.83	0.59
1:K:12:ASP:OD2	1:K:49:SER:HB2	2.01	0.59
1:A:52:LEU:O	1:A:56:ILE:HG13	2.01	0.59
1:E:158:ALA:HA	2:F:62:THR:HG21	1.84	0.59
2:J:351:ARG:O	2:J:351:ARG:HG3	2.03	0.59
2:P:468:MET:HE3	2:P:470:LEU:HD21	1.83	0.59
2:B:261:GLU:HG2	2:B:264:MET:HG3	1.85	0.59
2:D:261:GLU:HG2	2:D:264:MET:HG3	1.85	0.59
1:E:43:PRO:HG3	2:L:319:ASN:HD21	1.67	0.59
2:H:412:LEU:HD11	2:H:445:LEU:CD2	2.33	0.59
2:L:197:LEU:O	2:L:225:VAL:HA	2.02	0.59
2:N:65:PRO:HA	2:N:103:TRP:CZ3	2.38	0.59
2:P:91:LEU:O	2:P:567:HIS:HE1	1.86	0.58
2:B:519:TRP:NE1	4:B:1100:OGK:H01	2.18	0.58
1:C:12:ASP:OD2	1:C:49:SER:HB2	2.03	0.58
1:I:93:ILE:HD12	1:I:97:THR:CG2	2.26	0.58
2:J:357:GLY:HA2	2:J:415:ARG:NH2	2.12	0.58
2:N:404:ASN:HA	2:N:437:LYS:HD2	1.85	0.58
1:C:52:LEU:O	1:C:56:ILE:HG13	2.02	0.58
2:F:227:VAL:CG1	2:F:228:GLY:N	2.66	0.58
1:G:153:ARG:HG2	1:G:153:ARG:HH11	1.67	0.58
2:D:319:ASN:ND2	1:G:43:PRO:CG	2.65	0.58
2:L:547:SER:HB3	2:L:564:HIS:HB3	1.86	0.58
1:K:158:ALA:HA	2:L:62:THR:HG21	1.84	0.58
1:M:105:ALA:HB2	1:M:113:LEU:HD23	1.83	0.58
2:P:311:CYS:O	2:P:315:GLN:HB2	2.04	0.58
2:B:57:MET:HE3	2:B:62:THR:HG22	1.85	0.58
1:E:137:PHE:CD1	2:F:17:VAL:HG21	2.39	0.58
2:F:80:LEU:HB2	2:F:122:MET:CE	2.33	0.58
2:J:233:LEU:O	2:J:236:VAL:HG23	2.04	0.58
2:P:197:LEU:O	2:P:225:VAL:HA	2.03	0.58
2:P:337:LEU:HD12	2:P:341:CYS:SG	2.44	0.58
2:B:63:ALA:HB1	2:B:67:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:GLY:HA2	2:F:415:ARG:NH2	2.12	0.58
2:J:533:MET:HE3	2:J:588:LEU:HD13	1.85	0.58
2:L:357:GLY:HA2	2:L:415:ARG:NH2	2.11	0.58
2:P:84:PRO:HB3	2:P:517:TYR:OH	2.04	0.58
2:B:227:VAL:HG13	2:B:228:GLY:N	2.19	0.58
2:F:388:SER:O	2:F:416:GLU:HG3	2.03	0.58
1:G:98:LEU:HD21	1:G:120:THR:HG22	1.85	0.58
2:H:311:CYS:HB3	2:H:336:VAL:CG2	2.22	0.58
4:J:5100:OGK:HN08	4:J:5100:OGK:C18	2.16	0.58
2:J:91:LEU:O	2:J:567:HIS:HE1	1.87	0.58
2:P:519:TRP:NE1	4:P:8100:OGK:H01	2.18	0.58
2:F:129:LEU:HD21	2:F:155:GLY:HA3	1.86	0.58
2:H:390:ILE:HD11	2:H:410:LEU:HD11	1.83	0.58
2:N:80:LEU:HB2	2:N:122:MET:CE	2.34	0.58
1:O:12:ASP:OD2	1:O:49:SER:HB2	2.04	0.58
2:J:40:VAL:O	2:J:41:CYS:HB3	2.03	0.58
2:L:282:PRO:HA	2:L:285:MET:HE2	1.85	0.58
2:P:272:LEU:HD21	2:P:275:LEU:HB3	1.84	0.58
2:P:519:TRP:HE1	4:P:8100:OGK:H01	1.67	0.58
2:D:440:ARG:HB3	2:D:467:TRP:CE3	2.37	0.58
1:E:158:ALA:HA	2:F:62:THR:CG2	2.34	0.58
1:G:12:ASP:OD2	1:G:49:SER:HB2	2.04	0.58
2:H:305:LEU:HD23	2:H:305:LEU:H	1.69	0.58
2:H:25:MET:HG2	2:H:47:ILE:HG22	1.86	0.58
2:H:519:TRP:CH2	2:H:567:HIS:CE1	2.92	0.58
2:P:399:GLY:O	2:P:434:GLY:HA3	2.03	0.58
2:B:444:TYR:HA	2:B:471:GLY:CA	2.30	0.58
2:D:129:LEU:HD21	2:D:155:GLY:HA3	1.85	0.58
2:D:227:VAL:HG13	2:D:228:GLY:N	2.19	0.58
2:D:547:SER:HB3	2:D:564:HIS:HB3	1.85	0.58
1:K:137:PHE:CD1	2:L:17:VAL:HG21	2.39	0.58
2:L:130:ASP:OD1	2:L:134:LYS:HE3	2.03	0.58
2:L:367:GLN:HB3	2:L:391:THR:CG2	2.32	0.58
2:B:129:LEU:HD21	2:B:155:GLY:HA3	1.85	0.57
2:B:477:ASP:OD2	2:B:504:ALA:HB2	2.04	0.57
2:F:446:ARG:HG2	2:F:447:GLN:H	1.69	0.57
2:H:38:SER:O	2:H:45:PHE:HB2	2.04	0.57
1:I:134:ARG:HB2	1:I:139:ILE:O	2.04	0.57
2:L:533:MET:HE3	2:L:588:LEU:HD13	1.85	0.57
2:D:533:MET:HE3	2:D:588:LEU:HD13	1.87	0.57
2:F:396:GLU:O	2:F:400:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:184:LEU:HD12	2:N:207:ILE:HB	1.86	0.57
2:P:101:THR:HG22	2:P:128:ASP:HB3	1.84	0.57
2:B:396:GLU:O	2:B:400:THR:HB	2.04	0.57
2:H:519:TRP:HE1	4:H:4100:OGK:C01	2.16	0.57
1:G:159:PHE:CE2	2:H:68:LEU:HD13	2.39	0.57
1:M:158:ALA:HA	2:N:62:THR:CG2	2.34	0.57
1:O:91:MET:SD	1:O:117:THR:HG22	2.44	0.57
2:H:444:TYR:CD1	2:H:471:GLY:HA2	2.39	0.57
2:J:197:LEU:O	2:J:225:VAL:HA	2.04	0.57
1:O:134:ARG:HB2	1:O:139:ILE:O	2.04	0.57
2:B:91:LEU:O	2:B:567:HIS:HE1	1.87	0.57
2:J:184:LEU:HD12	2:J:207:ILE:HB	1.86	0.57
2:B:519:TRP:HE1	4:B:1100:OGK:H01	1.70	0.57
2:B:101:THR:HG22	2:B:128:ASP:HB3	1.85	0.57
2:B:270:ARG:CB	1:O:107:TYR:CD1	2.88	0.57
2:D:233:LEU:O	2:D:236:VAL:HG23	2.04	0.57
2:F:55:VAL:HG23	2:F:75:LEU:HD21	1.87	0.57
2:D:365:VAL:HG23	2:D:387:VAL:HA	1.85	0.57
2:H:587:VAL:O	2:H:587:VAL:HG12	2.04	0.57
1:I:105:ALA:CB	1:I:114:LEU:HD13	2.33	0.57
2:N:590:GLU:HB3	2:N:591:PRO:CD	2.27	0.57
2:P:297:LYS:HG3	2:P:322:VAL:HB	1.85	0.57
2:B:547:SER:HB3	2:B:564:HIS:HB3	1.86	0.57
2:H:395:LEU:HB3	2:H:427:GLY:O	2.04	0.57
1:M:134:ARG:HB2	1:M:139:ILE:O	2.04	0.57
2:B:138:ASP:OD2	2:B:164:ARG:HG3	2.05	0.57
2:D:130:ASP:OD1	2:D:134:LYS:HE3	2.04	0.57
2:F:227:VAL:HG13	2:F:228:GLY:N	2.19	0.57
2:H:121:ARG:NH2	5:H:1103:PO4:O4	2.38	0.57
2:J:101:THR:CG2	2:J:128:ASP:OD1	2.53	0.57
2:J:344:LEU:HD23	2:J:380:LEU:HD21	1.87	0.57
2:L:93:PRO:HA	2:L:548:ARG:CB	2.26	0.57
2:N:191:ASN:HD21	2:N:194:LEU:H	1.50	0.57
1:O:48:THR:HG22	1:O:51:ILE:HB	1.87	0.57
1:O:158:ALA:HA	2:P:62:THR:HG21	1.87	0.57
2:H:95:ASN:ND2	2:H:95:ASN:N	2.44	0.57
2:J:84:PRO:HB3	2:J:517:TYR:OH	2.05	0.57
2:N:261:GLU:HG2	2:N:264:MET:HG3	1.87	0.57
2:P:40:VAL:O	2:P:41:CYS:HB3	2.02	0.57
1:A:48:THR:HG22	1:A:51:ILE:HB	1.86	0.56
1:E:134:ARG:HB2	1:E:139:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:407:ASP:OD1	2:H:440:ARG:HD2	2.05	0.56
2:H:542:ILE:CD1	2:H:588:LEU:HB2	2.35	0.56
1:I:160:GLU:HA	1:I:160:GLU:OE2	2.05	0.56
2:J:143:LEU:HD23	2:J:159:ILE:HD13	1.87	0.56
1:K:6:ILE:HD12	1:K:23:ALA:HB3	1.86	0.56
2:L:311:CYS:O	2:L:315:GLN:HB2	2.04	0.56
2:P:396:GLU:O	2:P:400:THR:HB	2.04	0.56
2:D:396:GLU:O	2:D:400:THR:HB	2.05	0.56
1:E:160:GLU:HA	1:E:160:GLU:OE2	2.05	0.56
2:F:91:LEU:O	2:F:567:HIS:HE1	1.88	0.56
2:H:225:VAL:HG21	2:H:238:PHE:HZ	1.70	0.56
2:J:101:THR:HG22	2:J:128:ASP:HB3	1.86	0.56
1:M:102:ILE:HD12	2:N:20:VAL:CG2	2.31	0.56
2:B:233:LEU:O	2:B:236:VAL:HG23	2.04	0.56
2:D:519:TRP:HE1	4:D:2100:OGK:H01	1.69	0.56
2:F:261:GLU:HG2	2:F:264:MET:HG3	1.87	0.56
2:F:311:CYS:O	2:F:315:GLN:HB2	2.06	0.56
2:F:443:PHE:CE2	2:F:445:LEU:HD11	2.40	0.56
2:H:365:VAL:CG2	2:H:387:VAL:HG13	2.34	0.56
2:L:519:TRP:NE1	4:L:6100:OGK:H01	2.20	0.56
2:N:223:VAL:O	2:N:245:LEU:HD12	2.06	0.56
2:N:547:SER:HB3	2:N:564:HIS:HB3	1.86	0.56
1:O:52:LEU:O	1:O:56:ILE:HG13	2.05	0.56
1:G:130:PRO:O	1:G:134:ARG:HG3	2.05	0.56
2:J:272:LEU:HD21	2:J:275:LEU:HB3	1.88	0.56
1:K:30:ALA:O	1:K:33:VAL:HG22	2.05	0.56
2:L:357:GLY:CA	2:L:415:ARG:HH22	2.13	0.56
2:P:521:GLN:HG3	2:P:567:HIS:HD2	1.69	0.56
2:J:565:PRO:HG2	3:U:201:LEU:HD21	1.86	0.56
2:P:350:GLU:HB3	3:X:209:LEU:HD21	1.86	0.56
1:M:58:TYR:CD2	1:M:113:LEU:HD13	2.40	0.56
2:P:227:VAL:CG1	2:P:228:GLY:N	2.68	0.56
2:P:54:HIS:HE1	2:P:56:THR:OG1	1.88	0.56
2:D:121:ARG:NH2	5:D:1103:PO4:O4	2.37	0.56
2:D:298:LEU:HD23	2:D:300:LEU:HD11	1.87	0.56
2:F:101:THR:CG2	2:F:128:ASP:OD1	2.54	0.56
2:H:276:GLY:HA3	2:H:299:ASP:HB3	1.87	0.56
2:H:411:VAL:CG1	2:H:444:TYR:HB3	2.35	0.56
2:H:82:GLY:HA3	2:H:122:MET:HG2	1.88	0.56
1:E:43:PRO:HG2	2:L:319:ASN:HD22	1.68	0.56
2:L:311:CYS:HB3	2:L:336:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:THR:HG22	1:C:51:ILE:HB	1.86	0.56
2:D:357:GLY:HA2	2:D:415:ARG:NH2	2.14	0.56
2:D:404:ASN:HA	2:D:437:LYS:HD2	1.86	0.56
2:F:482:GLU:O	2:F:485:ARG:HG2	2.05	0.56
2:H:334:LEU:HD22	2:H:373:LEU:HD22	1.85	0.56
2:H:447:GLN:HG3	2:H:447:GLN:O	2.05	0.56
1:I:30:ALA:O	1:I:33:VAL:HG22	2.06	0.56
2:N:396:GLU:O	2:N:400:THR:HB	2.05	0.56
2:N:40:VAL:O	2:N:41:CYS:HB3	2.04	0.56
2:N:477:ASP:OD2	2:N:504:ALA:HB2	2.05	0.56
2:P:404:ASN:HA	2:P:437:LYS:HD2	1.88	0.56
2:P:93:PRO:HA	2:P:548:ARG:CB	2.29	0.56
2:B:472:TYR:OH	3:Q:201:LEU:HB2	2.05	0.56
2:D:444:TYR:HA	2:D:471:GLY:CA	2.31	0.56
2:H:199:PHE:CE1	2:H:227:VAL:HG23	2.41	0.56
2:H:384:ALA:CB	2:H:409:ARG:HG3	2.35	0.56
2:L:337:LEU:HD12	2:L:341:CYS:SG	2.46	0.56
2:L:519:TRP:HE1	4:L:6100:OGK:H01	1.71	0.56
2:P:443:PHE:CE2	2:P:445:LEU:HD11	2.40	0.56
2:D:138:ASP:OD2	2:D:164:ARG:HG3	2.06	0.56
1:C:158:ALA:HA	2:D:62:THR:CG2	2.36	0.56
2:F:275:LEU:HD11	2:F:288:LEU:HD21	1.88	0.56
1:G:48:THR:HG22	1:G:51:ILE:HB	1.88	0.56
2:H:326:ARG:HA	2:H:350:GLU:O	2.05	0.56
2:H:343:GLN:H	2:H:343:GLN:CD	2.09	0.56
2:J:365:VAL:HG23	2:J:387:VAL:HA	1.87	0.56
2:B:40:VAL:O	2:B:41:CYS:HB3	2.06	0.56
2:F:191:ASN:HD21	2:F:194:LEU:H	1.53	0.56
2:H:285:MET:CG	2:H:286:PRO:HD3	2.34	0.56
2:H:469:LEU:HD21	4:H:4100:OGK:H05	1.88	0.56
2:L:396:GLU:O	2:L:400:THR:HB	2.06	0.56
2:N:321:GLU:HA	2:N:344:LEU:HA	1.87	0.56
2:N:344:LEU:HD23	2:N:380:LEU:HD21	1.86	0.56
2:N:468:MET:HE3	2:N:470:LEU:HD21	1.88	0.56
2:P:367:GLN:O	2:P:371:ILE:HG22	2.05	0.56
1:A:134:ARG:HB2	1:A:139:ILE:O	2.06	0.56
1:A:95:GLN:HE21	1:A:124:MET:HE3	1.71	0.56
2:B:310:HIS:O	2:B:314:ILE:HG12	2.05	0.56
2:D:411:VAL:HG22	2:D:444:TYR:HB3	1.87	0.56
2:F:184:LEU:HD12	2:F:207:ILE:HB	1.88	0.56
2:F:519:TRP:NE1	4:F:3100:OGK:H01	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:PRO:HA	2:F:548:ARG:CB	2.29	0.56
2:H:291:PHE:H	2:H:291:PHE:HD2	1.53	0.56
2:H:462:SER:N	2:H:463:PRO:HD3	2.20	0.56
1:I:12:ASP:OD2	1:I:49:SER:HB2	2.05	0.56
1:K:158:ALA:HA	2:L:62:THR:CG2	2.35	0.56
1:M:96:ALA:CB	2:N:14:VAL:HG12	2.34	0.56
2:B:55:VAL:HG23	2:B:75:LEU:HD21	1.88	0.55
1:C:30:ALA:O	1:C:33:VAL:HG22	2.05	0.55
2:H:390:ILE:HD12	2:H:410:LEU:HD21	1.88	0.55
1:G:125:ILE:HD11	2:H:44:TRP:HH2	1.71	0.55
2:L:272:LEU:HD21	2:L:275:LEU:HB3	1.87	0.55
2:L:399:GLY:O	2:L:434:GLY:HA3	2.06	0.55
2:N:546:PRO:HD3	2:N:584:THR:O	2.06	0.55
2:P:351:ARG:HG3	2:P:351:ARG:O	2.06	0.55
2:B:397:SER:O	2:B:400:THR:HG22	2.06	0.55
2:D:519:TRP:NE1	4:D:2100:OGK:H01	2.20	0.55
2:H:76:ARG:O	2:H:114:LEU:HD12	2.07	0.55
2:J:396:GLU:O	2:J:400:THR:HB	2.05	0.55
2:L:40:VAL:O	2:L:41:CYS:HB3	2.06	0.55
2:L:411:VAL:HG22	2:L:444:TYR:HB3	1.88	0.55
2:P:397:SER:O	2:P:400:THR:HG22	2.06	0.55
1:E:45:PRO:HG3	2:L:293:ALA:HB3	1.87	0.55
1:G:153:ARG:HH11	1:G:153:ARG:CG	2.19	0.55
2:H:366:SER:HB3	2:H:368:ARG:HG3	1.88	0.55
2:H:477:ASP:O	2:H:481:MET:HG2	2.06	0.55
2:J:282:PRO:HA	2:J:285:MET:HE2	1.88	0.55
4:L:6100:OGK:HN08	4:L:6100:OGK:C18	2.17	0.55
4:N:7100:OGK:C18	4:N:7100:OGK:N08	2.69	0.55
1:O:153:ARG:NH2	2:P:539:TYR:CE1	2.74	0.55
2:F:519:TRP:HE1	4:F:3100:OGK:H01	1.71	0.55
1:G:26:SER:OG	1:G:108:LEU:HB3	2.06	0.55
2:J:261:GLU:HG2	2:J:264:MET:HG3	1.89	0.55
1:A:158:ALA:HA	2:B:62:THR:HG21	1.88	0.55
1:I:6:ILE:HD12	1:I:23:ALA:HB3	1.88	0.55
2:L:101:THR:HG22	2:L:128:ASP:HB3	1.88	0.55
1:E:45:PRO:CD	2:L:294:GLN:HB2	2.37	0.55
2:L:398:ILE:HG23	2:L:402:LEU:HD11	1.89	0.55
1:A:6:ILE:HD12	1:A:23:ALA:HB3	1.87	0.55
2:B:296:ARG:NH2	1:O:37:CYS:SG	2.80	0.55
2:D:143:LEU:HD23	2:D:159:ILE:HD13	1.89	0.55
4:D:2100:OGK:HN08	4:D:2100:OGK:C18	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:310:HIS:O	2:F:314:ILE:CG1	2.55	0.55
2:J:446:ARG:HG2	2:J:447:GLN:H	1.71	0.55
2:J:95:ASN:O	2:J:582:PRO:HG3	2.06	0.55
1:K:48:THR:HG22	1:K:51:ILE:HB	1.88	0.55
2:P:101:THR:CG2	2:P:128:ASP:OD1	2.54	0.55
1:A:30:ALA:O	1:A:33:VAL:HG22	2.06	0.55
1:C:102:ILE:HG12	1:C:117:THR:HB	1.89	0.55
2:F:367:GLN:HB3	2:F:391:THR:CG2	2.34	0.55
2:H:232:ILE:HG13	2:H:253:LEU:HD21	1.89	0.55
2:H:374:ALA:HB2	2:H:398:ILE:HD12	1.88	0.55
2:J:311:CYS:O	2:J:315:GLN:HB2	2.06	0.55
1:O:105:ALA:CB	1:O:114:LEU:HD13	2.37	0.55
2:P:261:GLU:HG2	2:P:264:MET:HG3	1.89	0.55
2:P:310:HIS:O	2:P:314:ILE:CG1	2.55	0.55
2:B:197:LEU:O	2:B:225:VAL:HA	2.07	0.55
2:D:80:LEU:HB2	2:D:122:MET:CE	2.37	0.55
1:G:6:ILE:HD12	1:G:23:ALA:HB3	1.89	0.55
2:H:382:TYR:C	2:H:382:TYR:CD1	2.79	0.55
1:M:102:ILE:HB	2:N:20:VAL:HG21	1.89	0.55
1:M:30:ALA:O	1:M:33:VAL:HG22	2.07	0.55
1:O:48:THR:HG22	1:O:51:ILE:CG1	2.37	0.55
1:A:91:MET:O	1:A:93:ILE:N	2.40	0.55
2:B:547:SER:HB3	2:B:564:HIS:CG	2.42	0.55
2:J:130:ASP:OD1	2:J:134:LYS:HE3	2.06	0.55
2:J:444:TYR:HA	2:J:471:GLY:CA	2.32	0.55
2:N:365:VAL:HG23	2:N:387:VAL:HA	1.88	0.55
2:N:440:ARG:HB3	2:N:467:TRP:HE3	1.72	0.55
2:B:20:VAL:O	2:B:24:VAL:HG23	2.07	0.55
2:B:311:CYS:HB3	2:B:336:VAL:HG21	1.89	0.55
2:D:197:LEU:O	2:D:225:VAL:HA	2.06	0.55
1:G:129:THR:HG23	1:G:132:GLU:CD	2.27	0.55
2:D:319:ASN:HD22	1:G:43:PRO:HG2	1.71	0.55
2:H:232:ILE:HG13	2:H:253:LEU:CD2	2.37	0.55
2:J:298:LEU:HD23	2:J:300:LEU:HD11	1.88	0.55
2:L:57:MET:HE2	2:L:62:THR:HG22	1.88	0.55
2:N:397:SER:O	2:N:400:THR:HG22	2.07	0.55
1:O:30:ALA:O	1:O:33:VAL:HG22	2.06	0.55
2:B:101:THR:CG2	2:B:128:ASP:OD1	2.55	0.54
2:H:201:MET:HG3	2:H:302:TYR:CE1	2.41	0.54
2:L:444:TYR:HA	2:L:471:GLY:CA	2.34	0.54
2:L:63:ALA:HB1	2:L:67:ARG:HD2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:ILE:HD12	1:M:23:ALA:HB3	1.89	0.54
2:P:547:SER:HB3	2:P:564:HIS:CG	2.42	0.54
2:B:404:ASN:HA	2:B:437:LYS:HD2	1.89	0.54
2:F:298:LEU:HD23	2:F:300:LEU:HD11	1.88	0.54
2:H:104:VAL:HG21	2:H:128:ASP:CB	2.37	0.54
1:K:26:SER:OG	1:K:108:LEU:HB3	2.07	0.54
2:N:444:TYR:HA	2:N:471:GLY:CA	2.31	0.54
1:O:26:SER:OG	1:O:108:LEU:HB3	2.07	0.54
2:P:365:VAL:HG23	2:P:387:VAL:HA	1.89	0.54
2:F:357:GLY:CA	2:F:415:ARG:HH22	2.12	0.54
2:H:363:GLY:O	2:H:364:LEU:C	2.46	0.54
1:I:137:PHE:CD1	2:J:17:VAL:HG21	2.43	0.54
2:N:95:ASN:O	2:N:582:PRO:HG3	2.07	0.54
2:P:454:GLY:O	2:P:457:TYR:HB2	2.08	0.54
1:C:134:ARG:HB2	1:C:139:ILE:O	2.07	0.54
2:L:91:LEU:O	2:L:567:HIS:HE1	1.89	0.54
1:A:158:ALA:HA	2:B:62:THR:CG2	2.37	0.54
1:E:52:LEU:HD12	1:E:52:LEU:O	2.06	0.54
2:H:375:GLN:HG2	2:H:401:TYR:CE1	2.42	0.54
2:H:54:HIS:ND1	2:H:55:VAL:N	2.56	0.54
2:J:477:ASP:OD2	2:J:504:ALA:HB2	2.08	0.54
2:J:455:LEU:HD22	2:J:483:PHE:HB2	1.88	0.54
2:N:314:ILE:HD11	2:N:329:ILE:HD11	1.90	0.54
2:N:465:VAL:HG11	2:N:468:MET:HG3	1.89	0.54
2:N:533:MET:HE3	2:N:588:LEU:HD13	1.89	0.54
2:L:350:GLU:HB3	3:V:209:LEU:HD21	1.89	0.54
2:D:468:MET:HE3	2:D:470:LEU:HD21	1.90	0.54
1:A:145:PRO:HB2	2:D:539:TYR:CE2	2.42	0.54
2:F:547:SER:HB3	2:F:564:HIS:HB3	1.88	0.54
2:H:428:VAL:HG11	2:H:443:PHE:CE2	2.42	0.54
2:J:367:GLN:HG3	2:J:390:ILE:HA	1.89	0.54
2:L:547:SER:HB3	2:L:564:HIS:CG	2.43	0.54
1:M:99:PHE:CD2	2:N:16:THR:C	2.81	0.54
2:P:227:VAL:HG13	2:P:228:GLY:N	2.22	0.54
2:P:357:GLY:CA	2:P:415:ARG:HH22	2.12	0.54
1:A:58:TYR:CE1	1:A:62:HIS:CE1	2.96	0.54
2:F:519:TRP:CZ3	2:F:567:HIS:CG	2.95	0.54
2:H:506:ALA:HB1	2:H:535:MET:HB2	1.88	0.54
2:J:440:ARG:HB3	2:J:467:TRP:CE3	2.43	0.54
1:M:159:PHE:O	1:M:160:GLU:CB	2.47	0.54
1:M:160:GLU:HA	1:M:160:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:ASP:O	2:N:215:ILE:HG13	2.08	0.54
2:N:446:ARG:HG2	2:N:447:GLN:H	1.73	0.54
2:P:121:ARG:NH2	5:P:1103:PO4:O4	2.40	0.54
2:P:152:THR:HG22	2:P:177:SER:HB2	1.90	0.54
2:P:344:LEU:HD23	2:P:380:LEU:HD21	1.90	0.54
2:P:367:GLN:HB3	2:P:391:THR:CG2	2.34	0.54
1:A:137:PHE:HD1	2:B:17:VAL:HG21	1.72	0.54
2:H:153:THR:CG2	2:H:178:GLU:HA	2.38	0.54
2:H:266:LEU:HD13	2:H:267:VAL:N	2.22	0.54
2:N:78:LEU:HD12	2:N:79:LYS:H	1.72	0.54
1:A:160:GLU:OE2	1:A:160:GLU:HA	2.08	0.54
2:H:478:GLU:O	2:H:482:GLU:HG2	2.06	0.54
2:J:357:GLY:CA	2:J:415:ARG:HH22	2.13	0.54
2:L:153:THR:HG23	2:L:178:GLU:HA	1.90	0.54
2:N:55:VAL:CG2	2:N:75:LEU:HD21	2.37	0.54
1:C:93:ILE:HD12	1:C:97:THR:CG2	2.32	0.54
2:D:521:GLN:HG3	2:D:567:HIS:HD2	1.71	0.54
1:E:128:LYS:HB3	1:E:132:GLU:HB2	1.91	0.54
2:L:261:GLU:HG2	2:L:264:MET:HG3	1.90	0.54
2:L:490:LEU:HD11	2:L:493:LEU:HD13	1.90	0.54
2:N:54:HIS:HE1	2:N:56:THR:OG1	1.91	0.54
2:J:227:VAL:CG1	2:J:228:GLY:N	2.71	0.53
2:L:54:HIS:HE1	2:L:56:THR:OG1	1.90	0.53
2:N:320:LEU:HD21	2:N:323:LEU:HB2	1.90	0.53
2:N:357:GLY:CA	2:N:415:ARG:HH22	2.14	0.53
2:P:143:LEU:HD23	2:P:159:ILE:HD13	1.90	0.53
2:B:521:GLN:HG3	2:B:567:HIS:CD2	2.43	0.53
1:C:6:ILE:HD12	1:C:23:ALA:HB3	1.90	0.53
2:F:80:LEU:HB2	2:F:122:MET:HE1	1.90	0.53
1:I:48:THR:HG22	1:I:51:ILE:HB	1.91	0.53
2:P:221:SER:O	2:P:223:VAL:HG23	2.08	0.53
1:E:105:ALA:HB3	1:E:114:LEU:CD1	2.32	0.53
2:F:65:PRO:HA	2:F:103:TRP:CZ3	2.44	0.53
2:J:201:MET:HB3	3:U:211:ARG:HH12	1.74	0.53
1:K:134:ARG:HB2	1:K:139:ILE:O	2.09	0.53
2:L:101:THR:OG1	2:L:102:PRO:HD3	2.08	0.53
2:L:314:ILE:HD11	2:L:329:ILE:HD11	1.90	0.53
2:N:143:LEU:CD2	2:N:159:ILE:HD13	2.38	0.53
1:A:98:LEU:HD21	1:A:120:THR:HG22	1.90	0.53
2:B:501:SER:HA	2:B:524:ARG:HB2	1.91	0.53
1:C:48:THR:HG22	1:C:51:ILE:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:ARG:HB3	1:G:107:TYR:CD1	2.43	0.53
2:F:85:ARG:NH1	5:F:1101:PO4:O3	2.41	0.53
1:I:6:ILE:HG22	1:I:7:VAL:N	2.24	0.53
1:K:113:LEU:O	1:K:117:THR:HG23	2.08	0.53
2:B:294:GLN:NE2	1:O:107:TYR:OH	2.42	0.53
2:B:298:LEU:HB2	2:B:320:LEU:HD11	1.90	0.53
2:D:55:VAL:HG23	2:D:75:LEU:HD21	1.91	0.53
2:F:404:ASN:HA	2:F:437:LYS:HD2	1.89	0.53
2:H:111:LEU:C	2:H:113:GLN:H	2.10	0.53
2:H:43:ARG:HH21	2:H:47:ILE:HD11	1.73	0.53
2:H:98:GLY:O	2:H:122:MET:HE3	2.08	0.53
2:J:399:GLY:O	2:J:434:GLY:HA3	2.08	0.53
2:J:547:SER:HB3	2:J:564:HIS:CG	2.44	0.53
1:K:91:MET:O	1:K:93:ILE:N	2.40	0.53
2:L:465:VAL:HG11	2:L:468:MET:HG3	1.91	0.53
1:M:91:MET:O	1:M:93:ILE:N	2.40	0.53
2:N:367:GLN:HG3	2:N:390:ILE:HA	1.90	0.53
2:N:454:GLY:O	2:N:457:TYR:HB2	2.09	0.53
2:B:184:LEU:HD12	2:B:207:ILE:HB	1.90	0.53
2:B:367:GLN:HB3	2:B:391:THR:CG2	2.34	0.53
1:C:91:MET:O	1:C:93:ILE:N	2.41	0.53
2:F:444:TYR:HA	2:F:471:GLY:CA	2.32	0.53
1:I:153:ARG:HG2	1:I:157:TRP:CZ3	2.44	0.53
2:J:468:MET:HE3	2:J:470:LEU:HD21	1.91	0.53
2:L:121:ARG:NH2	5:L:1103:PO4:O4	2.42	0.53
1:M:87:ASP:OD2	1:M:116:LEU:HD22	2.09	0.53
2:B:80:LEU:HB2	2:B:122:MET:HE1	1.91	0.53
1:C:134:ARG:HH11	2:D:40:VAL:HA	1.74	0.53
2:D:63:ALA:HB1	2:D:67:ARG:HD2	1.91	0.53
2:F:367:GLN:HG3	2:F:390:ILE:HA	1.91	0.53
2:F:397:SER:O	2:F:400:THR:HG22	2.08	0.53
2:H:364:LEU:HD22	2:H:388:SER:N	2.24	0.53
2:H:423:PRO:HB3	2:H:425:ASP:OD2	2.09	0.53
2:L:367:GLN:HG3	2:L:390:ILE:HA	1.89	0.53
1:A:159:PHE:O	1:A:160:GLU:CB	2.52	0.53
2:D:101:THR:CG2	2:D:128:ASP:OD1	2.56	0.53
2:F:153:THR:HG23	2:F:178:GLU:HA	1.91	0.53
2:F:311:CYS:HB3	2:F:336:VAL:HG21	1.91	0.53
2:H:286:PRO:C	2:H:288:LEU:N	2.62	0.53
2:H:362:GLU:C	2:H:364:LEU:N	2.61	0.53
2:P:325:THR:O	2:P:349:ILE:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:HG22	1:A:51:ILE:CG1	2.39	0.53
2:D:443:PHE:CE2	2:D:445:LEU:HD11	2.44	0.53
2:D:455:LEU:HD22	2:D:483:PHE:HB2	1.90	0.53
1:E:26:SER:OG	1:E:108:LEU:HB3	2.09	0.53
1:E:11:SER:HA	1:E:45:PRO:HA	1.90	0.53
2:F:547:SER:HB3	2:F:564:HIS:CG	2.44	0.53
2:H:97:GLY:HA3	2:H:123:ILE:CD1	2.38	0.53
4:H:4100:OGK:C18	4:H:4100:OGK:HN08	2.21	0.53
1:K:160:GLU:OE2	1:K:160:GLU:HA	2.09	0.53
2:L:440:ARG:HB3	2:L:467:TRP:CE3	2.43	0.53
1:M:102:ILE:HB	2:N:20:VAL:CG2	2.39	0.53
2:N:519:TRP:CZ3	2:N:567:HIS:CG	2.97	0.53
2:B:367:GLN:HG3	2:B:390:ILE:HA	1.90	0.53
2:B:419:ILE:HD11	2:B:446:ARG:HH22	1.74	0.53
2:H:65:PRO:HG3	2:H:103:TRP:CD2	2.44	0.53
2:H:214:THR:HA	2:H:217:ARG:HG2	1.91	0.53
2:J:227:VAL:HG13	2:J:228:GLY:N	2.23	0.53
1:K:93:ILE:HD12	1:K:97:THR:CG2	2.28	0.53
2:L:80:LEU:HB2	2:L:122:MET:CE	2.39	0.53
1:M:134:ARG:CZ	1:M:141:ASN:HD22	2.22	0.53
2:N:197:LEU:O	2:N:225:VAL:HA	2.09	0.53
2:N:59:LEU:O	2:N:62:THR:HB	2.08	0.53
2:N:93:PRO:HA	2:N:548:ARG:CB	2.33	0.53
1:O:158:ALA:HA	2:P:62:THR:CG2	2.39	0.53
2:B:275:LEU:HD11	2:B:288:LEU:HD21	1.89	0.52
2:B:93:PRO:HA	2:B:548:ARG:CB	2.32	0.52
1:G:160:GLU:HB3	2:H:31:PRO:HB3	1.90	0.52
2:H:111:LEU:O	2:H:113:GLN:N	2.42	0.52
2:H:184:LEU:HD12	2:H:207:ILE:HB	1.91	0.52
2:H:187:LEU:HB3	2:H:215:ILE:HD11	1.90	0.52
1:I:58:TYR:CD2	1:I:113:LEU:HD13	2.44	0.52
2:J:422:LEU:HB3	2:J:423:PRO:HD3	1.90	0.52
2:B:399:GLY:O	2:B:434:GLY:HA3	2.09	0.52
2:H:280:MET:HE1	2:H:285:MET:HA	1.90	0.52
2:H:535:MET:CE	2:H:542:ILE:HG21	2.39	0.52
2:L:542:ILE:HD11	2:L:588:LEU:CD1	2.24	0.52
1:O:6:ILE:HD12	1:O:23:ALA:HB3	1.90	0.52
1:O:58:TYR:CD2	1:O:113:LEU:HD13	2.44	0.52
2:F:454:GLY:O	2:F:457:TYR:HB2	2.09	0.52
2:H:492:LYS:HZ3	2:H:516:ARG:HH11	1.57	0.52
2:H:494:GLU:HG2	2:H:519:TRP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:ARG:CZ	1:I:141:ASN:HD22	2.23	0.52
2:L:397:SER:O	2:L:400:THR:HG22	2.08	0.52
1:M:52:LEU:HD12	1:M:52:LEU:O	2.09	0.52
2:N:101:THR:HG22	2:N:128:ASP:HB3	1.90	0.52
2:N:138:ASP:OD2	2:N:164:ARG:HG3	2.09	0.52
2:P:411:VAL:HG22	2:P:444:TYR:HB3	1.91	0.52
1:C:11:SER:HA	1:C:45:PRO:HA	1.90	0.52
2:D:190:HIS:ND1	2:H:112:ARG:HD2	2.24	0.52
2:D:235:LEU:O	2:D:238:PHE:HB3	2.10	0.52
2:D:54:HIS:HE1	2:D:56:THR:OG1	1.92	0.52
2:F:337:LEU:HD12	2:F:341:CYS:SG	2.49	0.52
2:H:192:THR:HG22	2:H:218:ASN:O	2.10	0.52
2:H:354:ASP:O	2:H:354:ASP:OD2	2.28	0.52
1:I:159:PHE:O	1:I:160:GLU:CB	2.49	0.52
2:J:456:SER:HB2	2:J:482:GLU:HB3	1.91	0.52
2:L:344:LEU:HD23	2:L:380:LEU:HD21	1.91	0.52
1:M:99:PHE:HB2	2:N:15:ALA:HB3	1.90	0.52
1:M:102:ILE:CD1	2:N:20:VAL:CG2	2.88	0.52
2:N:233:LEU:O	2:N:236:VAL:HG23	2.08	0.52
2:P:546:PRO:HD3	2:P:584:THR:O	2.08	0.52
1:C:160:GLU:HA	1:C:160:GLU:OE2	2.09	0.52
2:D:519:TRP:CZ3	2:D:567:HIS:CG	2.97	0.52
2:F:289:PHE:HB2	2:F:290:PRO:HD3	1.91	0.52
1:G:48:THR:HG22	1:G:51:ILE:CG1	2.39	0.52
2:H:365:VAL:HG21	2:H:387:VAL:CA	2.39	0.52
2:H:402:LEU:HD13	2:H:405:LEU:HG	1.92	0.52
2:J:232:ILE:HD12	2:J:252:SER:H	1.74	0.52
2:P:55:VAL:CG2	2:P:75:LEU:HD21	2.37	0.52
1:C:26:SER:OG	1:C:108:LEU:HB3	2.10	0.52
2:D:547:SER:HB3	2:D:564:HIS:CG	2.43	0.52
2:L:446:ARG:HG2	2:L:447:GLN:H	1.74	0.52
2:N:547:SER:HB3	2:N:564:HIS:CG	2.44	0.52
1:O:160:GLU:HA	1:O:160:GLU:OE2	2.10	0.52
1:O:137:PHE:HD1	2:P:17:VAL:HG21	1.72	0.52
2:P:275:LEU:HD11	2:P:288:LEU:HD21	1.91	0.52
2:P:501:SER:HA	2:P:524:ARG:HB2	1.92	0.52
2:D:446:ARG:HG2	2:D:447:GLN:H	1.74	0.52
2:H:170:LEU:HD23	2:H:170:LEU:C	2.30	0.52
1:I:158:ALA:HA	2:J:62:THR:HG21	1.90	0.52
2:L:235:LEU:O	2:L:238:PHE:HB3	2.10	0.52
2:L:545:ILE:HG22	2:L:546:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:325:THR:O	2:N:349:ILE:HA	2.09	0.52
2:N:472:TYR:OH	3:W:201:LEU:HB2	2.10	0.52
2:P:446:ARG:HG2	2:P:447:GLN:H	1.74	0.52
2:B:454:GLY:O	2:B:457:TYR:HB2	2.10	0.52
2:D:275:LEU:HD11	2:D:288:LEU:HD21	1.92	0.52
2:D:375:GLN:HG2	2:D:401:TYR:CE1	2.45	0.52
2:F:521:GLN:HG3	2:F:567:HIS:CD2	2.45	0.52
1:K:153:ARG:NH2	2:L:539:TYR:CE1	2.78	0.52
2:L:521:GLN:HG3	2:L:567:HIS:CD2	2.44	0.52
2:N:130:ASP:OD1	2:N:134:LYS:HE3	2.09	0.52
2:N:456:SER:HB2	2:N:482:GLU:HB3	1.92	0.52
2:B:54:HIS:HE1	2:B:56:THR:OG1	1.92	0.52
2:D:85:ARG:NH2	4:D:2100:OGK:O07	2.35	0.52
2:D:311:CYS:HB3	2:D:336:VAL:HG21	1.91	0.52
2:D:367:GLN:HG3	2:D:390:ILE:HA	1.92	0.52
2:F:411:VAL:HG22	2:F:444:TYR:HB3	1.92	0.52
2:F:533:MET:HE3	2:F:588:LEU:HD13	1.91	0.52
2:H:225:VAL:CG2	2:H:245:LEU:HD11	2.40	0.52
2:J:275:LEU:HD11	2:J:288:LEU:HD21	1.90	0.52
2:J:305:LEU:O	2:J:305:LEU:HD23	2.10	0.52
2:J:465:VAL:HG11	2:J:468:MET:HG3	1.91	0.52
2:J:521:GLN:HG3	2:J:567:HIS:CD2	2.45	0.52
2:P:419:ILE:CD1	2:P:446:ARG:HH22	2.23	0.52
4:B:1100:OGK:C18	4:B:1100:OGK:HN08	2.19	0.52
2:B:337:LEU:HD12	2:B:341:CYS:SG	2.50	0.52
1:C:137:PHE:CD1	2:D:17:VAL:HG21	2.45	0.52
2:F:422:LEU:HB3	2:F:423:PRO:HD3	1.92	0.52
2:H:306:GLU:O	2:H:310:HIS:HD2	1.92	0.52
2:H:328:VAL:HG12	2:H:359:GLU:HG2	1.92	0.52
2:J:80:LEU:HB2	2:J:122:MET:CE	2.39	0.52
2:J:85:ARG:NH2	4:J:5100:OGK:O07	2.33	0.52
2:J:93:PRO:HA	2:J:548:ARG:CB	2.33	0.52
2:L:404:ASN:HA	2:L:437:LYS:HD2	1.92	0.52
2:N:298:LEU:HB2	2:N:320:LEU:HD11	1.92	0.52
2:P:407:ASP:OD1	2:P:440:ARG:HD2	2.10	0.52
2:D:191:ASN:ND2	2:D:194:LEU:H	2.07	0.51
2:D:519:TRP:CZ3	2:D:567:HIS:ND1	2.79	0.51
1:E:93:ILE:HD12	1:E:97:THR:CG2	2.29	0.51
2:F:235:LEU:O	2:F:238:PHE:HB3	2.10	0.51
1:G:151:VAL:CG1	2:H:39:LEU:HD21	2.40	0.51
2:H:302:TYR:N	2:H:302:TYR:CD2	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:532:LEU:HD11	2:H:568:ILE:HD13	1.92	0.51
1:M:137:PHE:HD1	2:N:17:VAL:HG21	1.74	0.51
2:N:101:THR:CG2	2:N:128:ASP:OD1	2.58	0.51
2:N:310:HIS:O	2:N:314:ILE:CG1	2.58	0.51
2:P:367:GLN:HG3	2:P:390:ILE:HA	1.92	0.51
2:P:456:SER:HB2	2:P:482:GLU:HB3	1.92	0.51
2:P:80:LEU:HB2	2:P:122:MET:CE	2.40	0.51
2:B:367:GLN:O	2:B:371:ILE:HG22	2.09	0.51
2:H:411:VAL:CG2	4:H:4100:OGK:H16A	2.40	0.51
2:L:477:ASP:OD2	2:L:504:ALA:HB2	2.10	0.51
1:M:112:ASN:C	1:M:114:LEU:N	2.62	0.51
2:N:456:SER:CB	2:N:482:GLU:HB3	2.40	0.51
2:P:233:LEU:O	2:P:236:VAL:HG23	2.11	0.51
2:P:251:GLY:O	2:P:278:SER:HB2	2.10	0.51
2:B:446:ARG:HG2	2:B:447:GLN:H	1.75	0.51
2:F:233:LEU:O	2:F:236:VAL:HG23	2.09	0.51
2:P:101:THR:OG1	2:P:102:PRO:HD3	2.10	0.51
2:P:398:ILE:HG23	2:P:402:LEU:HD11	1.92	0.51
1:A:11:SER:HA	1:A:45:PRO:HA	1.92	0.51
2:B:455:LEU:HD22	2:B:483:PHE:HB2	1.91	0.51
2:D:298:LEU:HB2	2:D:320:LEU:HD11	1.93	0.51
1:C:158:ALA:HA	2:D:62:THR:HG21	1.91	0.51
2:F:63:ALA:HB1	2:F:67:ARG:HD2	1.91	0.51
2:H:406:CYS:HA	2:H:438:LEU:HA	1.92	0.51
2:H:418:ARG:HG2	2:H:446:ARG:NH1	2.25	0.51
2:H:455:LEU:HD21	2:H:473:VAL:CG2	2.40	0.51
2:J:235:LEU:O	2:J:238:PHE:HB3	2.10	0.51
1:M:87:ASP:HB3	1:M:116:LEU:HD21	1.92	0.51
2:B:143:LEU:CD2	2:B:159:ILE:HD13	2.40	0.51
2:D:93:PRO:HA	2:D:548:ARG:CB	2.32	0.51
1:E:48:THR:HG22	1:E:51:ILE:CG1	2.40	0.51
2:H:424:LEU:O	2:H:426:ASN:N	2.43	0.51
2:H:65:PRO:HA	2:H:103:TRP:CZ3	2.44	0.51
2:N:153:THR:HG23	2:N:178:GLU:HA	1.93	0.51
2:N:337:LEU:HD12	2:N:341:CYS:SG	2.51	0.51
1:O:48:THR:CG2	1:O:51:ILE:HG12	2.41	0.51
1:A:105:ALA:HB2	1:A:113:LEU:HD23	1.92	0.51
1:A:52:LEU:HD12	1:A:52:LEU:O	2.10	0.51
2:F:255:GLU:HG3	2:F:255:GLU:O	2.11	0.51
2:F:546:PRO:HD3	2:F:584:THR:O	2.08	0.51
2:H:382:TYR:CD2	2:H:407:ASP:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:THR:HG22	1:I:51:ILE:CG1	2.40	0.51
2:J:311:CYS:HB3	2:J:336:VAL:HG21	1.91	0.51
1:M:48:THR:HG22	1:M:51:ILE:CG1	2.40	0.51
2:N:542:ILE:CD1	2:N:588:LEU:HD12	2.28	0.51
1:A:134:ARG:HH11	2:B:40:VAL:HA	1.75	0.51
1:A:153:ARG:NH2	2:B:539:TYR:CE1	2.79	0.51
2:D:422:LEU:HB3	2:D:423:PRO:HD3	1.93	0.51
2:H:278:SER:C	2:H:280:MET:H	2.13	0.51
2:H:496:ARG:HD2	4:H:4100:OGK:H23A	1.92	0.51
2:J:501:SER:HA	2:J:524:ARG:HB2	1.92	0.51
2:P:247:GLU:HA	2:P:274:ARG:O	2.11	0.51
2:P:63:ALA:HB1	2:P:67:ARG:HD2	1.91	0.51
2:F:298:LEU:HB2	2:F:320:LEU:HD11	1.92	0.51
2:H:306:GLU:OE2	2:H:306:GLU:HA	2.09	0.51
1:K:137:PHE:HD1	2:L:17:VAL:HG21	1.76	0.51
1:K:48:THR:HG22	1:K:51:ILE:CG1	2.41	0.51
2:L:519:TRP:HH2	2:L:567:HIS:CE1	2.29	0.51
2:L:78:LEU:HD12	2:L:79:LYS:H	1.76	0.51
2:P:191:ASN:ND2	2:P:194:LEU:H	2.06	0.51
2:P:232:ILE:HD12	2:P:252:SER:H	1.76	0.51
2:D:310:HIS:O	2:D:314:ILE:HG12	2.11	0.51
2:F:367:GLN:O	2:F:371:ILE:HG22	2.10	0.51
1:O:91:MET:CE	1:O:117:THR:HG22	2.41	0.51
2:P:78:LEU:HD12	2:P:79:LYS:H	1.74	0.51
2:B:272:LEU:HD21	2:B:275:LEU:HB3	1.93	0.51
2:F:272:LEU:HD21	2:F:275:LEU:HB3	1.92	0.51
2:F:305:LEU:O	2:F:305:LEU:HD23	2.11	0.51
2:F:501:SER:HA	2:F:524:ARG:HB2	1.93	0.51
2:H:414:ASP:HB3	2:H:446:ARG:HH21	1.76	0.51
2:N:422:LEU:HB3	2:N:423:PRO:HD3	1.93	0.51
1:O:11:SER:HA	1:O:45:PRO:HA	1.92	0.51
1:O:91:MET:O	1:O:93:ILE:N	2.44	0.51
2:B:153:THR:HG23	2:B:178:GLU:HA	1.92	0.50
2:B:255:GLU:HG3	2:B:255:GLU:O	2.11	0.50
2:B:305:LEU:O	2:B:305:LEU:HD23	2.11	0.50
2:B:320:LEU:HD21	2:B:323:LEU:HB2	1.93	0.50
2:B:546:PRO:HD3	2:B:584:THR:O	2.11	0.50
2:B:519:TRP:HH2	2:B:567:HIS:CE1	2.29	0.50
2:D:272:LEU:HD21	2:D:275:LEU:HB3	1.92	0.50
2:H:365:VAL:HG21	2:H:387:VAL:CG1	2.39	0.50
2:H:390:ILE:HD11	2:H:412:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:409:ARG:HD2	4:H:4100:OGK:H13A	1.92	0.50
1:M:153:ARG:HG2	1:M:157:TRP:CZ3	2.46	0.50
2:B:482:GLU:O	2:B:485:ARG:HG2	2.11	0.50
1:C:134:ARG:NH1	2:D:40:VAL:HA	2.26	0.50
2:F:143:LEU:CD2	2:F:159:ILE:HD13	2.41	0.50
2:F:542:ILE:CD1	2:F:588:LEU:HD12	2.30	0.50
2:B:357:GLY:CA	2:B:415:ARG:HH22	2.12	0.50
2:F:398:ILE:O	2:F:402:LEU:HD12	2.12	0.50
2:H:291:PHE:N	2:H:291:PHE:CD2	2.79	0.50
2:H:370:LEU:HB2	2:H:394:SER:HB3	1.93	0.50
2:F:110:ASN:HA	2:L:190:HIS:HE1	1.77	0.50
2:L:482:GLU:O	2:L:485:ARG:HG2	2.11	0.50
2:P:153:THR:HG23	2:P:178:GLU:HA	1.92	0.50
2:P:289:PHE:HB2	2:P:290:PRO:HD3	1.92	0.50
2:P:65:PRO:HA	2:P:103:TRP:CZ3	2.46	0.50
1:C:91:MET:O	1:C:93:ILE:HG12	2.12	0.50
2:D:456:SER:HB2	2:D:482:GLU:HB3	1.94	0.50
2:F:95:ASN:O	2:F:582:PRO:HG3	2.12	0.50
2:H:230:PHE:CB	2:H:235:LEU:HD21	2.41	0.50
2:H:432:LEU:HD11	2:H:458:ILE:HD13	1.93	0.50
2:H:87:ALA:HB2	2:H:92:ILE:HB	1.93	0.50
1:I:158:ALA:HA	2:J:62:THR:CG2	2.41	0.50
1:K:128:LYS:HB3	1:K:132:GLU:HB2	1.93	0.50
2:P:159:ILE:HD12	2:P:166:ILE:HD11	1.93	0.50
2:B:80:LEU:HB2	2:B:122:MET:CE	2.41	0.50
2:B:130:ASP:OD1	2:B:134:LYS:HE3	2.12	0.50
2:B:440:ARG:HB3	2:B:467:TRP:CE3	2.45	0.50
2:H:145:LEU:O	2:H:171:MET:HA	2.10	0.50
2:J:519:TRP:HH2	2:J:567:HIS:CE1	2.30	0.50
2:L:233:LEU:O	2:L:236:VAL:HG23	2.11	0.50
2:N:523:TYR:CE2	2:N:568:ILE:HD11	2.47	0.50
2:D:20:VAL:O	2:D:24:VAL:HG23	2.11	0.50
2:H:464:ASN:O	2:H:466:ARG:HD2	2.11	0.50
2:J:419:ILE:HD11	2:J:446:ARG:HH22	1.75	0.50
1:K:105:ALA:HB2	1:K:113:LEU:HD23	1.93	0.50
2:P:422:LEU:HB3	2:P:423:PRO:HD3	1.93	0.50
1:A:128:LYS:HB3	1:A:132:GLU:HB2	1.94	0.50
2:B:159:ILE:HD12	2:B:166:ILE:HD11	1.94	0.50
1:E:48:THR:HG22	1:E:51:ILE:CB	2.41	0.50
2:F:477:ASP:OD2	2:F:504:ALA:HB2	2.12	0.50
2:J:289:PHE:HB2	2:J:290:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:289:PHE:HD1	2:P:316:LYS:HD2	1.73	0.50
2:F:465:VAL:HG11	2:F:468:MET:HG3	1.93	0.50
2:H:392:ASN:ND2	2:H:422:LEU:HD13	2.26	0.50
1:I:128:LYS:HB3	1:I:132:GLU:HB2	1.94	0.50
2:J:398:ILE:HG23	2:J:402:LEU:HD11	1.94	0.50
1:K:26:SER:HB3	1:K:29:ILE:HG13	1.93	0.50
2:B:232:ILE:HD12	2:B:252:SER:H	1.76	0.50
2:F:197:LEU:O	2:F:225:VAL:HA	2.12	0.50
2:F:232:ILE:HD12	2:F:252:SER:H	1.76	0.50
1:G:113:LEU:O	1:G:117:THR:HG23	2.11	0.50
2:H:289:PHE:N	2:H:290:PRO:CD	2.74	0.50
2:H:282:PRO:HB3	2:H:309:ASP:OD2	2.11	0.50
2:H:367:GLN:N	2:H:367:GLN:CD	2.65	0.50
2:H:496:ARG:HB2	4:H:4100:OGK:H01A	1.94	0.50
2:L:320:LEU:HD21	2:L:323:LEU:HB2	1.93	0.50
1:M:130:PRO:O	1:M:134:ARG:HG2	2.12	0.50
2:N:227:VAL:CG1	2:N:228:GLY:N	2.74	0.50
2:P:482:GLU:O	2:P:485:ARG:HG2	2.12	0.50
2:B:310:HIS:O	2:B:314:ILE:CG1	2.58	0.49
2:D:310:HIS:O	2:D:314:ILE:CG1	2.60	0.49
2:D:407:ASP:OD1	2:D:440:ARG:HD2	2.12	0.49
1:G:11:SER:HA	1:G:45:PRO:HA	1.94	0.49
2:H:191:ASN:ND2	2:H:194:LEU:H	2.08	0.49
2:H:516:ARG:HA	2:H:572:TYR:HD1	1.75	0.49
2:J:164:ARG:HH21	2:N:136:ARG:HH21	1.60	0.49
2:J:54:HIS:HE1	2:J:56:THR:OG1	1.95	0.49
2:J:80:LEU:HB2	2:J:122:MET:HE1	1.94	0.49
1:K:91:MET:O	1:K:93:ILE:HG12	2.12	0.49
1:O:113:LEU:HG	1:O:113:LEU:O	2.12	0.49
2:P:419:ILE:HD11	2:P:446:ARG:HH22	1.75	0.49
2:P:465:VAL:HG11	2:P:468:MET:HG3	1.94	0.49
2:P:80:LEU:HB2	2:P:122:MET:HE1	1.94	0.49
2:D:398:ILE:HG23	2:D:402:LEU:HD11	1.94	0.49
2:H:97:GLY:CA	2:H:123:ILE:HD11	2.42	0.49
2:H:191:ASN:ND2	2:H:193:SER:H	2.10	0.49
2:H:289:PHE:N	2:H:290:PRO:HD2	2.27	0.49
2:L:310:HIS:O	2:L:314:ILE:HG12	2.12	0.49
1:M:102:ILE:CB	2:N:20:VAL:CG2	2.90	0.49
1:O:134:ARG:CZ	1:O:141:ASN:HD22	2.25	0.49
2:P:477:ASP:OD2	2:P:504:ALA:HB2	2.12	0.49
2:N:565:PRO:HG2	3:W:201:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:CZ	1:C:141:ASN:HD22	2.24	0.49
1:E:91:MET:O	1:E:93:ILE:N	2.45	0.49
2:H:357:GLY:C	2:H:359:GLU:N	2.66	0.49
2:H:387:VAL:HG11	2:H:390:ILE:CD1	2.39	0.49
2:J:519:TRP:CZ3	2:J:567:HIS:CG	3.01	0.49
1:K:132:GLU:O	1:K:136:THR:HG23	2.12	0.49
2:P:138:ASP:OD2	2:P:164:ARG:HG3	2.12	0.49
2:B:350:GLU:HB3	3:Q:209:LEU:CD2	2.40	0.49
1:A:134:ARG:NH1	2:B:40:VAL:HA	2.27	0.49
1:C:58:TYR:CE1	1:C:62:HIS:CE1	3.00	0.49
2:D:65:PRO:HA	2:D:103:TRP:CZ3	2.48	0.49
2:L:519:TRP:CZ3	2:L:567:HIS:CG	3.00	0.49
2:N:357:GLY:HA2	2:N:415:ARG:NH2	2.14	0.49
2:P:159:ILE:HG13	2:P:160:VAL:N	2.26	0.49
2:P:468:MET:CE	2:P:470:LEU:HD11	2.42	0.49
1:A:91:MET:O	1:A:93:ILE:HG12	2.13	0.49
2:B:519:TRP:CZ3	2:B:567:HIS:CG	3.00	0.49
2:H:487:CYS:HB3	2:H:490:LEU:HB2	1.95	0.49
2:H:492:LYS:HZ3	2:H:516:ARG:NH1	2.09	0.49
1:I:91:MET:O	1:I:93:ILE:N	2.42	0.49
2:N:116:SER:CB	2:N:142:THR:HG23	2.36	0.49
2:B:419:ILE:CD1	2:B:446:ARG:HH22	2.26	0.49
2:D:211:ASP:O	2:D:215:ILE:HG13	2.12	0.49
1:G:10:SER:OG	1:G:11:SER:N	2.46	0.49
2:H:428:VAL:CG1	2:H:443:PHE:CZ	2.96	0.49
2:J:159:ILE:HD12	2:J:166:ILE:HD11	1.94	0.49
2:J:404:ASN:HA	2:J:437:LYS:HD2	1.94	0.49
2:J:443:PHE:CE2	2:J:445:LEU:HD11	2.48	0.49
2:J:411:VAL:HG22	2:J:444:TYR:HB3	1.93	0.49
1:K:134:ARG:HH11	2:L:40:VAL:HA	1.76	0.49
2:L:80:LEU:HB2	2:L:122:MET:HE1	1.95	0.49
1:M:48:THR:HG22	1:M:51:ILE:CB	2.42	0.49
2:N:159:ILE:HG13	2:N:160:VAL:N	2.27	0.49
2:N:375:GLN:HG2	2:N:401:TYR:CE1	2.48	0.49
2:P:248:PHE:CD2	2:P:248:PHE:C	2.86	0.49
1:A:26:SER:OG	1:A:108:LEU:HB3	2.13	0.49
1:C:128:LYS:HB3	1:C:132:GLU:HB2	1.95	0.49
2:D:519:TRP:HH2	2:D:567:HIS:CE1	2.31	0.49
2:F:295:ILE:HG21	2:F:298:LEU:CD1	2.41	0.49
2:F:407:ASP:OD1	2:F:440:ARG:HD2	2.12	0.49
2:H:83:LYS:O	2:H:121:ARG:NH1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:223:VAL:O	2:L:245:LEU:HD12	2.13	0.49
2:N:235:LEU:O	2:N:238:PHE:HB3	2.12	0.49
2:N:289:PHE:HB2	2:N:290:PRO:HD3	1.94	0.49
1:O:128:LYS:HB3	1:O:132:GLU:HB2	1.94	0.49
2:P:320:LEU:HD21	2:P:323:LEU:HB2	1.93	0.49
2:B:546:PRO:O	2:B:547:SER:HB2	2.13	0.49
2:H:332:ARG:O	2:H:336:VAL:HG23	2.13	0.49
2:H:431:LEU:HD23	2:H:432:LEU:N	2.27	0.49
2:H:450:LEU:CG	2:H:454:GLY:HA3	2.43	0.49
2:H:450:LEU:HD11	2:H:454:GLY:CA	2.39	0.49
2:J:482:GLU:O	2:J:485:ARG:HG2	2.13	0.49
2:J:490:LEU:HD11	2:J:493:LEU:HD13	1.94	0.49
2:L:227:VAL:HG13	2:L:228:GLY:H	1.76	0.49
2:L:255:GLU:HG3	2:L:255:GLU:O	2.13	0.49
2:N:170:LEU:HD23	2:N:170:LEU:C	2.33	0.49
2:N:400:THR:O	2:N:403:LYS:HE2	2.12	0.49
1:O:10:SER:OG	1:O:11:SER:N	2.46	0.49
1:O:153:ARG:HG2	1:O:157:TRP:CZ3	2.48	0.49
2:P:255:GLU:O	2:P:255:GLU:HG3	2.13	0.49
2:D:247:GLU:HA	2:D:274:ARG:O	2.12	0.49
2:D:482:GLU:O	2:D:485:ARG:HG2	2.12	0.49
2:F:409:ARG:HD3	4:F:3100:OGK:H13A	1.93	0.49
2:H:153:THR:HG23	2:H:178:GLU:HA	1.95	0.49
1:I:134:ARG:HH11	2:J:40:VAL:HA	1.77	0.49
2:L:275:LEU:HD11	2:L:288:LEU:HD21	1.93	0.49
2:N:469:LEU:HA	2:N:494:GLU:O	2.11	0.49
2:P:130:ASP:OD1	2:P:134:LYS:HE3	2.12	0.49
2:F:490:LEU:HD11	2:F:493:LEU:HD13	1.95	0.49
2:H:259:MET:N	2:H:260:PRO:HD3	2.28	0.49
2:H:385:VAL:HG12	2:H:387:VAL:HG23	1.95	0.49
2:H:57:MET:HB2	2:H:80:LEU:HD23	1.95	0.49
2:J:153:THR:HG23	2:J:178:GLU:HA	1.94	0.49
2:L:298:LEU:HB2	2:L:320:LEU:HD11	1.94	0.49
2:N:311:CYS:CB	2:N:336:VAL:HG21	2.43	0.49
2:B:321:GLU:HA	2:B:344:LEU:HA	1.94	0.48
2:D:153:THR:HG23	2:D:178:GLU:HA	1.95	0.48
2:D:57:MET:CE	2:D:62:THR:HG22	2.43	0.48
2:F:538:PRO:O	2:F:539:TYR:HB2	2.13	0.48
2:H:43:ARG:NH2	2:H:47:ILE:HD11	2.28	0.48
2:J:397:SER:O	2:J:400:THR:HG22	2.13	0.48
1:K:159:PHE:O	1:K:160:GLU:CB	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:ARG:NH1	2:L:40:VAL:HA	2.28	0.48
2:L:538:PRO:O	2:L:539:TYR:HB2	2.13	0.48
2:N:152:THR:HG22	2:N:177:SER:HB2	1.95	0.48
2:N:546:PRO:O	2:N:547:SER:HB2	2.12	0.48
2:N:96:TRP:O	2:N:578:ARG:NH2	2.41	0.48
2:H:526:SER:O	2:H:527:MET:C	2.52	0.48
2:J:400:THR:O	2:J:403:LYS:HE2	2.13	0.48
1:K:58:TYR:CD2	1:K:113:LEU:HD13	2.47	0.48
2:L:501:SER:HA	2:L:524:ARG:HB2	1.95	0.48
2:L:546:PRO:HD3	2:L:584:THR:O	2.11	0.48
2:N:482:GLU:O	2:N:485:ARG:HG2	2.13	0.48
2:N:57:MET:CE	2:N:62:THR:HG22	2.43	0.48
1:A:48:THR:CG2	1:A:51:ILE:HG12	2.43	0.48
2:B:176:PHE:CZ	2:B:204:PHE:CZ	3.01	0.48
2:B:282:PRO:HA	2:B:285:MET:CE	2.44	0.48
2:D:255:GLU:O	2:D:255:GLU:HG3	2.13	0.48
2:F:247:GLU:HA	2:F:274:ARG:O	2.13	0.48
2:F:519:TRP:CZ3	2:F:567:HIS:ND1	2.81	0.48
2:H:326:ARG:O	2:H:329:ILE:HG22	2.12	0.48
2:H:85:ARG:NH1	5:H:1101:PO4:O2	2.45	0.48
2:J:255:GLU:HG3	2:J:255:GLU:O	2.12	0.48
2:L:419:ILE:CD1	2:L:446:ARG:HH22	2.27	0.48
2:P:519:TRP:CZ3	2:P:567:HIS:CG	3.01	0.48
2:B:247:GLU:HA	2:B:274:ARG:O	2.14	0.48
2:D:397:SER:O	2:D:400:THR:HG22	2.13	0.48
2:D:399:GLY:O	2:D:434:GLY:HA3	2.13	0.48
1:E:134:ARG:HH11	2:F:40:VAL:HA	1.78	0.48
2:F:152:THR:HG22	2:F:177:SER:HB2	1.95	0.48
2:F:231:GLU:HG2	2:F:254:ASN:HD22	1.78	0.48
2:F:46:LYS:HE3	2:F:46:LYS:HB2	1.61	0.48
2:H:454:GLY:O	2:H:457:TYR:HB2	2.12	0.48
2:J:546:PRO:HD3	2:J:584:THR:O	2.14	0.48
2:L:519:TRP:CZ3	2:L:567:HIS:ND1	2.82	0.48
2:L:578:ARG:HG3	2:L:578:ARG:H	1.44	0.48
1:M:128:LYS:HB2	1:M:133:ILE:CD1	2.43	0.48
2:N:419:ILE:CD1	2:N:446:ARG:HH22	2.26	0.48
1:O:48:THR:HG22	1:O:51:ILE:CB	2.43	0.48
2:P:456:SER:CB	2:P:482:GLU:HB3	2.43	0.48
2:B:539:TYR:OH	1:C:146:GLU:HA	2.13	0.48
1:C:153:ARG:NH2	2:D:539:TYR:CE1	2.81	0.48
2:D:305:LEU:HD23	2:D:305:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:454:GLY:O	2:D:457:TYR:HB2	2.14	0.48
2:D:296:ARG:NH2	1:G:37:CYS:SG	2.87	0.48
2:H:476:SER:C	2:H:478:GLU:H	2.16	0.48
2:H:486:GLY:O	2:H:487:CYS:C	2.51	0.48
1:I:111:LYS:O	1:I:115:ASP:HB2	2.12	0.48
2:J:454:GLY:O	2:J:457:TYR:HB2	2.14	0.48
2:J:519:TRP:CZ3	2:J:567:HIS:ND1	2.82	0.48
2:L:85:ARG:NH1	5:L:1101:PO4:O3	2.46	0.48
2:L:454:GLY:O	2:L:457:TYR:HB2	2.13	0.48
2:N:159:ILE:HD12	2:N:166:ILE:HD11	1.95	0.48
2:N:501:SER:HA	2:N:524:ARG:HB2	1.95	0.48
1:G:48:THR:CG2	1:G:51:ILE:HG12	2.44	0.48
1:G:137:PHE:HB3	2:H:17:VAL:CG2	2.43	0.48
2:H:364:LEU:HD21	2:H:386:TYR:O	2.13	0.48
2:H:391:THR:C	2:H:393:GLU:N	2.67	0.48
2:J:295:ILE:HG21	2:J:298:LEU:CD1	2.43	0.48
2:J:546:PRO:O	2:J:547:SER:HB2	2.13	0.48
2:L:398:ILE:O	2:L:402:LEU:HD12	2.12	0.48
2:N:80:LEU:HB2	2:N:122:MET:HE2	1.95	0.48
2:B:170:LEU:HD23	2:B:170:LEU:C	2.34	0.48
2:B:477:ASP:N	2:B:477:ASP:OD1	2.46	0.48
2:D:546:PRO:HD3	2:D:584:THR:O	2.13	0.48
1:E:153:ARG:HG2	1:E:157:TRP:CZ3	2.49	0.48
2:F:101:THR:HG22	2:F:128:ASP:HB3	1.95	0.48
2:F:127:LEU:HD21	2:F:131:ARG:NH2	2.28	0.48
2:F:446:ARG:HG2	2:F:447:GLN:N	2.28	0.48
2:H:316:LYS:O	2:H:318:PRO:HD3	2.14	0.48
2:H:431:LEU:CD2	2:H:432:LEU:HD23	2.43	0.48
2:J:456:SER:CB	2:J:482:GLU:HB3	2.43	0.48
1:A:105:ALA:HB3	1:A:114:LEU:HD13	1.94	0.48
2:D:465:VAL:HG11	2:D:468:MET:HG3	1.96	0.48
2:H:21:ILE:HD12	2:H:24:VAL:HB	1.95	0.48
2:H:542:ILE:HD11	2:H:588:LEU:HD12	1.96	0.48
2:H:57:MET:HE2	2:H:62:THR:HG22	1.95	0.48
1:I:26:SER:HB3	1:I:29:ILE:HG13	1.96	0.48
2:J:121:ARG:NH2	5:J:1103:PO4:O4	2.47	0.48
2:L:289:PHE:HD1	2:L:316:LYS:HD2	1.73	0.48
2:L:477:ASP:OD1	2:L:477:ASP:N	2.47	0.48
2:L:456:SER:HB2	2:L:482:GLU:HB3	1.94	0.48
1:M:11:SER:HA	1:M:45:PRO:HA	1.96	0.48
2:N:419:ILE:HD11	2:N:446:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:545:ILE:HG22	2:N:546:PRO:CD	2.44	0.48
2:P:176:PHE:CZ	2:P:204:PHE:CZ	3.02	0.48
2:D:176:PHE:CZ	2:D:204:PHE:CZ	3.01	0.48
1:E:134:ARG:CZ	1:E:141:ASN:HD22	2.26	0.48
2:H:492:LYS:HZ1	2:H:516:ARG:NH1	2.10	0.48
2:L:251:GLY:O	2:L:278:SER:HB2	2.13	0.48
2:N:282:PRO:HA	2:N:285:MET:CE	2.43	0.48
2:N:392:ASN:HD21	2:N:424:LEU:HA	1.77	0.48
1:A:48:THR:HG22	1:A:51:ILE:CB	2.43	0.48
2:D:321:GLU:HA	2:D:344:LEU:HA	1.96	0.48
2:F:523:TYR:CE2	2:F:568:ILE:HD11	2.49	0.48
2:F:96:TRP:O	2:F:578:ARG:NH2	2.42	0.48
1:G:6:ILE:HG22	1:G:7:VAL:N	2.28	0.48
2:H:170:LEU:HB2	2:H:198:ASN:HB3	1.95	0.48
2:H:365:VAL:HG21	2:H:387:VAL:HA	1.95	0.48
2:H:477:ASP:OD2	2:H:501:SER:OG	2.23	0.48
1:K:11:SER:HA	1:K:45:PRO:HA	1.95	0.48
2:L:127:LEU:HD21	2:L:131:ARG:NH2	2.29	0.48
2:L:419:ILE:HD11	2:L:446:ARG:HH22	1.79	0.48
2:N:387:VAL:O	2:N:413:LEU:HD22	2.14	0.48
2:P:170:LEU:HD23	2:P:170:LEU:C	2.34	0.48
2:P:521:GLN:HG3	2:P:567:HIS:CD2	2.48	0.48
2:B:519:TRP:CZ3	2:B:567:HIS:ND1	2.82	0.47
2:D:367:GLN:O	2:D:371:ILE:HG22	2.14	0.47
1:E:48:THR:HG23	1:E:51:ILE:H	1.79	0.47
2:H:412:LEU:HD12	2:H:445:LEU:CA	2.44	0.47
2:J:545:ILE:HG22	2:J:546:PRO:CD	2.43	0.47
1:E:45:PRO:CB	2:L:291:PHE:HA	2.44	0.47
2:L:298:LEU:HD23	2:L:300:LEU:HD11	1.95	0.47
2:L:367:GLN:O	2:L:371:ILE:HG22	2.14	0.47
2:N:191:ASN:ND2	2:N:194:LEU:H	2.12	0.47
2:N:443:PHE:CE2	2:N:445:LEU:HD11	2.48	0.47
1:O:134:ARG:HH11	2:P:40:VAL:HA	1.78	0.47
2:B:227:VAL:HG13	2:B:228:GLY:H	1.78	0.47
2:D:295:ILE:HG21	2:D:298:LEU:CD1	2.43	0.47
2:H:247:GLU:HA	2:H:274:ARG:O	2.14	0.47
2:H:364:LEU:HD22	2:H:365:VAL:HG22	1.96	0.47
1:I:48:THR:CG2	1:I:51:ILE:HG12	2.43	0.47
2:J:164:ARG:HD2	2:N:112:ARG:CZ	2.45	0.47
2:J:298:LEU:HB2	2:J:320:LEU:HD11	1.96	0.47
2:L:456:SER:CB	2:L:482:GLU:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:289:PHE:HD1	2:N:316:LYS:HD2	1.76	0.47
2:N:351:ARG:O	2:N:351:ARG:HG3	2.14	0.47
2:N:519:TRP:CZ3	2:N:567:HIS:ND1	2.82	0.47
1:C:48:THR:CG2	1:C:51:ILE:HG12	2.44	0.47
2:D:232:ILE:HD12	2:D:252:SER:H	1.79	0.47
2:D:412:LEU:HD12	2:D:412:LEU:C	2.35	0.47
2:D:477:ASP:OD2	2:D:504:ALA:HB2	2.12	0.47
1:G:120:THR:O	1:G:124:MET:HG3	2.14	0.47
2:H:114:LEU:O	2:H:136:ARG:NH1	2.48	0.47
2:H:204:PHE:O	2:H:206:LYS:N	2.47	0.47
2:H:64:THR:O	2:H:65:PRO:C	2.51	0.47
2:J:247:GLU:HA	2:J:274:ARG:O	2.14	0.47
2:J:63:ALA:HB1	2:J:67:ARG:HD2	1.96	0.47
1:M:48:THR:CG2	1:M:51:ILE:HG12	2.45	0.47
2:N:171:MET:O	2:N:174:SER:HB2	2.14	0.47
2:N:176:PHE:CZ	2:N:204:PHE:CZ	3.02	0.47
2:N:490:LEU:HD11	2:N:493:LEU:HD13	1.96	0.47
2:B:248:PHE:CD2	2:B:248:PHE:C	2.87	0.47
2:D:501:SER:HA	2:D:524:ARG:HB2	1.96	0.47
2:D:565:PRO:HG2	3:R:201:LEU:HD21	1.97	0.47
2:F:297:LYS:HE3	2:F:297:LYS:HB2	1.65	0.47
2:H:280:MET:HG2	2:H:280:MET:O	2.14	0.47
1:I:11:SER:HA	1:I:45:PRO:HA	1.95	0.47
2:J:446:ARG:HG2	2:J:447:GLN:N	2.29	0.47
2:L:545:ILE:HG22	2:L:546:PRO:N	2.30	0.47
2:N:247:GLU:HA	2:N:274:ARG:O	2.14	0.47
2:N:248:PHE:CD2	2:N:248:PHE:C	2.87	0.47
2:N:297:LYS:HE3	2:N:297:LYS:HB2	1.62	0.47
2:P:440:ARG:HB3	2:P:467:TRP:CE3	2.45	0.47
2:B:422:LEU:HB3	2:B:423:PRO:HD3	1.96	0.47
2:B:465:VAL:HG11	2:B:468:MET:HG3	1.95	0.47
2:D:289:PHE:HD1	2:D:316:LYS:HD2	1.73	0.47
1:E:105:ALA:HB2	1:E:113:LEU:HD23	1.96	0.47
1:E:132:GLU:O	1:E:136:THR:HG23	2.15	0.47
2:F:138:ASP:OD2	2:F:164:ARG:HG3	2.14	0.47
2:H:315:GLN:HG3	2:H:340:TYR:CE1	2.50	0.47
2:H:89:PHE:CE2	4:H:4100:OGK:H04A	2.50	0.47
2:J:398:ILE:C	2:J:400:THR:H	2.17	0.47
1:K:134:ARG:CZ	1:K:141:ASN:HD22	2.28	0.47
2:D:80:LEU:HB2	2:D:122:MET:HE1	1.96	0.47
2:F:375:GLN:HG2	2:F:401:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:262:LYS:HD2	2:H:263:TYR:CE1	2.49	0.47
2:H:269:PRO:O	2:H:270:ARG:C	2.52	0.47
2:H:53:GLU:O	2:H:75:LEU:HD22	2.15	0.47
1:I:52:LEU:HD12	1:I:52:LEU:O	2.14	0.47
2:P:477:ASP:OD1	2:P:477:ASP:N	2.48	0.47
2:P:543:GLU:OE2	2:P:578:ARG:HD3	2.13	0.47
1:C:26:SER:HB3	1:C:29:ILE:HG13	1.96	0.47
2:J:285:MET:N	2:J:286:PRO:CD	2.78	0.47
2:J:57:MET:CE	2:J:62:THR:HG22	2.43	0.47
2:L:247:GLU:HA	2:L:274:ARG:O	2.13	0.47
2:L:339:GLN:HA	2:L:342:LYS:HE2	1.96	0.47
1:C:52:LEU:HD12	1:C:52:LEU:O	2.14	0.47
2:D:320:LEU:HD21	2:D:323:LEU:HB2	1.97	0.47
2:D:95:ASN:O	2:D:582:PRO:HG3	2.15	0.47
2:H:153:THR:HG23	2:H:177:SER:O	2.15	0.47
2:H:52:ARG:NH1	2:H:72:PHE:HZ	2.11	0.47
2:H:532:LEU:O	2:H:534:GLN:N	2.48	0.47
2:L:543:GLU:OE2	2:L:578:ARG:HD3	2.15	0.47
2:P:398:ILE:O	2:P:402:LEU:HD12	2.14	0.47
2:P:546:PRO:O	2:P:547:SER:HB2	2.15	0.47
2:B:468:MET:CE	2:B:470:LEU:HD11	2.45	0.47
1:E:26:SER:HB3	1:E:29:ILE:HG13	1.97	0.47
2:F:113:GLN:HE22	2:L:192:THR:HG21	1.80	0.47
1:G:105:ALA:HB2	1:G:113:LEU:HD23	1.97	0.47
2:H:352:GLY:O	2:H:353:ALA:HB2	2.15	0.47
2:H:367:GLN:CA	2:H:367:GLN:OE1	2.62	0.47
1:I:35:ASP:CB	2:N:243:ALA:HB1	2.42	0.47
2:J:223:VAL:O	2:J:245:LEU:HD12	2.14	0.47
2:J:472:TYR:CD2	2:J:497:GLY:O	2.68	0.47
2:P:298:LEU:HB2	2:P:320:LEU:HD11	1.96	0.47
2:P:321:GLU:HA	2:P:344:LEU:HA	1.97	0.47
2:P:444:TYR:HA	2:P:471:GLY:CA	2.37	0.47
1:C:48:THR:HG22	1:C:51:ILE:CB	2.44	0.47
2:D:190:HIS:HE1	2:H:110:ASN:HA	1.80	0.47
2:D:289:PHE:HB2	2:D:290:PRO:HD3	1.97	0.47
2:F:400:THR:O	2:F:403:LYS:HE2	2.15	0.47
1:G:58:TYR:CE1	1:G:62:HIS:CE1	3.03	0.47
2:H:168:THR:HB	2:H:196:VAL:HG13	1.96	0.47
2:H:187:LEU:HA	2:H:187:LEU:HD23	1.72	0.47
2:H:468:MET:HG3	2:H:490:LEU:HD21	1.96	0.47
2:J:289:PHE:HD1	2:J:316:LYS:HD2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:325:THR:O	2:J:349:ILE:HA	2.15	0.47
1:M:132:GLU:O	1:M:136:THR:HG23	2.14	0.47
2:N:20:VAL:O	2:N:24:VAL:HG23	2.15	0.47
1:C:114:LEU:C	1:C:116:LEU:H	2.17	0.47
2:F:440:ARG:HB3	2:F:467:TRP:CE3	2.48	0.47
2:H:58:ALA:HA	2:H:81:LYS:HD2	1.97	0.47
2:J:310:HIS:O	2:J:314:ILE:CG1	2.63	0.47
1:I:134:ARG:NH1	2:J:40:VAL:HA	2.30	0.47
2:L:297:LYS:HB2	2:L:297:LYS:HE3	1.64	0.47
2:D:477:ASP:N	2:D:477:ASP:OD1	2.47	0.46
2:F:320:LEU:HD21	2:F:323:LEU:HB2	1.96	0.46
1:G:134:ARG:HH11	2:H:40:VAL:HA	1.80	0.46
2:H:197:LEU:O	2:H:225:VAL:HA	2.15	0.46
2:H:230:PHE:HD1	2:H:235:LEU:HD21	1.78	0.46
2:H:284:GLU:O	2:H:287:ILE:HG23	2.15	0.46
1:I:91:MET:O	1:I:93:ILE:HG12	2.14	0.46
2:J:191:ASN:ND2	2:J:194:LEU:H	2.11	0.46
2:L:546:PRO:O	2:L:547:SER:HB2	2.15	0.46
2:L:523:TYR:CE2	2:L:568:ILE:HD11	2.50	0.46
1:M:137:PHE:HD1	2:N:17:VAL:CG2	2.27	0.46
2:B:357:GLY:HA2	2:B:415:ARG:NH2	2.12	0.46
2:F:159:ILE:HG13	2:F:160:VAL:N	2.29	0.46
2:H:31:PRO:O	2:H:35:ASP:HB2	2.16	0.46
2:H:78:LEU:CD1	2:H:79:LYS:H	2.11	0.46
2:H:92:ILE:HG23	2:H:93:PRO:HD2	1.97	0.46
1:K:108:LEU:HD12	1:K:110:ILE:CD1	2.40	0.46
1:M:128:LYS:HB3	1:M:132:GLU:HB2	1.96	0.46
2:P:519:TRP:HH2	2:P:567:HIS:CE1	2.32	0.46
2:P:519:TRP:CZ3	2:P:567:HIS:ND1	2.83	0.46
2:B:590:GLU:O	2:B:591:PRO:C	2.54	0.46
1:C:114:LEU:C	1:C:116:LEU:N	2.68	0.46
1:E:6:ILE:HG22	1:E:7:VAL:N	2.30	0.46
2:F:396:GLU:HG2	2:F:430:SER:OG	2.15	0.46
2:J:396:GLU:HG2	2:J:430:SER:OG	2.16	0.46
2:L:65:PRO:HA	2:L:103:TRP:CZ3	2.50	0.46
2:P:311:CYS:CB	2:P:336:VAL:HG21	2.46	0.46
2:P:373:LEU:HD12	2:P:377:CYS:SG	2.54	0.46
2:P:85:ARG:NH1	5:P:1101:PO4:O3	2.48	0.46
2:B:456:SER:HB2	2:B:482:GLU:HB3	1.98	0.46
2:B:545:ILE:HG22	2:B:546:PRO:CD	2.45	0.46
1:E:137:PHE:HD1	2:F:17:VAL:HG21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:266:LEU:HA	2:F:266:LEU:HD13	1.81	0.46
1:G:91:MET:O	1:G:93:ILE:N	2.47	0.46
2:H:148:CYS:O	2:H:174:SER:HA	2.16	0.46
2:H:469:LEU:HA	2:H:494:GLU:O	2.14	0.46
1:M:58:TYR:CE1	1:M:62:HIS:CE1	3.04	0.46
2:N:227:VAL:HG13	2:N:228:GLY:N	2.30	0.46
2:N:338:ALA:O	2:N:376:GLY:HA3	2.15	0.46
2:N:490:LEU:O	2:N:514:SER:HB2	2.14	0.46
2:P:285:MET:N	2:P:286:PRO:CD	2.79	0.46
2:B:85:ARG:NH1	5:B:1101:PO4:O3	2.49	0.46
1:C:159:PHE:O	1:C:160:GLU:CB	2.52	0.46
1:E:42:VAL:HG22	1:E:42:VAL:O	2.15	0.46
1:G:26:SER:C	1:G:28:THR:H	2.19	0.46
1:G:48:THR:HG22	1:G:51:ILE:CB	2.45	0.46
1:G:48:THR:HG23	1:G:51:ILE:H	1.80	0.46
2:H:450:LEU:HD21	2:H:455:LEU:N	2.30	0.46
2:J:310:HIS:O	2:J:314:ILE:HG12	2.16	0.46
2:J:373:LEU:HD12	2:J:377:CYS:SG	2.55	0.46
2:L:143:LEU:CD2	2:L:159:ILE:HD13	2.43	0.46
2:L:232:ILE:HD12	2:L:252:SER:H	1.80	0.46
2:L:310:HIS:O	2:L:314:ILE:CG1	2.64	0.46
2:L:422:LEU:HB3	2:L:423:PRO:HD3	1.97	0.46
2:L:446:ARG:HG2	2:L:447:GLN:N	2.31	0.46
1:M:99:PHE:CB	2:N:15:ALA:HB1	2.45	0.46
2:N:398:ILE:O	2:N:402:LEU:HD12	2.16	0.46
2:N:468:MET:CE	2:N:470:LEU:HD11	2.46	0.46
2:P:235:LEU:O	2:P:238:PHE:HB3	2.14	0.46
2:B:270:ARG:O	1:O:107:TYR:HE1	1.98	0.46
1:C:153:ARG:HG2	1:C:157:TRP:CZ3	2.50	0.46
2:D:282:PRO:HA	2:D:285:MET:CE	2.45	0.46
2:D:285:MET:N	2:D:286:PRO:CD	2.79	0.46
2:F:191:ASN:ND2	2:F:194:LEU:H	2.13	0.46
4:F:3100:OGK:N08	4:F:3100:OGK:C18	2.77	0.46
1:G:125:ILE:HD11	2:H:44:TRP:CH2	2.51	0.46
2:H:29:THR:HG23	2:H:30:ASP:N	2.31	0.46
2:H:298:LEU:HD13	2:H:300:LEU:HD11	1.96	0.46
1:I:106:ASN:ND2	2:J:23:GLN:NE2	2.63	0.46
2:J:419:ILE:CD1	2:J:446:ARG:HH22	2.28	0.46
2:L:46:LYS:HE3	2:L:46:LYS:HB2	1.60	0.46
2:D:299:ASP:OD2	2:D:301:LEU:HB2	2.16	0.46
2:F:344:LEU:HD23	2:F:380:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:456:SER:CB	2:F:482:GLU:HB3	2.46	0.46
1:G:160:GLU:HG3	2:H:52:ARG:NH2	2.18	0.46
2:J:46:LYS:HB2	2:J:46:LYS:HE3	1.55	0.46
2:L:198:ASN:C	2:L:198:ASN:OD1	2.53	0.46
2:L:367:GLN:CB	2:L:391:THR:HG22	2.39	0.46
2:P:57:MET:CE	2:P:62:THR:HG22	2.46	0.46
2:B:367:GLN:CB	2:B:391:THR:HG22	2.41	0.46
2:B:539:TYR:CE2	1:C:145:PRO:HB2	2.51	0.46
2:J:367:GLN:O	2:J:371:ILE:HG22	2.15	0.46
1:K:52:LEU:HD12	1:K:52:LEU:O	2.16	0.46
2:J:294:GLN:NE2	1:M:107:TYR:OH	2.49	0.46
1:M:46:ASN:HB2	1:M:107:TYR:CZ	2.51	0.46
1:O:134:ARG:NH1	2:P:40:VAL:HA	2.31	0.46
2:B:191:ASN:ND2	2:B:194:LEU:H	2.11	0.46
2:B:253:LEU:CD1	2:B:280:MET:HB2	2.42	0.46
2:B:289:PHE:N	2:B:290:PRO:CD	2.79	0.46
2:B:398:ILE:O	2:B:402:LEU:HD12	2.16	0.46
1:C:137:PHE:HD1	2:D:17:VAL:HG21	1.79	0.46
2:D:419:ILE:HD11	2:D:446:ARG:HH22	1.81	0.46
2:F:101:THR:N	2:F:102:PRO:CD	2.79	0.46
2:F:121:ARG:NH2	5:F:1103:PO4:O4	2.48	0.46
2:H:291:PHE:N	2:H:291:PHE:HD2	2.11	0.46
2:L:101:THR:CG2	2:L:128:ASP:OD1	2.63	0.46
2:P:282:PRO:HA	2:P:285:MET:CE	2.43	0.46
2:P:545:ILE:HG22	2:P:546:PRO:CD	2.45	0.46
2:F:392:ASN:HD21	2:F:424:LEU:HA	1.80	0.46
2:H:253:LEU:HD12	2:H:280:MET:HB2	1.97	0.46
2:H:285:MET:HE1	2:H:309:ASP:HB3	1.98	0.46
2:H:390:ILE:CD1	2:H:410:LEU:HD11	2.45	0.46
2:H:501:SER:HB2	2:H:503:ARG:NH2	2.31	0.46
2:J:538:PRO:O	2:J:539:TYR:HB2	2.16	0.46
2:L:248:PHE:CD2	2:L:248:PHE:C	2.89	0.46
2:L:325:THR:O	2:L:349:ILE:HA	2.16	0.46
1:O:159:PHE:O	1:O:160:GLU:CB	2.51	0.46
2:P:446:ARG:HG2	2:P:447:GLN:N	2.31	0.46
2:D:412:LEU:HD12	2:D:412:LEU:O	2.15	0.45
2:F:170:LEU:C	2:F:170:LEU:HD23	2.36	0.45
2:F:468:MET:CE	2:F:470:LEU:HD11	2.46	0.45
1:G:26:SER:HB3	1:G:29:ILE:HG13	1.97	0.45
2:H:80:LEU:HD11	2:H:103:TRP:CD2	2.51	0.45
2:H:129:LEU:HD23	2:H:155:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:LEU:HD21	2:H:262:LYS:HG2	1.97	0.45
1:I:102:ILE:CG2	1:I:118:CYS:SG	3.03	0.45
2:J:20:VAL:O	2:J:24:VAL:HG23	2.16	0.45
2:N:339:GLN:HA	2:N:342:LYS:HE2	1.98	0.45
2:N:545:ILE:HG22	2:N:546:PRO:HD2	1.98	0.45
2:N:546:PRO:HB2	2:N:547:SER:H	1.67	0.45
2:P:542:ILE:CD1	2:P:588:LEU:HD12	2.32	0.45
2:B:289:PHE:HD1	2:B:316:LYS:HD2	1.75	0.45
2:B:327:ASN:HD22	2:B:327:ASN:N	2.13	0.45
2:B:351:ARG:O	2:B:351:ARG:HG3	2.16	0.45
2:B:436:LYS:HB3	2:B:436:LYS:HE2	1.72	0.45
2:D:116:SER:CB	2:D:142:THR:HG23	2.40	0.45
2:F:398:ILE:HG23	2:F:402:LEU:HD11	1.97	0.45
2:H:365:VAL:CG2	2:H:388:SER:H	2.29	0.45
1:I:58:TYR:CE1	1:I:62:HIS:CE1	3.04	0.45
2:N:496:ARG:NH2	3:W:201:LEU:HD22	2.31	0.45
2:D:468:MET:CE	2:D:470:LEU:HD11	2.46	0.45
2:F:387:VAL:O	2:F:413:LEU:HD22	2.17	0.45
2:F:436:LYS:HB3	2:F:436:LYS:HE2	1.72	0.45
1:G:130:PRO:HG3	2:H:39:LEU:HB2	1.98	0.45
1:G:52:LEU:O	1:G:52:LEU:HD12	2.16	0.45
2:J:176:PHE:CZ	2:J:204:PHE:CZ	3.04	0.45
5:N:1102:PO4:O3	3:W:206:ARG:NH2	2.45	0.45
2:P:409:ARG:HD3	4:P:8100:OGK:H13A	1.98	0.45
2:B:101:THR:HG22	2:B:128:ASP:CB	2.46	0.45
2:D:96:TRP:O	2:D:578:ARG:NH2	2.42	0.45
1:E:159:PHE:O	1:E:160:GLU:CB	2.51	0.45
2:F:351:ARG:O	2:F:351:ARG:HG3	2.15	0.45
2:F:490:LEU:HA	2:F:490:LEU:HD23	1.74	0.45
1:G:93:ILE:HD12	1:G:97:THR:CG2	2.36	0.45
2:L:305:LEU:HD23	2:L:305:LEU:O	2.16	0.45
4:L:6100:OGK:N08	4:L:6100:OGK:C18	2.79	0.45
2:P:387:VAL:O	2:P:413:LEU:HD22	2.17	0.45
2:B:65:PRO:HA	2:B:103:TRP:CZ3	2.52	0.45
2:B:338:ALA:O	2:B:376:GLY:HA3	2.17	0.45
2:D:456:SER:CB	2:D:482:GLU:HB3	2.47	0.45
1:E:19:GLU:N	1:E:19:GLU:OE1	2.47	0.45
1:E:58:TYR:CE1	1:E:62:HIS:CE1	3.04	0.45
2:F:367:GLN:CB	2:F:391:THR:HG22	2.41	0.45
2:F:472:TYR:CD2	2:F:497:GLY:O	2.70	0.45
2:H:243:ALA:C	2:H:245:LEU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:418:ARG:HB3	2:H:421:ASP:HB2	1.99	0.45
2:H:487:CYS:HB2	2:H:512:LEU:CD2	2.46	0.45
2:H:503:ARG:HG2	2:H:504:ALA:N	2.31	0.45
2:J:546:PRO:O	2:J:547:SER:CB	2.65	0.45
1:M:91:MET:SD	1:M:117:THR:HG22	2.55	0.45
1:M:137:PHE:CD1	2:N:17:VAL:CG2	2.99	0.45
1:M:6:ILE:HG22	1:M:7:VAL:N	2.31	0.45
2:N:255:GLU:O	2:N:255:GLU:HG3	2.16	0.45
2:P:523:TYR:CE2	2:P:568:ILE:HD11	2.52	0.45
1:E:10:SER:OG	1:E:11:SER:N	2.48	0.45
1:E:134:ARG:NH1	2:F:40:VAL:HA	2.32	0.45
1:E:48:THR:CG2	1:E:51:ILE:HG12	2.46	0.45
2:F:519:TRP:HH2	2:F:567:HIS:CE1	2.34	0.45
2:L:159:ILE:HD12	2:L:166:ILE:HD11	1.98	0.45
2:L:57:MET:CE	2:L:62:THR:HG22	2.47	0.45
1:M:91:MET:O	1:M:93:ILE:HG12	2.16	0.45
1:O:48:THR:HG23	1:O:51:ILE:H	1.82	0.45
1:O:91:MET:O	1:O:93:ILE:HG12	2.17	0.45
1:C:42:VAL:HA	1:C:43:PRO:HD3	1.79	0.45
2:D:327:ASN:HD22	2:D:327:ASN:N	2.15	0.45
2:D:446:ARG:HG2	2:D:447:GLN:N	2.32	0.45
2:F:456:SER:HB2	2:F:482:GLU:HB3	1.98	0.45
2:H:351:ARG:HG3	2:H:359:GLU:OE2	2.16	0.45
1:I:125:ILE:HG23	1:I:133:ILE:CD1	2.39	0.45
2:J:127:LEU:HD21	2:J:131:ARG:NH2	2.32	0.45
2:L:563:GLU:O	2:L:563:GLU:HG3	2.17	0.45
2:D:127:LEU:HB2	2:N:126:ASP:HB3	1.99	0.45
2:N:440:ARG:HB3	2:N:467:TRP:CE3	2.51	0.45
2:N:446:ARG:HG2	2:N:447:GLN:N	2.32	0.45
2:P:285:MET:N	2:P:286:PRO:HD2	2.32	0.45
2:B:289:PHE:HB2	2:B:290:PRO:HD3	1.97	0.45
2:B:351:ARG:HD3	2:B:413:LEU:HD11	1.98	0.45
2:B:545:ILE:HB	2:B:567:HIS:HB2	1.98	0.45
2:D:248:PHE:CD2	2:D:248:PHE:C	2.90	0.45
2:D:400:THR:O	2:D:403:LYS:HE2	2.17	0.45
2:D:357:GLY:CA	2:D:415:ARG:HH22	2.14	0.45
2:H:387:VAL:HG12	2:H:390:ILE:HD13	1.95	0.45
1:I:102:ILE:HG12	1:I:117:THR:CB	2.47	0.45
1:I:46:ASN:HB2	1:I:107:TYR:CZ	2.52	0.45
2:J:187:LEU:HA	2:J:187:LEU:HD23	1.82	0.45
1:K:6:ILE:HG22	1:K:7:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:282:PRO:HA	2:L:285:MET:CE	2.47	0.45
2:L:419:ILE:O	2:L:420:THR:O	2.34	0.45
1:M:102:ILE:CB	2:N:20:VAL:HG21	2.47	0.45
3:X:201:LEU:HD23	3:X:201:LEU:HA	1.80	0.45
2:D:289:PHE:N	2:D:290:PRO:CD	2.80	0.45
2:D:523:TYR:CE2	2:D:568:ILE:HD11	2.52	0.45
1:G:42:VAL:O	1:G:42:VAL:HG22	2.17	0.45
2:H:91:LEU:O	2:H:567:HIS:HE1	2.00	0.45
1:I:102:ILE:HG12	1:I:117:THR:HB	1.99	0.45
2:J:198:ASN:OD1	2:J:198:ASN:C	2.55	0.45
2:N:407:ASP:OD1	2:N:440:ARG:HD2	2.17	0.45
1:O:137:PHE:HD1	2:P:17:VAL:CG2	2.29	0.45
1:C:6:ILE:HG22	1:C:7:VAL:N	2.32	0.45
2:D:159:ILE:HD12	2:D:166:ILE:HD11	1.99	0.45
2:D:351:ARG:HG3	2:D:351:ARG:O	2.16	0.45
2:F:546:PRO:O	2:F:547:SER:HB2	2.17	0.45
2:F:89:PHE:CD1	3:S:206:ARG:HA	2.52	0.45
1:G:42:VAL:HA	1:G:43:PRO:HD3	1.79	0.45
2:H:275:LEU:C	2:H:275:LEU:HD12	2.37	0.45
2:H:400:THR:C	2:H:403:LYS:HE2	2.37	0.45
2:H:53:GLU:O	2:H:75:LEU:CD2	2.65	0.45
2:H:96:TRP:HE3	2:H:97:GLY:N	2.15	0.45
2:L:412:LEU:HD12	2:L:412:LEU:C	2.37	0.45
2:L:55:VAL:CG2	2:L:75:LEU:HD21	2.44	0.45
2:L:544:LEU:HD11	2:L:588:LEU:HD11	1.99	0.45
1:M:99:PHE:CZ	2:N:17:VAL:HG22	2.52	0.45
2:N:429:ARG:O	2:N:433:ILE:HD12	2.17	0.45
1:O:6:ILE:HG22	1:O:7:VAL:N	2.32	0.45
2:B:311:CYS:CB	2:B:336:VAL:HG21	2.47	0.44
2:B:412:LEU:HD12	2:B:412:LEU:C	2.37	0.44
2:D:490:LEU:HD11	2:D:493:LEU:HD13	1.98	0.44
2:D:546:PRO:O	2:D:547:SER:HB2	2.16	0.44
2:D:578:ARG:HG3	2:D:578:ARG:H	1.46	0.44
2:F:20:VAL:O	2:F:24:VAL:HG23	2.18	0.44
2:F:251:GLY:O	2:F:278:SER:HB2	2.17	0.44
2:H:467:TRP:HZ3	2:H:494:GLU:HG3	1.82	0.44
2:J:285:MET:N	2:J:286:PRO:HD2	2.32	0.44
2:J:490:LEU:HD23	2:J:490:LEU:HA	1.79	0.44
1:K:42:VAL:HA	1:K:43:PRO:HD3	1.81	0.44
1:K:48:THR:CG2	1:K:51:ILE:HG12	2.48	0.44
2:N:367:GLN:CB	2:N:391:THR:HG22	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:398:ILE:HG23	2:N:402:LEU:HD11	1.99	0.44
2:P:120:ARG:NH2	5:P:1103:PO4:O4	2.48	0.44
2:P:339:GLN:HA	2:P:342:LYS:HE2	1.99	0.44
2:B:419:ILE:O	2:B:420:THR:O	2.35	0.44
2:B:392:ASN:HD21	2:B:424:LEU:HA	1.82	0.44
2:B:59:LEU:O	2:B:62:THR:HB	2.17	0.44
2:D:398:ILE:C	2:D:400:THR:H	2.20	0.44
1:E:153:ARG:NH2	2:F:539:TYR:CE1	2.85	0.44
2:F:544:LEU:HD11	2:F:588:LEU:HD11	2.00	0.44
2:H:97:GLY:HA3	2:H:123:ILE:HD11	1.98	0.44
2:J:321:GLU:HA	2:J:344:LEU:HA	1.99	0.44
2:J:419:ILE:O	2:J:420:THR:C	2.55	0.44
2:L:373:LEU:HD12	2:L:377:CYS:SG	2.57	0.44
2:L:443:PHE:CE2	2:L:445:LEU:HD11	2.52	0.44
2:L:468:MET:CE	2:L:470:LEU:HD11	2.48	0.44
2:N:46:LYS:HE3	2:N:46:LYS:HB2	1.54	0.44
2:P:375:GLN:HG2	2:P:401:TYR:CE1	2.52	0.44
2:P:367:GLN:CB	2:P:391:THR:HG22	2.42	0.44
3:W:201:LEU:HA	3:W:202:PRO:HD3	1.83	0.44
2:D:419:ILE:CD1	2:D:446:ARG:HH22	2.29	0.44
2:D:521:GLN:HG3	2:D:567:HIS:CD2	2.50	0.44
2:F:545:ILE:HG22	2:F:546:PRO:CD	2.47	0.44
2:H:409:ARG:HA	2:H:442:ALA:O	2.18	0.44
2:H:410:LEU:HD13	2:H:411:VAL:O	2.18	0.44
2:H:87:ALA:HB2	2:H:92:ILE:CG1	2.47	0.44
2:N:519:TRP:HH2	2:N:567:HIS:CE1	2.35	0.44
2:N:80:LEU:HB2	2:N:122:MET:HE1	1.97	0.44
1:O:26:SER:HB3	1:O:29:ILE:HG13	1.98	0.44
1:O:58:TYR:CE1	1:O:62:HIS:CE1	3.05	0.44
1:O:91:MET:HE3	1:O:117:THR:HG22	1.98	0.44
2:P:545:ILE:HG22	2:P:546:PRO:HD2	1.99	0.44
2:P:96:TRP:O	2:P:578:ARG:NH2	2.44	0.44
1:A:95:GLN:NE2	1:A:124:MET:HE3	2.32	0.44
2:B:546:PRO:HB2	2:B:547:SER:H	1.68	0.44
4:D:2100:OGK:N08	4:D:2100:OGK:H18A	2.26	0.44
2:D:351:ARG:HD3	2:D:413:LEU:HD11	1.98	0.44
2:D:545:ILE:HB	2:D:567:HIS:HB2	1.99	0.44
1:E:107:TYR:CD1	2:L:270:ARG:HB3	2.52	0.44
2:F:419:ILE:CD1	2:F:446:ARG:HH22	2.31	0.44
2:H:423:PRO:HA	2:H:449:GLY:O	2.18	0.44
2:J:380:LEU:HA	2:J:380:LEU:HD23	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:191:ASN:ND2	2:L:194:LEU:H	2.12	0.44
2:L:338:ALA:O	2:L:376:GLY:HA3	2.17	0.44
2:L:400:THR:O	2:L:403:LYS:HE2	2.18	0.44
2:P:101:THR:HG22	2:P:128:ASP:CB	2.47	0.44
2:P:168:THR:CB	2:P:196:VAL:HG13	2.26	0.44
2:P:396:GLU:HG2	2:P:430:SER:OG	2.16	0.44
2:D:533:MET:CE	2:D:588:LEU:HD13	2.47	0.44
2:H:101:THR:HB	2:H:102:PRO:HD3	1.98	0.44
2:H:97:GLY:CA	2:H:123:ILE:CD1	2.96	0.44
2:H:208:SER:HA	2:H:209:PRO:HD2	1.82	0.44
1:I:148:GLU:HG2	1:I:152:ARG:HH12	1.83	0.44
2:J:304:LEU:HA	2:J:304:LEU:HD12	1.71	0.44
2:J:338:ALA:O	2:J:376:GLY:HA3	2.17	0.44
2:J:419:ILE:O	2:J:420:THR:O	2.36	0.44
2:J:539:TYR:OH	1:K:146:GLU:HA	2.18	0.44
1:O:137:PHE:CD1	2:P:17:VAL:CG2	3.01	0.44
2:D:297:LYS:HE3	2:D:297:LYS:HB2	1.68	0.44
2:D:344:LEU:HD23	2:D:380:LEU:HD21	1.98	0.44
2:D:419:ILE:O	2:D:420:THR:C	2.56	0.44
2:H:511:LYS:HB2	2:H:511:LYS:HE2	1.66	0.44
2:H:535:MET:HG2	2:H:535:MET:O	2.17	0.44
2:J:299:ASP:OD2	2:J:301:LEU:HB2	2.18	0.44
2:J:392:ASN:HD21	2:J:424:LEU:HA	1.82	0.44
4:J:5100:OGK:C18	4:J:5100:OGK:N08	2.79	0.44
2:J:85:ARG:NH1	5:J:1101:PO4:O3	2.50	0.44
2:N:231:GLU:HG2	2:N:254:ASN:HD22	1.82	0.44
2:P:65:PRO:HB3	2:P:103:TRP:CE3	2.52	0.44
2:P:314:ILE:HD11	2:P:329:ILE:HD11	1.99	0.44
2:P:419:ILE:O	2:P:420:THR:C	2.56	0.44
2:P:538:PRO:O	2:P:539:TYR:HB2	2.18	0.44
1:A:137:PHE:HD1	2:B:17:VAL:CG2	2.31	0.44
2:D:75:LEU:HA	2:D:75:LEU:HD23	1.81	0.44
2:F:55:VAL:CG2	2:F:75:LEU:HD21	2.48	0.44
2:H:225:VAL:HG21	2:H:238:PHE:CZ	2.53	0.44
2:H:275:LEU:C	2:H:275:LEU:CD1	2.86	0.44
2:H:423:PRO:CB	2:H:425:ASP:OD2	2.65	0.44
2:J:263:TYR:O	2:J:266:LEU:HD23	2.18	0.44
1:I:153:ARG:NH2	2:J:539:TYR:CE1	2.86	0.44
1:K:48:THR:HG22	1:K:51:ILE:CB	2.47	0.44
2:L:321:GLU:HA	2:L:344:LEU:HA	1.98	0.44
2:L:545:ILE:HG22	2:L:546:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:96:ALA:CB	2:N:14:VAL:CG1	2.95	0.44
1:M:99:PHE:HB2	2:N:15:ALA:HB1	2.00	0.44
2:N:382:TYR:CD2	2:N:407:ASP:HB3	2.53	0.44
2:N:419:ILE:O	2:N:420:THR:C	2.56	0.44
2:N:83:LYS:O	2:N:121:ARG:NH1	2.46	0.44
2:P:419:ILE:O	2:P:420:THR:O	2.36	0.44
4:P:8100:OGK:C18	4:P:8100:OGK:N08	2.75	0.44
2:B:545:ILE:HG22	2:B:546:PRO:HD2	2.00	0.44
2:D:127:LEU:HD21	2:D:131:ARG:NH2	2.33	0.44
2:D:266:LEU:HD13	2:D:266:LEU:HA	1.80	0.44
2:D:319:ASN:HD21	1:G:43:PRO:HG3	1.82	0.44
2:D:46:LYS:HB2	2:D:46:LYS:HE3	1.55	0.44
1:E:129:THR:HB	1:E:130:PRO:HD2	2.00	0.44
2:F:230:PHE:O	2:F:252:SER:HB3	2.18	0.44
2:F:419:ILE:O	2:F:420:THR:C	2.56	0.44
1:G:148:GLU:HG3	1:G:152:ARG:NH1	2.33	0.44
2:J:543:GLU:OE2	2:J:578:ARG:HD3	2.16	0.44
2:J:78:LEU:HD12	2:J:79:LYS:H	1.83	0.44
2:L:276:GLY:HA3	2:L:299:ASP:HB3	2.00	0.44
2:N:101:THR:N	2:N:102:PRO:CD	2.81	0.44
2:N:85:ARG:NH1	5:N:1101:PO4:O3	2.51	0.44
1:C:58:TYR:CD2	1:C:113:LEU:HD13	2.52	0.44
2:H:101:THR:N	2:H:102:PRO:CD	2.81	0.44
2:H:189:GLN:C	2:H:190:HIS:ND1	2.71	0.44
2:H:289:PHE:CE1	2:H:316:LYS:HD3	2.53	0.44
2:H:519:TRP:CH2	2:H:567:HIS:ND1	2.86	0.44
1:I:34:GLU:O	2:N:271:LYS:HE3	2.18	0.44
2:J:468:MET:CE	2:J:470:LEU:HD11	2.48	0.44
2:L:176:PHE:CZ	2:L:204:PHE:CZ	3.06	0.44
2:L:75:LEU:HD23	2:L:75:LEU:HA	1.83	0.44
1:O:52:LEU:O	1:O:52:LEU:HD12	2.17	0.44
2:B:18:ASP:OD2	2:B:43:ARG:HD2	2.17	0.43
2:B:419:ILE:O	2:B:420:THR:C	2.56	0.43
2:B:446:ARG:HG2	2:B:447:GLN:N	2.33	0.43
1:C:48:THR:HG23	1:C:51:ILE:H	1.83	0.43
2:D:538:PRO:O	2:D:539:TYR:HB2	2.18	0.43
2:D:165:LYS:NZ	2:H:139:ASP:OD1	2.43	0.43
2:H:390:ILE:HD11	2:H:412:LEU:HD21	2.00	0.43
2:H:411:VAL:HG13	2:H:444:TYR:CB	2.40	0.43
1:I:108:LEU:HD12	1:I:110:ILE:CD1	2.43	0.43
2:J:545:ILE:HG22	2:J:546:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:184:LEU:HA	2:N:184:LEU:HD23	1.86	0.43
2:N:251:GLY:O	2:N:278:SER:HB2	2.18	0.43
2:N:305:LEU:HD23	2:N:305:LEU:O	2.18	0.43
2:N:398:ILE:C	2:N:400:THR:H	2.20	0.43
2:N:436:LYS:HE2	2:N:436:LYS:HB3	1.75	0.43
2:P:125:SER:O	2:P:129:LEU:HD22	2.18	0.43
2:B:373:LEU:HD12	2:B:377:CYS:SG	2.58	0.43
2:B:57:MET:CE	2:B:62:THR:HG22	2.48	0.43
2:D:209:PRO:HD3	2:D:230:PHE:HE2	1.83	0.43
2:D:233:LEU:HD23	2:D:233:LEU:HA	1.78	0.43
2:F:419:ILE:O	2:F:420:THR:O	2.36	0.43
2:F:590:GLU:O	2:F:591:PRO:C	2.57	0.43
2:H:166:ILE:CG2	2:H:167:LYS:N	2.80	0.43
2:H:512:LEU:HA	2:H:513:PRO:HD3	1.71	0.43
1:I:10:SER:OG	1:I:11:SER:N	2.50	0.43
1:I:48:THR:HG22	1:I:51:ILE:CB	2.48	0.43
2:J:320:LEU:HD21	2:J:323:LEU:HB2	1.99	0.43
1:A:27:GLN:HA	1:A:30:ALA:HB3	2.00	0.43
2:F:578:ARG:HG3	2:F:578:ARG:H	1.51	0.43
2:H:196:VAL:O	2:H:196:VAL:HG22	2.17	0.43
2:H:266:LEU:HD13	2:H:267:VAL:H	1.82	0.43
1:K:137:PHE:HD1	2:L:17:VAL:CG2	2.31	0.43
2:L:116:SER:CB	2:L:142:THR:HG23	2.43	0.43
2:L:392:ASN:HD21	2:L:424:LEU:HA	1.84	0.43
2:N:519:TRP:HA	2:N:568:ILE:O	2.18	0.43
1:A:146:GLU:HA	2:D:539:TYR:OH	2.18	0.43
4:B:1100:OGK:C18	4:B:1100:OGK:N08	2.79	0.43
2:B:125:SER:O	2:B:129:LEU:HD22	2.19	0.43
2:B:235:LEU:O	2:B:238:PHE:HB3	2.18	0.43
2:D:85:ARG:NH1	5:D:1101:PO4:O3	2.51	0.43
2:F:248:PHE:C	2:F:248:PHE:CD2	2.91	0.43
2:H:318:PRO:C	2:H:320:LEU:H	2.22	0.43
2:H:542:ILE:HD12	2:H:543:GLU:N	2.33	0.43
1:M:101:LEU:HD23	1:M:101:LEU:HA	1.80	0.43
1:M:26:SER:HB3	1:M:29:ILE:HG13	2.00	0.43
2:N:546:PRO:O	2:N:547:SER:CB	2.66	0.43
2:P:398:ILE:C	2:P:400:THR:H	2.20	0.43
1:A:6:ILE:HG22	1:A:7:VAL:N	2.34	0.43
4:B:1100:OGK:H18A	4:B:1100:OGK:N08	2.24	0.43
2:B:325:THR:O	2:B:349:ILE:HA	2.19	0.43
2:B:519:TRP:C	2:B:519:TRP:CD1	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LEU:O	1:C:117:THR:CG2	2.65	0.43
2:F:176:PHE:CZ	2:F:204:PHE:CZ	3.07	0.43
2:F:321:GLU:HA	2:F:344:LEU:HA	1.99	0.43
2:J:231:GLU:HG2	2:J:254:ASN:HD22	1.83	0.43
2:J:18:ASP:OD2	2:J:43:ARG:HD2	2.19	0.43
2:J:55:VAL:CG2	2:J:75:LEU:HD21	2.47	0.43
2:L:351:ARG:O	2:L:351:ARG:HG3	2.19	0.43
2:L:95:ASN:O	2:L:582:PRO:HG3	2.18	0.43
2:N:289:PHE:N	2:N:290:PRO:CD	2.81	0.43
1:O:101:LEU:HD23	1:O:101:LEU:HA	1.88	0.43
1:O:128:LYS:HB2	1:O:133:ILE:CD1	2.49	0.43
1:O:42:VAL:HG22	1:O:42:VAL:O	2.18	0.43
2:P:289:PHE:N	2:P:290:PRO:CD	2.81	0.43
2:P:343:GLN:NE2	2:P:343:GLN:HA	2.33	0.43
3:R:201:LEU:HD23	3:R:201:LEU:HA	1.85	0.43
2:B:59:LEU:HD22	2:B:61:TYR:H	1.83	0.43
2:D:227:VAL:HG13	2:D:228:GLY:H	1.80	0.43
2:D:485:ARG:HE	2:D:485:ARG:HB3	1.69	0.43
2:D:563:GLU:O	2:D:563:GLU:HG3	2.19	0.43
2:F:545:ILE:HG22	2:F:546:PRO:HD2	2.00	0.43
2:H:444:TYR:CD1	2:H:471:GLY:CA	3.01	0.43
2:J:248:PHE:CD2	2:J:248:PHE:C	2.92	0.43
2:J:308:GLU:O	2:J:312:THR:HG23	2.18	0.43
1:K:58:TYR:CE1	1:K:62:HIS:CE1	3.06	0.43
2:L:152:THR:HG22	2:L:177:SER:HB2	2.01	0.43
2:L:311:CYS:CB	2:L:336:VAL:HG21	2.48	0.43
2:L:398:ILE:C	2:L:400:THR:H	2.22	0.43
2:N:304:LEU:HD12	2:N:304:LEU:HA	1.71	0.43
2:B:157:LEU:HD12	2:B:157:LEU:O	2.19	0.43
2:B:159:ILE:HG13	2:B:160:VAL:N	2.29	0.43
2:B:398:ILE:C	2:B:400:THR:H	2.22	0.43
1:C:8:LEU:HD23	1:C:42:VAL:CG1	2.49	0.43
2:D:546:PRO:O	2:D:547:SER:CB	2.67	0.43
2:D:542:ILE:CD1	2:D:588:LEU:HD12	2.29	0.43
1:E:107:TYR:HE1	2:L:270:ARG:O	2.02	0.43
2:F:419:ILE:HD11	2:F:446:ARG:HH22	1.84	0.43
2:F:502:GLU:HG3	2:F:525:ALA:HA	2.00	0.43
2:H:207:ILE:H	2:H:207:ILE:HG12	1.59	0.43
2:H:301:LEU:HB3	2:H:302:TYR:CD2	2.53	0.43
2:H:367:GLN:HA	2:H:367:GLN:OE1	2.18	0.43
2:J:266:LEU:HA	2:J:266:LEU:HD13	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:407:ASP:OD1	2:J:440:ARG:HD2	2.19	0.43
2:L:304:LEU:HD12	2:L:304:LEU:HA	1.75	0.43
2:L:351:ARG:HD3	2:L:413:LEU:HD11	2.00	0.43
1:M:42:VAL:HA	1:M:43:PRO:HD3	1.79	0.43
3:S:201:LEU:HD23	3:S:201:LEU:HA	1.79	0.43
1:A:10:SER:OG	1:A:11:SER:N	2.52	0.43
1:A:48:THR:HG23	1:A:51:ILE:H	1.84	0.43
2:B:116:SER:CB	2:B:142:THR:HG23	2.40	0.43
2:D:519:TRP:HZ3	2:D:567:HIS:ND1	2.15	0.43
2:D:59:LEU:O	2:D:62:THR:HB	2.18	0.43
2:F:125:SER:O	2:F:128:ASP:OD2	2.37	0.43
2:H:129:LEU:HA	2:H:129:LEU:HD12	1.69	0.43
2:H:444:TYR:CE1	2:H:471:GLY:HA2	2.54	0.43
2:H:480:LEU:HD22	2:H:500:PHE:CD1	2.53	0.43
2:J:59:LEU:HD22	2:J:61:TYR:H	1.84	0.43
2:L:419:ILE:O	2:L:420:THR:C	2.56	0.43
1:M:148:GLU:HG2	1:M:152:ARG:HH12	1.83	0.43
2:N:412:LEU:HD12	2:N:412:LEU:O	2.18	0.43
2:N:411:VAL:HG22	2:N:444:TYR:HB3	1.99	0.43
2:N:490:LEU:HD23	2:N:490:LEU:HA	1.82	0.43
2:P:46:LYS:HB2	2:P:46:LYS:HE3	1.54	0.43
1:A:108:LEU:HD12	1:A:110:ILE:CD1	2.42	0.43
5:B:1102:PO4:O3	3:Q:206:ARG:NH2	2.49	0.43
2:B:201:MET:HB3	3:Q:211:ARG:HH12	1.82	0.43
2:B:233:LEU:HA	2:B:233:LEU:HD23	1.80	0.43
2:B:411:VAL:HG22	2:B:444:TYR:HB3	2.01	0.43
2:D:190:HIS:CD2	2:H:112:ARG:NH1	2.86	0.43
2:F:65:PRO:HB3	2:F:103:TRP:CE3	2.54	0.43
2:H:298:LEU:HD22	2:H:300:LEU:CG	2.45	0.43
2:H:325:THR:OG1	2:H:326:ARG:N	2.51	0.43
2:H:385:VAL:CG1	2:H:387:VAL:HG23	2.48	0.43
2:H:412:LEU:CD1	2:H:445:LEU:CD2	2.97	0.43
1:I:132:GLU:O	1:I:136:THR:HG23	2.19	0.43
2:J:233:LEU:HA	2:J:233:LEU:HD23	1.81	0.43
2:J:542:ILE:CD1	2:J:588:LEU:HD12	2.29	0.43
2:F:136:ARG:HH21	2:L:164:ARG:HH21	1.65	0.43
1:M:153:ARG:CG	1:M:157:TRP:CZ3	3.02	0.43
2:N:380:LEU:HA	2:N:380:LEU:HD23	1.77	0.43
2:N:396:GLU:HG2	2:N:430:SER:OG	2.18	0.43
1:M:134:ARG:HH11	2:N:40:VAL:HA	1.82	0.43
2:N:472:TYR:CD2	2:N:497:GLY:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:HIS:HE1	2:P:110:ASN:HA	1.84	0.43
2:P:227:VAL:HG13	2:P:228:GLY:H	1.82	0.43
3:U:201:LEU:HA	3:U:201:LEU:HD23	1.85	0.43
2:B:375:GLN:HG2	2:B:401:TYR:CE1	2.53	0.43
2:B:538:PRO:O	2:B:539:TYR:HB2	2.19	0.43
2:B:55:VAL:CG2	2:B:75:LEU:HD21	2.49	0.43
2:D:590:GLU:O	2:D:591:PRO:C	2.56	0.43
1:E:128:LYS:HB2	1:E:133:ILE:CD1	2.49	0.43
1:E:42:VAL:HA	1:E:43:PRO:HD3	1.79	0.43
1:E:91:MET:O	1:E:93:ILE:HG12	2.18	0.43
2:F:311:CYS:CB	2:F:336:VAL:HG21	2.49	0.43
1:G:58:TYR:CD2	1:G:113:LEU:HD13	2.54	0.43
2:H:362:GLU:O	2:H:364:LEU:N	2.52	0.43
2:H:97:GLY:HA3	2:H:123:ILE:HD12	1.99	0.43
2:J:58:ALA:O	2:J:81:LYS:HB2	2.19	0.43
1:M:42:VAL:O	1:M:42:VAL:HG22	2.18	0.43
2:D:580:ASP:HA	2:N:206:LYS:HE3	2.01	0.43
2:N:351:ARG:HD3	2:N:413:LEU:HD11	2.00	0.43
2:L:565:PRO:HG2	3:V:201:LEU:HD21	1.99	0.43
1:A:95:GLN:NE2	1:A:124:MET:CE	2.82	0.42
2:D:263:TYR:O	2:D:266:LEU:HD23	2.19	0.42
2:D:343:GLN:NE2	2:D:343:GLN:HA	2.34	0.42
2:D:546:PRO:HB2	2:D:547:SER:H	1.72	0.42
2:F:519:TRP:CH2	2:F:567:HIS:CG	3.07	0.42
2:H:316:LYS:C	2:H:318:PRO:HD3	2.40	0.42
2:H:437:LYS:HB3	2:H:437:LYS:HE2	1.80	0.42
2:H:450:LEU:HG	2:H:454:GLY:HA3	2.01	0.42
1:I:27:GLN:HA	1:I:30:ALA:HB3	2.01	0.42
1:I:42:VAL:HG22	1:I:42:VAL:O	2.18	0.42
2:J:308:GLU:HG3	2:J:332:ARG:NH2	2.28	0.42
2:J:545:ILE:HG22	2:J:546:PRO:N	2.34	0.42
2:L:231:GLU:HG2	2:L:254:ASN:HD22	1.83	0.42
2:P:578:ARG:HG3	2:P:578:ARG:H	1.44	0.42
1:A:26:SER:HB3	1:A:29:ILE:HG13	2.01	0.42
2:B:198:ASN:OD1	2:B:198:ASN:C	2.57	0.42
2:B:344:LEU:HD23	2:B:380:LEU:HD21	2.01	0.42
2:B:46:LYS:HB2	2:B:46:LYS:HE3	1.51	0.42
2:B:523:TYR:CE2	2:B:568:ILE:HD11	2.54	0.42
2:D:311:CYS:CB	2:D:336:VAL:HG21	2.50	0.42
1:E:26:SER:C	1:E:28:THR:H	2.22	0.42
1:E:45:PRO:HD2	2:L:294:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:303:ALA:O	2:H:326:ARG:NH2	2.52	0.42
2:H:304:LEU:HD22	2:H:304:LEU:HA	1.48	0.42
2:H:310:HIS:O	2:H:314:ILE:CG1	2.49	0.42
2:J:544:LEU:HD11	2:J:588:LEU:HD11	2.01	0.42
1:K:26:SER:C	1:K:28:THR:H	2.21	0.42
2:P:338:ALA:O	2:P:376:GLY:HA3	2.19	0.42
2:B:396:GLU:HG2	2:B:430:SER:OG	2.19	0.42
1:C:27:GLN:HA	1:C:30:ALA:HB3	2.00	0.42
2:D:231:GLU:HG2	2:D:254:ASN:HD22	1.84	0.42
2:D:380:LEU:HD23	2:D:380:LEU:HA	1.71	0.42
2:D:78:LEU:HD12	2:D:79:LYS:H	1.85	0.42
2:F:198:ASN:OD1	2:F:198:ASN:C	2.56	0.42
1:G:102:ILE:HG12	1:G:117:THR:OG1	2.18	0.42
1:G:46:ASN:HB2	1:G:107:TYR:CZ	2.54	0.42
2:H:168:THR:CG2	2:H:196:VAL:HG13	2.50	0.42
2:H:20:VAL:O	2:H:24:VAL:HG23	2.20	0.42
2:H:542:ILE:HD12	2:H:542:ILE:C	2.39	0.42
2:J:101:THR:N	2:J:102:PRO:CD	2.82	0.42
2:J:289:PHE:N	2:J:290:PRO:CD	2.82	0.42
2:J:297:LYS:HB2	2:J:297:LYS:HE3	1.62	0.42
2:L:299:ASP:OD2	2:L:301:LEU:HB2	2.18	0.42
2:N:412:LEU:HD12	2:N:412:LEU:C	2.40	0.42
2:N:465:VAL:CG1	2:N:468:MET:HG3	2.48	0.42
1:A:148:GLU:HG2	1:A:152:ARG:HH12	1.84	0.42
2:B:398:ILE:HG23	2:B:402:LEU:HD11	2.02	0.42
2:B:519:TRP:CH2	2:B:567:HIS:CE1	3.07	0.42
4:D:2100:OGK:N08	4:D:2100:OGK:C18	2.81	0.42
1:E:46:ASN:HB2	1:E:107:TYR:CZ	2.54	0.42
2:F:452:ASP:OD1	2:F:478:GLU:HB2	2.19	0.42
2:H:208:SER:O	2:H:211:ASP:N	2.50	0.42
2:H:350:GLU:CB	2:H:386:TYR:CD1	3.02	0.42
2:H:505:ILE:C	2:H:507:ALA:N	2.73	0.42
2:J:367:GLN:CB	2:J:391:THR:HG22	2.37	0.42
1:M:87:ASP:HB3	1:M:116:LEU:CD2	2.49	0.42
2:N:232:ILE:HD12	2:N:252:SER:H	1.83	0.42
2:N:280:MET:HG2	2:N:280:MET:O	2.19	0.42
2:N:477:ASP:N	2:N:477:ASP:OD1	2.52	0.42
2:N:544:LEU:HD11	2:N:588:LEU:CD1	2.50	0.42
2:P:20:VAL:O	2:P:24:VAL:HG23	2.19	0.42
2:P:546:PRO:O	2:P:547:SER:CB	2.67	0.42
4:P:8100:OGK:N08	4:P:8100:OGK:H18A	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:201:LEU:HA	3:V:202:PRO:HD3	1.82	0.42
2:B:95:ASN:O	2:B:582:PRO:HG3	2.20	0.42
2:D:299:ASP:C	2:D:301:LEU:H	2.23	0.42
1:E:137:PHE:CD1	2:F:17:VAL:CG2	3.02	0.42
2:F:221:SER:O	2:F:223:VAL:HG23	2.20	0.42
2:F:544:LEU:HD11	2:F:588:LEU:CD1	2.50	0.42
2:F:542:ILE:CG1	2:F:588:LEU:HB2	2.49	0.42
2:H:136:ARG:O	2:H:139:ASP:HB2	2.19	0.42
2:H:412:LEU:O	2:H:414:ASP:N	2.53	0.42
1:I:48:THR:HG23	1:I:51:ILE:H	1.85	0.42
2:J:563:GLU:O	2:J:563:GLU:HG3	2.19	0.42
2:J:590:GLU:O	2:J:591:PRO:C	2.57	0.42
1:K:48:THR:HG23	1:K:51:ILE:H	1.85	0.42
2:L:221:SER:O	2:L:223:VAL:HG23	2.18	0.42
2:L:20:VAL:O	2:L:24:VAL:HG23	2.19	0.42
1:M:134:ARG:NE	1:M:141:ASN:HB2	2.34	0.42
2:N:127:LEU:HD21	2:N:131:ARG:NH2	2.34	0.42
2:P:431:LEU:C	2:P:431:LEU:HD12	2.39	0.42
1:A:134:ARG:CZ	1:A:141:ASN:HD22	2.32	0.42
2:B:295:ILE:HG21	2:B:298:LEU:CD1	2.47	0.42
2:B:456:SER:CB	2:B:482:GLU:HB3	2.49	0.42
2:B:490:LEU:HD11	2:B:493:LEU:HD13	2.01	0.42
2:D:125:SER:O	2:D:129:LEU:HD22	2.20	0.42
2:D:436:LYS:HE2	2:D:436:LYS:HB3	1.74	0.42
2:F:227:VAL:HG13	2:F:228:GLY:H	1.84	0.42
2:H:194:LEU:HA	2:H:194:LEU:HD12	1.77	0.42
2:H:242:ALA:HB1	2:H:245:LEU:HB2	2.02	0.42
2:H:362:GLU:HB3	2:H:363:GLY:H	1.52	0.42
2:H:518:LEU:HB3	2:H:570:ALA:HB3	2.02	0.42
2:J:65:PRO:HA	2:J:103:TRP:CZ3	2.54	0.42
1:I:137:PHE:HD1	2:J:17:VAL:HG21	1.83	0.42
2:J:350:GLU:HB3	3:U:209:LEU:CD2	2.46	0.42
2:L:431:LEU:HD12	2:L:431:LEU:O	2.19	0.42
2:L:519:TRP:CD1	2:L:519:TRP:C	2.90	0.42
1:M:48:THR:HG23	1:M:51:ILE:H	1.84	0.42
1:A:98:LEU:CD2	1:A:120:THR:HG22	2.49	0.42
1:A:137:PHE:CD1	2:B:17:VAL:CG2	3.03	0.42
1:A:153:ARG:HG2	1:A:157:TRP:CZ3	2.54	0.42
2:B:299:ASP:OD2	2:B:301:LEU:HB2	2.19	0.42
1:C:132:GLU:O	1:C:136:THR:HG23	2.20	0.42
2:F:339:GLN:HA	2:F:342:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:347:LEU:HD11	2:F:349:ILE:HD11	2.01	0.42
2:F:469:LEU:HA	2:F:494:GLU:O	2.19	0.42
2:F:563:GLU:HG3	2:F:563:GLU:O	2.20	0.42
2:H:115:LYS:O	2:H:141:GLU:N	2.51	0.42
2:H:320:LEU:HD12	2:H:321:GLU:H	1.84	0.42
1:I:101:LEU:HB3	1:I:117:THR:HG21	2.01	0.42
1:I:128:LYS:HB2	1:I:133:ILE:CD1	2.50	0.42
2:J:101:THR:HG22	2:J:128:ASP:CB	2.48	0.42
2:J:59:LEU:O	2:J:62:THR:HB	2.20	0.42
2:L:253:LEU:CD1	2:L:280:MET:HB2	2.46	0.42
2:L:308:GLU:O	2:L:312:THR:HG23	2.20	0.42
2:L:452:ASP:OD1	2:L:478:GLU:HB2	2.20	0.42
2:N:299:ASP:OD2	2:N:301:LEU:HB2	2.19	0.42
1:O:48:THR:HG22	1:O:51:ILE:HG12	2.01	0.42
2:P:231:GLU:HG2	2:P:254:ASN:HD22	1.84	0.42
2:P:431:LEU:HD12	2:P:431:LEU:O	2.20	0.42
2:P:59:LEU:O	2:P:62:THR:HB	2.19	0.42
2:D:101:THR:HG22	2:D:128:ASP:CB	2.48	0.42
2:F:159:ILE:HD12	2:F:166:ILE:HD11	2.00	0.42
2:F:211:ASP:O	2:F:215:ILE:HG13	2.19	0.42
2:F:78:LEU:HD12	2:F:79:LYS:H	1.84	0.42
1:G:101:LEU:HA	1:G:101:LEU:HD23	1.82	0.42
1:G:91:MET:O	1:G:93:ILE:HG12	2.19	0.42
2:H:503:ARG:HE	2:H:503:ARG:H	1.66	0.42
2:H:535:MET:HE1	2:H:542:ILE:HG21	2.01	0.42
2:J:325:THR:OG1	2:J:326:ARG:N	2.53	0.42
1:M:10:SER:OG	1:M:11:SER:N	2.52	0.42
2:B:270:ARG:CB	1:O:107:TYR:HD1	2.31	0.42
1:A:8:LEU:HD23	1:A:42:VAL:CG1	2.50	0.42
2:B:546:PRO:O	2:B:547:SER:CB	2.66	0.42
2:F:289:PHE:HD1	2:F:316:LYS:HD2	1.76	0.42
2:H:213:GLU:HA	2:H:238:PHE:HB2	2.01	0.42
2:H:390:ILE:HG12	2:H:390:ILE:H	1.64	0.42
2:J:477:ASP:N	2:J:477:ASP:OD1	2.53	0.42
1:K:135:THR:HG22	1:K:136:THR:N	2.34	0.42
2:L:412:LEU:HD12	2:L:412:LEU:O	2.19	0.42
2:N:429:ARG:HG2	2:N:433:ILE:HD12	2.02	0.42
1:O:59:CYS:O	1:O:63:VAL:HG23	2.19	0.42
2:P:563:GLU:HG3	2:P:563:GLU:O	2.20	0.42
2:D:431:LEU:HD12	2:D:431:LEU:C	2.39	0.42
2:F:380:LEU:HD23	2:F:380:LEU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:285:MET:O	2:H:287:ILE:N	2.53	0.42
2:H:462:SER:HB2	2:H:465:VAL:HB	2.02	0.42
1:M:99:PHE:CE2	2:N:17:VAL:N	2.88	0.42
2:N:419:ILE:O	2:N:420:THR:O	2.37	0.42
2:P:392:ASN:ND2	2:P:421:ASP:OD1	2.48	0.42
1:A:102:ILE:HG12	1:A:117:THR:HB	2.02	0.41
2:B:272:LEU:C	2:B:272:LEU:CD2	2.88	0.41
2:B:300:LEU:HD12	2:B:323:LEU:HD11	2.02	0.41
2:D:296:ARG:HH12	1:G:32:MET:HG3	1.85	0.41
2:D:396:GLU:HG2	2:D:430:SER:OG	2.20	0.41
2:D:419:ILE:O	2:D:420:THR:O	2.38	0.41
2:D:543:GLU:OE2	2:D:578:ARG:HD3	2.20	0.41
2:F:314:ILE:HD11	2:F:329:ILE:HD11	2.01	0.41
2:H:100:VAL:O	2:H:100:VAL:HG13	2.19	0.41
2:H:188:ALA:HB1	2:H:214:THR:OG1	2.20	0.41
2:L:396:GLU:HG2	2:L:430:SER:OG	2.19	0.41
2:L:546:PRO:O	2:L:547:SER:CB	2.67	0.41
1:M:134:ARG:NH1	2:N:40:VAL:HA	2.35	0.41
2:N:326:ARG:HA	2:N:350:GLU:O	2.20	0.41
1:A:48:THR:HG22	1:A:51:ILE:HG12	2.03	0.41
2:B:223:VAL:O	2:B:245:LEU:HD12	2.20	0.41
2:D:337:LEU:HD12	2:D:341:CYS:SG	2.60	0.41
2:F:282:PRO:HA	2:F:285:MET:CE	2.48	0.41
2:F:285:MET:N	2:F:286:PRO:CD	2.81	0.41
2:H:184:LEU:HD23	2:H:184:LEU:HA	1.69	0.41
2:H:428:VAL:CG2	2:H:429:ARG:N	2.83	0.41
1:I:101:LEU:HA	1:I:101:LEU:HD23	1.83	0.41
2:J:143:LEU:CD2	2:J:159:ILE:HD13	2.50	0.41
2:J:314:ILE:HD11	2:J:329:ILE:HD11	2.01	0.41
2:L:285:MET:N	2:L:286:PRO:CD	2.83	0.41
2:L:308:GLU:HG3	2:L:332:ARG:NH2	2.26	0.41
2:P:253:LEU:CD1	2:P:280:MET:HB2	2.49	0.41
3:Q:201:LEU:HA	3:Q:201:LEU:HD23	1.85	0.41
2:B:348:ARG:HG3	2:B:384:ALA:HB3	2.02	0.41
2:B:563:GLU:O	2:B:563:GLU:HG3	2.21	0.41
1:E:134:ARG:NE	1:E:141:ASN:HB2	2.35	0.41
2:H:87:ALA:HB2	2:H:92:ILE:CB	2.50	0.41
1:I:106:ASN:HB2	1:I:114:LEU:HD11	2.02	0.41
1:I:129:THR:HB	1:I:130:PRO:HD2	2.03	0.41
1:I:19:GLU:OE1	1:I:19:GLU:N	2.51	0.41
2:J:322:VAL:HG13	2:J:346:ARG:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:75:LEU:HD23	2:J:75:LEU:HA	1.83	0.41
1:K:46:ASN:HB2	1:K:107:TYR:CZ	2.55	0.41
2:L:209:PRO:HD3	2:L:230:PHE:HE2	1.84	0.41
1:M:27:GLN:HA	1:M:30:ALA:HB3	2.02	0.41
2:N:107:ILE:HA	2:N:111:LEU:HB2	2.02	0.41
2:N:358:MET:HG3	2:N:364:LEU:HG	2.01	0.41
2:N:502:GLU:HG3	2:N:525:ALA:HA	2.03	0.41
2:N:544:LEU:HD11	2:N:588:LEU:HD11	2.01	0.41
1:O:105:ALA:HB2	1:O:113:LEU:HD23	2.02	0.41
1:O:125:ILE:HG23	1:O:133:ILE:CD1	2.44	0.41
1:C:105:ALA:HB2	1:C:113:LEU:HD23	2.02	0.41
2:D:325:THR:O	2:D:349:ILE:HA	2.20	0.41
2:F:343:GLN:NE2	2:F:343:GLN:HA	2.35	0.41
2:H:347:LEU:CD2	2:H:373:LEU:HD21	2.50	0.41
2:H:395:LEU:HB3	2:H:427:GLY:C	2.40	0.41
2:L:125:SER:O	2:L:129:LEU:HD22	2.20	0.41
2:L:289:PHE:N	2:L:290:PRO:CD	2.82	0.41
2:N:590:GLU:O	2:N:591:PRO:C	2.57	0.41
2:P:83:LYS:HA	2:P:84:PRO:HD3	1.86	0.41
1:A:132:GLU:O	1:A:136:THR:HG23	2.20	0.41
2:B:266:LEU:HD13	2:B:266:LEU:HA	1.83	0.41
2:D:187:LEU:HD23	2:D:187:LEU:HA	1.88	0.41
2:F:54:HIS:HE1	2:F:56:THR:OG1	2.03	0.41
2:H:124:VAL:CG1	2:H:129:LEU:HD13	2.51	0.41
2:H:411:VAL:HG23	4:H:4100:OGK:H16A	2.02	0.41
1:K:137:PHE:CD1	2:L:17:VAL:CG2	3.03	0.41
2:L:289:PHE:HB2	2:L:290:PRO:HD3	2.01	0.41
1:M:125:ILE:HG23	1:M:133:ILE:CD1	2.39	0.41
2:N:519:TRP:HZ3	2:N:567:HIS:ND1	2.18	0.41
1:O:102:ILE:HD12	2:P:20:VAL:HG21	2.02	0.41
2:P:308:GLU:O	2:P:312:THR:HG23	2.21	0.41
2:P:328:VAL:CG2	2:P:359:GLU:HB2	2.43	0.41
2:P:436:LYS:HB3	2:P:436:LYS:HE2	1.74	0.41
2:P:490:LEU:HD11	2:P:493:LEU:HD13	2.03	0.41
2:P:89:PHE:CD1	3:X:206:ARG:HA	2.56	0.41
1:A:114:LEU:HA	1:A:114:LEU:HD12	1.97	0.41
1:A:101:LEU:HB3	1:A:117:THR:HG21	2.01	0.41
2:D:285:MET:N	2:D:286:PRO:HD2	2.36	0.41
2:F:311:CYS:SG	2:F:333:GLY:HA2	2.60	0.41
2:H:111:LEU:C	2:H:113:GLN:N	2.74	0.41
2:H:365:VAL:HG21	2:H:387:VAL:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:HIS:O	2:H:55:VAL:HG23	2.20	0.41
2:L:519:TRP:CH2	2:L:567:HIS:CE1	3.08	0.41
2:L:590:GLU:O	2:L:591:PRO:C	2.57	0.41
1:O:153:ARG:NH2	2:P:539:TYR:HE1	2.19	0.41
2:B:231:GLU:HG2	2:B:254:ASN:HD22	1.86	0.41
2:H:315:GLN:HG3	2:H:340:TYR:CZ	2.55	0.41
1:I:134:ARG:NE	1:I:141:ASN:HB2	2.36	0.41
2:J:209:PRO:HD3	2:J:230:PHE:HE2	1.85	0.41
2:J:409:ARG:HD3	4:J:5100:OGK:H13A	2.01	0.41
1:K:8:LEU:HD23	1:K:42:VAL:CG1	2.50	0.41
2:L:431:LEU:HD12	2:L:431:LEU:C	2.41	0.41
2:N:308:GLU:HG3	2:N:332:ARG:NH2	2.30	0.41
2:P:545:ILE:HB	2:P:567:HIS:HB2	2.01	0.41
1:C:137:PHE:HD1	2:D:17:VAL:CG2	2.34	0.41
2:D:405:LEU:HA	2:D:405:LEU:HD23	1.88	0.41
2:D:429:ARG:HG2	2:D:433:ILE:HD12	2.02	0.41
2:H:168:THR:HG22	2:H:196:VAL:HG13	2.01	0.41
2:H:408:PHE:C	2:H:409:ARG:HG2	2.41	0.41
2:H:52:ARG:HH11	2:H:72:PHE:HE2	1.69	0.41
2:J:124:VAL:CG1	2:J:129:LEU:HD13	2.50	0.41
2:L:101:THR:N	2:L:102:PRO:CD	2.84	0.41
2:N:121:ARG:NH2	5:N:1103:PO4:O4	2.54	0.41
2:N:496:ARG:HA	2:N:521:GLN:O	2.19	0.41
2:N:586:ARG:NH2	2:N:588:LEU:HD21	2.35	0.41
2:P:198:ASN:OD1	2:P:198:ASN:C	2.59	0.41
2:P:490:LEU:HA	2:P:490:LEU:HD23	1.72	0.41
2:P:590:GLU:O	2:P:591:PRO:C	2.58	0.41
2:B:519:TRP:HA	2:B:568:ILE:O	2.21	0.41
2:B:78:LEU:HD12	2:B:79:LYS:H	1.86	0.41
1:G:129:THR:OG1	1:G:132:GLU:HG3	2.21	0.41
2:H:170:LEU:HA	2:H:198:ASN:O	2.20	0.41
2:H:468:MET:HE2	2:H:470:LEU:HD21	2.02	0.41
2:H:59:LEU:O	2:H:62:THR:HB	2.21	0.41
2:J:191:ASN:ND2	2:J:192:THR:N	2.68	0.41
2:J:405:LEU:HA	2:J:405:LEU:HD23	1.85	0.41
2:J:545:ILE:HB	2:J:567:HIS:HB2	2.03	0.41
2:L:533:MET:CE	2:L:588:LEU:HD13	2.51	0.41
2:N:398:ILE:HG22	2:N:431:LEU:HD13	2.02	0.41
2:B:314:ILE:HD11	2:B:329:ILE:HD11	2.03	0.41
2:B:328:VAL:CG2	2:B:359:GLU:HB2	2.45	0.41
1:C:99:PHE:CE2	2:D:17:VAL:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:545:ILE:HG22	2:D:546:PRO:CD	2.51	0.41
2:F:338:ALA:O	2:F:376:GLY:HA3	2.21	0.41
1:G:148:GLU:HG3	1:G:152:ARG:HH11	1.85	0.41
2:H:391:THR:O	2:H:393:GLU:N	2.54	0.41
2:H:455:LEU:HD21	2:H:473:VAL:HG21	2.03	0.41
2:H:584:THR:HG22	2:H:584:THR:O	2.21	0.41
2:H:92:ILE:HD11	2:H:519:TRP:CZ3	2.56	0.41
2:J:412:LEU:C	2:J:412:LEU:HD12	2.41	0.41
2:L:490:LEU:HD23	2:L:490:LEU:HA	1.77	0.41
2:N:308:GLU:O	2:N:312:THR:HG23	2.21	0.41
1:O:46:ASN:HB2	1:O:107:TYR:CZ	2.56	0.41
2:P:392:ASN:HD21	2:P:424:LEU:HA	1.85	0.41
1:A:141:ASN:OD1	1:A:141:ASN:C	2.58	0.41
1:A:26:SER:C	1:A:28:THR:H	2.24	0.41
1:C:125:ILE:HG23	1:C:133:ILE:CD1	2.44	0.41
2:D:489:ASN:HA	2:D:489:ASN:HD22	1.65	0.41
2:F:480:LEU:HB2	2:F:500:PHE:CE2	2.56	0.41
1:G:147:GLU:HG3	1:G:147:GLU:H	1.60	0.41
2:H:352:GLY:O	2:H:353:ALA:CB	2.69	0.41
2:H:70:ARG:O	2:H:72:PHE:N	2.54	0.41
2:H:98:GLY:C	2:H:122:MET:HE3	2.41	0.41
2:J:328:VAL:CG2	2:J:359:GLU:HB2	2.45	0.41
2:J:367:GLN:NE2	2:J:389:ASP:OD1	2.54	0.41
2:J:519:TRP:C	2:J:519:TRP:CD1	2.92	0.41
2:L:436:LYS:HE2	2:L:436:LYS:HB3	1.70	0.41
1:O:114:LEU:HD12	1:O:114:LEU:HA	1.91	0.41
2:B:152:THR:HG22	2:B:177:SER:HB2	2.03	0.40
2:B:533:MET:CE	2:B:588:LEU:HD13	2.47	0.40
1:C:10:SER:OG	1:C:11:SER:N	2.54	0.40
1:C:158:ALA:HA	2:D:62:THR:HG23	2.03	0.40
2:D:404:ASN:HB3	2:D:437:LYS:HD2	2.03	0.40
2:D:533:MET:C	2:D:535:MET:H	2.25	0.40
2:F:263:TYR:O	2:F:266:LEU:HD23	2.20	0.40
1:G:130:PRO:HD3	2:H:36:SER:CB	2.50	0.40
2:H:120:ARG:O	2:H:122:MET:HG3	2.20	0.40
1:I:26:SER:C	1:I:28:THR:H	2.25	0.40
2:J:533:MET:C	2:J:535:MET:H	2.24	0.40
1:K:114:LEU:C	1:K:116:LEU:N	2.73	0.40
2:L:266:LEU:HA	2:L:266:LEU:HD13	1.83	0.40
2:L:327:ASN:HD22	2:L:327:ASN:N	2.18	0.40
2:L:409:ARG:HD3	4:L:6100:OGK:H13A	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:563:GLU:HG3	2:N:563:GLU:O	2.21	0.40
2:P:101:THR:N	2:P:102:PRO:CD	2.84	0.40
2:P:266:LEU:HA	2:P:266:LEU:HD13	1.86	0.40
2:P:276:GLY:HA3	2:P:299:ASP:HB3	2.02	0.40
2:P:305:LEU:HD23	2:P:305:LEU:O	2.19	0.40
2:P:399:GLY:HA3	2:P:431:LEU:HA	2.04	0.40
2:B:304:LEU:HD12	2:B:304:LEU:HA	1.72	0.40
2:B:489:ASN:HD22	2:B:489:ASN:HA	1.66	0.40
2:D:490:LEU:HD23	2:D:490:LEU:HA	1.74	0.40
1:E:130:PRO:O	1:E:134:ARG:HG2	2.20	0.40
2:F:118:HIS:C	2:F:118:HIS:CD2	2.94	0.40
2:B:127:LEU:HB2	2:F:126:ASP:HB3	2.03	0.40
2:F:392:ASN:ND2	2:F:421:ASP:OD1	2.54	0.40
2:F:429:ARG:HG2	2:F:433:ILE:HD12	2.04	0.40
2:F:55:VAL:HG21	2:F:72:PHE:CD1	2.56	0.40
2:H:274:ARG:HA	2:H:297:LYS:HB3	2.03	0.40
2:H:32:LYS:HD3	2:H:32:LYS:HA	1.81	0.40
2:J:436:LYS:HE2	2:J:436:LYS:HB3	1.77	0.40
2:N:285:MET:N	2:N:286:PRO:CD	2.85	0.40
2:N:545:ILE:HG22	2:N:546:PRO:N	2.36	0.40
2:N:55:VAL:HG21	2:N:72:PHE:CD1	2.56	0.40
2:P:232:ILE:O	2:P:235:LEU:HB2	2.21	0.40
2:P:95:ASN:O	2:P:582:PRO:HG3	2.21	0.40
3:W:201:LEU:HA	3:W:201:LEU:HD23	1.81	0.40
2:B:263:TYR:O	2:B:266:LEU:HD23	2.21	0.40
2:B:545:ILE:HG22	2:B:546:PRO:N	2.36	0.40
2:B:83:LYS:HA	2:B:84:PRO:HD3	1.86	0.40
2:F:289:PHE:N	2:F:290:PRO:CD	2.84	0.40
2:F:398:ILE:C	2:F:400:THR:H	2.25	0.40
1:I:153:ARG:CG	1:I:157:TRP:CZ3	3.04	0.40
2:L:519:TRP:HZ3	2:L:567:HIS:ND1	2.20	0.40
1:I:146:GLU:HA	2:L:539:TYR:OH	2.22	0.40
2:N:328:VAL:CG2	2:N:359:GLU:HB2	2.41	0.40
2:N:501:SER:O	2:N:505:ILE:HG12	2.21	0.40
2:P:107:ILE:HA	2:P:111:LEU:HB2	2.03	0.40
2:P:100:VAL:HG11	2:P:124:VAL:HG22	2.03	0.40
2:P:184:LEU:HA	2:P:184:LEU:HD23	1.85	0.40
2:P:187:LEU:HA	2:P:187:LEU:HD23	1.85	0.40
2:P:327:ASN:N	2:P:327:ASN:HD22	2.20	0.40
2:P:351:ARG:HD3	2:P:413:LEU:HD11	2.03	0.40
2:P:519:TRP:HZ3	2:P:567:HIS:ND1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:ASN:ND2	1:O:43:PRO:HG2	2.36	0.40
1:E:26:SER:CB	1:E:29:ILE:HG13	2.51	0.40
2:F:308:GLU:HG3	2:F:332:ARG:NH2	2.28	0.40
1:G:135:THR:HG22	1:G:136:THR:HG23	2.04	0.40
2:H:191:ASN:ND2	2:H:193:SER:N	2.70	0.40
4:H:4100:OGK:N08	4:H:4100:OGK:C18	2.84	0.40
1:K:114:LEU:C	1:K:116:LEU:H	2.25	0.40
1:K:26:SER:CB	1:K:29:ILE:HG13	2.50	0.40
2:L:343:GLN:NE2	2:L:343:GLN:HA	2.36	0.40
2:N:124:VAL:O	2:N:151:PHE:HB3	2.20	0.40
2:N:538:PRO:O	2:N:539:TYR:HB2	2.21	0.40
1:O:132:GLU:O	1:O:136:THR:HG23	2.22	0.40
1:O:148:GLU:HG2	1:O:152:ARG:HH12	1.85	0.40
2:P:263:TYR:O	2:P:266:LEU:HD23	2.21	0.40
2:B:285:MET:N	2:B:286:PRO:CD	2.85	0.40
1:E:148:GLU:HG2	1:E:152:ARG:HH12	1.86	0.40
2:F:398:ILE:HG22	2:F:431:LEU:HD13	2.03	0.40
2:F:519:TRP:HZ3	2:F:567:HIS:ND1	2.17	0.40
2:H:191:ASN:HD22	2:H:191:ASN:C	2.24	0.40
2:H:374:ALA:CB	2:H:398:ILE:HD12	2.49	0.40
2:H:453:LEU:O	2:H:456:SER:HB3	2.21	0.40
2:H:80:LEU:CD1	2:H:103:TRP:CG	3.05	0.40
2:J:253:LEU:CD1	2:J:280:MET:HB2	2.49	0.40
2:J:375:GLN:HG2	2:J:401:TYR:CE1	2.56	0.40
2:N:289:PHE:N	2:N:290:PRO:HD2	2.37	0.40
2:N:398:ILE:CG2	2:N:431:LEU:HD13	2.52	0.40
2:N:492:LYS:HG3	2:N:517:TYR:CD2	2.57	0.40
1:O:61:ARG:HA	1:O:61:ARG:HD2	1.97	0.40
2:P:289:PHE:N	2:P:290:PRO:HD2	2.37	0.40
2:P:358:MET:HG3	2:P:364:LEU:HG	2.03	0.40
2:P:400:THR:O	2:P:403:LYS:HE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	3 23
1	C	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	3 23
1	E	140/160 (88%)	118 (84%)	17 (12%)	5 (4%)	3 23
1	G	140/160 (88%)	113 (81%)	21 (15%)	6 (4%)	2 19
1	I	140/160 (88%)	117 (84%)	17 (12%)	6 (4%)	2 19
1	K	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	3 23
1	M	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	3 23
1	O	140/160 (88%)	115 (82%)	19 (14%)	6 (4%)	2 19
2	B	564/592 (95%)	501 (89%)	57 (10%)	6 (1%)	14 47
2	D	564/592 (95%)	503 (89%)	53 (9%)	8 (1%)	11 41
2	F	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	13 45
2	H	558/592 (94%)	426 (76%)	95 (17%)	37 (7%)	1 10
2	J	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	13 45
2	L	564/592 (95%)	501 (89%)	55 (10%)	8 (1%)	11 41
2	N	564/592 (95%)	502 (89%)	55 (10%)	7 (1%)	13 45
2	P	564/592 (95%)	500 (89%)	58 (10%)	6 (1%)	14 47
3	Q	16/21 (76%)	15 (94%)	1 (6%)	0	100 100
3	R	16/21 (76%)	14 (88%)	2 (12%)	0	100 100
3	S	16/21 (76%)	14 (88%)	2 (12%)	0	100 100
3	U	16/21 (76%)	14 (88%)	2 (12%)	0	100 100
3	V	16/21 (76%)	14 (88%)	2 (12%)	0	100 100
3	W	16/21 (76%)	15 (94%)	1 (6%)	0	100 100
3	X	16/21 (76%)	14 (88%)	2 (12%)	0	100 100
All	All	5738/6163 (93%)	4968 (87%)	641 (11%)	129 (2%)	6 33

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
2	B	420	THR
2	B	546	PRO
2	D	420	THR

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Mol	Chain	Res	Type
2	D	546	PRO
2	F	420	THR
2	F	546	PRO
2	H	41	CYS
2	H	71	ARG
2	H	172	GLU
2	H	200	TYR
2	H	270	ARG
2	H	278	SER
2	H	357	GLY
2	H	364	LEU
2	H	425	ASP
2	H	525	ALA
2	H	526	SER
2	J	420	THR
2	J	546	PRO
1	K	92	LYS
2	L	420	THR
2	L	546	PRO
2	N	420	THR
2	N	546	PRO
2	P	420	THR
2	P	546	PRO
1	A	10	SER
1	A	13	GLY
1	A	36	ASP
1	A	126	LYS
2	B	547	SER
1	C	10	SER
1	C	13	GLY
1	C	36	ASP
1	C	92	LYS
1	C	126	LYS
2	D	547	SER
1	E	10	SER
1	E	13	GLY
1	E	36	ASP
1	E	92	LYS
1	E	126	LYS
1	G	10	SER
1	G	13	GLY
1	G	36	ASP

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Mol	Chain	Res	Type
1	G	92	LYS
1	G	128	LYS
2	H	97	GLY
2	H	228	GLY
2	H	271	LYS
2	H	279	TYR
2	H	353	ALA
2	H	365	VAL
2	H	392	ASN
2	H	449	GLY
2	H	528	THR
1	I	10	SER
1	I	13	GLY
1	I	36	ASP
1	I	92	LYS
1	I	126	LYS
2	J	547	SER
1	K	10	SER
1	K	36	ASP
1	K	126	LYS
2	L	547	SER
1	M	10	SER
1	M	13	GLY
1	M	36	ASP
1	M	92	LYS
1	M	126	LYS
1	O	10	SER
1	O	36	ASP
1	O	92	LYS
1	O	126	LYS
2	P	547	SER
2	B	590	GLU
2	D	590	GLU
2	F	20	VAL
2	F	547	SER
2	F	590	GLU
2	H	70	ARG
2	H	319	ASN
2	H	499	CYS
2	H	533	MET
2	H	577	GLN
2	H	582	PRO

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Mol	Chain	Res	Type
2	J	590	GLU
1	K	13	GLY
2	L	590	GLU
2	N	547	SER
2	N	590	GLU
1	O	13	GLY
2	P	590	GLU
2	B	20	VAL
2	D	20	VAL
2	D	112	ARG
2	H	112	ARG
2	H	137	ALA
2	H	269	PRO
2	H	305	LEU
2	H	358	MET
2	H	538	PRO
2	L	112	ARG
2	N	290	PRO
2	P	20	VAL
2	D	290	PRO
2	H	206	LYS
1	I	137	PHE
2	J	20	VAL
2	J	290	PRO
2	L	20	VAL
2	L	290	PRO
2	N	20	VAL
1	O	27	GLN
2	P	290	PRO
2	F	290	PRO
1	G	153	ARG
2	H	209	PRO
2	H	276	GLY
2	H	20	VAL
2	H	286	PRO
2	B	591	PRO
2	D	591	PRO
2	N	591	PRO
2	F	591	PRO
2	J	591	PRO
2	L	591	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	127/137 (93%)	114 (90%)	13 (10%)	7 29
1	C	127/137 (93%)	115 (91%)	12 (9%)	8 32
1	E	127/137 (93%)	113 (89%)	14 (11%)	6 25
1	G	127/137 (93%)	113 (89%)	14 (11%)	6 25
1	I	127/137 (93%)	114 (90%)	13 (10%)	7 29
1	K	127/137 (93%)	114 (90%)	13 (10%)	7 29
1	M	127/137 (93%)	114 (90%)	13 (10%)	7 29
1	O	127/137 (93%)	113 (89%)	14 (11%)	6 25
2	B	500/523 (96%)	433 (87%)	67 (13%)	4 17
2	D	500/523 (96%)	432 (86%)	68 (14%)	3 17
2	F	500/523 (96%)	433 (87%)	67 (13%)	4 17
2	H	494/523 (94%)	397 (80%)	97 (20%)	1 6
2	J	500/523 (96%)	433 (87%)	67 (13%)	4 17
2	L	500/523 (96%)	431 (86%)	69 (14%)	3 16
2	N	500/523 (96%)	432 (86%)	68 (14%)	3 17
2	P	500/523 (96%)	434 (87%)	66 (13%)	4 18
3	Q	16/19 (84%)	16 (100%)	0	100 100
3	R	16/19 (84%)	16 (100%)	0	100 100
3	S	16/19 (84%)	16 (100%)	0	100 100
3	U	16/19 (84%)	16 (100%)	0	100 100
3	V	16/19 (84%)	16 (100%)	0	100 100
3	W	16/19 (84%)	16 (100%)	0	100 100
3	X	16/19 (84%)	16 (100%)	0	100 100
All	All	5122/5413 (95%)	4447 (87%)	675 (13%)	4 18

All (675) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	14	GLU
1	A	22	VAL
1	A	29	ILE
1	A	35	ASP
1	A	36	ASP
1	A	42	VAL
1	A	44	LEU
1	A	48	THR
1	A	81	ASP
1	A	125	ILE
1	A	153	ARG
1	A	160	GLU
2	B	16	THR
2	B	20	VAL
2	B	35	ASP
2	B	40	VAL
2	B	43	ARG
2	B	48	ASP
2	B	52	ARG
2	B	59	LEU
2	B	62	THR
2	B	64	THR
2	B	104	VAL
2	B	123	ILE
2	B	129	LEU
2	B	132	LEU
2	B	136	ARG
2	B	142	THR
2	B	159	ILE
2	B	166	ILE
2	B	168	THR
2	B	182	LYS
2	B	184	LEU
2	B	191	ASN
2	B	193	SER
2	B	196	VAL
2	B	214	THR
2	B	220	ARG
2	B	225	VAL
2	B	230	PHE
2	B	231	GLU
2	B	232	ILE

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Mol	Chain	Res	Type
2	B	270	ARG
2	B	272	LEU
2	B	275	LEU
2	B	284	GLU
2	B	301	LEU
2	B	304	LEU
2	B	305	LEU
2	B	312	THR
2	B	314	ILE
2	B	327	ASN
2	B	349	ILE
2	B	360	ASP
2	B	367	GLN
2	B	377	CYS
2	B	390	ILE
2	B	400	THR
2	B	402	LEU
2	B	404	ASN
2	B	405	LEU
2	B	412	LEU
2	B	418	ARG
2	B	422	LEU
2	B	447	GLN
2	B	453	LEU
2	B	455	LEU
2	B	477	ASP
2	B	481	MET
2	B	490	LEU
2	B	495	MET
2	B	503	ARG
2	B	510	THR
2	B	516	ARG
2	B	519	TRP
2	B	528	THR
2	B	537	ARG
2	B	542	ILE
2	B	578	ARG
1	C	8	LEU
1	C	14	GLU
1	C	29	ILE
1	C	35	ASP
1	C	36	ASP

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Mol	Chain	Res	Type
1	C	42	VAL
1	C	44	LEU
1	C	48	THR
1	C	125	ILE
1	C	150	GLU
1	C	153	ARG
1	C	160	GLU
2	D	16	THR
2	D	20	VAL
2	D	35	ASP
2	D	40	VAL
2	D	43	ARG
2	D	48	ASP
2	D	52	ARG
2	D	59	LEU
2	D	62	THR
2	D	64	THR
2	D	104	VAL
2	D	123	ILE
2	D	129	LEU
2	D	132	LEU
2	D	136	ARG
2	D	142	THR
2	D	159	ILE
2	D	166	ILE
2	D	168	THR
2	D	182	LYS
2	D	184	LEU
2	D	191	ASN
2	D	196	VAL
2	D	214	THR
2	D	220	ARG
2	D	225	VAL
2	D	230	PHE
2	D	231	GLU
2	D	232	ILE
2	D	270	ARG
2	D	272	LEU
2	D	275	LEU
2	D	284	GLU
2	D	301	LEU
2	D	304	LEU

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Mol	Chain	Res	Type
2	D	305	LEU
2	D	312	THR
2	D	314	ILE
2	D	327	ASN
2	D	349	ILE
2	D	360	ASP
2	D	367	GLN
2	D	377	CYS
2	D	390	ILE
2	D	400	THR
2	D	402	LEU
2	D	404	ASN
2	D	405	LEU
2	D	412	LEU
2	D	413	LEU
2	D	418	ARG
2	D	422	LEU
2	D	447	GLN
2	D	453	LEU
2	D	455	LEU
2	D	477	ASP
2	D	481	MET
2	D	490	LEU
2	D	495	MET
2	D	496	ARG
2	D	503	ARG
2	D	510	THR
2	D	516	ARG
2	D	519	TRP
2	D	528	THR
2	D	537	ARG
2	D	542	ILE
2	D	578	ARG
1	E	8	LEU
1	E	14	GLU
1	E	22	VAL
1	E	29	ILE
1	E	35	ASP
1	E	36	ASP
1	E	42	VAL
1	E	44	LEU
1	E	48	THR

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Mol	Chain	Res	Type
1	E	81	ASP
1	E	125	ILE
1	E	150	GLU
1	E	153	ARG
1	E	160	GLU
2	F	16	THR
2	F	20	VAL
2	F	35	ASP
2	F	40	VAL
2	F	43	ARG
2	F	48	ASP
2	F	52	ARG
2	F	59	LEU
2	F	62	THR
2	F	64	THR
2	F	104	VAL
2	F	123	ILE
2	F	129	LEU
2	F	132	LEU
2	F	136	ARG
2	F	142	THR
2	F	159	ILE
2	F	166	ILE
2	F	168	THR
2	F	182	LYS
2	F	184	LEU
2	F	191	ASN
2	F	196	VAL
2	F	201	MET
2	F	214	THR
2	F	220	ARG
2	F	225	VAL
2	F	231	GLU
2	F	232	ILE
2	F	270	ARG
2	F	272	LEU
2	F	275	LEU
2	F	284	GLU
2	F	301	LEU
2	F	304	LEU
2	F	305	LEU
2	F	312	THR

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Mol	Chain	Res	Type
2	F	314	ILE
2	F	327	ASN
2	F	349	ILE
2	F	360	ASP
2	F	367	GLN
2	F	377	CYS
2	F	390	ILE
2	F	400	THR
2	F	402	LEU
2	F	404	ASN
2	F	405	LEU
2	F	412	LEU
2	F	413	LEU
2	F	418	ARG
2	F	422	LEU
2	F	447	GLN
2	F	453	LEU
2	F	455	LEU
2	F	477	ASP
2	F	481	MET
2	F	490	LEU
2	F	495	MET
2	F	503	ARG
2	F	510	THR
2	F	516	ARG
2	F	519	TRP
2	F	528	THR
2	F	537	ARG
2	F	542	ILE
2	F	578	ARG
1	G	8	LEU
1	G	14	GLU
1	G	22	VAL
1	G	35	ASP
1	G	36	ASP
1	G	42	VAL
1	G	44	LEU
1	G	48	THR
1	G	81	ASP
1	G	129	THR
1	G	133	ILE
1	G	144	THR

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Mol	Chain	Res	Type
1	G	150	GLU
1	G	153	ARG
2	H	14	VAL
2	H	17	VAL
2	H	20	VAL
2	H	21	ILE
2	H	35	ASP
2	H	40	VAL
2	H	46	LYS
2	H	52	ARG
2	H	59	LEU
2	H	62	THR
2	H	64	THR
2	H	71	ARG
2	H	75	LEU
2	H	76	ARG
2	H	77	SER
2	H	85	ARG
2	H	95	ASN
2	H	100	VAL
2	H	111	LEU
2	H	128	ASP
2	H	132	LEU
2	H	136	ARG
2	H	140	LEU
2	H	142	THR
2	H	159	ILE
2	H	166	ILE
2	H	168	THR
2	H	170	LEU
2	H	171	MET
2	H	175	SER
2	H	184	LEU
2	H	190	HIS
2	H	191	ASN
2	H	192	THR
2	H	193	SER
2	H	194	LEU
2	H	196	VAL
2	H	203	GLU
2	H	214	THR
2	H	225	VAL

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Mol	Chain	Res	Type
2	H	231	GLU
2	H	233	LEU
2	H	238	PHE
2	H	255	GLU
2	H	266	LEU
2	H	272	LEU
2	H	275	LEU
2	H	284	GLU
2	H	291	PHE
2	H	298	LEU
2	H	301	LEU
2	H	302	TYR
2	H	304	LEU
2	H	305	LEU
2	H	313	LEU
2	H	315	GLN
2	H	316	LYS
2	H	325	THR
2	H	326	ARG
2	H	343	GLN
2	H	345	LYS
2	H	348	ARG
2	H	364	LEU
2	H	365	VAL
2	H	370	LEU
2	H	377	CYS
2	H	382	TYR
2	H	388	SER
2	H	389	ASP
2	H	390	ILE
2	H	394	SER
2	H	396	GLU
2	H	398	ILE
2	H	402	LEU
2	H	403	LYS
2	H	409	ARG
2	H	410	LEU
2	H	411	VAL
2	H	415	ARG
2	H	422	LEU
2	H	453	LEU
2	H	467	TRP

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Mol	Chain	Res	Type
2	H	477	ASP
2	H	485	ARG
2	H	490	LEU
2	H	503	ARG
2	H	511	LYS
2	H	516	ARG
2	H	519	TRP
2	H	534	GLN
2	H	542	ILE
2	H	547	SER
2	H	548	ARG
2	H	568	ILE
2	H	579	THR
2	H	583	THR
2	H	589	LYS
1	I	8	LEU
1	I	14	GLU
1	I	22	VAL
1	I	35	ASP
1	I	36	ASP
1	I	42	VAL
1	I	44	LEU
1	I	48	THR
1	I	81	ASP
1	I	125	ILE
1	I	150	GLU
1	I	153	ARG
1	I	160	GLU
2	J	16	THR
2	J	20	VAL
2	J	35	ASP
2	J	40	VAL
2	J	43	ARG
2	J	48	ASP
2	J	52	ARG
2	J	59	LEU
2	J	62	THR
2	J	64	THR
2	J	104	VAL
2	J	129	LEU
2	J	132	LEU
2	J	136	ARG

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Mol	Chain	Res	Type
2	J	142	THR
2	J	159	ILE
2	J	166	ILE
2	J	168	THR
2	J	182	LYS
2	J	184	LEU
2	J	191	ASN
2	J	196	VAL
2	J	214	THR
2	J	217	ARG
2	J	220	ARG
2	J	225	VAL
2	J	227	VAL
2	J	230	PHE
2	J	231	GLU
2	J	232	ILE
2	J	272	LEU
2	J	275	LEU
2	J	284	GLU
2	J	301	LEU
2	J	304	LEU
2	J	305	LEU
2	J	312	THR
2	J	314	ILE
2	J	327	ASN
2	J	341	CYS
2	J	349	ILE
2	J	360	ASP
2	J	367	GLN
2	J	377	CYS
2	J	390	ILE
2	J	400	THR
2	J	402	LEU
2	J	404	ASN
2	J	405	LEU
2	J	413	LEU
2	J	418	ARG
2	J	422	LEU
2	J	447	GLN
2	J	453	LEU
2	J	455	LEU
2	J	477	ASP

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Mol	Chain	Res	Type
2	J	481	MET
2	J	490	LEU
2	J	495	MET
2	J	503	ARG
2	J	510	THR
2	J	516	ARG
2	J	519	TRP
2	J	528	THR
2	J	537	ARG
2	J	542	ILE
2	J	578	ARG
1	K	8	LEU
1	K	14	GLU
1	K	22	VAL
1	K	29	ILE
1	K	35	ASP
1	K	36	ASP
1	K	42	VAL
1	K	44	LEU
1	K	48	THR
1	K	125	ILE
1	K	150	GLU
1	K	153	ARG
1	K	160	GLU
2	L	16	THR
2	L	20	VAL
2	L	35	ASP
2	L	40	VAL
2	L	43	ARG
2	L	48	ASP
2	L	52	ARG
2	L	59	LEU
2	L	62	THR
2	L	64	THR
2	L	104	VAL
2	L	123	ILE
2	L	129	LEU
2	L	132	LEU
2	L	136	ARG
2	L	142	THR
2	L	159	ILE
2	L	166	ILE

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Mol	Chain	Res	Type
2	L	168	THR
2	L	182	LYS
2	L	184	LEU
2	L	191	ASN
2	L	193	SER
2	L	196	VAL
2	L	201	MET
2	L	214	THR
2	L	220	ARG
2	L	225	VAL
2	L	227	VAL
2	L	231	GLU
2	L	232	ILE
2	L	270	ARG
2	L	272	LEU
2	L	275	LEU
2	L	284	GLU
2	L	301	LEU
2	L	304	LEU
2	L	305	LEU
2	L	312	THR
2	L	314	ILE
2	L	327	ASN
2	L	341	CYS
2	L	349	ILE
2	L	360	ASP
2	L	367	GLN
2	L	377	CYS
2	L	390	ILE
2	L	400	THR
2	L	402	LEU
2	L	404	ASN
2	L	405	LEU
2	L	413	LEU
2	L	418	ARG
2	L	422	LEU
2	L	447	GLN
2	L	453	LEU
2	L	455	LEU
2	L	477	ASP
2	L	481	MET
2	L	490	LEU

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Mol	Chain	Res	Type
2	L	495	MET
2	L	503	ARG
2	L	510	THR
2	L	516	ARG
2	L	519	TRP
2	L	528	THR
2	L	537	ARG
2	L	542	ILE
2	L	578	ARG
1	M	8	LEU
1	M	14	GLU
1	M	22	VAL
1	M	35	ASP
1	M	36	ASP
1	M	42	VAL
1	M	44	LEU
1	M	48	THR
1	M	81	ASP
1	M	125	ILE
1	M	150	GLU
1	M	153	ARG
1	M	160	GLU
2	N	16	THR
2	N	20	VAL
2	N	35	ASP
2	N	40	VAL
2	N	43	ARG
2	N	48	ASP
2	N	52	ARG
2	N	59	LEU
2	N	62	THR
2	N	64	THR
2	N	104	VAL
2	N	123	ILE
2	N	129	LEU
2	N	132	LEU
2	N	136	ARG
2	N	142	THR
2	N	159	ILE
2	N	166	ILE
2	N	168	THR
2	N	184	LEU

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Mol	Chain	Res	Type
2	N	191	ASN
2	N	196	VAL
2	N	201	MET
2	N	214	THR
2	N	217	ARG
2	N	220	ARG
2	N	225	VAL
2	N	230	PHE
2	N	231	GLU
2	N	232	ILE
2	N	270	ARG
2	N	272	LEU
2	N	275	LEU
2	N	284	GLU
2	N	301	LEU
2	N	304	LEU
2	N	305	LEU
2	N	312	THR
2	N	314	ILE
2	N	327	ASN
2	N	341	CYS
2	N	349	ILE
2	N	360	ASP
2	N	365	VAL
2	N	367	GLN
2	N	377	CYS
2	N	390	ILE
2	N	400	THR
2	N	402	LEU
2	N	404	ASN
2	N	405	LEU
2	N	418	ARG
2	N	422	LEU
2	N	447	GLN
2	N	453	LEU
2	N	455	LEU
2	N	477	ASP
2	N	481	MET
2	N	490	LEU
2	N	495	MET
2	N	503	ARG
2	N	510	THR

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Mol	Chain	Res	Type
2	N	516	ARG
2	N	519	TRP
2	N	528	THR
2	N	537	ARG
2	N	542	ILE
2	N	578	ARG
1	O	8	LEU
1	O	14	GLU
1	O	22	VAL
1	O	29	ILE
1	O	35	ASP
1	O	36	ASP
1	O	42	VAL
1	O	44	LEU
1	O	48	THR
1	O	81	ASP
1	O	125	ILE
1	O	150	GLU
1	O	153	ARG
1	O	160	GLU
2	P	16	THR
2	P	20	VAL
2	P	35	ASP
2	P	40	VAL
2	P	43	ARG
2	P	48	ASP
2	P	52	ARG
2	P	59	LEU
2	P	62	THR
2	P	64	THR
2	P	104	VAL
2	P	123	ILE
2	P	129	LEU
2	P	132	LEU
2	P	136	ARG
2	P	142	THR
2	P	159	ILE
2	P	168	THR
2	P	182	LYS
2	P	184	LEU
2	P	191	ASN
2	P	196	VAL

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Mol	Chain	Res	Type
2	P	214	THR
2	P	220	ARG
2	P	225	VAL
2	P	230	PHE
2	P	231	GLU
2	P	232	ILE
2	P	270	ARG
2	P	272	LEU
2	P	275	LEU
2	P	284	GLU
2	P	301	LEU
2	P	304	LEU
2	P	305	LEU
2	P	312	THR
2	P	314	ILE
2	P	327	ASN
2	P	341	CYS
2	P	349	ILE
2	P	360	ASP
2	P	367	GLN
2	P	377	CYS
2	P	390	ILE
2	P	400	THR
2	P	402	LEU
2	P	404	ASN
2	P	405	LEU
2	P	418	ARG
2	P	422	LEU
2	P	447	GLN
2	P	453	LEU
2	P	455	LEU
2	P	477	ASP
2	P	481	MET
2	P	490	LEU
2	P	495	MET
2	P	496	ARG
2	P	503	ARG
2	P	510	THR
2	P	516	ARG
2	P	519	TRP
2	P	528	THR
2	P	537	ARG

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Mol	Chain	Res	Type
2	P	542	ILE
2	P	578	ARG

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

Mol	Chain	Res	Type
1	A	46	ASN
1	A	62	HIS
1	A	95	GLN
2	B	54	HIS
2	B	74	ASN
2	B	109	ASN
2	B	191	ASN
2	B	254	ASN
2	B	294	GLN
2	B	319	ASN
2	B	327	ASN
2	B	343	GLN
2	B	460	GLN
2	B	489	ASN
2	B	564	HIS
2	B	567	HIS
1	C	46	ASN
1	C	62	HIS
2	D	54	HIS
2	D	74	ASN
2	D	109	ASN
2	D	190	HIS
2	D	191	ASN
2	D	254	ASN
2	D	294	GLN
2	D	319	ASN
2	D	327	ASN
2	D	343	GLN
2	D	460	GLN
2	D	489	ASN
2	D	564	HIS
2	D	567	HIS
1	E	46	ASN
1	E	62	HIS
1	E	95	GLN
2	F	54	HIS

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Mol	Chain	Res	Type
2	F	74	ASN
2	F	109	ASN
2	F	113	GLN
2	F	191	ASN
2	F	254	ASN
2	F	327	ASN
2	F	343	GLN
2	F	460	GLN
2	F	489	ASN
2	F	564	HIS
2	F	567	HIS
1	G	46	ASN
1	G	62	HIS
2	H	23	GLN
2	H	74	ASN
2	H	95	ASN
2	H	110	ASN
2	H	191	ASN
2	H	310	HIS
2	H	375	GLN
2	H	392	ASN
2	H	447	GLN
2	H	460	GLN
2	H	489	ASN
2	H	530	GLN
2	H	577	GLN
1	I	46	ASN
1	I	62	HIS
1	I	106	ASN
2	J	23	GLN
2	J	54	HIS
2	J	109	ASN
2	J	191	ASN
2	J	254	ASN
2	J	294	GLN
2	J	327	ASN
2	J	343	GLN
2	J	460	GLN
2	J	489	ASN
2	J	564	HIS
2	J	567	HIS
1	K	46	ASN

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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	L	1103	-	4,4,4	4.19	4 (100%)	6,6,6	0.76	0
5	PO4	L	1104	-	4,4,4	4.37	4 (100%)	6,6,6	0.57	0
5	PO4	D	1101	-	4,4,4	3.95	4 (100%)	6,6,6	1.04	0
4	OGK	B	1100	-	22,25,25	6.42	9 (40%)	25,38,38	2.54	12 (48%)
5	PO4	B	1101	-	4,4,4	4.08	4 (100%)	6,6,6	0.81	0
5	PO4	H	1104	-	4,4,4	4.32	4 (100%)	6,6,6	1.10	0
5	PO4	F	1104	-	4,4,4	4.44	4 (100%)	6,6,6	0.67	0
5	PO4	N	1103	-	4,4,4	4.16	3 (75%)	6,6,6	1.34	1 (16%)
5	PO4	B	1104	-	4,4,4	4.16	4 (100%)	6,6,6	0.69	0
5	PO4	P	1101	-	4,4,4	4.13	4 (100%)	6,6,6	0.82	0
4	OGK	J	5100	-	22,25,25	6.51	9 (40%)	25,38,38	2.62	12 (48%)
5	PO4	L	1102	-	4,4,4	4.23	4 (100%)	6,6,6	0.34	0
5	PO4	N	1102	-	4,4,4	4.29	4 (100%)	6,6,6	0.52	0
5	PO4	F	1102	-	4,4,4	4.53	4 (100%)	6,6,6	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PO4	J	1103	-	4,4,4	4.13	4 (100%)	6,6,6	0.64	0
4	OGK	P	8100	-	22,25,25	6.50	8 (36%)	25,38,38	2.56	10 (40%)
4	OGK	D	2100	-	22,25,25	6.52	8 (36%)	25,38,38	2.61	11 (44%)
5	PO4	B	1103	-	4,4,4	4.18	4 (100%)	6,6,6	0.46	0
5	PO4	H	1102	-	4,4,4	4.28	4 (100%)	6,6,6	0.79	0
5	PO4	N	1101	-	4,4,4	4.45	3 (75%)	6,6,6	1.46	1 (16%)
5	PO4	H	1101	-	4,4,4	4.38	4 (100%)	6,6,6	0.63	0
5	PO4	F	1101	-	4,4,4	4.17	4 (100%)	6,6,6	1.22	0
4	OGK	H	4100	-	22,25,25	6.37	9 (40%)	25,38,38	2.60	12 (48%)
5	PO4	P	1102	-	4,4,4	4.19	4 (100%)	6,6,6	0.56	0
5	PO4	D	1103	-	4,4,4	4.29	4 (100%)	6,6,6	0.71	0
5	PO4	H	1103	-	4,4,4	4.46	4 (100%)	6,6,6	0.61	0
5	PO4	J	1102	-	4,4,4	4.25	4 (100%)	6,6,6	0.58	0
4	OGK	L	6100	-	22,25,25	6.35	9 (40%)	25,38,38	2.52	11 (44%)
4	OGK	F	3100	-	22,25,25	6.43	8 (36%)	25,38,38	2.52	9 (36%)
5	PO4	L	1101	-	4,4,4	4.20	4 (100%)	6,6,6	0.86	0
5	PO4	P	1104	-	4,4,4	4.21	4 (100%)	6,6,6	0.73	0
5	PO4	J	1104	-	4,4,4	4.22	4 (100%)	6,6,6	0.66	0
5	PO4	P	1103	-	4,4,4	4.12	4 (100%)	6,6,6	0.73	0
4	OGK	N	7100	-	22,25,25	6.13	8 (36%)	25,38,38	2.57	9 (36%)
5	PO4	D	1104	-	4,4,4	4.20	4 (100%)	6,6,6	0.79	0
5	PO4	F	1103	-	4,4,4	4.19	4 (100%)	6,6,6	0.75	0
5	PO4	B	1102	-	4,4,4	4.22	4 (100%)	6,6,6	0.58	0
5	PO4	D	1102	-	4,4,4	4.17	4 (100%)	6,6,6	0.32	0
5	PO4	J	1101	-	4,4,4	4.08	4 (100%)	6,6,6	0.97	0
5	PO4	N	1104	-	4,4,4	4.28	4 (100%)	6,6,6	0.69	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	B	1100	-	-	4/13/52/52	0/3/3/3
4	OGK	P	8100	-	-	4/13/52/52	0/3/3/3
4	OGK	J	5100	-	-	3/13/52/52	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OGK	D	2100	-	-	3/13/52/52	0/3/3/3
4	OGK	L	6100	-	-	3/13/52/52	0/3/3/3
4	OGK	F	3100	-	-	4/13/52/52	0/3/3/3
4	OGK	H	4100	-	1/1/9/10	4/13/52/52	0/3/3/3
4	OGK	N	7100	-	-	4/13/52/52	0/3/3/3

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5100	OGK	C13-C09	-21.82	1.27	1.51
4	D	2100	OGK	C13-C09	-21.72	1.27	1.51
4	P	8100	OGK	C13-C09	-21.47	1.28	1.51
4	F	3100	OGK	C13-C09	-21.42	1.28	1.51
4	B	1100	OGK	C13-C09	-21.18	1.28	1.51
4	L	6100	OGK	C13-C09	-21.16	1.28	1.51
4	H	4100	OGK	C13-C09	-20.94	1.28	1.51
4	N	7100	OGK	C13-C09	-20.18	1.29	1.51
4	P	8100	OGK	C09-C14	-17.95	1.33	1.52
4	D	2100	OGK	C09-C14	-17.77	1.33	1.52
4	J	5100	OGK	C09-C14	-17.54	1.34	1.52
4	F	3100	OGK	C09-C14	-17.45	1.34	1.52
4	B	1100	OGK	C09-C14	-17.35	1.34	1.52
4	L	6100	OGK	C09-C14	-17.22	1.34	1.52
4	H	4100	OGK	C09-C14	-17.19	1.34	1.52
4	N	7100	OGK	C09-C14	-16.45	1.35	1.52
4	B	1100	OGK	C13-C14	-7.53	1.31	1.50
4	D	2100	OGK	C13-C14	-7.37	1.32	1.50
4	B	1100	OGK	C06-N08	7.28	1.49	1.34
4	H	4100	OGK	C13-C14	-7.25	1.32	1.50
4	J	5100	OGK	C13-C14	-7.19	1.32	1.50
4	F	3100	OGK	C06-N08	7.15	1.49	1.34
4	L	6100	OGK	C13-C14	-7.14	1.32	1.50
4	P	8100	OGK	C06-N08	7.09	1.49	1.34
4	F	3100	OGK	C13-C14	-7.05	1.33	1.50
4	P	8100	OGK	C13-C14	-6.95	1.33	1.50
4	N	7100	OGK	C06-N08	6.85	1.48	1.34
5	F	1102	PO4	P-O1	6.84	1.66	1.50
4	D	2100	OGK	C06-N08	6.81	1.48	1.34
4	N	7100	OGK	C13-C14	-6.68	1.33	1.50
5	F	1104	PO4	P-O1	6.67	1.66	1.50
5	J	1104	PO4	P-O1	6.67	1.66	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1104	PO4	P-O1	6.54	1.66	1.50
4	J	5100	OGK	C06-N08	6.46	1.47	1.34
5	H	1103	PO4	P-O1	6.46	1.66	1.50
4	L	6100	OGK	C06-N08	6.41	1.47	1.34
4	H	4100	OGK	C06-N08	6.39	1.47	1.34
5	B	1102	PO4	P-O1	6.36	1.65	1.50
5	N	1102	PO4	P-O1	6.33	1.65	1.50
5	N	1103	PO4	P-O1	6.32	1.65	1.50
5	J	1103	PO4	P-O1	6.31	1.65	1.50
5	L	1103	PO4	P-O1	6.30	1.65	1.50
5	D	1103	PO4	P-O1	6.29	1.65	1.50
5	P	1104	PO4	P-O1	6.28	1.65	1.50
5	D	1102	PO4	P-O1	6.23	1.65	1.50
5	N	1101	PO4	P-O1	6.22	1.65	1.50
5	H	1102	PO4	P-O1	6.22	1.65	1.50
5	N	1104	PO4	P-O1	6.21	1.65	1.50
5	P	1103	PO4	P-O1	6.19	1.65	1.50
5	J	1102	PO4	P-O1	6.19	1.65	1.50
5	F	1101	PO4	P-O1	6.18	1.65	1.50
5	F	1103	PO4	P-O1	6.18	1.65	1.50
5	D	1104	PO4	P-O1	6.18	1.65	1.50
5	B	1104	PO4	P-O1	6.16	1.65	1.50
5	P	1102	PO4	P-O1	6.14	1.65	1.50
5	H	1104	PO4	P-O1	6.14	1.65	1.50
5	H	1101	PO4	P-O1	6.14	1.65	1.50
5	B	1103	PO4	P-O1	6.14	1.65	1.50
5	P	1101	PO4	P-O1	6.13	1.65	1.50
5	L	1102	PO4	P-O1	6.10	1.65	1.50
5	B	1101	PO4	P-O1	5.96	1.64	1.50
5	J	1101	PO4	P-O1	5.88	1.64	1.50
5	L	1101	PO4	P-O1	5.84	1.64	1.50
5	D	1101	PO4	P-O1	5.65	1.64	1.50
4	H	4100	OGK	C23-C22	5.00	1.61	1.53
5	N	1101	PO4	P-O3	4.66	1.68	1.54
4	N	7100	OGK	C23-C22	4.38	1.60	1.53
5	H	1104	PO4	P-O3	4.13	1.67	1.54
5	N	1101	PO4	P-O4	4.04	1.66	1.54
5	N	1104	PO4	P-O4	4.04	1.66	1.54
5	H	1103	PO4	P-O3	3.97	1.66	1.54
5	H	1101	PO4	P-O3	3.94	1.66	1.54
5	L	1104	PO4	P-O4	3.92	1.66	1.54
5	B	1103	PO4	P-O3	3.88	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1104	PO4	P-O4	3.85	1.66	1.54
5	H	1101	PO4	P-O4	3.85	1.66	1.54
5	H	1102	PO4	P-O4	3.84	1.66	1.54
5	F	1103	PO4	P-O4	3.81	1.66	1.54
5	L	1101	PO4	P-O3	3.79	1.66	1.54
5	N	1102	PO4	P-O4	3.79	1.66	1.54
5	F	1102	PO4	P-O3	3.78	1.66	1.54
5	P	1102	PO4	P-O3	3.77	1.65	1.54
5	J	1102	PO4	P-O3	3.76	1.65	1.54
5	F	1104	PO4	P-O4	3.75	1.65	1.54
5	F	1104	PO4	P-O3	3.74	1.65	1.54
5	D	1104	PO4	P-O3	3.74	1.65	1.54
5	J	1101	PO4	P-O4	3.74	1.65	1.54
5	L	1101	PO4	P-O4	3.73	1.65	1.54
5	H	1103	PO4	P-O4	3.72	1.65	1.54
5	L	1102	PO4	P-O3	3.70	1.65	1.54
5	B	1101	PO4	P-O3	3.70	1.65	1.54
5	N	1103	PO4	P-O3	3.69	1.65	1.54
5	N	1104	PO4	P-O3	3.69	1.65	1.54
4	P	8100	OGK	C23-C22	3.63	1.59	1.53
5	N	1102	PO4	P-O3	3.63	1.65	1.54
5	P	1104	PO4	P-O4	3.61	1.65	1.54
5	J	1101	PO4	P-O3	3.61	1.65	1.54
5	L	1103	PO4	P-O3	3.61	1.65	1.54
5	F	1102	PO4	P-O4	3.58	1.65	1.54
5	L	1104	PO4	P-O3	3.58	1.65	1.54
5	D	1102	PO4	P-O4	3.57	1.65	1.54
5	F	1103	PO4	P-O3	3.57	1.65	1.54
5	B	1102	PO4	P-O4	3.56	1.65	1.54
5	D	1104	PO4	P-O4	3.56	1.65	1.54
4	F	3100	OGK	C18-C17	-3.55	1.44	1.54
5	P	1104	PO4	P-O3	3.52	1.65	1.54
5	J	1102	PO4	P-O4	3.51	1.65	1.54
5	P	1103	PO4	P-O4	3.50	1.65	1.54
5	P	1101	PO4	P-O3	3.50	1.65	1.54
5	P	1103	PO4	P-O3	3.50	1.65	1.54
4	L	6100	OGK	C23-C22	3.50	1.59	1.53
5	J	1104	PO4	P-O3	3.49	1.65	1.54
4	B	1100	OGK	C18-C17	-3.49	1.44	1.54
5	H	1102	PO4	P-O3	3.48	1.65	1.54
5	P	1102	PO4	P-O4	3.47	1.65	1.54
5	B	1104	PO4	P-O3	3.47	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1103	PO4	P-O4	3.47	1.65	1.54
5	D	1101	PO4	P-O4	3.46	1.65	1.54
5	L	1102	PO4	P-O4	3.46	1.65	1.54
5	D	1103	PO4	P-O3	3.45	1.65	1.54
4	P	8100	OGK	C18-C17	-3.41	1.45	1.54
5	B	1102	PO4	P-O3	3.39	1.64	1.54
5	J	1103	PO4	P-O3	3.38	1.64	1.54
5	F	1101	PO4	P-O3	3.38	1.64	1.54
4	B	1100	OGK	C23-C22	3.37	1.58	1.53
4	J	5100	OGK	C18-C17	-3.37	1.45	1.54
5	D	1103	PO4	P-O4	3.37	1.64	1.54
5	B	1104	PO4	P-O4	3.35	1.64	1.54
5	P	1101	PO4	P-O4	3.34	1.64	1.54
5	F	1101	PO4	P-O4	3.34	1.64	1.54
5	D	1103	PO4	P-O2	-3.28	1.44	1.54
4	D	2100	OGK	C23-C22	3.28	1.58	1.53
4	D	2100	OGK	C18-C17	-3.27	1.45	1.54
4	J	5100	OGK	C23-C22	3.26	1.58	1.53
5	D	1101	PO4	P-O3	3.26	1.64	1.54
4	H	4100	OGK	C18-C17	-3.25	1.45	1.54
4	N	7100	OGK	C18-C17	-3.24	1.45	1.54
5	J	1104	PO4	P-O4	3.17	1.64	1.54
5	L	1103	PO4	P-O4	3.09	1.63	1.54
5	J	1103	PO4	P-O4	3.09	1.63	1.54
5	D	1102	PO4	P-O3	3.06	1.63	1.54
5	B	1103	PO4	P-O4	3.06	1.63	1.54
4	L	6100	OGK	C18-C17	-3.02	1.46	1.54
5	B	1101	PO4	P-O4	2.97	1.63	1.54
4	J	5100	OGK	C05-C06	2.96	1.56	1.51
4	D	2100	OGK	C05-C06	2.96	1.56	1.51
5	H	1101	PO4	P-O2	-2.96	1.45	1.54
5	B	1101	PO4	P-O2	-2.96	1.45	1.54
5	D	1102	PO4	P-O2	-2.96	1.45	1.54
5	L	1102	PO4	P-O2	-2.94	1.45	1.54
5	F	1101	PO4	P-O2	-2.94	1.45	1.54
4	B	1100	OGK	C09-N08	2.89	1.50	1.45
4	N	7100	OGK	C09-N08	2.88	1.50	1.45
4	L	6100	OGK	C05-C06	2.86	1.56	1.51
5	H	1103	PO4	P-O2	-2.85	1.46	1.54
5	F	1102	PO4	P-O2	-2.85	1.46	1.54
4	F	3100	OGK	C23-C22	2.85	1.58	1.53
5	L	1101	PO4	P-O2	-2.84	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1104	PO4	P-O2	-2.84	1.46	1.54
5	B	1103	PO4	P-O2	-2.82	1.46	1.54
5	L	1103	PO4	P-O2	-2.80	1.46	1.54
5	D	1101	PO4	P-O2	-2.80	1.46	1.54
4	L	6100	OGK	C09-N08	2.78	1.50	1.45
4	H	4100	OGK	C05-C06	2.77	1.56	1.51
5	H	1102	PO4	P-O2	-2.77	1.46	1.54
5	J	1103	PO4	P-O2	-2.72	1.46	1.54
5	P	1101	PO4	P-O2	-2.72	1.46	1.54
5	J	1102	PO4	P-O2	-2.72	1.46	1.54
4	F	3100	OGK	C09-N08	2.69	1.50	1.45
4	J	5100	OGK	C09-N08	2.66	1.50	1.45
4	P	8100	OGK	C05-C06	2.64	1.56	1.51
5	B	1102	PO4	P-O2	-2.55	1.46	1.54
5	F	1104	PO4	P-O2	-2.52	1.47	1.54
5	P	1102	PO4	P-O2	-2.49	1.47	1.54
4	J	5100	OGK	O07-C06	-2.49	1.18	1.23
5	P	1104	PO4	P-O2	-2.48	1.47	1.54
5	N	1102	PO4	P-O2	-2.46	1.47	1.54
4	D	2100	OGK	O07-C06	-2.45	1.18	1.23
4	H	4100	OGK	C09-N08	2.45	1.50	1.45
5	D	1104	PO4	P-O2	-2.38	1.47	1.54
4	F	3100	OGK	C05-C06	2.37	1.55	1.51
4	H	4100	OGK	O07-C06	-2.37	1.18	1.23
5	L	1104	PO4	P-O2	-2.31	1.47	1.54
4	L	6100	OGK	O07-C06	-2.30	1.18	1.23
5	H	1104	PO4	P-O2	-2.29	1.47	1.54
5	J	1101	PO4	P-O2	-2.26	1.47	1.54
5	P	1103	PO4	P-O2	-2.24	1.47	1.54
4	N	7100	OGK	C05-C06	2.21	1.55	1.51
4	B	1100	OGK	O07-C06	-2.21	1.19	1.23
5	N	1104	PO4	P-O2	-2.20	1.48	1.54
5	F	1103	PO4	P-O2	-2.16	1.48	1.54
5	J	1104	PO4	P-O2	-2.11	1.48	1.54
4	P	8100	OGK	C09-N08	2.10	1.49	1.45
4	B	1100	OGK	C05-C06	2.07	1.55	1.51

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	7100	OGK	C04-C05-C17	6.21	121.81	110.07
4	J	5100	OGK	C13-C14-C09	-5.99	57.22	60.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1100	OGK	C04-C05-C17	5.79	121.01	110.07
4	F	3100	OGK	C13-C14-C09	-5.78	57.33	60.30
4	P	8100	OGK	C04-C05-C17	5.76	120.95	110.07
4	P	8100	OGK	C13-C14-C09	-5.70	57.37	60.30
4	J	5100	OGK	C04-C05-C17	5.69	120.82	110.07
4	D	2100	OGK	C13-C14-C09	-5.58	57.43	60.30
4	F	3100	OGK	C04-C05-C17	5.57	120.60	110.07
4	L	6100	OGK	C04-C05-C17	5.56	120.58	110.07
4	L	6100	OGK	C13-C14-C09	-5.54	57.45	60.30
4	D	2100	OGK	C04-C05-C17	5.44	120.35	110.07
4	N	7100	OGK	C13-C14-C09	-5.43	57.51	60.30
4	L	6100	OGK	C05-C04-C03	5.40	119.91	109.35
4	P	8100	OGK	C05-C04-C03	5.26	119.63	109.35
4	H	4100	OGK	C23-C03-C02	5.25	121.43	112.47
4	H	4100	OGK	C13-C14-C09	-5.20	57.63	60.30
4	D	2100	OGK	C05-C04-C03	5.16	119.42	109.35
4	B	1100	OGK	C13-C14-C09	-5.05	57.70	60.30
4	J	5100	OGK	C05-C04-C03	4.86	118.84	109.35
4	B	1100	OGK	C05-C04-C03	4.81	118.74	109.35
4	F	3100	OGK	C05-C04-C03	4.71	118.55	109.35
4	N	7100	OGK	C05-C04-C03	4.47	118.08	109.35
4	N	7100	OGK	C18-C17-C22	4.36	109.22	104.04
4	B	1100	OGK	O07-C06-C05	-4.18	116.69	121.73
4	P	8100	OGK	C13-C09-C14	3.99	61.17	59.12
4	H	4100	OGK	C04-C05-C17	3.94	117.52	110.07
4	F	3100	OGK	C18-C17-C22	3.72	108.46	104.04
4	H	4100	OGK	C13-C09-N08	-3.72	112.35	117.69
4	J	5100	OGK	C18-C17-C22	3.67	108.41	104.04
4	H	4100	OGK	C22-C23-C03	3.61	116.40	109.35
4	D	2100	OGK	C04-C03-C02	-3.46	106.58	112.47
4	F	3100	OGK	C13-C09-C14	3.44	60.89	59.12
4	H	4100	OGK	C23-C03-C04	3.35	115.98	109.65
4	J	5100	OGK	C13-C09-C14	3.35	60.84	59.12
4	H	4100	OGK	C14-C09-N08	-3.30	108.61	117.62
4	D	2100	OGK	C18-C17-C22	3.23	107.87	104.04
4	N	7100	OGK	C13-C09-C14	3.19	60.76	59.12
4	D	2100	OGK	C13-C09-N08	-3.17	113.14	117.69
4	J	5100	OGK	C04-C03-C02	-3.10	107.20	112.47
4	F	3100	OGK	C14-C09-N08	-3.09	109.17	117.62
4	D	2100	OGK	C14-C09-N08	-3.09	109.19	117.62
4	L	6100	OGK	C04-C03-C02	-3.08	107.22	112.47
4	H	4100	OGK	C18-C17-C22	3.06	107.68	104.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2100	OGK	C13-C09-C14	2.98	60.65	59.12
4	L	6100	OGK	C13-C09-C14	2.98	60.65	59.12
4	P	8100	OGK	C18-C17-C22	2.92	107.50	104.04
4	P	8100	OGK	C14-C09-N08	-2.90	109.70	117.62
4	F	3100	OGK	C13-C09-N08	-2.89	113.54	117.69
4	B	1100	OGK	C05-C06-N08	2.88	120.19	116.25
4	J	5100	OGK	C14-C09-N08	-2.84	109.85	117.62
4	L	6100	OGK	C14-C09-N08	-2.84	109.88	117.62
4	P	8100	OGK	C04-C03-C02	-2.82	107.67	112.47
4	N	7100	OGK	C14-C09-N08	-2.82	109.93	117.62
4	H	4100	OGK	C05-C04-C03	2.80	114.82	109.35
4	B	1100	OGK	C14-C09-N08	-2.79	110.00	117.62
4	L	6100	OGK	C18-C17-C22	2.73	107.28	104.04
4	P	8100	OGK	C13-C09-N08	-2.72	113.79	117.69
4	L	6100	OGK	C13-C09-N08	-2.71	113.80	117.69
4	B	1100	OGK	C04-C03-C02	-2.71	107.86	112.47
4	P	8100	OGK	O07-C06-C05	-2.68	118.50	121.73
4	B	1100	OGK	C15-C14-C13	-2.65	117.56	121.32
5	N	1103	PO4	O4-P-O1	-2.63	101.28	110.89
4	J	5100	OGK	C05-C06-N08	2.61	119.82	116.25
4	N	7100	OGK	C13-C09-N08	-2.59	113.97	117.69
4	H	4100	OGK	C13-C09-C14	2.57	60.44	59.12
4	B	1100	OGK	C13-C09-N08	-2.55	114.03	117.69
4	B	1100	OGK	C09-C13-C14	2.53	62.10	60.84
4	J	5100	OGK	C13-C09-N08	-2.52	114.07	117.69
4	D	2100	OGK	C05-C06-N08	2.51	119.69	116.25
4	F	3100	OGK	O07-C06-C05	-2.49	118.73	121.73
4	J	5100	OGK	O07-C06-N08	-2.47	117.86	123.14
4	L	6100	OGK	C05-C06-N08	2.34	119.44	116.25
4	F	3100	OGK	C04-C03-C02	-2.32	108.52	112.47
4	D	2100	OGK	C15-C14-C13	-2.29	118.07	121.32
4	L	6100	OGK	O07-C06-N08	-2.25	118.33	123.14
4	J	5100	OGK	C09-C13-C14	2.22	61.94	60.84
4	H	4100	OGK	C09-C13-C14	2.20	61.93	60.84
4	N	7100	OGK	C22-C23-C03	2.18	113.60	109.35
4	D	2100	OGK	C09-C13-C14	2.17	61.92	60.84
4	B	1100	OGK	C18-C17-C22	2.13	106.57	104.04
4	L	6100	OGK	C09-C13-C14	2.13	61.90	60.84
4	J	5100	OGK	C22-C23-C03	2.12	113.48	109.35
4	B	1100	OGK	C13-C09-C14	2.10	60.20	59.12
4	P	8100	OGK	C05-C06-N08	2.10	119.12	116.25
5	N	1101	PO4	O3-P-O2	2.09	114.68	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	4100	OGK	C19-C20-C22	-2.08	105.53	109.05
4	N	7100	OGK	O07-C06-C05	-2.07	119.23	121.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	4100	OGK	C03

All (29) torsion outliers are listed below:

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

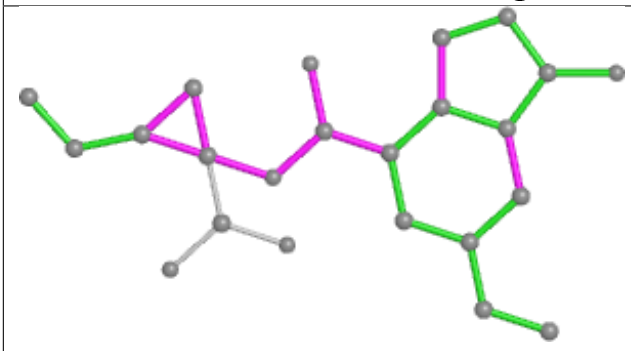
There are no ring outliers.

27 monomers are involved in 85 short contacts:

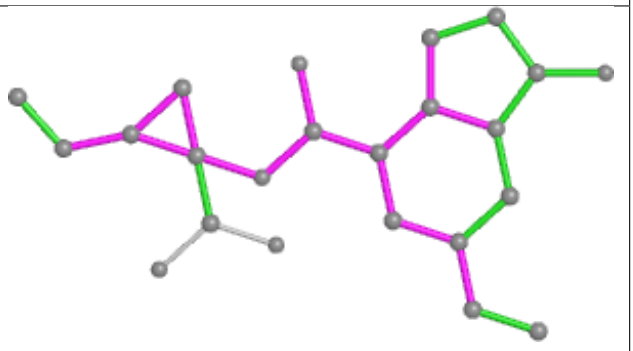
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1103	PO4	1	0
5	D	1101	PO4	1	0
4	B	1100	OGK	7	0
5	B	1101	PO4	1	0
5	N	1103	PO4	1	0
5	P	1101	PO4	1	0
4	J	5100	OGK	7	0
5	N	1102	PO4	1	0
5	J	1103	PO4	1	0
4	P	8100	OGK	8	0
4	D	2100	OGK	7	0
5	B	1103	PO4	1	0
5	H	1102	PO4	1	0
5	N	1101	PO4	1	0
5	H	1101	PO4	1	0
5	F	1101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

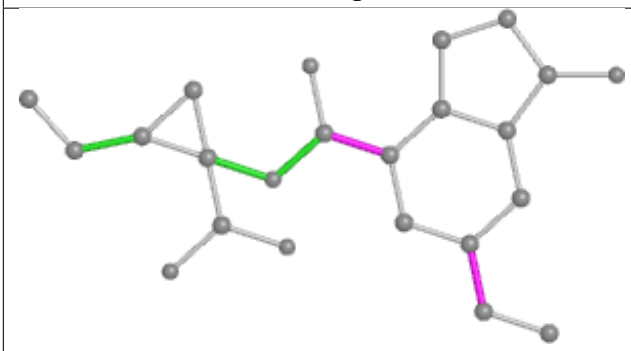
Ligand OGK B 1100



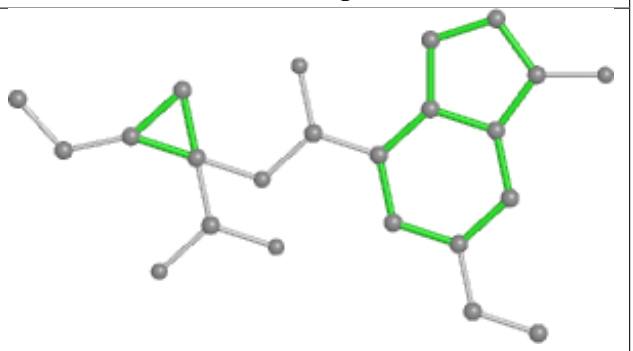
Bond lengths



Bond angles

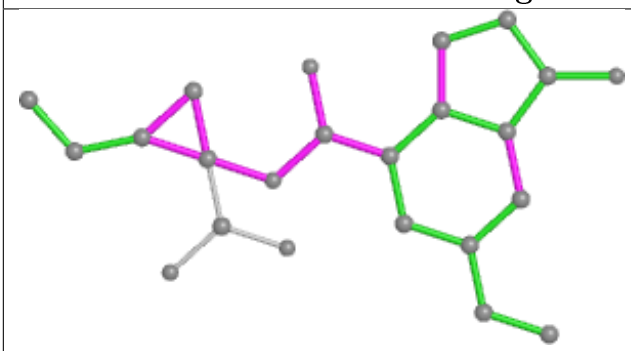


Torsions

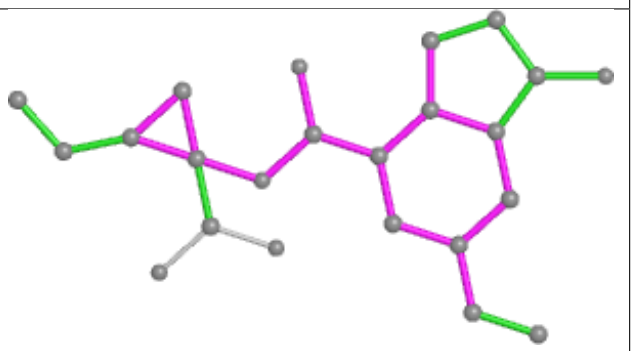


Rings

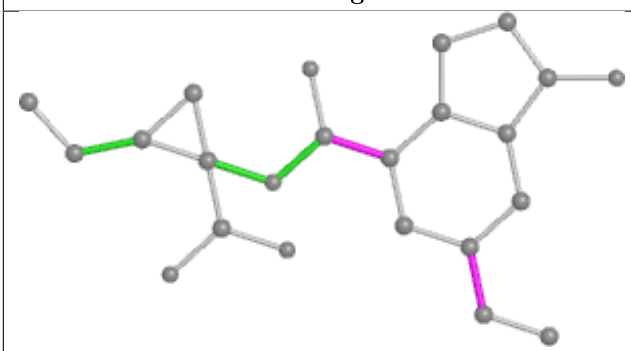
Ligand OGK J 5100



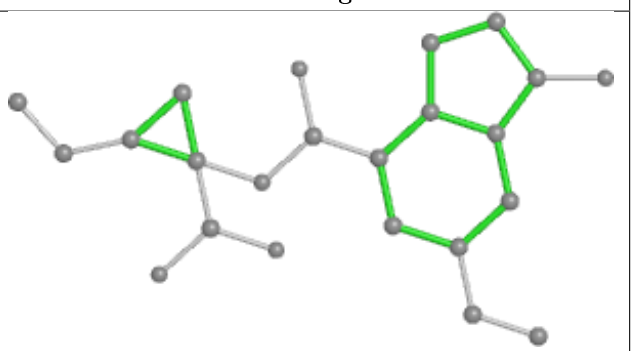
Bond lengths



Bond angles

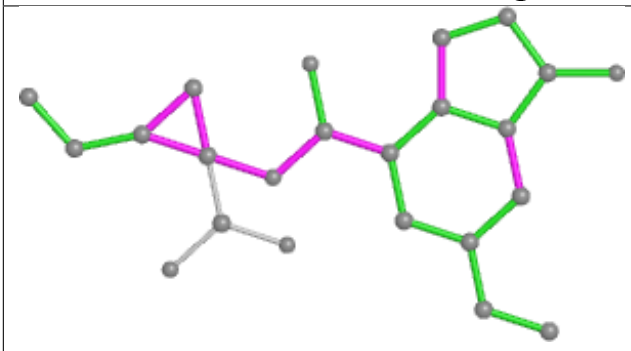


Torsions

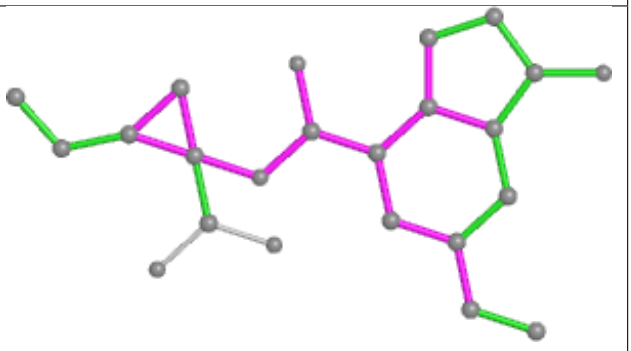


Rings

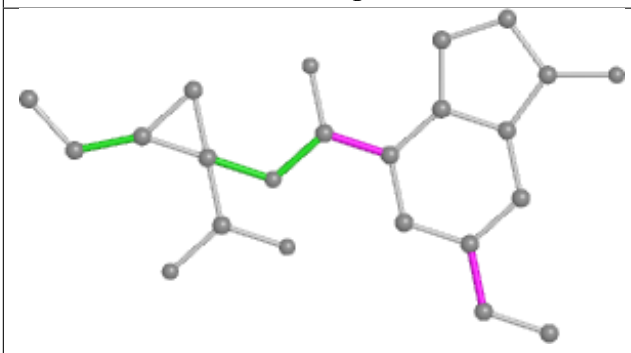
Ligand OGK P 8100



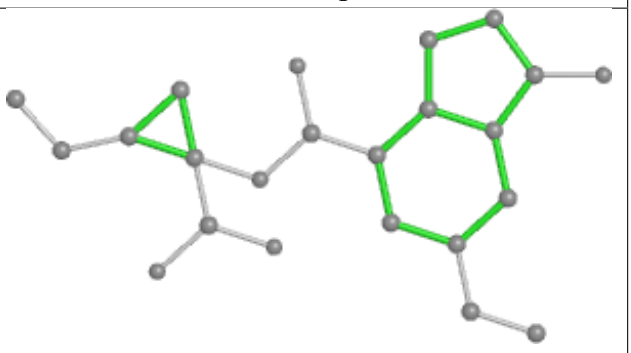
Bond lengths



Bond angles

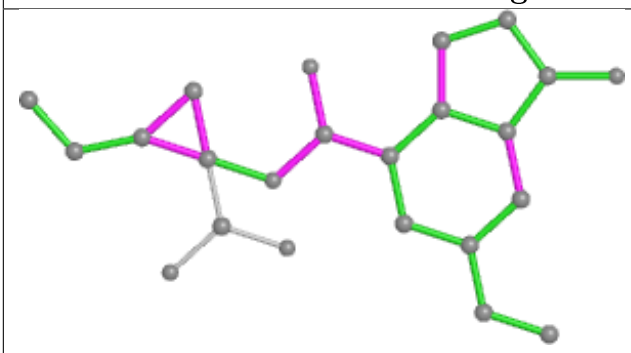


Torsions

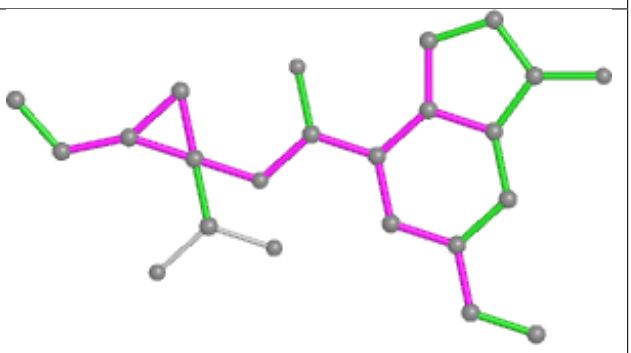


Rings

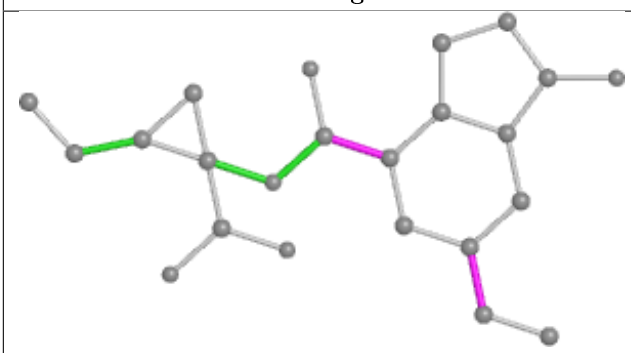
Ligand OGK D 2100



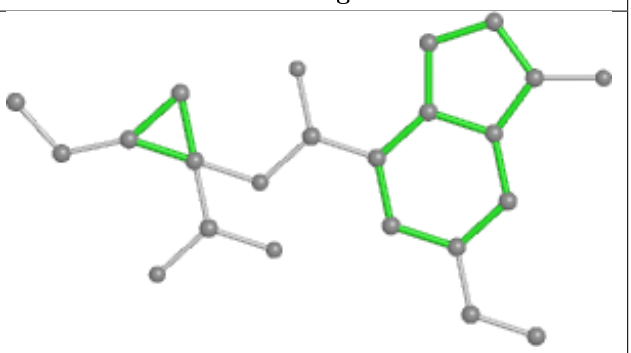
Bond lengths



Bond angles

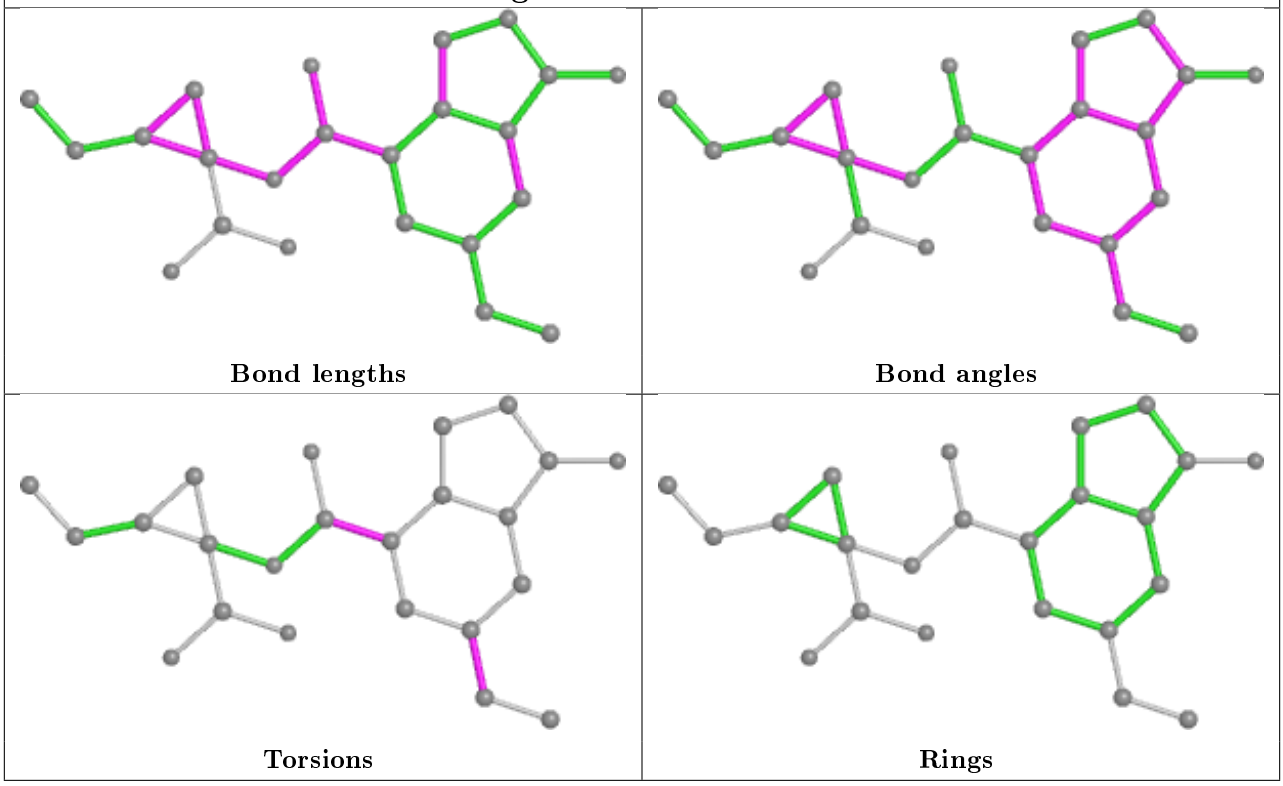


Torsions

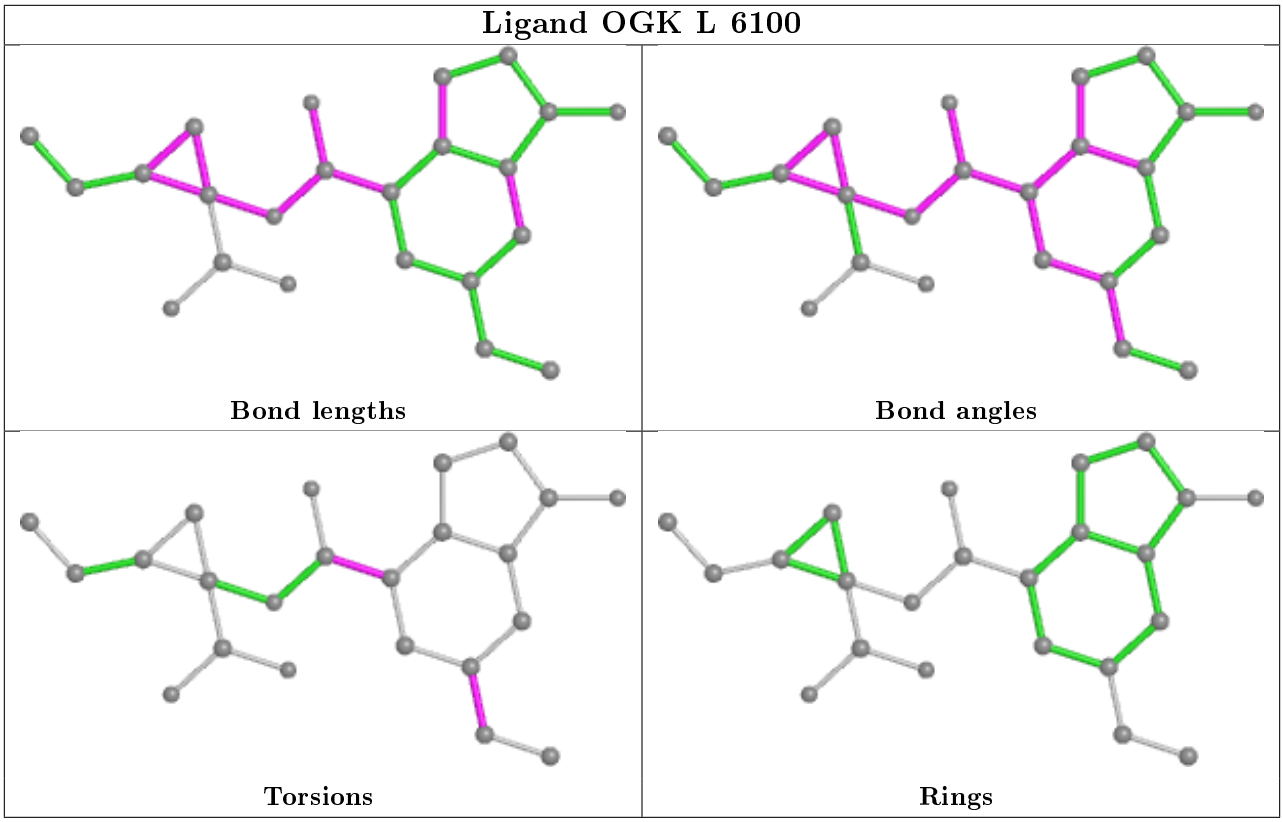


Rings

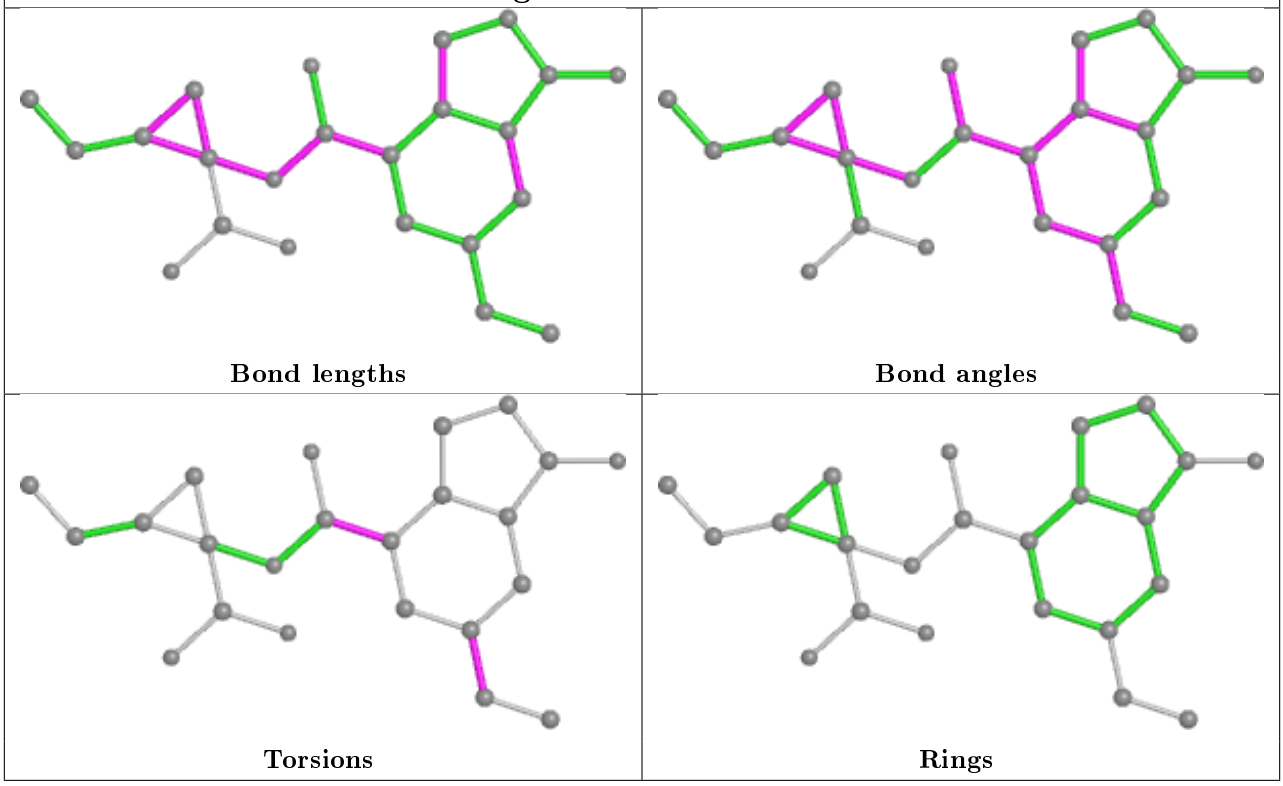
Ligand OGK H 4100



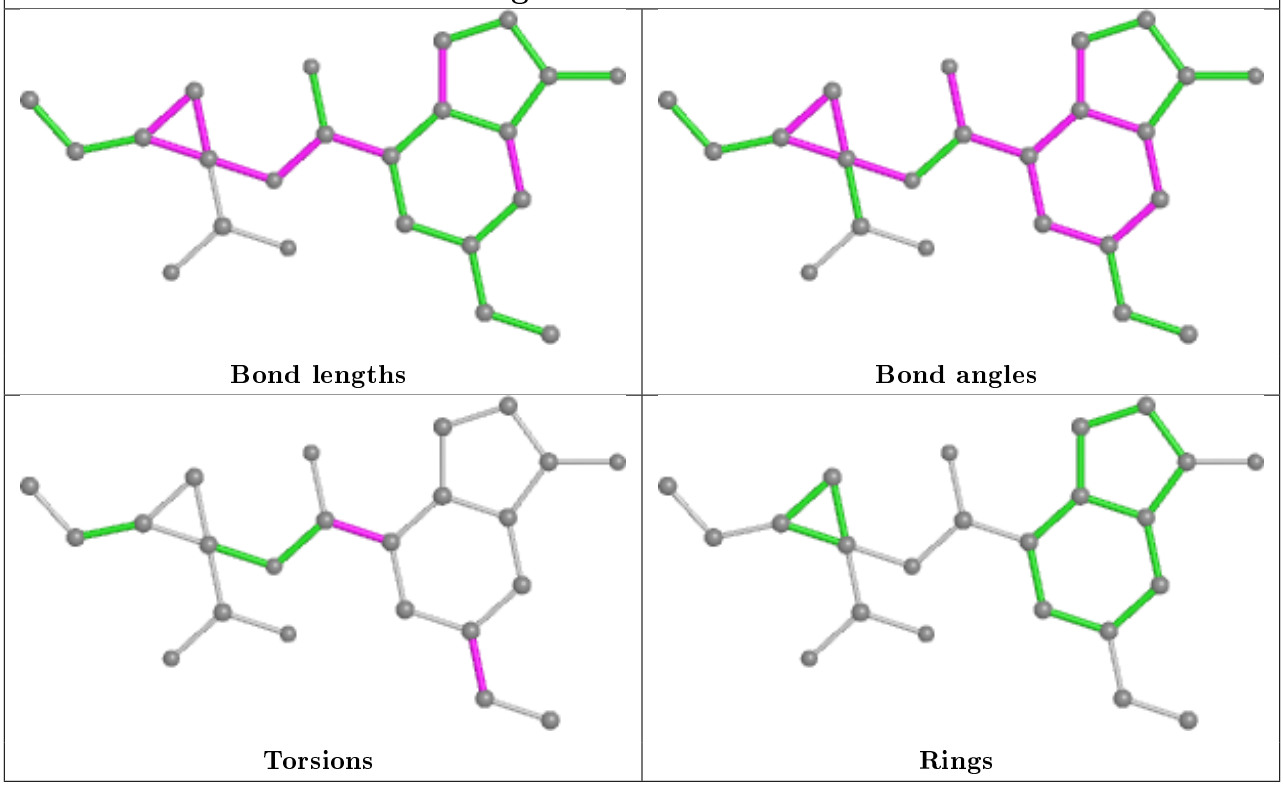
Ligand OGK L 6100



Ligand OGK F 3100



Ligand OGK N 7100



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	144/160 (90%)	0.49	7 (4%) 29 29	50, 100, 151, 168	0
1	C	144/160 (90%)	0.55	9 (6%) 20 21	50, 102, 153, 170	0
1	E	144/160 (90%)	0.33	6 (4%) 36 36	54, 101, 151, 171	0
1	G	144/160 (90%)	0.14	2 (1%) 75 75	49, 96, 149, 170	0
1	I	144/160 (90%)	0.37	6 (4%) 36 36	50, 100, 150, 170	0
1	K	144/160 (90%)	0.63	17 (11%) 4 4	53, 102, 152, 170	0
1	M	144/160 (90%)	0.67	14 (9%) 7 8	55, 102, 152, 175	0
1	O	144/160 (90%)	0.63	17 (11%) 4 4	51, 101, 151, 173	0
2	B	568/592 (95%)	-0.15	8 (1%) 75 75	38, 76, 136, 201	0
2	D	568/592 (95%)	-0.04	8 (1%) 75 75	38, 75, 135, 200	0
2	F	568/592 (95%)	-0.08	16 (2%) 53 52	40, 79, 136, 202	0
2	H	562/592 (94%)	-0.23	12 (2%) 63 63	34, 73, 127, 191	0
2	J	568/592 (95%)	-0.14	9 (1%) 72 71	39, 77, 136, 204	0
2	L	568/592 (95%)	-0.14	9 (1%) 72 71	41, 79, 135, 202	0
2	N	568/592 (95%)	0.39	41 (7%) 15 16	41, 82, 137, 206	0
2	P	568/592 (95%)	-0.09	14 (2%) 57 56	40, 80, 138, 204	0
3	Q	18/21 (85%)	-0.13	0 100 100	72, 93, 116, 143	0
3	R	18/21 (85%)	-0.08	0 100 100	71, 88, 115, 145	0
3	S	18/21 (85%)	-0.34	0 100 100	73, 93, 117, 143	0
3	U	18/21 (85%)	-0.16	0 100 100	71, 88, 112, 143	0
3	V	18/21 (85%)	0.01	1 (5%) 24 25	75, 93, 115, 143	0
3	W	18/21 (85%)	0.26	1 (5%) 24 25	80, 96, 119, 143	0
3	X	18/21 (85%)	-0.10	1 (5%) 24 25	76, 91, 119, 143	0
All	All	5816/6163 (94%)	0.05	198 (3%) 45 44	34, 82, 141, 206	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	591	PRO	8.5
2	B	549	ARG	6.2
2	N	590	GLU	6.1
2	P	592	ILE	5.9
2	P	12	SER	5.9
2	N	360	ASP	5.9
2	N	592	ILE	5.8
2	J	360	ASP	5.8
2	F	547	SER	5.4
1	M	80	ASP	5.3
2	P	362	GLU	5.3
2	D	360	ASP	5.0
2	L	359	GLU	4.9
1	O	80	ASP	4.8
2	N	359	GLU	4.7
2	F	355	GLU	4.7
1	M	115	ASP	4.6
2	P	547	SER	4.4
2	N	355	GLU	4.4
1	A	24	LEU	4.3
2	H	356	GLN	4.3
2	P	591	PRO	4.2
2	H	355	GLU	4.2
2	L	592	ILE	4.2
2	D	12	SER	4.1
2	J	592	ILE	4.1
2	H	352	GLY	4.0
2	F	356	GLN	4.0
2	N	373	LEU	4.0
3	V	200	GLU	4.0
2	L	356	GLN	4.0
2	N	354	ASP	4.0
2	N	356	GLN	3.9
2	N	358	MET	3.8
2	J	549	ARG	3.7
2	F	546	PRO	3.7
2	P	356	GLN	3.7
2	F	592	ILE	3.7
2	L	360	ASP	3.6
1	K	6	ILE	3.6
2	F	12	SER	3.5
3	X	200	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	P	548	ARG	3.5
2	D	592	ILE	3.4
3	W	200	GLU	3.4
2	N	389	ASP	3.4
2	F	591	PRO	3.3
2	B	356	GLN	3.3
2	N	266	LEU	3.3
2	H	12	SER	3.2
1	O	116	LEU	3.2
1	A	59	CYS	3.2
2	J	548	ARG	3.2
2	F	360	ASP	3.2
1	M	87	ASP	3.2
1	M	63	VAL	3.2
2	L	12	SER	3.1
1	M	116	LEU	3.1
1	I	38	VAL	3.1
2	P	549	ARG	3.1
2	B	359	GLU	3.1
1	I	35	ASP	3.1
1	A	20	GLU	3.1
2	F	359	GLU	3.0
1	A	21	ALA	3.0
1	O	88	ALA	3.0
1	E	138	ASN	3.0
1	O	5	LYS	3.0
2	H	420	THR	2.9
1	C	7	VAL	2.9
2	F	416	GLU	2.9
2	L	354	ASP	2.9
2	H	332	ARG	2.9
2	N	383	MET	2.9
2	N	15	ALA	2.9
2	B	360	ASP	2.9
1	O	55	VAL	2.8
2	N	12	SER	2.8
2	J	361	GLU	2.8
1	E	80	ASP	2.8
2	H	358	MET	2.8
2	P	420	THR	2.8
1	O	117	THR	2.8
1	A	41	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	38	VAL	2.8
2	L	548	ARG	2.7
2	N	474	GLY	2.7
1	O	21	ALA	2.7
2	B	592	ILE	2.7
2	F	590	GLU	2.7
1	K	59	CYS	2.7
1	A	6	ILE	2.7
1	O	56	ILE	2.7
2	J	358	MET	2.7
2	H	357	GLY	2.7
2	N	424	LEU	2.7
1	M	84	LYS	2.6
2	P	590	GLU	2.6
1	E	84	LYS	2.6
2	B	358	MET	2.6
2	P	546	PRO	2.6
2	F	549	ARG	2.6
1	C	59	CYS	2.6
2	N	291	PHE	2.6
1	M	20	GLU	2.6
1	M	6	ILE	2.6
1	K	25	GLU	2.6
2	J	356	GLN	2.5
2	B	527	MET	2.5
2	H	353	ALA	2.5
1	C	115	ASP	2.5
1	M	37	CYS	2.5
1	K	22	VAL	2.5
1	K	8	LEU	2.5
2	D	548	ARG	2.5
1	C	45	PRO	2.5
1	K	87	ASP	2.5
1	M	123	ASP	2.5
1	C	40	ASN	2.5
1	C	66	ALA	2.5
2	P	258	GLY	2.4
1	K	20	GLU	2.4
2	F	358	MET	2.4
1	K	24	LEU	2.4
2	N	370	LEU	2.4
1	K	21	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	47	VAL	2.4
2	D	358	MET	2.4
1	I	39	ASP	2.4
2	N	306	GLU	2.4
1	K	80	ASP	2.4
1	E	82	ASP	2.4
1	O	89	ASP	2.4
2	F	361	GLU	2.4
1	K	82	ASP	2.4
2	B	355	GLU	2.4
1	O	87	ASP	2.4
1	O	52	LEU	2.4
2	N	588	LEU	2.4
1	M	17	GLU	2.4
2	J	591	PRO	2.4
2	N	256	ASP	2.3
2	F	588	LEU	2.3
1	O	84	LYS	2.3
1	C	20	GLU	2.3
1	O	86	TRP	2.3
2	N	290	PRO	2.3
2	N	462	SER	2.3
2	D	527	MET	2.3
2	F	548	ARG	2.3
2	H	361	GLU	2.3
2	N	548	ARG	2.3
1	O	112	ASN	2.3
1	O	63	VAL	2.3
1	K	43	PRO	2.3
2	N	416	GLU	2.3
2	N	298	LEU	2.3
2	N	334	LEU	2.3
2	L	549	ARG	2.3
2	N	449	GLY	2.3
2	N	527	MET	2.3
1	E	19	GLU	2.2
2	N	363	GLY	2.2
2	P	359	GLU	2.2
1	M	83	LEU	2.2
2	H	362	GLU	2.2
2	N	420	THR	2.2
2	D	549	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	57	GLU	2.2
1	K	15	SER	2.2
1	I	6	ILE	2.2
2	H	527	MET	2.2
2	N	313	LEU	2.2
2	N	402	LEU	2.2
1	C	87	ASP	2.2
1	I	7	VAL	2.2
2	N	361	GLU	2.2
1	C	63	VAL	2.1
1	K	9	LYS	2.1
2	N	287	ILE	2.1
1	O	67	ALA	2.1
1	K	17	GLU	2.1
1	A	22	VAL	2.1
2	N	434	GLY	2.1
1	K	5	LYS	2.1
1	G	90	PHE	2.1
1	O	115	ASP	2.1
2	P	588	LEU	2.1
2	N	435	CYS	2.0
2	N	349	ILE	2.0
2	N	398	ILE	2.0
1	K	81	ASP	2.0
2	J	258	GLY	2.0
1	M	91	MET	2.0
2	L	362	GLU	2.0
1	G	80	ASP	2.0
2	N	589	LYS	2.0
2	D	429	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	H	1104	5/5	0.87	0.36	54,57,114,134	0
5	PO4	N	1101	5/5	0.87	0.31	51,59,80,82	0
4	OGK	N	7100	23/23	0.87	0.26	65,79,100,104	0
5	PO4	F	1102	5/5	0.88	0.29	64,90,96,109	0
5	PO4	D	1104	5/5	0.88	0.24	72,73,107,122	0
5	PO4	L	1104	5/5	0.89	0.27	76,78,119,123	0
5	PO4	N	1103	5/5	0.90	0.37	56,56,74,85	0
5	PO4	N	1104	5/5	0.90	0.35	82,83,118,122	0
5	PO4	J	1104	5/5	0.92	0.33	76,81,112,117	0
5	PO4	B	1104	5/5	0.92	0.24	68,79,102,119	0
5	PO4	N	1102	5/5	0.92	0.35	78,90,92,113	0
5	PO4	P	1104	5/5	0.92	0.26	73,75,110,121	0
4	OGK	H	4100	23/23	0.93	0.25	44,71,85,98	0
5	PO4	F	1104	5/5	0.93	0.19	72,81,117,120	0
5	PO4	P	1102	5/5	0.94	0.20	72,87,98,108	0
5	PO4	L	1103	5/5	0.94	0.32	52,56,69,89	0
5	PO4	H	1102	5/5	0.94	0.33	58,59,72,88	0
5	PO4	J	1102	5/5	0.95	0.39	67,86,95,104	0
4	OGK	L	6100	23/23	0.95	0.23	62,71,90,92	0
4	OGK	F	3100	23/23	0.95	0.24	64,72,91,94	0
4	OGK	B	1100	23/23	0.95	0.23	62,73,87,93	0
5	PO4	L	1101	5/5	0.96	0.32	48,58,74,76	0
4	OGK	P	8100	23/23	0.96	0.25	64,75,88,90	0
4	OGK	D	2100	23/23	0.96	0.25	60,72,81,86	0
4	OGK	J	5100	23/23	0.96	0.24	59,67,88,93	0
5	PO4	L	1102	5/5	0.96	0.36	73,82,96,100	0
5	PO4	F	1103	5/5	0.96	0.28	53,57,73,86	0
5	PO4	B	1102	5/5	0.96	0.24	70,84,93,100	0
5	PO4	F	1101	5/5	0.96	0.24	52,58,68,88	0
5	PO4	D	1101	5/5	0.97	0.29	51,55,63,80	0
5	PO4	H	1103	5/5	0.97	0.20	38,47,52,77	0
5	PO4	B	1101	5/5	0.97	0.22	58,59,65,75	0
5	PO4	J	1103	5/5	0.97	0.26	53,53,64,77	0
5	PO4	D	1102	5/5	0.97	0.24	66,79,93,93	0
5	PO4	J	1101	5/5	0.97	0.26	50,55,74,79	0
5	PO4	P	1103	5/5	0.97	0.23	50,58,73,85	0
5	PO4	D	1103	5/5	0.98	0.30	48,52,55,81	0

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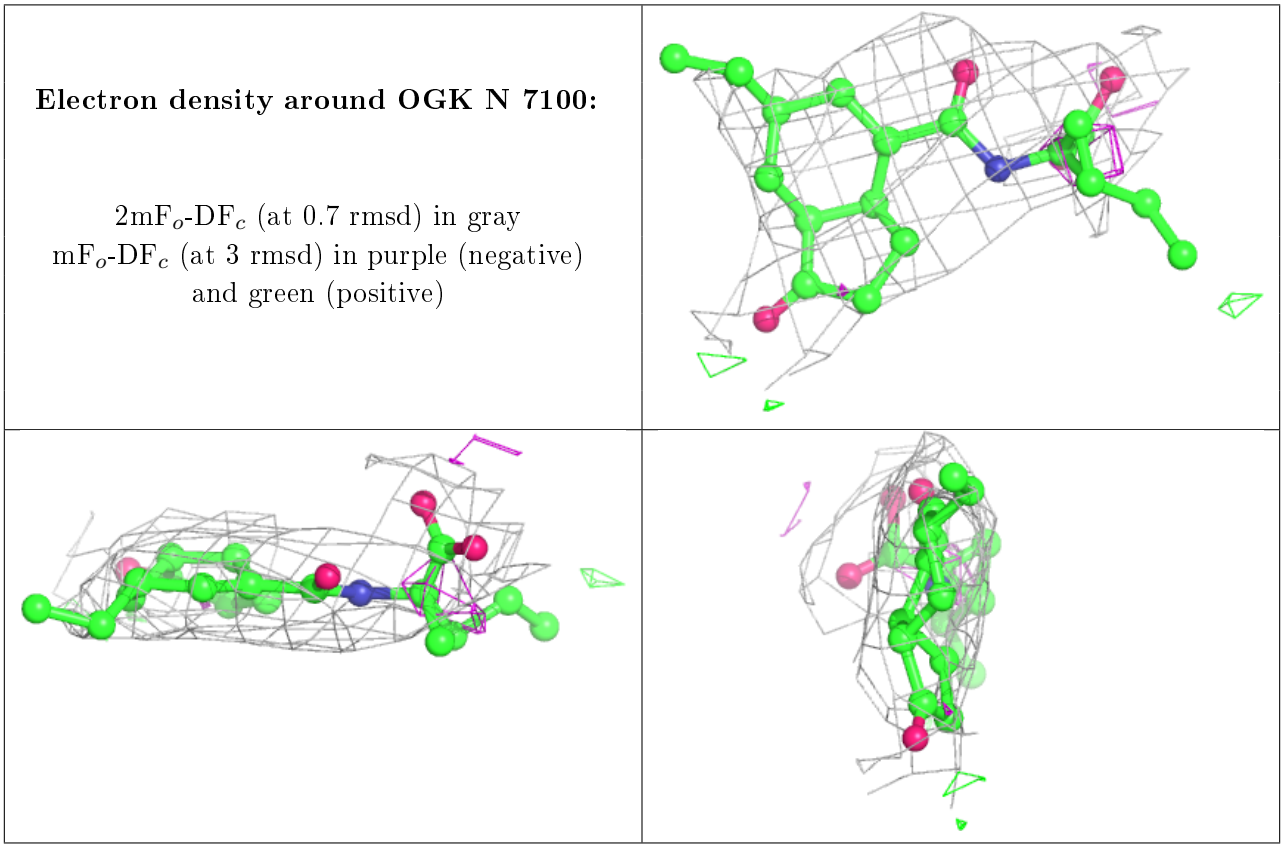
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	P	1101	5/5	0.98	0.28	57,62,74,75	0
5	PO4	B	1103	5/5	0.98	0.28	54,54,61,76	0
5	PO4	H	1101	5/5	0.98	0.21	36,45,63,88	0

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

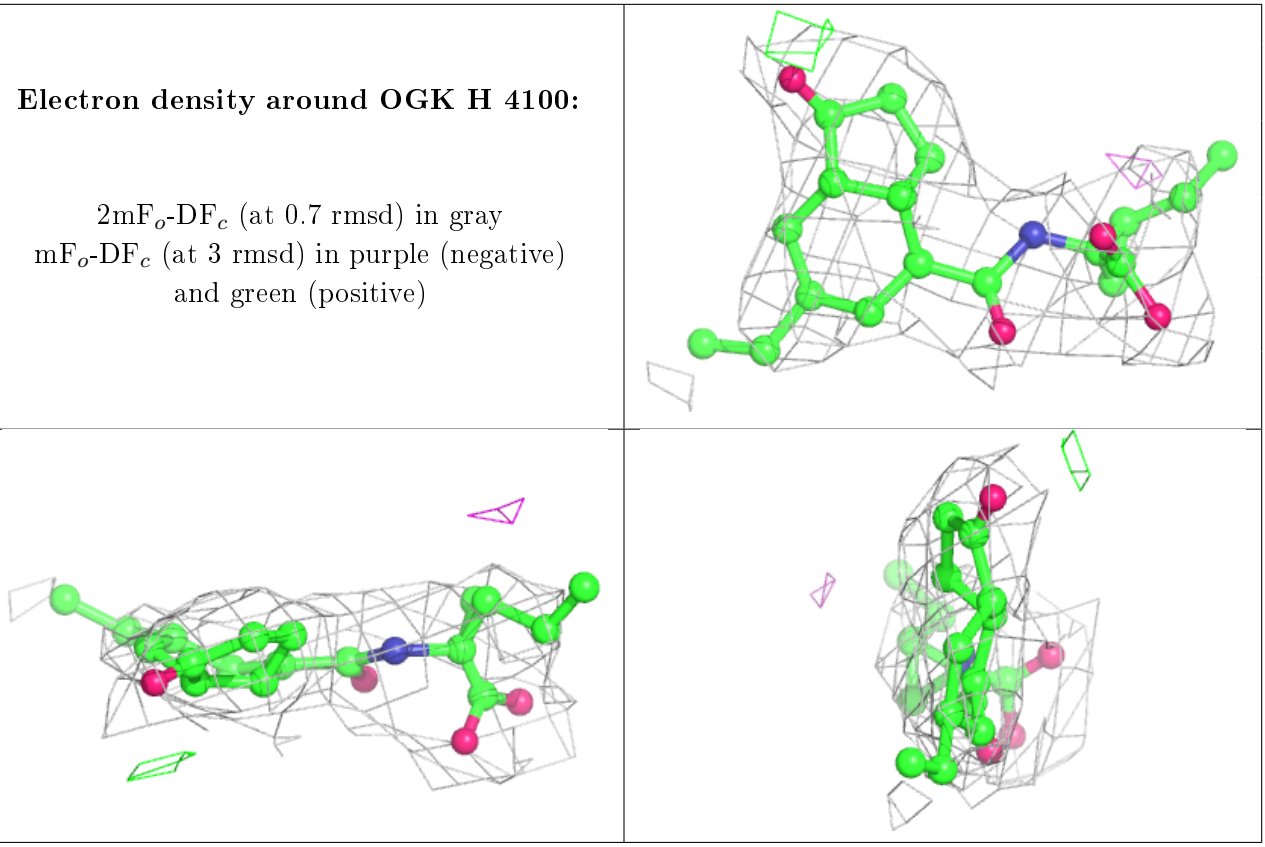
Electron density around OGK N 7100:

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



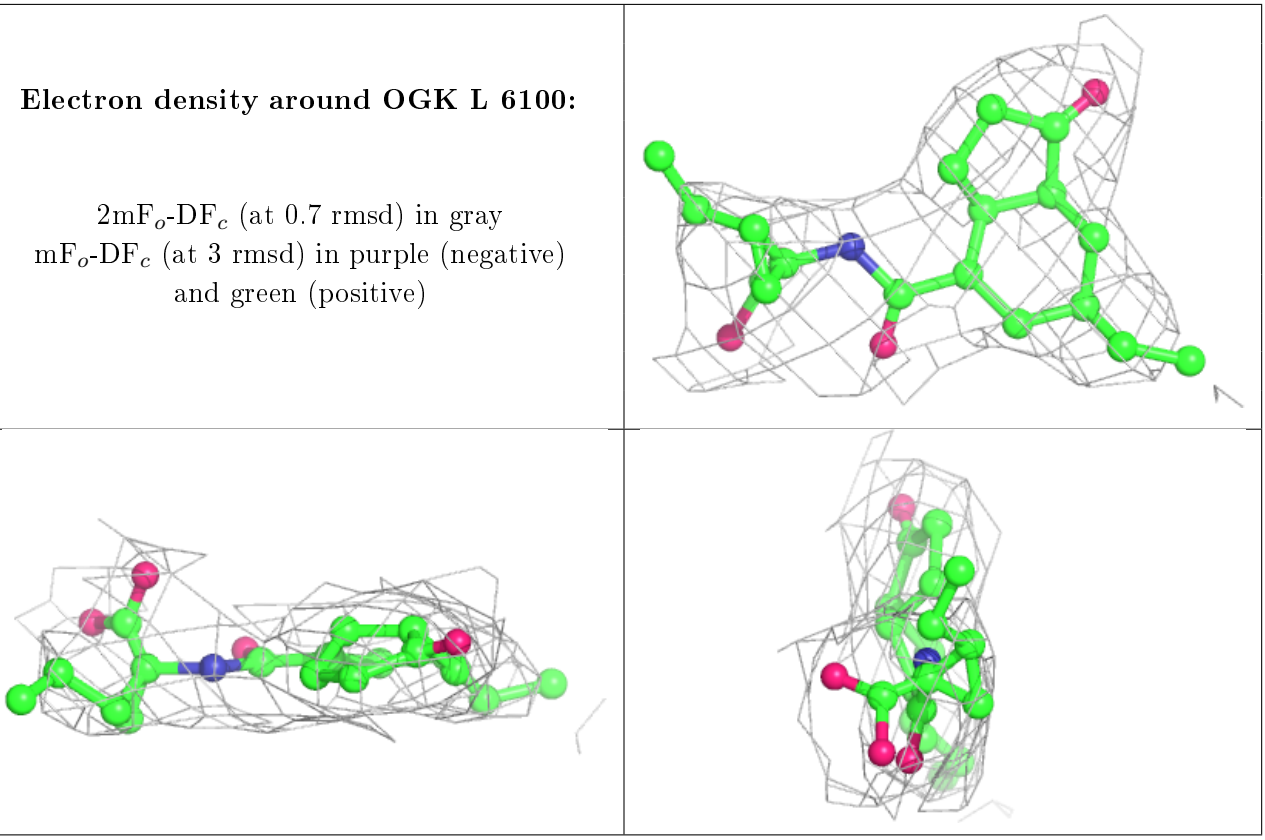
Electron density around OGK H 4100:

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



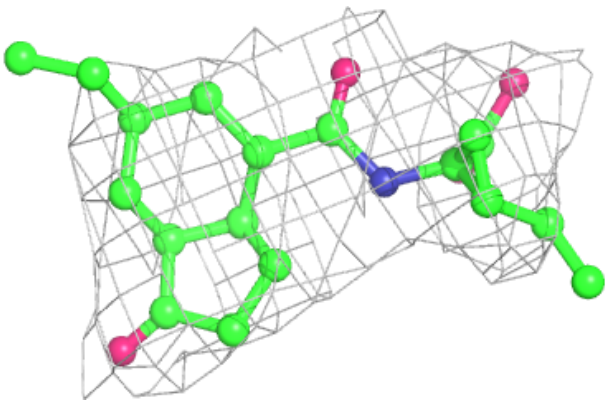
Electron density around OGK L 6100:

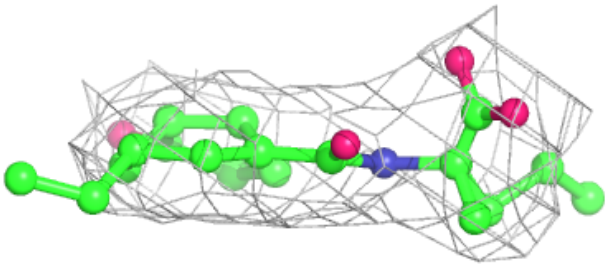
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

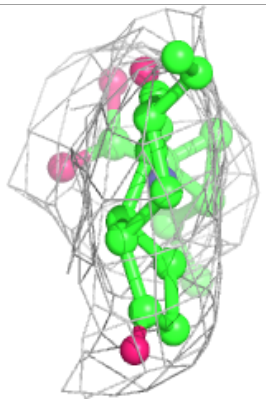


Electron density around OGK F 3100:

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

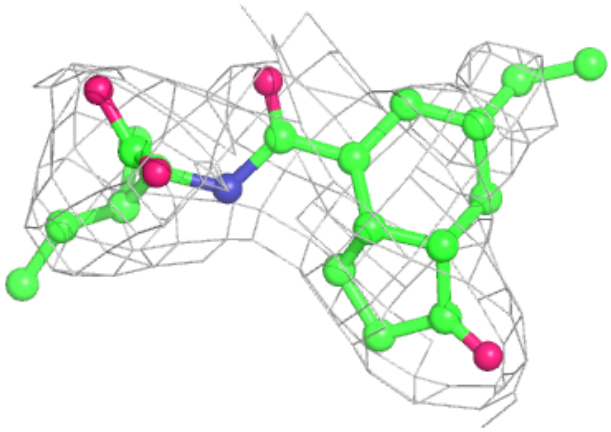


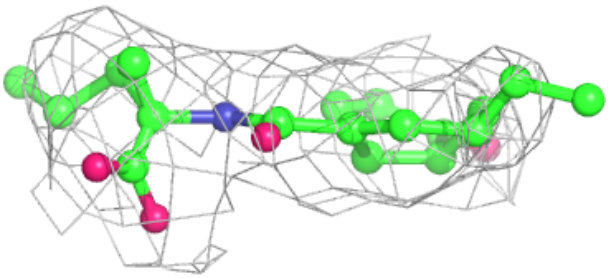


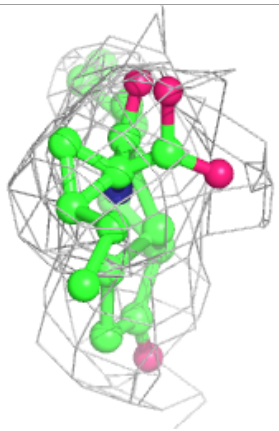


Electron density around OGK B 1100:

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

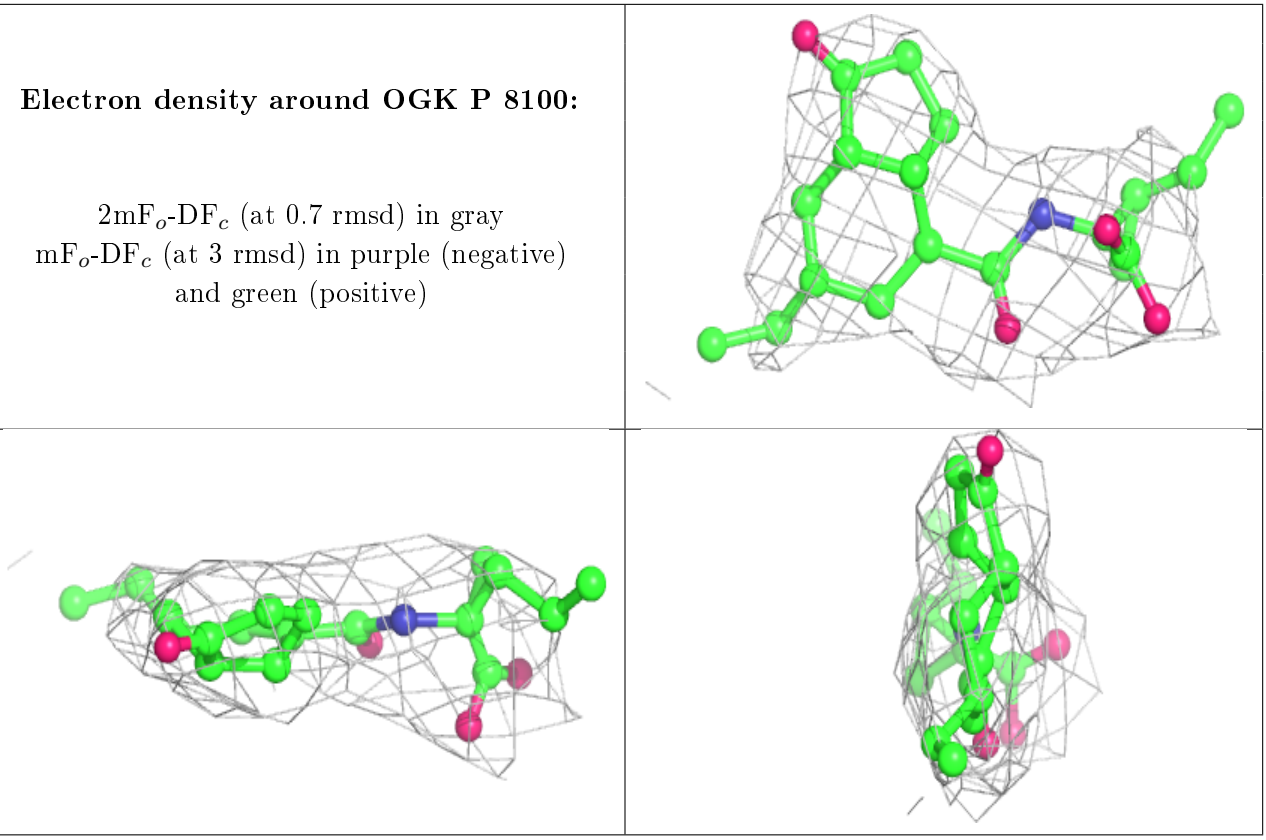






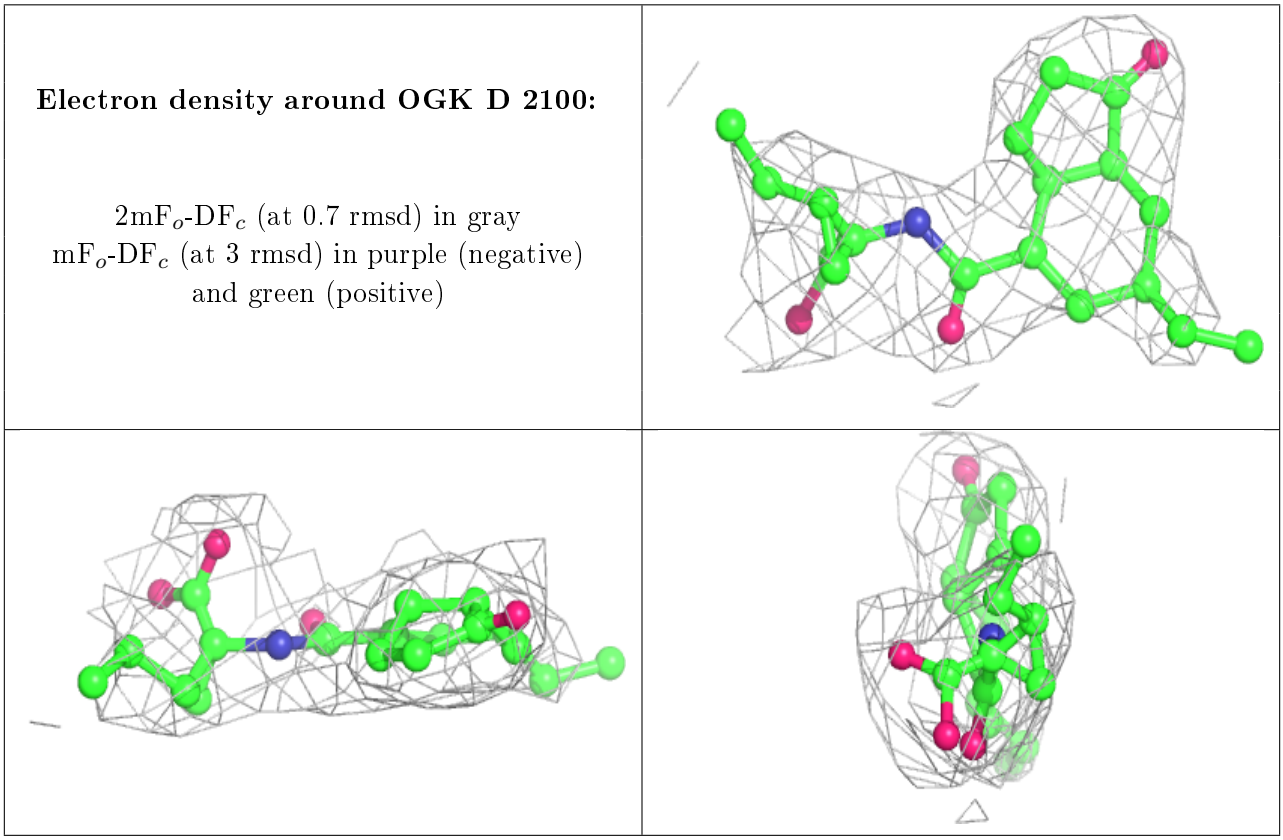
Electron density around OGK P 8100:

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



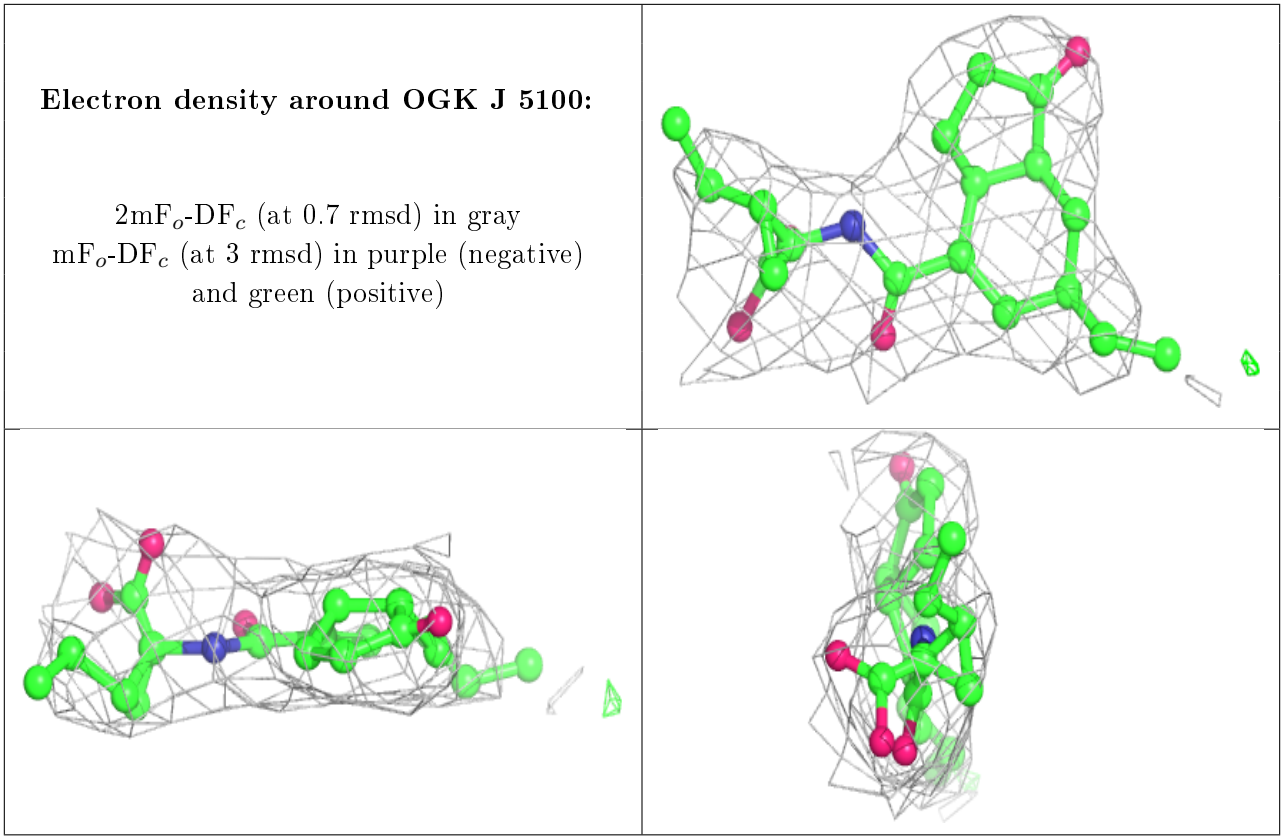
Electron density around OGK D 2100:

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



Electron density around OGK J 5100:

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



6.5 Other polymers

There are no such residues in this entry.