Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:38 AM BST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

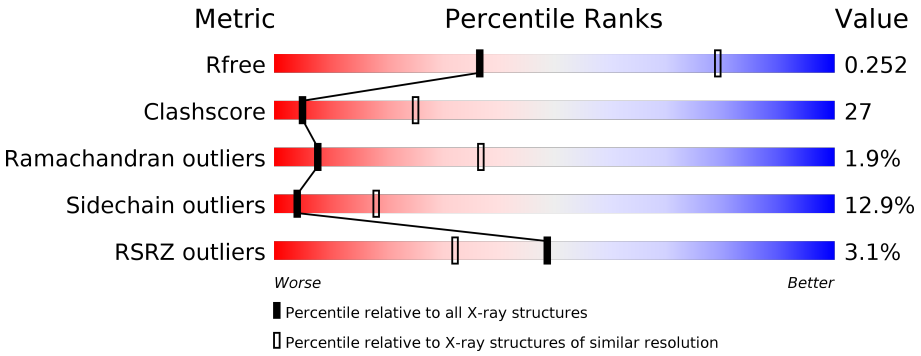
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	3% 49% 36% 5% 10%
1	C	160	5% 49% 34% 6% 10%
1	E	160	54% 29% 7% 10%
1	G	160	53% 31% 7% 10%
1	I	160	5% 48% 34% 8% • 10%
1	K	160	6% 52% 31% 7% 10%

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Mol	Chain	Length	Quality of chain
1	M	160	11% 47% 37% 6% 10%
1	O	160	10% 51% 33% 6% 10%
2	B	592	2% 53% 35% 7%
2	D	592	2% 52% 36% 7%
2	F	592	3% 53% 36% 7%
2	H	592	% 33% 47% 14% 5%
2	J	592	2% 51% 38% 7%
2	L	592	2% 53% 36% 7%
2	N	592	5% 51% 38% 7%
2	P	592	3% 52% 37% 8%
3	Q	21	57% 29% 14%
3	R	21	5% 57% 29% 14%
3	S	21	57% 29% 14%
3	U	21	57% 29% 14%
3	V	21	5% 57% 29% 14%
3	W	21	5% 62% 24% 14%
3	X	21	5% 52% 33% 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	7JA	B	1100	-	-	X	-
4	7JA	D	1100	-	-	X	-
4	7JA	F	1100	-	-	X	-
4	7JA	H	1100	-	-	X	-
4	7JA	J	1100	-	-	X	-
4	7JA	L	1100	-	-	X	-
4	7JA	N	1100	-	-	X	-
4	7JA	P	1100	-	-	X	-

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

2 Entry composition

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

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

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

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

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

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

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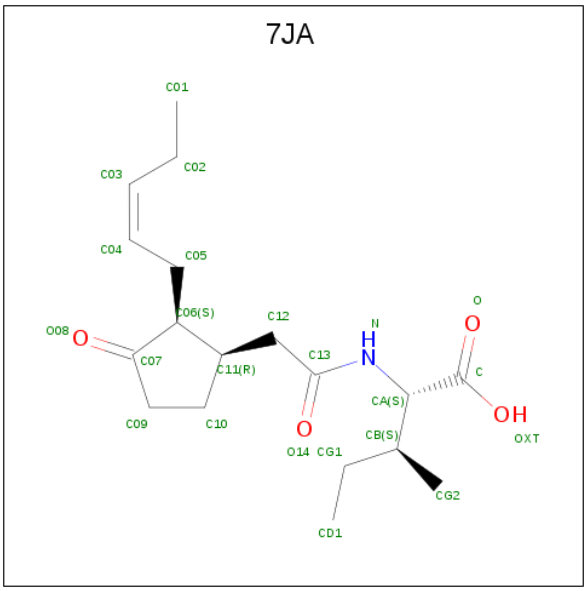
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	P	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

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

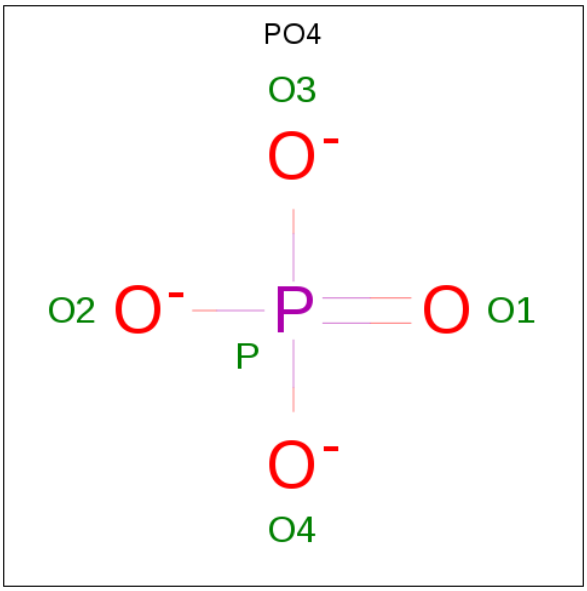
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156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

- Molecule 4 is N-({(1R,2S)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetyl)-L-isoleucine (three-letter code: 7JA) (formula: $C_{18}H_{29}NO_4$).



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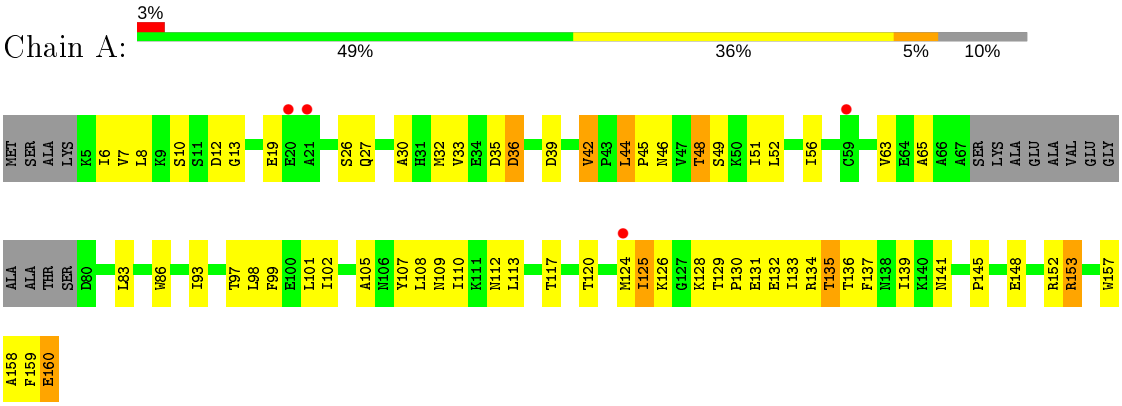
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	N	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0
5	P	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

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

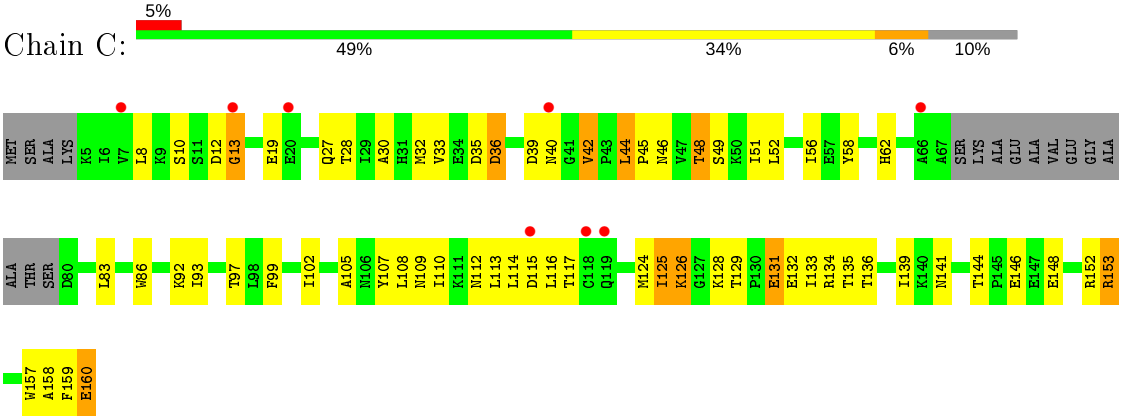
- Molecule 1: SKP1-like protein 1A

Chain A:



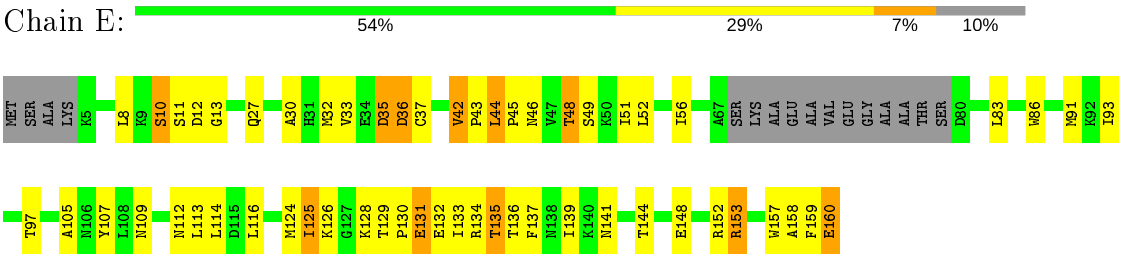
- Molecule 1: SKP1-like protein 1A

Chain C:



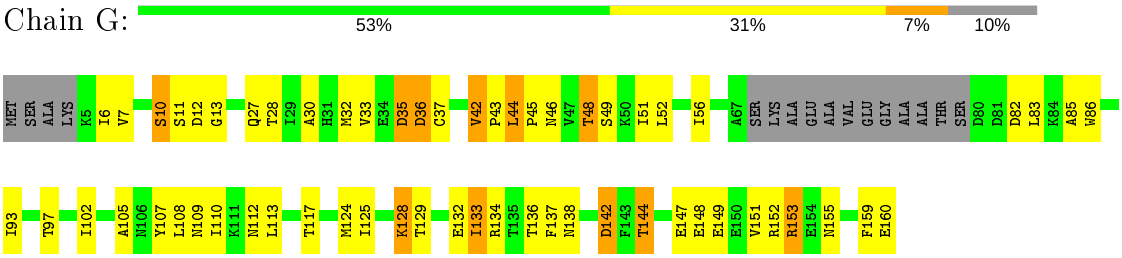
- Molecule 1: SKP1-like protein 1A

Chain E:



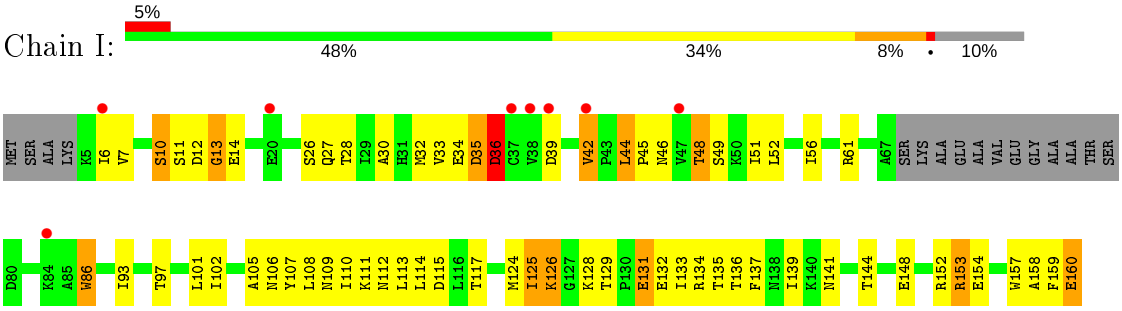
- Molecule 1: SKP1-like protein 1A

Chain G:



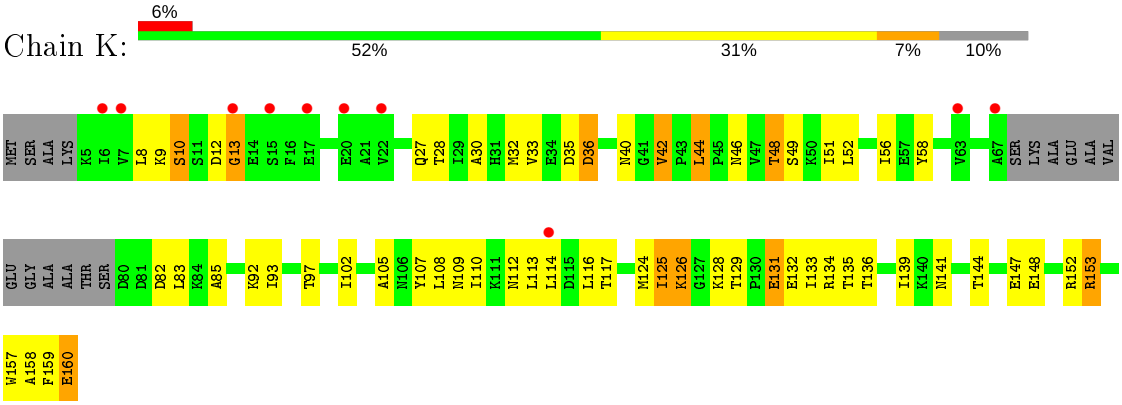
• Molecule 1: SKP1-like protein 1A

Chain I:



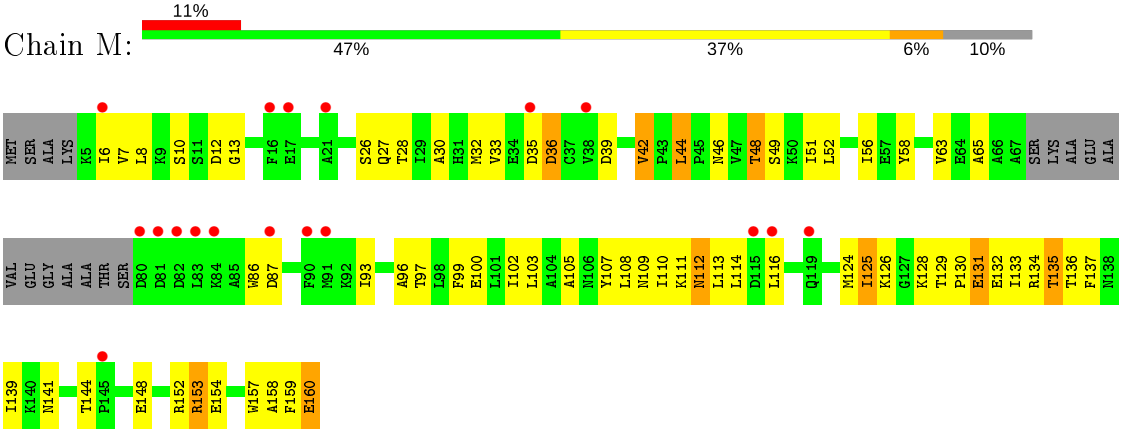
• Molecule 1: SKP1-like protein 1A

Chain K:

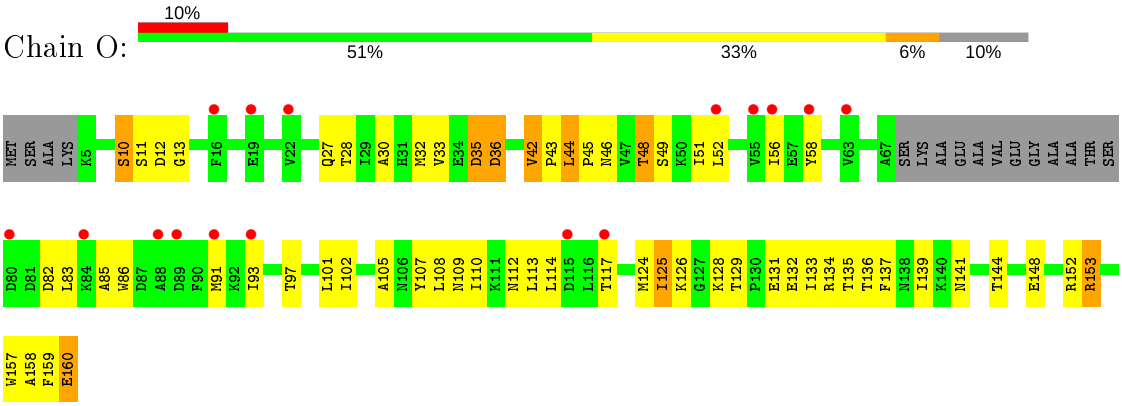


• Molecule 1: SKP1-like protein 1A

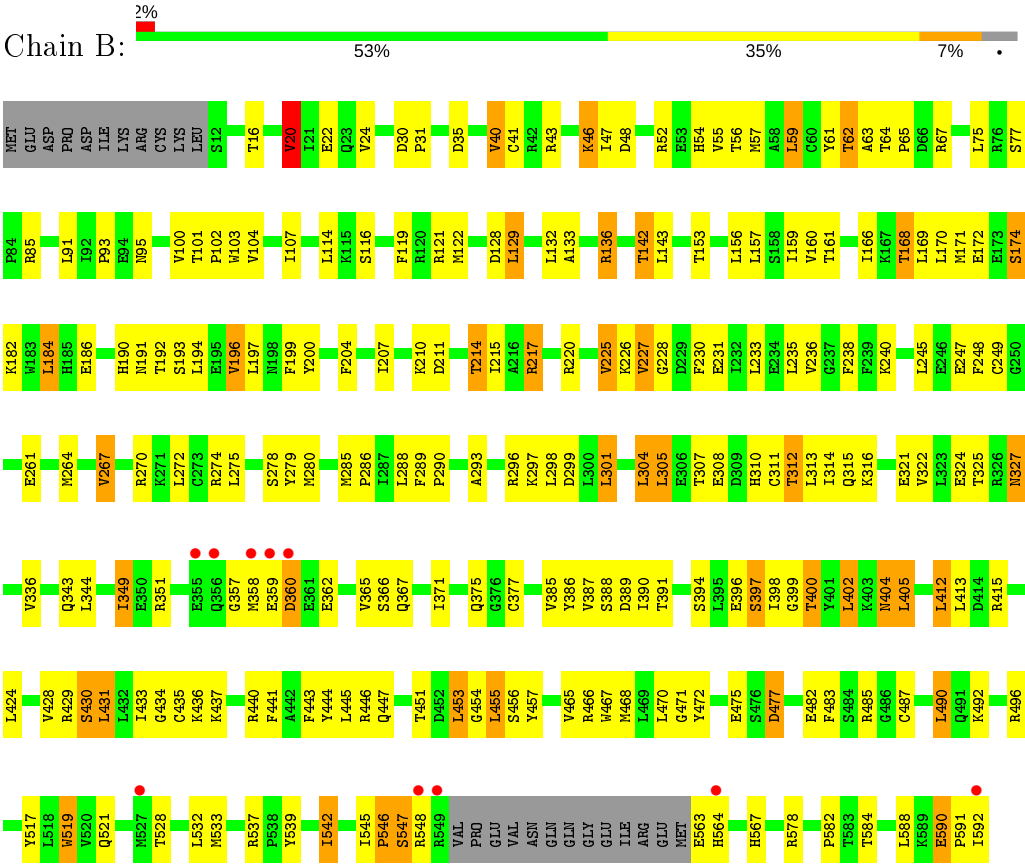
Chain M:



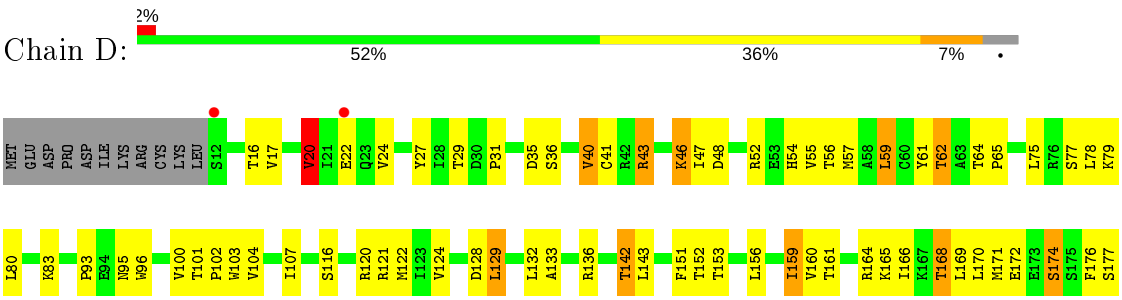
• Molecule 1: SKP1-like protein 1A

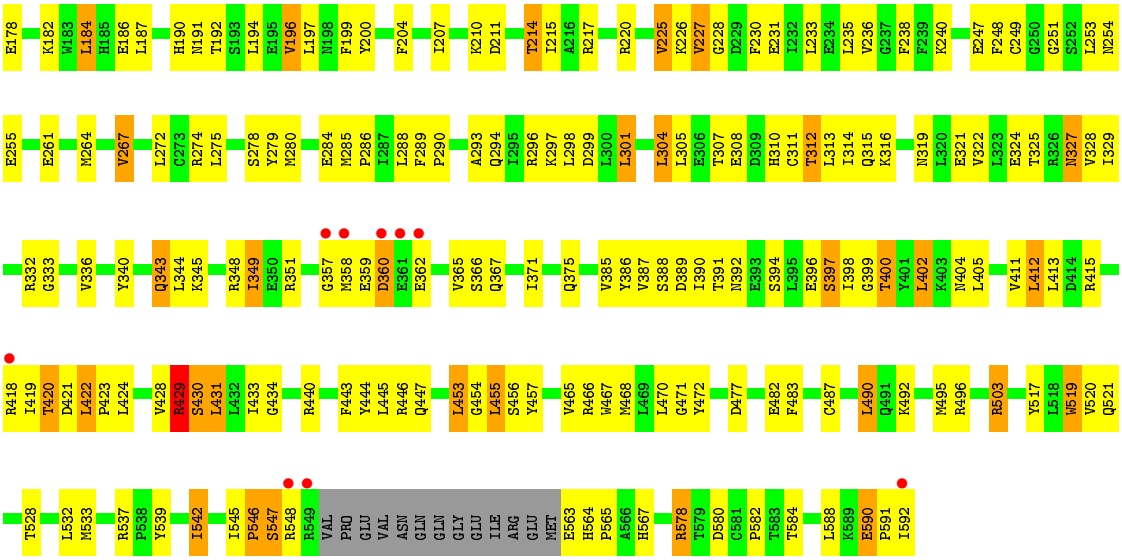


- Molecule 2: Coronatine-insensitive protein 1



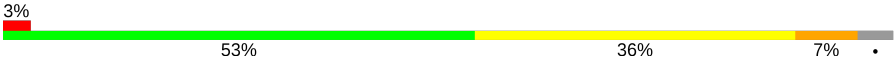
- Molecule 2: Coronatine-insensitive protein 1

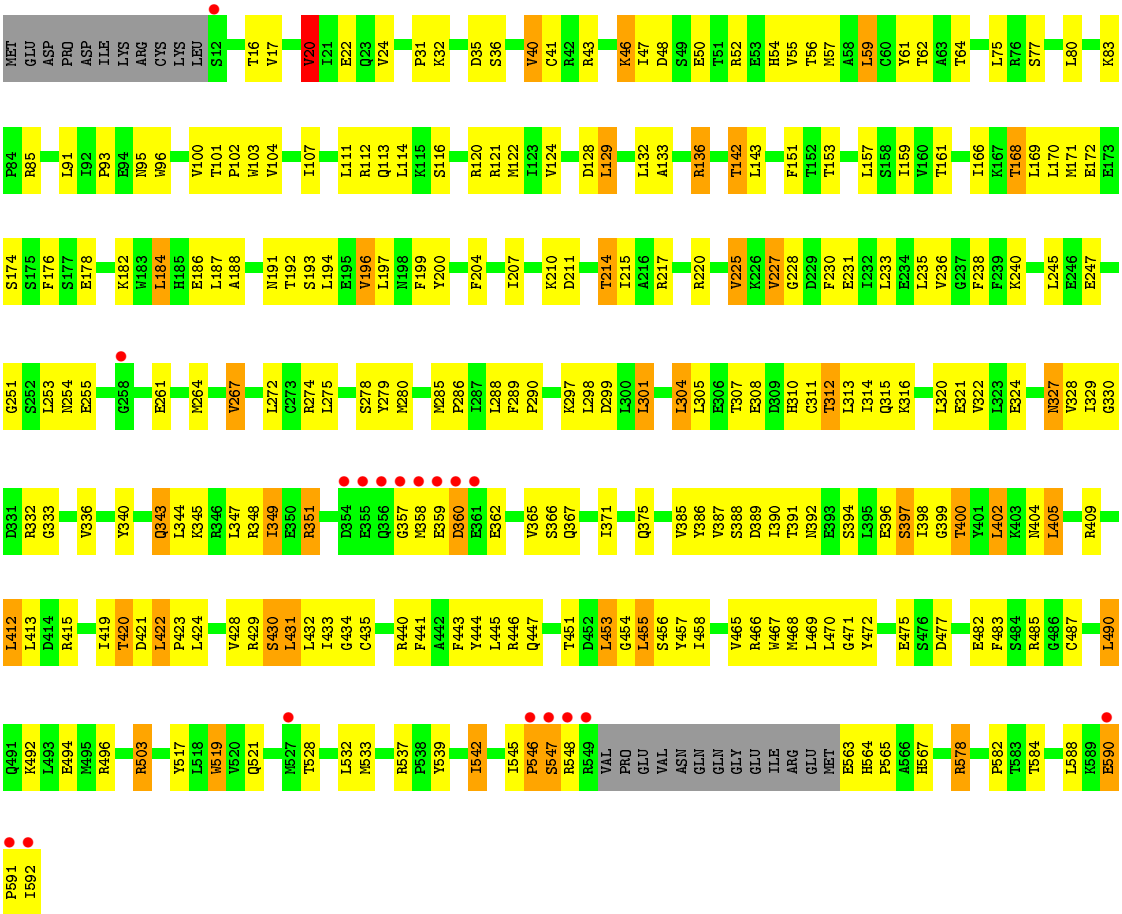




• Molecule 2: Coronatine-insensitive protein 1

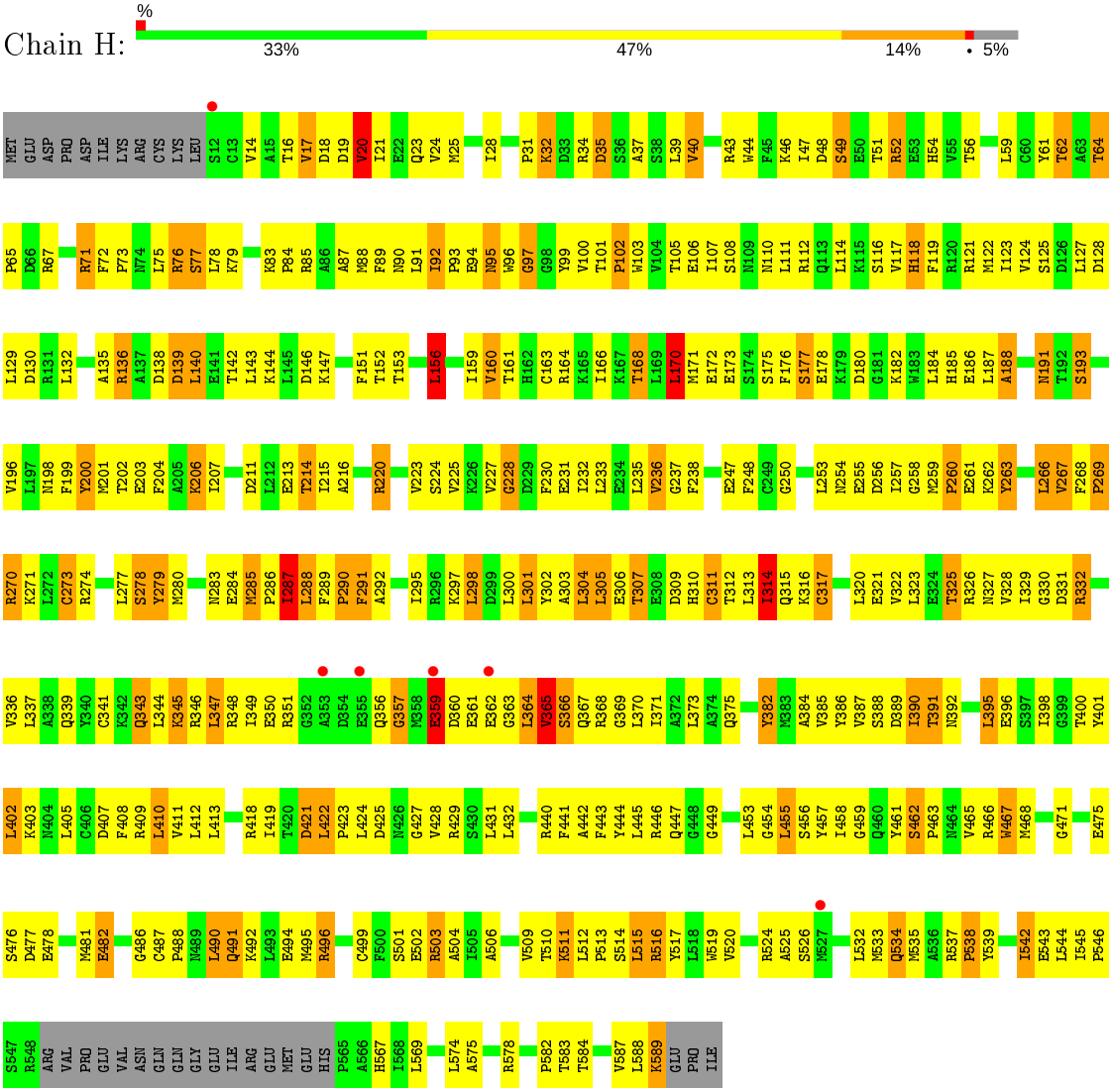
Chain F:





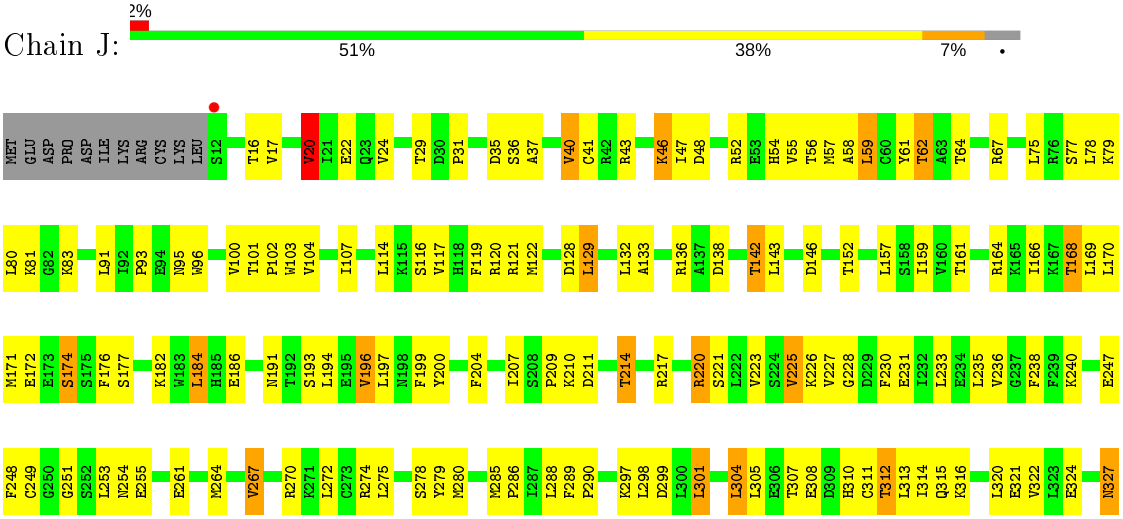
• Molecule 2: Coronatine-insensitive protein 1

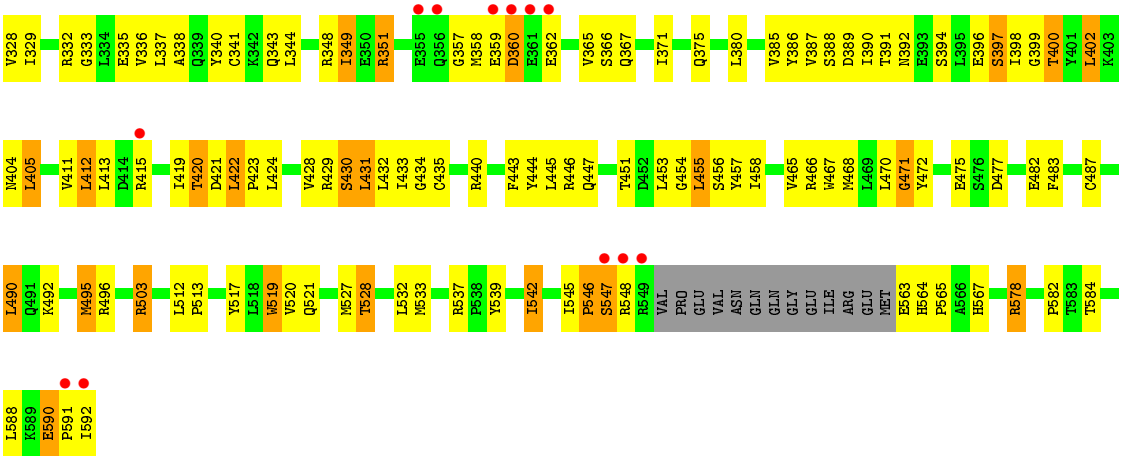
Chain H:



- Molecule 2: Coronatine-insensitive protein 1

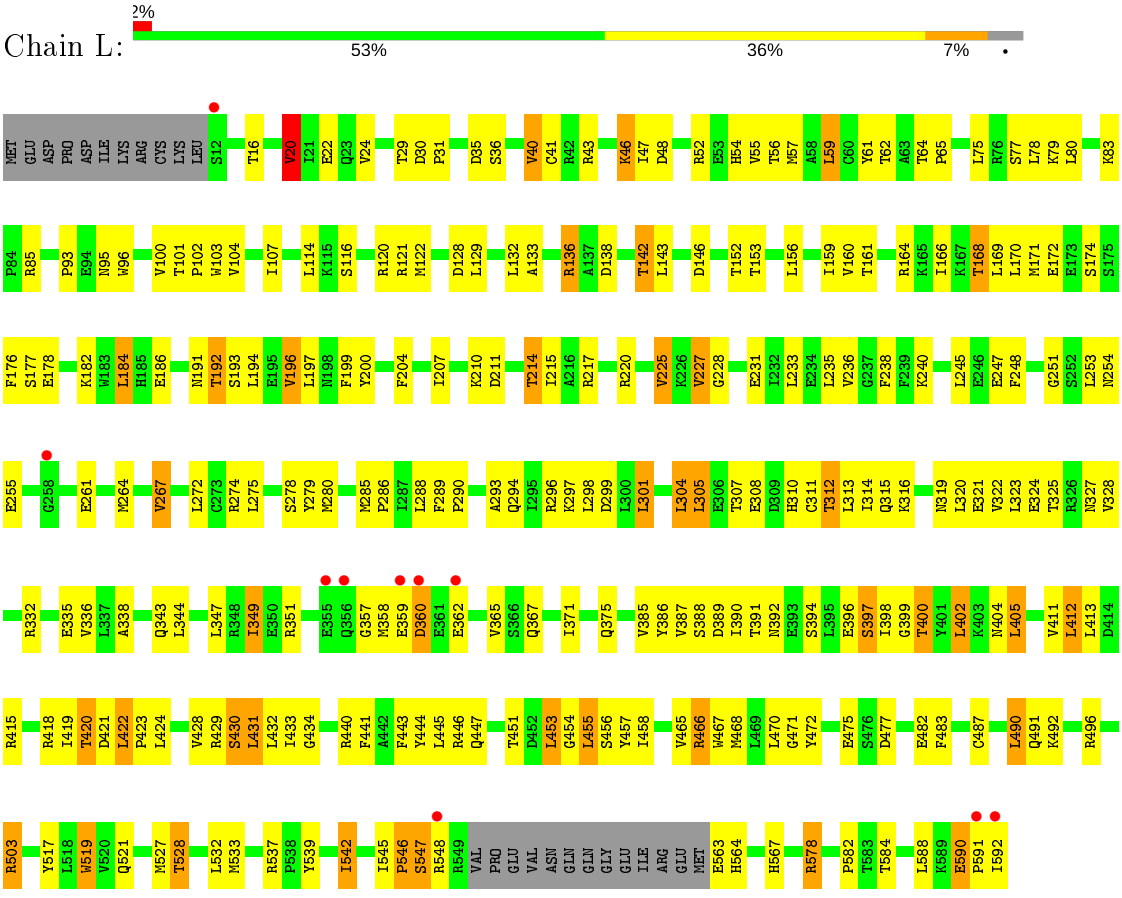
Chain J:





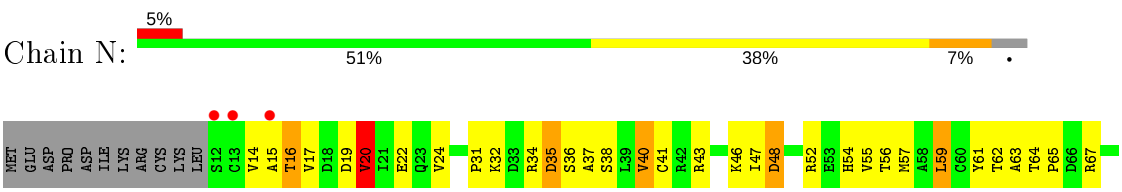
• Molecule 2: Coronatine-insensitive protein 1

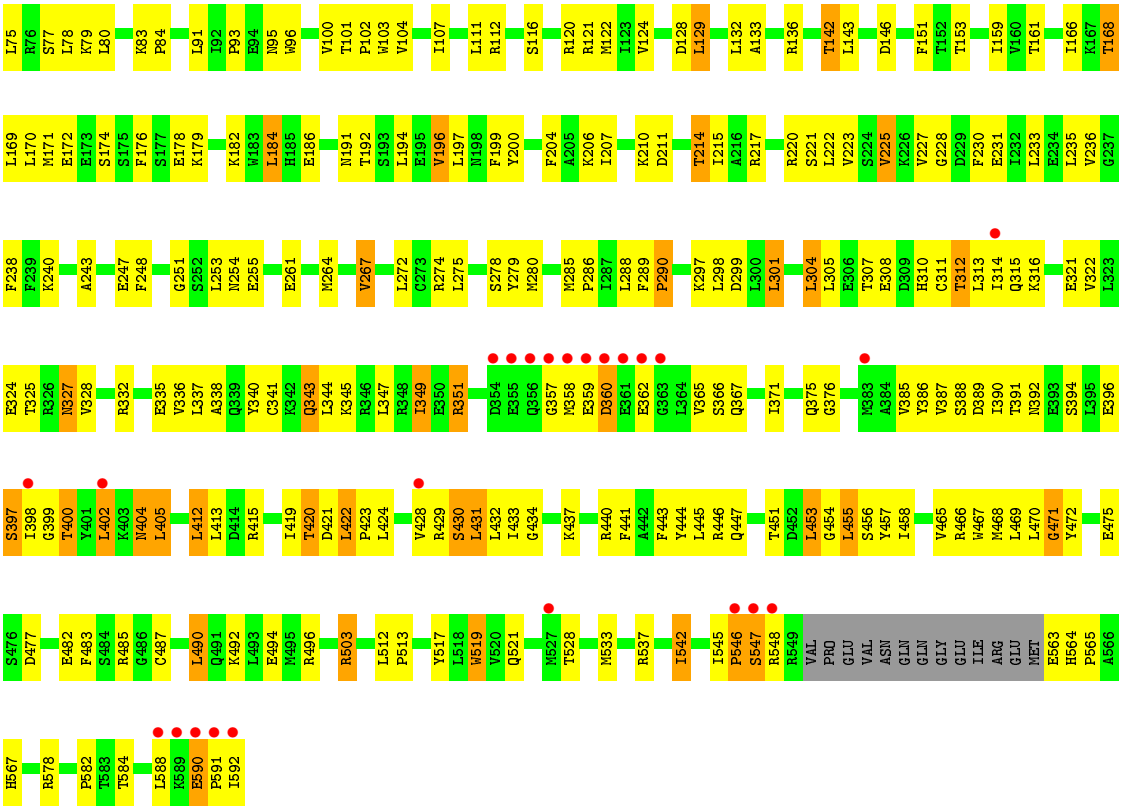
Chain L:



• Molecule 2: Coronatine-insensitive protein 1

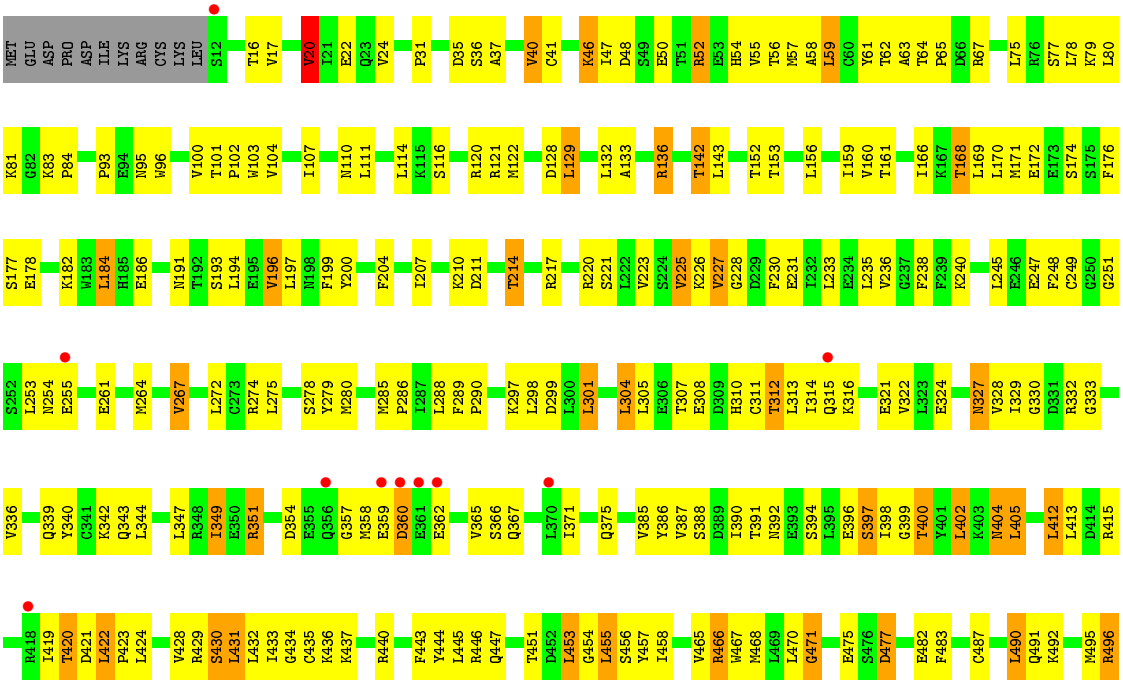
Chain N:

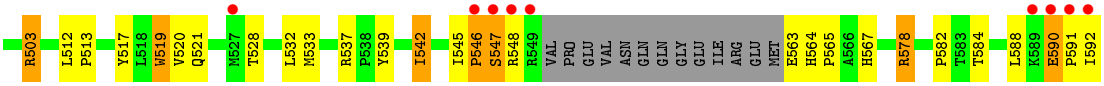




• Molecule 2: Coronatine-insensitive protein 1

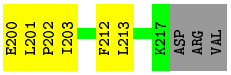
Chain P:





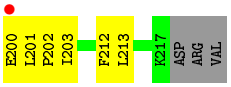
• Molecule 3: JAZ1 incomplete degron peptide

Chain Q:



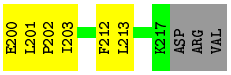
• Molecule 3: JAZ1 incomplete degron peptide

Chain R:



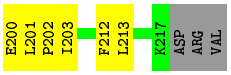
• Molecule 3: JAZ1 incomplete degron peptide

Chain S:



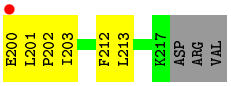
• Molecule 3: JAZ1 incomplete degron peptide

Chain U:



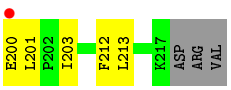
• Molecule 3: JAZ1 incomplete degron peptide

Chain V:



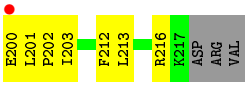
• Molecule 3: JAZ1 incomplete degron peptide

Chain W:



• Molecule 3: JAZ1 incomplete degron peptide

Chain X:


E200
L201
P202
I203
F212
L213
R216
K217
ASP
ARG
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.35Å 220.82Å 148.67Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	49.68 – 3.18 49.68 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (49.68-3.18) 91.1 (49.68-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.215 , 0.263 0.204 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.0	EDS
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)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, 7JA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.48	0/1162	0.60	0/1571
1	C	0.56	0/1162	0.63	0/1571
1	E	0.53	0/1162	0.63	0/1571
1	G	0.55	0/1162	0.69	0/1571
1	I	0.49	0/1162	0.61	0/1571
1	K	0.48	0/1162	0.61	0/1571
1	M	0.52	0/1162	0.61	0/1571
1	O	0.51	0/1162	0.60	0/1571
2	B	0.60	1/4623 (0.0%)	0.71	1/6238 (0.0%)
2	D	0.58	0/4623	0.71	2/6238 (0.0%)
2	F	0.53	0/4623	0.71	1/6238 (0.0%)
2	H	0.63	0/4566	0.87	3/6161 (0.0%)
2	J	0.54	0/4623	0.70	1/6238 (0.0%)
2	L	0.52	0/4623	0.70	1/6238 (0.0%)
2	N	0.61	0/4623	0.72	1/6238 (0.0%)
2	P	0.54	0/4623	0.70	1/6238 (0.0%)
3	Q	0.50	0/158	0.58	0/208
3	R	0.44	0/158	0.60	0/208
3	S	0.41	0/158	0.57	0/208
3	U	0.47	0/158	0.56	0/208
3	V	0.44	0/158	0.57	0/208
3	W	0.48	0/158	0.60	0/208
3	X	0.47	0/158	0.55	0/208
All	All	0.56	1/47329 (0.0%)	0.71	11/63851 (0.0%)

All (1) bond length outliers are listed below:

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

All (11) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

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

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

All (2545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:357:GLY:HA2	2:J:415:ARG:HH22	1.49	0.77
2:L:308:GLU:HG3	2:L:332:ARG:HH22	1.50	0.77
2:F:419:ILE:HD11	2:F:446:ARG:HH22	1.49	0.77
1:G:155:ASN:HB3	2:H:35:ASP:OD2	1.85	0.77
2:N:455:LEU:HD22	2:N:483:PHE:HB2	1.67	0.77
2:D:308:GLU:HG3	2:D:332:ARG:HH22	1.50	0.77
2:H:178:GLU:OE1	2:H:206:LYS:HB3	1.84	0.77
2:D:429:ARG:O	2:D:433:ILE:HG13	1.84	0.77
2:B:440:ARG:HB3	2:B:467:TRP:HE3	1.50	0.76
1:O:159:PHE:O	1:O:160:GLU:HB2	1.84	0.76
2:D:519:TRP:HE1	4:D:1100:7JA:C01	1.98	0.76
2:J:419:ILE:HD11	2:J:446:ARG:HH22	1.48	0.76
2:F:455:LEU:HD22	2:F:483:PHE:HB2	1.67	0.76
2:H:92:ILE:HD13	2:H:93:PRO:HD2	1.67	0.76
1:O:113:LEU:HG	1:O:113:LEU:O	1.83	0.76
2:P:80:LEU:HB2	2:P:122:MET:CE	2.15	0.76
2:L:349:ILE:HG13	2:L:385:VAL:HG22	1.67	0.76
2:J:398:ILE:HG23	2:J:402:LEU:HD11	1.68	0.76
2:B:546:PRO:HG2	2:B:584:THR:HB	1.65	0.76
2:B:80:LEU:HB2	2:B:122:MET:HE1	1.65	0.76
2:D:419:ILE:HD11	2:D:446:ARG:HH22	1.49	0.76
2:L:357:GLY:HA2	2:L:415:ARG:HH22	1.50	0.76
2:H:331:ASP:OD2	2:H:366:SER:HB2	1.84	0.76
1:O:125:ILE:HG23	1:O:133:ILE:HD12	1.67	0.76
2:F:443:PHE:CE2	2:F:445:LEU:HD11	2.21	0.75
2:H:285:MET:HE1	2:H:309:ASP:HB3	1.69	0.75
2:H:373:LEU:HD12	2:H:373:LEU:O	1.85	0.75
2:J:240:LYS:HG3	2:J:267:VAL:HG21	1.67	0.75
2:F:59:LEU:HD22	2:F:61:TYR:H	1.49	0.75
2:F:286:PRO:HA	2:F:289:PHE:CE2	2.21	0.75
2:H:323:LEU:CD1	2:H:325:THR:HG22	2.16	0.75
1:M:159:PHE:O	1:M:160:GLU:HB2	1.84	0.75
1:M:112:ASN:C	1:M:114:LEU:H	1.89	0.75
2:N:349:ILE:HG13	2:N:385:VAL:HG22	1.68	0.75
2:H:519:TRP:HE1	4:H:1100:7JA:C01	1.90	0.75
2:H:519:TRP:CH2	2:H:567:HIS:ND1	2.53	0.75
4:P:1100:7JA:C04	4:P:1100:7JA:H12A	2.16	0.75
2:L:455:LEU:HD22	2:L:483:PHE:HB2	1.68	0.75
2:P:310:HIS:O	2:P:314:ILE:HG12	1.87	0.75
2:H:400:THR:O	2:H:403:LYS:HE2	1.87	0.75
1:A:160:GLU:OE2	1:A:160:GLU:HA	1.86	0.75

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:299:ASP:OD2	2:J:301:LEU:HB2	1.94	0.68
2:F:349:ILE:HG13	2:F:385:VAL:HG22	1.75	0.68
2:H:492:LYS:HZ3	2:H:516:ARG:HH11	1.39	0.68
1:I:159:PHE:O	1:I:160:GLU:HB2	1.92	0.68
2:N:391:THR:HG23	2:N:394:SER:H	1.58	0.68
2:N:59:LEU:HD22	2:N:61:TYR:H	1.56	0.68
2:P:143:LEU:HD23	2:P:159:ILE:HD13	1.74	0.68
2:P:251:GLY:O	2:P:278:SER:HB2	1.93	0.68
2:J:563:GLU:O	2:J:563:GLU:HG3	1.93	0.68
2:N:440:ARG:HB3	2:N:467:TRP:HE3	1.58	0.68
2:B:210:LYS:O	2:B:214:THR:HG22	1.93	0.68
2:B:240:LYS:HG3	2:B:267:VAL:HG21	1.76	0.68
2:B:328:VAL:HG22	2:B:359:GLU:HB2	1.74	0.68
2:B:351:ARG:HD3	2:B:413:LEU:HD11	1.75	0.68
2:D:419:ILE:HD13	2:D:446:ARG:HH12	1.59	0.68
2:D:545:ILE:HB	2:D:567:HIS:HB2	1.73	0.68
2:H:367:GLN:O	2:H:371:ILE:HG13	1.93	0.68
2:J:357:GLY:CA	2:J:415:ARG:HH22	2.07	0.68
1:M:102:ILE:HD13	2:N:20:VAL:HG22	1.75	0.68
2:J:164:ARG:CD	2:N:112:ARG:HG2	2.23	0.68
2:H:428:VAL:HG23	2:H:429:ARG:N	2.08	0.68
2:F:55:VAL:HG23	2:F:75:LEU:HD21	1.75	0.68
2:H:278:SER:O	2:H:280:MET:N	2.26	0.68
4:N:1100:7JA:H12	4:N:1100:7JA:C04	2.05	0.68
1:O:48:THR:HG22	1:O:51:ILE:HB	1.76	0.68
2:D:455:LEU:HD22	2:D:483:PHE:HB2	1.74	0.68
2:L:80:LEU:HB2	2:L:122:MET:HE1	1.76	0.68
2:P:349:ILE:HG13	2:P:385:VAL:HG22	1.75	0.68
2:L:210:LYS:O	2:L:214:THR:HG22	1.92	0.68
2:P:443:PHE:CE2	2:P:445:LEU:HD11	2.29	0.68
2:B:487:CYS:HB3	2:B:490:LEU:HB2	1.75	0.68
2:F:251:GLY:O	2:F:278:SER:HB2	1.93	0.68
2:P:191:ASN:HD21	2:P:194:LEU:H	1.40	0.68
2:D:289:PHE:CD1	2:D:316:LYS:HD2	2.29	0.67
2:L:468:MET:HE3	2:L:470:LEU:HD21	1.75	0.67
2:L:563:GLU:O	2:L:563:GLU:HG3	1.94	0.67
2:N:307:THR:HG21	2:N:362:GLU:HB2	1.76	0.67
3:W:203:ILE:HD12	3:W:203:ILE:H	1.59	0.67
2:J:424:LEU:O	2:J:428:VAL:HG23	1.94	0.67
2:L:391:THR:HG23	2:L:394:SER:H	1.59	0.67
1:G:132:GLU:O	1:G:136:THR:HG23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:THR:HB	2:H:196:VAL:HG13	1.76	0.67
2:N:367:GLN:O	2:N:371:ILE:HG22	1.95	0.67
2:N:487:CYS:HB3	2:N:490:LEU:HB2	1.76	0.67
2:H:443:PHE:CE2	2:H:445:LEU:HD11	2.29	0.67
2:L:311:CYS:HB3	2:L:336:VAL:HG21	1.77	0.67
2:N:545:ILE:HB	2:N:567:HIS:HB2	1.75	0.67
2:H:232:ILE:HG13	2:H:253:LEU:CD2	2.25	0.67
2:J:365:VAL:HG23	2:J:387:VAL:HA	1.77	0.67
2:J:455:LEU:HD22	2:J:483:PHE:HB2	1.76	0.67
2:P:357:GLY:CA	2:P:415:ARG:HH22	2.07	0.67
2:B:563:GLU:O	2:B:563:GLU:HG3	1.94	0.67
1:E:125:ILE:HG23	1:E:133:ILE:HD12	1.77	0.67
1:G:30:ALA:O	1:G:33:VAL:HG22	1.94	0.67
2:H:347:LEU:HD12	2:H:348:ARG:H	1.59	0.67
2:J:191:ASN:HD21	2:J:194:LEU:H	1.42	0.67
1:M:102:ILE:HD13	2:N:20:VAL:CG2	2.23	0.67
2:B:365:VAL:HG23	2:B:387:VAL:HA	1.75	0.67
1:E:45:PRO:HG3	2:L:293:ALA:HB3	1.75	0.67
2:F:286:PRO:HA	2:F:289:PHE:CD2	2.30	0.67
2:H:441:PHE:CZ	2:H:443:PHE:CD1	2.83	0.67
2:P:468:MET:HE3	2:P:470:LEU:HD21	1.77	0.67
1:A:48:THR:HG22	1:A:51:ILE:HB	1.77	0.67
2:B:533:MET:HE3	2:B:588:LEU:HD13	1.76	0.67
2:D:307:THR:HG21	2:D:362:GLU:HB2	1.77	0.67
2:J:184:LEU:HD12	2:J:207:ILE:HB	1.74	0.67
2:J:545:ILE:HB	2:J:567:HIS:HB2	1.75	0.67
1:I:158:ALA:HA	2:J:62:THR:HG21	1.77	0.67
2:L:431:LEU:HD12	2:L:431:LEU:O	1.95	0.67
2:P:289:PHE:CD1	2:P:316:LYS:HD2	2.29	0.67
2:D:95:ASN:O	2:D:582:PRO:HG3	1.95	0.67
1:G:48:THR:CG2	1:G:51:ILE:H	2.07	0.67
2:H:542:ILE:HD11	2:H:588:LEU:HB2	1.76	0.67
2:B:519:TRP:HH2	2:B:567:HIS:CE1	2.13	0.66
2:L:357:GLY:CA	2:L:415:ARG:HH22	2.07	0.66
2:D:349:ILE:HG13	2:D:385:VAL:HG22	1.77	0.66
2:F:311:CYS:HB3	2:F:336:VAL:HG21	1.77	0.66
2:P:93:PRO:HA	2:P:548:ARG:CB	2.22	0.66
2:B:357:GLY:CA	2:B:415:ARG:HH22	2.08	0.66
2:B:55:VAL:HG23	2:B:75:LEU:HD21	1.77	0.66
2:F:289:PHE:CD1	2:F:316:LYS:HD2	2.31	0.66
2:J:251:GLY:O	2:J:278:SER:HB2	1.96	0.66

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:563:GLU:HG3	2:N:563:GLU:O	1.97	0.64
2:P:431:LEU:O	2:P:431:LEU:HD12	1.97	0.64
2:D:412:LEU:HD12	2:D:412:LEU:O	1.98	0.64
2:F:424:LEU:O	2:F:428:VAL:HG23	1.97	0.64
2:H:143:LEU:HD12	2:H:144:LYS:H	1.62	0.64
1:I:30:ALA:O	1:I:33:VAL:HG22	1.97	0.64
2:N:431:LEU:HD12	2:N:431:LEU:C	2.17	0.64
2:F:468:MET:HE3	2:F:470:LEU:HD21	1.78	0.64
2:L:121:ARG:NH2	5:L:1103:PO4:O4	2.31	0.64
1:M:102:ILE:HG21	2:N:20:VAL:HG23	1.78	0.64
2:N:519:TRP:HH2	2:N:567:HIS:CE1	2.16	0.64
2:B:299:ASP:OD2	2:B:301:LEU:HB2	1.98	0.64
2:B:54:HIS:HE1	2:B:56:THR:OG1	1.80	0.64
2:D:55:VAL:HG23	2:D:75:LEU:HD21	1.79	0.64
1:E:113:LEU:HG	1:E:113:LEU:O	1.98	0.64
2:L:487:CYS:HB3	2:L:490:LEU:HB2	1.80	0.64
2:B:310:HIS:O	2:B:314:ILE:HG12	1.98	0.64
2:H:291:PHE:N	2:H:291:PHE:CD2	2.65	0.64
2:H:327:ASN:CG	2:H:351:ARG:HB2	2.18	0.63
2:H:85:ARG:NH2	4:H:1100:7JA:O14	2.31	0.63
2:L:191:ASN:HD21	2:L:194:LEU:H	1.46	0.63
2:L:286:PRO:HA	2:L:289:PHE:CD2	2.33	0.63
1:M:131:GLU:HA	1:M:131:GLU:OE2	1.97	0.63
1:K:48:THR:HG22	1:K:51:ILE:HB	1.78	0.63
2:L:80:LEU:HB2	2:L:122:MET:HE2	1.79	0.63
2:J:231:GLU:HG2	2:J:254:ASN:HD22	1.62	0.63
2:F:93:PRO:HA	2:F:548:ARG:CB	2.26	0.63
2:L:365:VAL:HG23	2:L:387:VAL:HA	1.78	0.63
2:B:286:PRO:HA	2:B:289:PHE:CD2	2.34	0.63
2:D:159:ILE:HD12	2:D:166:ILE:HD11	1.81	0.63
2:D:294:GLN:NE2	1:G:107:TYR:OH	2.31	0.63
2:J:487:CYS:HB3	2:J:490:LEU:HB2	1.80	0.63
2:P:227:VAL:HG13	2:P:228:GLY:N	2.13	0.63
2:B:412:LEU:HD12	2:B:412:LEU:O	1.99	0.63
2:F:519:TRP:HH2	2:F:567:HIS:CE1	2.17	0.63
1:K:102:ILE:CG1	1:K:117:THR:HB	2.27	0.63
1:M:102:ILE:CG2	2:N:20:VAL:HG23	2.28	0.63
2:H:143:LEU:HD12	2:H:144:LYS:N	2.14	0.63
2:H:307:THR:HB	2:H:328:VAL:O	1.99	0.63
2:B:440:ARG:HB3	2:B:467:TRP:CE3	2.34	0.63
2:D:424:LEU:O	2:D:428:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:GLY:CA	2:F:415:ARG:HH22	2.10	0.63
2:F:391:THR:HG23	2:F:394:SER:H	1.64	0.63
2:H:542:ILE:CD1	2:H:588:LEU:HB2	2.29	0.63
2:L:519:TRP:HH2	2:L:567:HIS:CE1	2.16	0.63
1:M:100:GLU:HG2	2:N:15:ALA:CB	2.29	0.63
2:N:365:VAL:HG23	2:N:387:VAL:HA	1.81	0.63
1:O:48:THR:CG2	1:O:51:ILE:H	2.12	0.63
3:Q:203:ILE:HD12	3:Q:203:ILE:H	1.63	0.63
2:H:95:ASN:O	2:H:582:PRO:HG3	1.98	0.63
2:J:307:THR:HG21	2:J:362:GLU:HB2	1.79	0.63
2:L:310:HIS:O	2:L:314:ILE:HG12	1.99	0.63
2:P:199:PHE:CE1	2:P:227:VAL:HG22	2.33	0.63
2:B:431:LEU:C	2:B:431:LEU:HD12	2.19	0.62
2:F:307:THR:HG21	2:F:362:GLU:HB2	1.80	0.62
2:N:310:HIS:O	2:N:314:ILE:HG12	1.98	0.62
2:N:301:LEU:HD23	2:N:324:GLU:HB3	1.81	0.62
2:P:299:ASP:OD2	2:P:301:LEU:HB2	1.98	0.62
2:B:184:LEU:HD12	2:B:207:ILE:HB	1.79	0.62
2:B:289:PHE:CD1	2:B:316:LYS:HD2	2.33	0.62
2:B:454:GLY:O	2:B:457:TYR:HB2	1.97	0.62
2:D:231:GLU:HG2	2:D:254:ASN:HD22	1.64	0.62
2:N:396:GLU:O	2:N:400:THR:HB	1.98	0.62
2:B:545:ILE:HB	2:B:567:HIS:HB2	1.80	0.62
2:D:357:GLY:CA	2:D:415:ARG:HH22	2.11	0.62
2:J:286:PRO:HA	2:J:289:PHE:CD2	2.35	0.62
1:M:96:ALA:CB	2:N:14:VAL:CG1	2.76	0.62
2:B:251:GLY:O	2:B:278:SER:HB2	1.99	0.62
2:H:284:GLU:O	2:H:287:ILE:HD13	1.99	0.62
2:H:442:ALA:CB	4:H:1100:7JA:CD1	2.75	0.62
2:L:542:ILE:CD1	2:L:588:LEU:HD12	2.27	0.62
2:H:125:SER:O	2:H:129:LEU:HB2	2.00	0.62
2:H:365:VAL:HG21	2:H:387:VAL:HG13	1.81	0.62
2:H:409:ARG:HB3	4:H:1100:7JA:HD1	1.80	0.62
2:L:121:ARG:HH22	5:L:1103:PO4:P	2.23	0.62
2:L:424:LEU:O	2:L:428:VAL:HG23	1.99	0.62
1:M:100:GLU:HG2	2:N:15:ALA:HB2	1.81	0.62
2:H:258:GLY:C	2:H:260:PRO:HD3	2.20	0.62
1:K:48:THR:CG2	1:K:51:ILE:H	2.13	0.62
2:H:322:VAL:CG1	2:H:323:LEU:N	2.62	0.62
2:J:310:HIS:O	2:J:314:ILE:HG12	1.98	0.62
2:J:431:LEU:HD12	2:J:431:LEU:C	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:231:GLU:HG2	2:N:254:ASN:HD22	1.64	0.62
2:B:371:ILE:O	2:B:375:GLN:HG3	2.00	0.62
2:D:227:VAL:HG13	2:D:228:GLY:N	2.15	0.62
2:D:310:HIS:O	2:D:314:ILE:HG12	1.99	0.62
2:H:144:LYS:HG2	2:H:170:LEU:HD13	1.82	0.62
2:F:50:GLU:OE1	2:L:217:ARG:NH1	2.33	0.62
1:M:99:PHE:CE2	2:N:17:VAL:N	2.68	0.62
2:P:351:ARG:HD3	2:P:413:LEU:HD11	1.82	0.62
2:B:93:PRO:HA	2:B:548:ARG:CB	2.27	0.62
1:C:113:LEU:O	1:C:117:THR:HG23	1.99	0.62
2:F:297:LYS:HE2	2:F:322:VAL:HG21	1.82	0.62
2:H:78:LEU:HD12	2:H:79:LYS:H	1.63	0.62
2:J:412:LEU:HD12	2:J:412:LEU:O	1.99	0.62
1:M:87:ASP:OD2	1:M:116:LEU:HD22	2.00	0.62
1:A:48:THR:CG2	1:A:51:ILE:H	2.13	0.61
2:B:533:MET:CE	2:B:588:LEU:HD13	2.29	0.61
2:H:25:MET:HA	2:H:28:ILE:HD12	1.82	0.61
2:H:443:PHE:HE2	2:H:445:LEU:HD11	1.65	0.61
2:L:211:ASP:HA	2:L:214:THR:HG23	1.82	0.61
2:L:412:LEU:O	2:L:412:LEU:HD12	1.98	0.61
2:D:519:TRP:CH2	2:D:567:HIS:ND1	2.68	0.61
2:H:431:LEU:HD23	2:H:431:LEU:C	2.20	0.61
2:L:93:PRO:HA	2:L:548:ARG:CB	2.25	0.61
2:P:546:PRO:O	2:P:547:SER:HB2	2.01	0.61
2:B:391:THR:HG23	2:B:394:SER:H	1.65	0.61
2:D:171:MET:O	2:D:174:SER:HB2	1.99	0.61
1:E:107:TYR:OH	2:L:294:GLN:NE2	2.33	0.61
2:H:225:VAL:O	2:H:248:PHE:HA	2.00	0.61
2:D:367:GLN:O	2:D:371:ILE:HG22	1.99	0.61
2:J:419:ILE:HD13	2:J:446:ARG:NH1	2.15	0.61
2:D:211:ASP:HA	2:D:214:THR:HG23	1.81	0.61
2:F:440:ARG:HB3	2:F:467:TRP:HE3	1.65	0.61
2:J:233:LEU:O	2:J:236:VAL:HG23	2.00	0.61
1:K:158:ALA:HA	2:L:62:THR:HG21	1.81	0.61
2:N:444:TYR:HA	2:N:471:GLY:CA	2.28	0.61
2:D:431:LEU:O	2:D:431:LEU:HD12	1.99	0.61
2:L:299:ASP:OD2	2:L:301:LEU:HB2	2.00	0.61
1:M:99:PHE:HB2	2:N:15:ALA:CB	2.31	0.61
2:N:311:CYS:HB3	2:N:336:VAL:HG21	1.82	0.61
2:J:533:MET:HE3	2:J:588:LEU:HD13	1.82	0.61
1:M:48:THR:CG2	1:M:51:ILE:H	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:412:LEU:HD12	2:N:412:LEU:O	2.01	0.61
2:B:397:SER:O	2:B:400:THR:HG22	2.00	0.61
2:P:80:LEU:HB2	2:P:122:MET:HE2	1.82	0.61
1:O:158:ALA:HA	2:P:62:THR:HG21	1.82	0.61
1:C:48:THR:CG2	1:C:51:ILE:H	2.11	0.60
2:D:143:LEU:HD23	2:D:159:ILE:HD13	1.83	0.60
2:F:419:ILE:HD13	2:F:446:ARG:NH1	2.16	0.60
2:H:395:LEU:H	2:H:395:LEU:CD2	2.13	0.60
2:J:391:THR:HG23	2:J:394:SER:H	1.65	0.60
2:P:371:ILE:O	2:P:375:GLN:HG3	2.01	0.60
2:P:456:SER:CB	2:P:482:GLU:HB3	2.31	0.60
2:P:54:HIS:HE1	2:P:56:THR:OG1	1.83	0.60
2:L:472:TYR:OH	3:V:201:LEU:HB2	2.00	0.60
2:H:386:TYR:CE1	4:H:1100:7JA:HG2B	2.36	0.60
2:H:533:MET:C	2:H:535:MET:H	2.05	0.60
4:J:1100:7JA:H04	4:J:1100:7JA:H12A	1.73	0.60
2:N:386:TYR:CE1	4:N:1100:7JA:CG2	2.81	0.60
2:B:227:VAL:HG13	2:B:228:GLY:N	2.16	0.60
2:H:361:GLU:HA	2:H:364:LEU:HD12	1.81	0.60
2:L:351:ARG:HD3	2:L:413:LEU:HD11	1.83	0.60
2:D:293:ALA:HB3	1:G:45:PRO:HG3	1.84	0.60
2:H:477:ASP:OD2	2:H:504:ALA:HB2	2.01	0.60
1:I:131:GLU:OE2	1:I:131:GLU:HA	2.01	0.60
2:J:95:ASN:O	2:J:582:PRO:HG3	2.01	0.60
2:J:93:PRO:HA	2:J:548:ARG:CB	2.30	0.60
2:N:143:LEU:HD23	2:N:159:ILE:HD13	1.82	0.60
1:A:30:ALA:O	1:A:33:VAL:HG22	2.01	0.60
2:H:386:TYR:CZ	4:H:1100:7JA:HG2B	2.37	0.60
1:G:153:ARG:NH2	2:H:539:TYR:HE1	1.99	0.60
2:N:211:ASP:O	2:N:215:ILE:HG13	2.02	0.60
2:P:456:SER:HB3	2:P:482:GLU:HB3	1.83	0.60
1:C:30:ALA:O	1:C:33:VAL:HG22	2.00	0.60
1:M:30:ALA:O	1:M:33:VAL:HG22	2.01	0.60
2:N:133:ALA:HB2	2:N:159:ILE:HG22	1.84	0.60
2:N:521:GLN:HG3	2:N:567:HIS:HD2	1.66	0.60
2:P:159:ILE:HD12	2:P:166:ILE:HD11	1.83	0.60
2:H:285:MET:HG2	2:H:286:PRO:HD3	1.83	0.60
2:L:54:HIS:HD2	2:L:77:SER:OG	1.84	0.60
1:M:99:PHE:CZ	2:N:17:VAL:HG22	2.37	0.60
2:D:472:TYR:OH	3:R:201:LEU:HB2	2.02	0.60
2:D:184:LEU:HD12	2:D:207:ILE:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:407:ASP:OD1	2:H:440:ARG:HD2	2.01	0.60
2:J:367:GLN:O	2:J:371:ILE:HG22	2.01	0.60
2:N:397:SER:O	2:N:400:THR:HG22	2.02	0.60
2:B:231:GLU:HG2	2:B:254:ASN:HD22	1.66	0.60
1:K:30:ALA:O	1:K:33:VAL:HG22	2.00	0.60
2:B:211:ASP:HA	2:B:214:THR:HG23	1.84	0.60
2:L:231:GLU:HG2	2:L:254:ASN:ND2	2.17	0.60
1:M:112:ASN:C	1:M:114:LEU:N	2.55	0.60
1:O:131:GLU:OE2	1:O:131:GLU:HA	2.02	0.60
2:D:419:ILE:HD13	2:D:446:ARG:NH1	2.17	0.59
2:H:259:MET:C	2:H:261:GLU:H	2.06	0.59
2:H:262:LYS:HD2	2:H:263:TYR:CE1	2.36	0.59
2:H:343:GLN:CD	2:H:343:GLN:H	2.05	0.59
2:H:92:ILE:HG22	2:H:93:PRO:O	2.02	0.59
2:N:121:ARG:NH2	5:N:1103:PO4:O4	2.35	0.59
2:N:54:HIS:HE1	2:N:56:THR:OG1	1.85	0.59
2:F:386:TYR:CE1	4:F:1100:7JA:CG2	2.83	0.59
2:P:231:GLU:HG2	2:P:254:ASN:HD22	1.67	0.59
2:P:391:THR:HG23	2:P:394:SER:H	1.65	0.59
2:P:412:LEU:HD12	2:P:412:LEU:O	2.01	0.59
2:B:279:TYR:HA	2:B:304:LEU:HD22	1.83	0.59
2:D:440:ARG:HB3	2:D:467:TRP:CE3	2.35	0.59
2:H:347:LEU:HD11	2:H:349:ILE:HG13	1.83	0.59
1:M:27:GLN:HB2	1:M:109:ASN:HB3	1.83	0.59
2:B:121:ARG:NH2	5:B:1103:PO4:O4	2.36	0.59
1:C:131:GLU:HA	1:C:131:GLU:OE2	2.00	0.59
2:F:261:GLU:HG2	2:F:264:MET:HG3	1.84	0.59
2:F:431:LEU:HD12	2:F:431:LEU:O	2.01	0.59
2:N:456:SER:CB	2:N:482:GLU:HB3	2.32	0.59
2:B:217:ARG:NH1	2:P:50:GLU:OE1	2.36	0.59
2:P:351:ARG:HG3	2:P:351:ARG:O	2.03	0.59
2:P:487:CYS:HB3	2:P:490:LEU:HB2	1.83	0.59
2:F:112:ARG:HG3	2:L:164:ARG:HE	1.68	0.59
2:H:125:SER:HB3	2:H:127:LEU:H	1.66	0.59
2:H:402:LEU:HD13	2:H:405:LEU:HG	1.85	0.59
2:L:297:LYS:HE2	2:L:322:VAL:HG21	1.83	0.59
2:L:367:GLN:O	2:L:371:ILE:HG22	2.01	0.59
2:F:472:TYR:OH	3:S:201:LEU:HB2	2.02	0.59
2:J:468:MET:HE3	2:J:470:LEU:HD21	1.83	0.59
1:K:105:ALA:HB2	1:K:113:LEU:HD23	1.85	0.59
2:N:546:PRO:O	2:N:547:SER:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:THR:CG2	1:I:51:ILE:H	2.15	0.59
2:N:170:LEU:HD23	2:N:170:LEU:C	2.23	0.59
1:C:158:ALA:HA	2:D:62:THR:HG21	1.84	0.59
2:F:227:VAL:HG13	2:F:228:GLY:N	2.17	0.59
2:H:191:ASN:ND2	2:H:193:SER:H	2.01	0.59
2:H:375:GLN:HG2	2:H:401:TYR:CD1	2.38	0.59
2:N:468:MET:HE3	2:N:470:LEU:HD21	1.85	0.59
2:J:164:ARG:NE	2:N:112:ARG:HG2	2.18	0.59
2:L:533:MET:HE3	2:L:588:LEU:HD13	1.85	0.59
1:M:153:ARG:HG2	1:M:157:TRP:CZ3	2.37	0.59
1:M:158:ALA:HA	2:N:62:THR:HG21	1.83	0.59
2:N:275:LEU:HD11	2:N:288:LEU:HD21	1.84	0.59
2:P:103:TRP:O	2:P:107:ILE:HG13	2.03	0.59
2:P:279:TYR:HA	2:P:304:LEU:HD22	1.84	0.59
2:B:424:LEU:O	2:B:428:VAL:HG23	2.02	0.58
1:C:12:ASP:O	1:K:40:ASN:CB	2.50	0.58
2:D:311:CYS:HB3	2:D:336:VAL:HG21	1.83	0.58
2:F:456:SER:HB3	2:F:482:GLU:HB3	1.85	0.58
2:D:546:PRO:O	2:D:547:SER:HB2	2.02	0.58
2:F:533:MET:CE	2:F:588:LEU:HD13	2.33	0.58
2:H:233:LEU:O	2:H:236:VAL:HG23	2.03	0.58
2:J:143:LEU:HD23	2:J:159:ILE:HD13	1.85	0.58
2:J:546:PRO:O	2:J:547:SER:HB2	2.03	0.58
2:L:159:ILE:HD12	2:L:166:ILE:HD11	1.84	0.58
2:L:54:HIS:HE1	2:L:56:THR:OG1	1.84	0.58
2:N:261:GLU:HG2	2:N:264:MET:HG3	1.85	0.58
1:A:102:ILE:HG13	1:A:117:THR:HB	1.84	0.58
2:B:367:GLN:O	2:B:371:ILE:HG22	2.04	0.58
2:H:371:ILE:CG2	2:H:375:GLN:HE21	2.14	0.58
2:H:392:ASN:HD21	2:H:422:LEU:HD13	1.68	0.58
2:J:422:LEU:HB3	2:J:423:PRO:HD3	1.85	0.58
2:J:440:ARG:HB3	2:J:467:TRP:CE3	2.36	0.58
2:P:301:LEU:HD23	2:P:324:GLU:HB3	1.85	0.58
1:C:27:GLN:HB2	1:C:109:ASN:HB3	1.85	0.58
2:F:80:LEU:HB2	2:F:122:MET:HE2	1.85	0.58
2:N:159:ILE:HD12	2:N:166:ILE:HD11	1.86	0.58
2:N:199:PHE:CE1	2:N:227:VAL:HG22	2.38	0.58
2:N:424:LEU:O	2:N:428:VAL:HG23	2.02	0.58
1:C:132:GLU:O	1:C:136:THR:HG23	2.03	0.58
2:H:509:VAL:HG21	2:H:535:MET:SD	2.43	0.58
1:M:148:GLU:HG2	1:M:152:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:MET:SD	1:O:117:THR:HG22	2.44	0.58
2:B:161:THR:HG22	2:B:186:GLU:HG2	1.86	0.58
1:A:158:ALA:HA	2:B:62:THR:HG21	1.85	0.58
1:C:48:THR:HG22	1:C:51:ILE:N	2.14	0.58
1:C:102:ILE:HG21	2:D:20:VAL:CG2	2.34	0.58
2:F:546:PRO:HG2	2:F:584:THR:CB	2.32	0.58
2:H:310:HIS:O	2:H:314:ILE:HG12	2.03	0.58
2:P:172:GLU:HG3	2:P:200:TYR:HB3	1.85	0.58
2:F:40:VAL:O	2:F:41:CYS:HB3	2.02	0.58
1:I:35:ASP:HB3	2:N:243:ALA:HB1	1.85	0.58
2:L:419:ILE:HD13	2:L:446:ARG:NH1	2.19	0.58
2:L:95:ASN:O	2:L:582:PRO:HG3	2.02	0.58
1:C:48:THR:HG22	1:C:51:ILE:HB	1.85	0.58
2:D:286:PRO:HA	2:D:289:PHE:CD2	2.38	0.58
1:E:153:ARG:HG2	1:E:157:TRP:CZ3	2.39	0.58
2:F:159:ILE:HD12	2:F:166:ILE:HD11	1.85	0.58
2:H:37:ALA:O	2:H:40:VAL:HG13	2.03	0.58
2:H:487:CYS:N	2:H:488:PRO:HD3	2.18	0.58
2:N:546:PRO:HG2	2:N:584:THR:CB	2.30	0.58
2:P:419:ILE:HD13	2:P:446:ARG:NH1	2.19	0.58
2:F:275:LEU:HD11	2:F:288:LEU:HD21	1.86	0.58
2:H:125:SER:HB3	2:H:127:LEU:N	2.18	0.58
2:H:382:TYR:C	2:H:382:TYR:CD1	2.77	0.58
2:N:440:ARG:HB3	2:N:467:TRP:CE3	2.39	0.58
2:B:159:ILE:HD11	2:B:169:LEU:HD13	1.86	0.58
2:F:133:ALA:HB2	2:F:159:ILE:HG22	1.86	0.58
2:H:99:TYR:CE2	2:H:123:ILE:HD12	2.39	0.58
2:J:431:LEU:HD12	2:J:431:LEU:O	2.04	0.58
2:L:307:THR:HG22	2:L:360:ASP:OD2	2.04	0.58
1:M:128:LYS:HB2	1:M:133:ILE:CD1	2.34	0.58
2:P:440:ARG:HB3	2:P:467:TRP:CE3	2.36	0.58
2:B:159:ILE:HD12	2:B:166:ILE:HD11	1.86	0.57
2:B:253:LEU:HD12	2:B:280:MET:HB2	1.86	0.57
2:D:386:TYR:CE1	4:D:1100:7JA:CG2	2.83	0.57
2:L:227:VAL:CG1	2:L:228:GLY:N	2.66	0.57
2:L:545:ILE:HB	2:L:567:HIS:HB2	1.85	0.57
2:N:431:LEU:HD12	2:N:431:LEU:O	2.04	0.57
2:D:454:GLY:O	2:D:457:TYR:HB2	2.04	0.57
2:J:227:VAL:HG13	2:J:228:GLY:N	2.19	0.57
2:P:133:ALA:HB2	2:P:159:ILE:HG22	1.85	0.57
2:P:397:SER:O	2:P:400:THR:HG22	2.04	0.57

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:386:TYR:HD2	2:H:413:LEU:HD21	1.70	0.56
2:J:519:TRP:CH2	2:J:567:HIS:ND1	2.73	0.56
1:C:40:ASN:HB3	1:K:13:GLY:O	2.04	0.56
2:L:592:ILE:HD12	2:L:592:ILE:H	1.70	0.56
2:N:533:MET:HE3	2:N:588:LEU:HD13	1.86	0.56
1:G:102:ILE:HG12	1:G:117:THR:OG1	2.06	0.56
2:H:136:ARG:NE	2:H:136:ARG:HA	2.19	0.56
2:H:216:ALA:HB2	2:H:238:PHE:CD1	2.40	0.56
2:J:54:HIS:HD2	2:J:77:SER:OG	1.88	0.56
2:L:386:TYR:CE1	4:L:1100:7JA:CG2	2.83	0.56
1:M:105:ALA:HB2	1:M:113:LEU:HD23	1.86	0.56
2:N:210:LYS:O	2:N:214:THR:HG22	2.05	0.56
1:C:52:LEU:O	1:C:56:ILE:HG13	2.06	0.56
2:D:121:ARG:HH22	5:D:1103:PO4:P	2.28	0.56
2:L:440:ARG:HB3	2:L:467:TRP:CE3	2.40	0.56
2:N:95:ASN:O	2:N:582:PRO:HG3	2.05	0.56
1:O:153:ARG:NH2	2:P:539:TYR:CE1	2.73	0.56
2:F:199:PHE:CE1	2:F:227:VAL:HG22	2.40	0.56
2:H:431:LEU:HD22	2:H:432:LEU:HD23	1.88	0.56
2:H:87:ALA:HB2	2:H:92:ILE:HB	1.87	0.56
2:J:159:ILE:HD12	2:J:166:ILE:HD11	1.86	0.56
2:J:231:GLU:HG2	2:J:254:ASN:ND2	2.20	0.56
2:J:547:SER:HB3	2:J:564:HIS:HB2	1.86	0.56
2:P:275:LEU:HD11	2:P:288:LEU:HD21	1.87	0.56
2:D:519:TRP:CZ3	2:D:567:HIS:ND1	2.73	0.56
2:D:533:MET:CE	2:D:588:LEU:HD13	2.36	0.56
2:H:444:TYR:HA	2:H:471:GLY:CA	2.31	0.56
2:J:396:GLU:HG2	2:J:430:SER:OG	2.06	0.56
2:N:171:MET:O	2:N:174:SER:HB2	2.06	0.56
2:B:444:TYR:HA	2:B:471:GLY:CA	2.30	0.56
1:G:124:MET:O	1:G:128:LYS:HE2	2.05	0.56
2:J:351:ARG:HD3	2:J:413:LEU:HD11	1.86	0.56
1:K:131:GLU:HA	1:K:131:GLU:OE2	2.05	0.56
2:N:57:MET:HE3	2:N:62:THR:HG22	1.87	0.56
2:B:547:SER:HB3	2:B:564:HIS:HB2	1.88	0.56
2:H:542:ILE:CD1	2:H:542:ILE:C	2.69	0.56
2:J:308:GLU:O	2:J:312:THR:HG23	2.06	0.56
2:J:456:SER:CB	2:J:482:GLU:HB3	2.36	0.56
2:L:199:PHE:CE1	2:L:227:VAL:HG22	2.41	0.56
2:L:547:SER:HB3	2:L:564:HIS:HB2	1.88	0.56
1:A:132:GLU:O	1:A:136:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:371:ILE:O	2:D:375:GLN:HG3	2.06	0.56
2:F:521:GLN:HG3	2:F:567:HIS:HD2	1.71	0.56
2:H:101:THR:HB	2:H:102:PRO:CD	2.36	0.56
2:H:170:LEU:HB2	2:H:198:ASN:HB3	1.88	0.56
2:J:261:GLU:HG2	2:J:264:MET:HG3	1.87	0.56
2:J:592:ILE:H	2:J:592:ILE:HD12	1.70	0.56
2:L:143:LEU:HD23	2:L:159:ILE:HD13	1.88	0.56
2:N:351:ARG:HD3	2:N:413:LEU:HD11	1.87	0.56
1:O:148:GLU:HG2	1:O:152:ARG:HH12	1.70	0.56
2:F:546:PRO:HD3	2:F:584:THR:O	2.06	0.56
2:H:156:LEU:O	2:H:160:VAL:HG22	2.05	0.56
2:H:542:ILE:HD12	2:H:543:GLU:N	2.21	0.56
2:L:386:TYR:HE1	4:L:1100:7JA:HG2	1.63	0.56
1:M:124:MET:O	1:M:128:LYS:HE2	2.04	0.56
1:M:99:PHE:HB2	2:N:15:ALA:HB3	1.88	0.56
1:O:27:GLN:HB2	1:O:109:ASN:HB3	1.86	0.56
2:P:307:THR:HG21	2:P:362:GLU:HB2	1.86	0.56
2:P:307:THR:HG22	2:P:360:ASP:OD2	2.06	0.56
2:D:412:LEU:HD12	2:D:412:LEU:C	2.25	0.56
2:D:456:SER:HB3	2:D:482:GLU:HB3	1.88	0.56
1:E:129:THR:O	1:E:133:ILE:HG12	2.06	0.56
2:F:412:LEU:O	2:F:412:LEU:HD12	2.05	0.56
2:H:259:MET:O	2:H:261:GLU:N	2.38	0.56
2:H:533:MET:HE1	2:H:588:LEU:HB3	1.88	0.56
1:I:27:GLN:HB2	1:I:109:ASN:HB3	1.88	0.56
2:J:456:SER:HB3	2:J:482:GLU:HB3	1.88	0.56
2:F:170:LEU:C	2:F:170:LEU:HD23	2.26	0.55
2:H:304:LEU:HD13	2:H:304:LEU:O	2.05	0.55
2:H:428:VAL:CG2	2:H:429:ARG:N	2.68	0.55
2:H:47:ILE:O	2:H:51:THR:HG23	2.05	0.55
2:L:170:LEU:HD23	2:L:170:LEU:C	2.26	0.55
2:N:546:PRO:HD3	2:N:584:THR:O	2.05	0.55
2:P:121:ARG:NH2	5:P:1103:PO4:O4	2.38	0.55
2:B:227:VAL:CG1	2:B:228:GLY:N	2.70	0.55
2:B:412:LEU:HD12	2:B:412:LEU:C	2.27	0.55
2:D:261:GLU:HG2	2:D:264:MET:HG3	1.87	0.55
2:F:533:MET:HE3	2:F:588:LEU:HD13	1.87	0.55
2:D:296:ARG:HH22	1:G:35:ASP:HB2	1.71	0.55
2:H:136:ARG:HG3	2:H:136:ARG:HH11	1.71	0.55
1:I:108:LEU:HD12	1:I:110:ILE:HD11	1.87	0.55
2:J:521:GLN:HG3	2:J:567:HIS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:521:GLN:HG3	2:J:567:HIS:CD2	2.42	0.55
2:N:472:TYR:OH	3:W:201:LEU:HB2	2.06	0.55
1:O:129:THR:O	1:O:133:ILE:HG12	2.06	0.55
2:D:301:LEU:HD23	2:D:324:GLU:HB3	1.88	0.55
2:H:322:VAL:HG12	2:H:323:LEU:N	2.19	0.55
2:J:121:ARG:NH2	5:J:1103:PO4:O4	2.39	0.55
2:N:327:ASN:HD22	2:N:328:VAL:N	2.04	0.55
2:N:80:LEU:HB2	2:N:122:MET:HE1	1.87	0.55
2:B:307:THR:HG22	2:B:360:ASP:OD2	2.05	0.55
1:E:105:ALA:HB2	1:E:113:LEU:HD23	1.88	0.55
2:L:533:MET:CE	2:L:588:LEU:HD13	2.36	0.55
2:L:546:PRO:O	2:L:547:SER:HB2	2.05	0.55
2:P:170:LEU:HD23	2:P:170:LEU:C	2.27	0.55
2:B:519:TRP:CH2	2:B:567:HIS:ND1	2.75	0.55
1:E:148:GLU:HG2	1:E:152:ARG:HH12	1.70	0.55
2:F:592:ILE:H	2:F:592:ILE:HD12	1.71	0.55
1:G:27:GLN:HB2	1:G:109:ASN:HB3	1.88	0.55
2:J:297:LYS:HE2	2:J:322:VAL:HG21	1.89	0.55
1:M:159:PHE:O	1:M:160:GLU:CB	2.52	0.55
2:N:172:GLU:HG3	2:N:200:TYR:HB3	1.89	0.55
1:A:153:ARG:HG2	1:A:157:TRP:CZ3	2.41	0.55
2:B:396:GLU:O	2:B:400:THR:HB	2.06	0.55
2:F:211:ASP:O	2:F:215:ILE:HG13	2.07	0.55
2:H:291:PHE:N	2:H:291:PHE:HD2	2.02	0.55
1:K:108:LEU:HD12	1:K:110:ILE:HD11	1.89	0.55
1:K:134:ARG:HH11	2:L:40:VAL:HA	1.72	0.55
2:N:519:TRP:NE1	4:N:1100:7JA:C01	2.61	0.55
2:H:286:PRO:O	2:H:288:LEU:N	2.40	0.55
2:H:305:LEU:CD2	2:H:305:LEU:H	2.14	0.55
2:H:419:ILE:HG13	2:H:419:ILE:O	2.06	0.55
2:H:84:PRO:HB3	2:H:517:TYR:OH	2.07	0.55
2:H:533:MET:CE	2:H:588:LEU:HD13	2.37	0.55
1:I:128:LYS:HB2	1:I:133:ILE:CD1	2.37	0.55
2:J:172:GLU:HG3	2:J:200:TYR:HB3	1.88	0.55
2:J:412:LEU:C	2:J:412:LEU:HD12	2.27	0.55
2:J:57:MET:HE3	2:J:62:THR:HG22	1.89	0.55
1:K:132:GLU:O	1:K:136:THR:HG23	2.06	0.55
1:M:102:ILE:HD12	2:N:20:VAL:CG2	2.24	0.55
1:O:113:LEU:O	1:O:113:LEU:CG	2.54	0.55
2:P:297:LYS:HE2	2:P:322:VAL:HG21	1.89	0.55
1:A:135:THR:HG22	1:A:136:THR:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:LEU:O	2:B:431:LEU:HD12	2.07	0.55
2:H:456:SER:OG	2:H:482:GLU:HB3	2.06	0.55
2:N:347:LEU:HD21	2:N:349:ILE:HD11	1.89	0.55
2:B:101:THR:CG2	2:B:128:ASP:OD1	2.51	0.55
2:F:521:GLN:HG3	2:F:567:HIS:CD2	2.42	0.55
1:G:159:PHE:O	1:G:160:GLU:HB2	2.05	0.55
2:D:296:ARG:NH2	1:G:37:CYS:SG	2.80	0.55
2:H:153:THR:HG23	2:H:178:GLU:HA	1.89	0.55
2:H:502:GLU:OE1	2:H:526:SER:HB2	2.07	0.55
2:J:419:ILE:CD1	2:J:446:ARG:HH12	2.20	0.55
2:P:191:ASN:ND2	2:P:194:LEU:H	2.04	0.55
1:A:102:ILE:HG12	1:A:117:THR:HB	1.87	0.55
2:B:275:LEU:HD11	2:B:288:LEU:HD21	1.89	0.55
2:D:93:PRO:HA	2:D:548:ARG:CB	2.28	0.55
1:E:132:GLU:O	1:E:136:THR:HG23	2.07	0.55
2:F:542:ILE:CD1	2:F:588:LEU:HD12	2.34	0.55
2:H:176:PHE:CZ	2:H:204:PHE:CZ	2.95	0.55
2:H:78:LEU:HD12	2:H:79:LYS:N	2.22	0.55
2:N:311:CYS:O	2:N:315:GLN:HB2	2.06	0.55
2:P:592:ILE:H	2:P:592:ILE:HD12	1.72	0.55
2:D:54:HIS:CD2	2:D:77:SER:OG	2.58	0.54
2:F:396:GLU:O	2:F:400:THR:HB	2.07	0.54
2:F:546:PRO:O	2:F:547:SER:HB2	2.06	0.54
2:H:138:ASP:OD2	2:H:164:ARG:HG3	2.07	0.54
2:H:284:GLU:CD	2:H:284:GLU:H	2.10	0.54
1:I:148:GLU:HG2	1:I:152:ARG:HH12	1.72	0.54
2:J:235:LEU:O	2:J:238:PHE:HB3	2.07	0.54
2:L:519:TRP:CH2	2:L:567:HIS:ND1	2.75	0.54
1:A:102:ILE:HG12	1:A:117:THR:CB	2.37	0.54
2:B:521:GLN:HG3	2:B:567:HIS:HD2	1.72	0.54
1:E:128:LYS:HB2	1:E:133:ILE:CD1	2.37	0.54
1:I:129:THR:O	1:I:133:ILE:HG12	2.06	0.54
1:I:26:SER:HG	1:I:108:LEU:HB3	1.72	0.54
1:M:125:ILE:HG23	1:M:133:ILE:CD1	2.36	0.54
2:N:419:ILE:HD13	2:N:446:ARG:NH1	2.21	0.54
1:A:99:PHE:HZ	1:A:137:PHE:HE1	1.55	0.54
1:C:134:ARG:HH11	2:D:40:VAL:HA	1.73	0.54
2:F:279:TYR:HA	2:F:304:LEU:HD22	1.89	0.54
2:H:232:ILE:HG13	2:H:253:LEU:HD23	1.89	0.54
2:H:49:SER:HB2	2:H:71:ARG:O	2.07	0.54
2:L:519:TRP:NE1	4:L:1100:7JA:C01	2.62	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:396:GLU:O	2:P:400:THR:HB	2.07	0.54
2:F:456:SER:CB	2:F:482:GLU:HB3	2.37	0.54
2:H:274:ARG:CG	2:H:297:LYS:HB3	2.27	0.54
2:H:83:LYS:HA	2:H:96:TRP:CZ3	2.43	0.54
1:C:12:ASP:OD2	1:C:49:SER:HB2	2.08	0.54
1:E:44:LEU:HD12	1:E:44:LEU:O	2.07	0.54
2:H:106:GLU:HA	2:H:106:GLU:OE1	2.08	0.54
1:M:48:THR:HG22	1:M:51:ILE:CB	2.38	0.54
1:O:128:LYS:HB2	1:O:133:ILE:CD1	2.38	0.54
4:D:1100:7JA:OXT	4:D:1100:7JA:CG2	2.53	0.54
1:E:135:THR:HG22	1:E:136:THR:N	2.21	0.54
2:F:253:LEU:HD12	2:F:280:MET:HB2	1.89	0.54
2:F:367:GLN:O	2:F:371:ILE:HG22	2.07	0.54
2:J:103:TRP:O	2:J:107:ILE:HG13	2.08	0.54
2:P:547:SER:HB3	2:P:564:HIS:HB2	1.90	0.54
2:P:519:TRP:CH2	2:P:567:HIS:ND1	2.76	0.54
2:B:255:GLU:HG3	2:B:255:GLU:O	2.08	0.54
2:H:492:LYS:NZ	2:H:516:ARG:NH1	2.54	0.54
2:J:357:GLY:HA2	2:J:415:ARG:NH2	2.20	0.54
2:L:396:GLU:O	2:L:400:THR:HB	2.07	0.54
2:B:297:LYS:HE2	2:B:322:VAL:HG21	1.90	0.54
2:H:391:THR:O	2:H:395:LEU:HD23	2.07	0.54
2:J:397:SER:O	2:J:400:THR:HG22	2.08	0.54
2:P:533:MET:CE	2:P:588:LEU:HD13	2.38	0.54
1:A:27:GLN:HB2	1:A:109:ASN:HB3	1.90	0.54
2:B:233:LEU:O	2:B:236:VAL:HG23	2.06	0.54
2:D:227:VAL:CG1	2:D:228:GLY:N	2.70	0.54
2:H:328:VAL:HG13	2:H:359:GLU:CG	2.37	0.54
1:I:105:ALA:HB2	1:I:113:LEU:HD23	1.89	0.54
1:I:48:THR:HG22	1:I:51:ILE:HB	1.90	0.54
2:J:101:THR:OG1	2:J:102:PRO:HD3	2.08	0.54
2:J:519:TRP:NE1	4:J:1100:7JA:C01	2.60	0.54
1:M:148:GLU:HG2	1:M:152:ARG:NH1	2.23	0.54
2:P:176:PHE:CZ	2:P:204:PHE:CZ	2.96	0.54
2:P:227:VAL:CG1	2:P:228:GLY:N	2.69	0.54
2:P:308:GLU:O	2:P:312:THR:HG23	2.08	0.54
2:P:424:LEU:O	2:P:428:VAL:HG23	2.07	0.54
2:D:121:ARG:NH2	5:D:1103:PO4:O4	2.41	0.54
2:D:456:SER:CB	2:D:482:GLU:HB3	2.38	0.54
2:D:492:LYS:HE3	2:D:517:TYR:CE2	2.43	0.54
2:D:54:HIS:HE1	2:D:56:THR:OG1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:CYS:SG	2:L:296:ARG:NH2	2.81	0.54
2:F:542:ILE:HG13	2:F:588:LEU:HB2	1.90	0.54
2:H:533:MET:CE	2:H:588:LEU:HB3	2.37	0.54
2:L:279:TYR:HA	2:L:304:LEU:HD22	1.90	0.54
2:N:307:THR:HG22	2:N:360:ASP:OD2	2.07	0.54
2:B:171:MET:O	2:B:174:SER:HB2	2.08	0.53
2:B:261:GLU:HG2	2:B:264:MET:HG3	1.90	0.53
2:B:357:GLY:HA2	2:B:415:ARG:NH2	2.23	0.53
2:D:159:ILE:HD11	2:D:169:LEU:HD13	1.90	0.53
2:D:422:LEU:HB3	2:D:423:PRO:HD3	1.89	0.53
2:F:227:VAL:CG1	2:F:228:GLY:N	2.72	0.53
2:H:118:HIS:HE1	2:H:146:ASP:OD2	1.90	0.53
1:I:132:GLU:O	1:I:136:THR:HG23	2.09	0.53
1:E:107:TYR:HE1	2:L:294:GLN:HE22	1.56	0.53
2:P:422:LEU:HB3	2:P:423:PRO:HD3	1.90	0.53
2:P:54:HIS:HD2	2:P:77:SER:OG	1.90	0.53
4:B:1100:7JA:O	4:B:1100:7JA:CG2	2.52	0.53
2:D:231:GLU:HG2	2:D:254:ASN:ND2	2.22	0.53
1:E:158:ALA:HA	2:F:62:THR:HG21	1.89	0.53
2:H:268:PHE:O	2:H:270:ARG:N	2.41	0.53
1:I:105:ALA:HB3	1:I:114:LEU:CD1	2.38	0.53
2:J:386:TYR:CE1	4:J:1100:7JA:CG2	2.86	0.53
1:A:48:THR:HG22	1:A:51:ILE:N	2.20	0.53
2:B:121:ARG:HH22	5:B:1103:PO4:P	2.32	0.53
2:H:390:ILE:HB	2:H:395:LEU:HD21	1.90	0.53
2:L:227:VAL:HG13	2:L:228:GLY:H	1.73	0.53
2:L:412:LEU:HD12	2:L:412:LEU:C	2.29	0.53
2:N:465:VAL:HG11	2:N:468:MET:HG3	1.90	0.53
2:N:547:SER:HB3	2:N:564:HIS:HB2	1.90	0.53
2:F:351:ARG:HG3	2:F:351:ARG:O	2.09	0.53
2:F:422:LEU:HB3	2:F:423:PRO:HD3	1.91	0.53
2:J:289:PHE:N	2:J:290:PRO:HD2	2.23	0.53
2:J:371:ILE:O	2:J:375:GLN:HG3	2.08	0.53
1:C:114:LEU:C	1:C:116:LEU:H	2.12	0.53
1:C:153:ARG:HG2	1:C:157:TRP:CZ3	2.44	0.53
1:C:159:PHE:O	1:C:160:GLU:CB	2.55	0.53
1:E:134:ARG:HH11	2:F:40:VAL:HA	1.74	0.53
1:E:27:GLN:HB2	1:E:109:ASN:HB3	1.90	0.53
2:H:18:ASP:OD2	2:H:43:ARG:NH1	2.34	0.53
1:I:102:ILE:CG1	1:I:117:THR:HB	2.38	0.53
2:L:542:ILE:CG1	2:L:588:LEU:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:545:ILE:HG22	2:N:546:PRO:N	2.24	0.53
2:P:412:LEU:C	2:P:412:LEU:HD12	2.28	0.53
2:B:103:TRP:O	2:B:107:ILE:HG13	2.08	0.53
2:B:191:ASN:ND2	2:B:194:LEU:H	2.06	0.53
2:B:456:SER:CB	2:B:482:GLU:HB3	2.38	0.53
1:I:52:LEU:O	1:I:56:ILE:HG13	2.09	0.53
2:F:113:GLN:HE22	2:L:192:THR:CB	2.21	0.53
2:L:465:VAL:HG11	2:L:468:MET:HG3	1.91	0.53
1:O:52:LEU:O	1:O:56:ILE:HG13	2.09	0.53
2:P:367:GLN:HB3	2:P:391:THR:HG22	1.91	0.53
2:P:521:GLN:HG3	2:P:567:HIS:HD2	1.73	0.53
2:P:533:MET:HE3	2:P:588:LEU:HD13	1.89	0.53
1:A:101:LEU:HB3	1:A:117:THR:HG21	1.91	0.53
2:D:235:LEU:O	2:D:238:PHE:HB3	2.09	0.53
2:D:396:GLU:HG2	2:D:430:SER:OG	2.08	0.53
1:E:159:PHE:O	1:E:160:GLU:CB	2.57	0.53
2:F:307:THR:HG22	2:F:360:ASP:OD2	2.09	0.53
2:F:547:SER:HB3	2:F:564:HIS:HB2	1.90	0.53
2:H:262:LYS:HD2	2:H:263:TYR:CZ	2.44	0.53
2:H:366:SER:C	2:H:368:ARG:N	2.60	0.53
2:H:365:VAL:HG12	2:H:370:LEU:HG	1.89	0.53
2:H:503:ARG:HE	2:H:503:ARG:H	1.57	0.53
2:L:255:GLU:HG3	2:L:255:GLU:O	2.08	0.53
2:L:289:PHE:N	2:L:290:PRO:HD2	2.24	0.53
2:L:547:SER:HB3	2:L:564:HIS:CB	2.39	0.53
1:A:159:PHE:O	1:A:160:GLU:CB	2.57	0.53
2:D:101:THR:OG1	2:N:179:LYS:NZ	2.42	0.53
2:D:397:SER:O	2:D:400:THR:HG22	2.09	0.53
1:E:48:THR:HG22	1:E:51:ILE:N	2.19	0.53
1:G:48:THR:HG22	1:G:51:ILE:CB	2.38	0.53
2:J:78:LEU:HD12	2:J:79:LYS:H	1.74	0.53
2:N:197:LEU:O	2:N:225:VAL:HA	2.09	0.53
2:P:78:LEU:HD12	2:P:79:LYS:H	1.73	0.53
2:B:231:GLU:HG2	2:B:254:ASN:ND2	2.24	0.53
2:B:95:ASN:O	2:B:582:PRO:HG3	2.08	0.53
2:D:161:THR:HG22	2:D:186:GLU:HG2	1.90	0.53
2:F:397:SER:O	2:F:400:THR:HG22	2.09	0.53
2:H:327:ASN:HD22	2:H:364:LEU:HD21	1.73	0.53
2:P:253:LEU:HD12	2:P:280:MET:HB2	1.91	0.53
2:B:422:LEU:HB3	2:B:423:PRO:HD3	1.91	0.53
2:B:456:SER:HB3	2:B:482:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLU:HG2	1:E:152:ARG:NH1	2.24	0.53
2:F:542:ILE:CG1	2:F:588:LEU:HB2	2.39	0.53
2:H:418:ARG:HB3	2:H:421:ASP:HB2	1.91	0.53
1:G:153:ARG:NH2	2:H:539:TYR:CE1	2.76	0.53
2:J:422:LEU:O	2:J:423:PRO:C	2.45	0.53
1:K:27:GLN:HB2	1:K:109:ASN:HB3	1.89	0.53
2:L:542:ILE:HG13	2:L:588:LEU:HB2	1.91	0.53
2:B:472:TYR:OH	3:Q:201:LEU:HB2	2.08	0.53
1:E:141:ASN:C	1:E:141:ASN:OD1	2.47	0.52
2:H:269:PRO:O	2:H:271:LYS:N	2.42	0.52
2:H:363:GLY:O	2:H:365:VAL:N	2.42	0.52
2:H:428:VAL:HG12	2:H:443:PHE:CE1	2.44	0.52
2:H:91:LEU:HD21	2:H:496:ARG:NH2	2.23	0.52
2:J:311:CYS:CB	2:J:336:VAL:HG21	2.38	0.52
2:J:547:SER:HB3	2:J:564:HIS:CB	2.38	0.52
2:L:371:ILE:O	2:L:375:GLN:HG3	2.08	0.52
2:N:121:ARG:HH22	5:N:1103:PO4:P	2.32	0.52
2:P:519:TRP:CZ3	2:P:567:HIS:ND1	2.77	0.52
1:A:12:ASP:OD2	1:A:49:SER:HB2	2.10	0.52
2:B:386:TYR:CE1	4:B:1100:7JA:CG2	2.87	0.52
1:C:148:GLU:HG2	1:C:152:ARG:HH12	1.74	0.52
2:J:545:ILE:HG22	2:J:546:PRO:N	2.25	0.52
1:K:46:ASN:HB2	1:K:107:TYR:CZ	2.44	0.52
2:F:161:THR:HG22	2:F:186:GLU:HG2	1.90	0.52
2:H:447:GLN:HG3	2:H:447:GLN:O	2.09	0.52
2:J:138:ASP:OD2	2:J:164:ARG:HG3	2.08	0.52
2:P:357:GLY:HA2	2:P:415:ARG:NH2	2.22	0.52
2:D:279:TYR:HA	2:D:304:LEU:HD22	1.89	0.52
2:F:396:GLU:HG2	2:F:430:SER:OG	2.09	0.52
2:F:54:HIS:HD2	2:F:77:SER:OG	1.93	0.52
2:J:170:LEU:HD23	2:J:170:LEU:C	2.30	0.52
2:J:171:MET:O	2:J:174:SER:HB2	2.09	0.52
4:L:1100:7JA:CG2	4:L:1100:7JA:OXT	2.55	0.52
1:M:87:ASP:HB3	1:M:116:LEU:HD21	1.92	0.52
1:O:148:GLU:HG2	1:O:152:ARG:NH1	2.24	0.52
2:P:386:TYR:CE1	4:P:1100:7JA:CG2	2.88	0.52
2:B:545:ILE:HG22	2:B:546:PRO:N	2.23	0.52
1:E:105:ALA:HB3	1:E:114:LEU:CD1	2.40	0.52
2:F:357:GLY:HA2	2:F:415:ARG:NH2	2.24	0.52
2:F:519:TRP:CH2	2:F:567:HIS:ND1	2.77	0.52
1:I:46:ASN:HB2	1:I:107:TYR:CZ	2.44	0.52

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:HIS:HD2	2:B:77:SER:OG	1.93	0.51
1:C:125:ILE:HG23	1:C:133:ILE:CD1	2.34	0.51
1:I:124:MET:O	1:I:128:LYS:HE2	2.09	0.51
2:J:367:GLN:HB3	2:J:391:THR:HG22	1.92	0.51
1:M:102:ILE:CB	2:N:20:VAL:CG2	2.87	0.51
1:M:44:LEU:HD12	1:M:44:LEU:O	2.11	0.51
1:O:134:ARG:HH11	2:P:40:VAL:HA	1.75	0.51
1:O:132:GLU:O	1:O:136:THR:HG23	2.09	0.51
2:P:399:GLY:O	2:P:434:GLY:HA3	2.10	0.51
2:P:542:ILE:HG13	2:P:588:LEU:HB2	1.92	0.51
2:D:365:VAL:CG2	2:D:387:VAL:HA	2.40	0.51
2:H:91:LEU:HD21	2:H:496:ARG:HH22	1.75	0.51
1:I:148:GLU:HG2	1:I:152:ARG:NH1	2.25	0.51
2:J:301:LEU:HD23	2:J:324:GLU:HB3	1.91	0.51
2:J:542:ILE:HG13	2:J:588:LEU:HB2	1.92	0.51
2:L:233:LEU:O	2:L:236:VAL:HG23	2.09	0.51
2:L:54:HIS:CD2	2:L:77:SER:OG	2.63	0.51
2:N:289:PHE:N	2:N:290:PRO:HD2	2.25	0.51
2:N:592:ILE:H	2:N:592:ILE:HD12	1.75	0.51
2:B:296:ARG:HH22	1:O:35:ASP:HB2	1.74	0.51
2:P:57:MET:HE3	2:P:62:THR:HG22	1.92	0.51
2:B:521:GLN:HG3	2:B:567:HIS:CD2	2.45	0.51
1:C:135:THR:HG22	1:C:136:THR:N	2.25	0.51
2:D:547:SER:HB3	2:D:564:HIS:CB	2.40	0.51
2:H:178:GLU:CD	2:H:206:LYS:HB3	2.30	0.51
2:H:199:PHE:CE1	2:H:227:VAL:CG2	2.92	0.51
2:J:197:LEU:O	2:J:225:VAL:HA	2.11	0.51
2:L:133:ALA:HB2	2:L:159:ILE:HG22	1.92	0.51
2:P:311:CYS:CB	2:P:336:VAL:HG21	2.41	0.51
2:P:396:GLU:HG2	2:P:430:SER:OG	2.10	0.51
2:B:176:PHE:CZ	2:B:204:PHE:CZ	2.99	0.51
2:D:592:ILE:H	2:D:592:ILE:HD12	1.76	0.51
2:F:301:LEU:HD23	2:F:324:GLU:HB3	1.93	0.51
2:F:419:ILE:CD1	2:F:446:ARG:HH12	2.23	0.51
1:G:108:LEU:HD12	1:G:110:ILE:HD11	1.93	0.51
2:H:256:ASP:OD2	2:H:259:MET:HG2	2.10	0.51
1:G:160:GLU:HG2	2:H:52:ARG:HH21	1.76	0.51
2:J:389:ASP:OD2	2:J:419:ILE:HG23	2.10	0.51
2:L:57:MET:HE3	2:L:62:THR:HG22	1.92	0.51
2:N:231:GLU:HG2	2:N:254:ASN:ND2	2.25	0.51
2:P:248:PHE:CD2	2:P:248:PHE:C	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:547:SER:HB3	2:P:564:HIS:CB	2.41	0.51
2:B:170:LEU:HD23	2:B:170:LEU:C	2.31	0.51
2:B:289:PHE:N	2:B:290:PRO:CD	2.73	0.51
1:C:108:LEU:HD12	1:C:110:ILE:HD11	1.92	0.51
1:E:124:MET:O	1:E:128:LYS:HE2	2.10	0.51
2:H:101:THR:HB	2:H:102:PRO:HD2	1.91	0.51
2:H:405:LEU:HD13	2:H:408:PHE:HB2	1.91	0.51
2:J:392:ASN:HD21	2:J:424:LEU:HA	1.75	0.51
2:L:65:PRO:HG3	2:L:103:TRP:CE2	2.46	0.51
2:N:357:GLY:HA2	2:N:415:ARG:NH2	2.24	0.51
2:P:519:TRP:NE1	4:P:1100:7JA:C01	2.65	0.51
2:B:157:LEU:O	2:B:161:THR:HG23	2.11	0.51
2:D:297:LYS:HE2	2:D:322:VAL:HG21	1.92	0.51
2:F:412:LEU:C	2:F:412:LEU:HD12	2.30	0.51
2:H:247:GLU:HA	2:H:274:ARG:O	2.10	0.51
2:H:459:GLY:O	2:H:486:GLY:HA3	2.10	0.51
1:I:105:ALA:HB3	1:I:114:LEU:HD12	1.92	0.51
2:L:357:GLY:HA2	2:L:415:ARG:NH2	2.21	0.51
2:L:521:GLN:HG3	2:L:567:HIS:HD2	1.75	0.51
1:M:135:THR:HG22	1:M:136:THR:N	2.25	0.51
1:A:48:THR:HG22	1:A:51:ILE:CB	2.40	0.51
1:C:129:THR:O	1:C:133:ILE:HG12	2.11	0.51
1:E:131:GLU:OE2	1:E:131:GLU:HA	2.11	0.51
2:F:172:GLU:HG3	2:F:200:TYR:HB3	1.91	0.51
2:J:519:TRP:CZ3	2:J:567:HIS:ND1	2.78	0.51
1:K:135:THR:HG22	1:K:136:THR:N	2.25	0.51
1:M:58:TYR:CD2	1:M:113:LEU:HD13	2.46	0.51
2:D:422:LEU:O	2:D:423:PRO:C	2.48	0.51
2:D:542:ILE:HG13	2:D:588:LEU:HB2	1.93	0.51
1:E:30:ALA:C	1:E:32:MET:H	2.15	0.51
2:F:171:MET:O	2:F:174:SER:HB2	2.10	0.51
1:G:153:ARG:HB3	2:H:574:LEU:HD21	1.93	0.51
2:H:124:VAL:O	2:H:151:PHE:HB3	2.11	0.51
2:J:227:VAL:CG1	2:J:228:GLY:N	2.73	0.51
2:L:289:PHE:N	2:L:290:PRO:CD	2.74	0.51
2:B:547:SER:HB3	2:B:564:HIS:CB	2.40	0.51
1:C:128:LYS:HB2	1:C:133:ILE:CD1	2.41	0.51
1:E:48:THR:HG22	1:E:51:ILE:CB	2.39	0.51
2:F:440:ARG:HB3	2:F:467:TRP:CE3	2.46	0.51
2:H:107:ILE:HG12	2:H:114:LEU:HD22	1.92	0.51
2:J:327:ASN:HD22	2:J:328:VAL:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:176:PHE:CZ	2:L:204:PHE:CZ	2.98	0.51
1:M:48:THR:HG22	1:M:51:ILE:N	2.21	0.51
1:M:99:PHE:CE2	2:N:16:THR:C	2.84	0.51
2:N:279:TYR:HA	2:N:304:LEU:HD22	1.93	0.51
2:B:293:ALA:HB3	1:O:45:PRO:HG3	1.93	0.51
2:P:521:GLN:HG3	2:P:567:HIS:CD2	2.45	0.51
2:B:539:TYR:OH	1:C:146:GLU:HA	2.10	0.51
2:F:328:VAL:CG2	2:F:359:GLU:HB2	2.41	0.51
2:F:482:GLU:O	2:F:485:ARG:HG2	2.11	0.51
1:G:28:THR:O	1:G:32:MET:HE2	2.11	0.51
2:H:337:LEU:HD11	2:H:344:LEU:HD22	1.93	0.51
2:H:542:ILE:HD11	2:H:588:LEU:CB	2.41	0.51
2:L:301:LEU:HD23	2:L:324:GLU:HB3	1.92	0.51
2:N:83:LYS:HA	2:N:96:TRP:CZ3	2.46	0.51
2:P:327:ASN:HD22	2:P:328:VAL:N	2.08	0.51
2:P:365:VAL:CG2	2:P:387:VAL:HA	2.41	0.51
2:B:57:MET:HE3	2:B:62:THR:HG22	1.92	0.50
1:G:151:VAL:HG12	2:H:39:LEU:HD21	1.86	0.50
2:L:422:LEU:HB3	2:L:423:PRO:HD3	1.93	0.50
2:N:227:VAL:HG13	2:N:228:GLY:N	2.26	0.50
1:O:102:ILE:HD12	2:P:20:VAL:HG21	1.91	0.50
2:B:351:ARG:HG3	2:B:351:ARG:O	2.11	0.50
2:F:22:GLU:HG2	2:F:47:ILE:CD1	2.41	0.50
2:F:547:SER:HB3	2:F:564:HIS:CB	2.42	0.50
2:H:232:ILE:HG13	2:H:253:LEU:HD21	1.93	0.50
2:H:332:ARG:O	2:H:336:VAL:HG23	2.11	0.50
1:I:102:ILE:HG13	1:I:117:THR:HB	1.94	0.50
1:I:106:ASN:N	1:I:114:LEU:HD13	2.26	0.50
2:J:191:ASN:ND2	2:J:194:LEU:HB2	2.27	0.50
2:J:40:VAL:O	2:J:41:CYS:HB3	2.11	0.50
1:K:125:ILE:HG23	1:K:133:ILE:CD1	2.38	0.50
2:N:159:ILE:HD11	2:N:169:LEU:HD13	1.92	0.50
2:N:255:GLU:O	2:N:255:GLU:HG3	2.11	0.50
1:A:52:LEU:O	1:A:56:ILE:HG13	2.11	0.50
2:D:253:LEU:HD12	2:D:280:MET:HB2	1.93	0.50
2:F:121:ARG:NH2	5:F:1103:PO4:O4	2.43	0.50
2:H:366:SER:HB3	2:H:368:ARG:CG	2.25	0.50
1:K:48:THR:HG22	1:K:51:ILE:CB	2.42	0.50
2:D:396:GLU:O	2:D:400:THR:HB	2.12	0.50
2:F:191:ASN:ND2	2:F:194:LEU:H	2.08	0.50
2:H:303:ALA:HB1	2:H:305:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:519:TRP:CZ3	2:L:567:HIS:ND1	2.79	0.50
2:N:253:LEU:HD12	2:N:280:MET:HB2	1.92	0.50
2:P:311:CYS:O	2:P:315:GLN:HB2	2.12	0.50
1:A:141:ASN:OD1	1:A:141:ASN:C	2.50	0.50
2:F:54:HIS:HE1	2:F:56:THR:OG1	1.95	0.50
2:H:76:ARG:HG2	2:H:76:ARG:HH11	1.76	0.50
2:J:191:ASN:ND2	2:J:194:LEU:H	2.08	0.50
1:M:12:ASP:OD2	1:M:49:SER:HB2	2.12	0.50
2:P:83:LYS:HA	2:P:96:TRP:CZ3	2.47	0.50
2:B:270:ARG:HB3	1:O:107:TYR:CD1	2.47	0.50
2:B:78:LEU:HD12	2:B:79:LYS:H	1.77	0.50
2:F:80:LEU:O	2:F:122:MET:HE2	2.12	0.50
2:H:587:VAL:O	2:H:587:VAL:HG12	2.10	0.50
1:I:48:THR:HG22	1:I:51:ILE:N	2.18	0.50
2:N:321:GLU:HA	2:N:344:LEU:HA	1.92	0.50
2:N:412:LEU:HD12	2:N:412:LEU:C	2.32	0.50
2:N:519:TRP:CZ3	2:N:567:HIS:ND1	2.80	0.50
2:N:54:HIS:HD2	2:N:77:SER:OG	1.94	0.50
2:B:399:GLY:O	2:B:434:GLY:HA3	2.12	0.50
1:G:52:LEU:O	1:G:56:ILE:HG13	2.11	0.50
1:I:101:LEU:HB3	1:I:117:THR:HG21	1.93	0.50
2:J:220:ARG:HH21	2:N:22:GLU:HB3	1.76	0.50
2:L:159:ILE:HD11	2:L:169:LEU:HD13	1.94	0.50
2:L:40:VAL:O	2:L:41:CYS:HB3	2.10	0.50
2:N:101:THR:OG1	2:N:102:PRO:HD3	2.12	0.50
2:N:35:ASP:O	2:N:38:SER:OG	2.29	0.50
2:D:197:LEU:O	2:D:225:VAL:HA	2.11	0.50
1:E:52:LEU:O	1:E:56:ILE:HG13	2.11	0.50
2:H:462:SER:HB2	2:H:465:VAL:HB	1.92	0.50
2:J:546:PRO:HG2	2:J:584:THR:CB	2.38	0.50
1:K:52:LEU:O	1:K:56:ILE:HG13	2.12	0.50
2:L:261:GLU:HG2	2:L:264:MET:HG3	1.94	0.50
2:L:311:CYS:CB	2:L:336:VAL:HG21	2.42	0.50
1:M:108:LEU:HD12	1:M:110:ILE:HD11	1.93	0.50
1:M:99:PHE:CD2	2:N:16:THR:O	2.65	0.50
2:P:261:GLU:HG2	2:P:264:MET:HG3	1.93	0.50
1:A:148:GLU:HG2	1:A:152:ARG:HH12	1.76	0.50
2:B:519:TRP:NE1	4:B:1100:7JA:C01	2.62	0.50
2:B:492:LYS:HE3	2:B:517:TYR:CE2	2.47	0.50
2:B:542:ILE:CG1	2:B:588:LEU:HB2	2.42	0.50
2:D:80:LEU:CB	2:D:122:MET:HE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:542:ILE:CG1	2:D:588:LEU:HB2	2.42	0.50
2:H:40:VAL:HG11	2:H:44:TRP:CE3	2.46	0.50
2:J:226:LYS:HA	2:J:249:CYS:O	2.12	0.50
1:I:158:ALA:HA	2:J:62:THR:CG2	2.42	0.50
2:L:503:ARG:NH1	2:L:503:ARG:HB3	2.27	0.50
2:P:156:LEU:O	2:P:160:VAL:HG22	2.12	0.50
2:B:386:TYR:HE1	4:B:1100:7JA:HG2	1.70	0.49
2:B:542:ILE:HG13	2:B:588:LEU:HB2	1.94	0.49
2:F:297:LYS:HG3	2:F:322:VAL:HB	1.92	0.49
2:F:22:GLU:HG2	2:F:47:ILE:HD13	1.94	0.49
2:H:100:VAL:CG2	2:H:119:PHE:CE1	2.95	0.49
2:H:331:ASP:OD1	2:H:366:SER:N	2.44	0.49
1:I:26:SER:OG	1:I:108:LEU:HB3	2.12	0.49
1:M:111:LYS:O	1:M:114:LEU:HB2	2.11	0.49
1:O:105:ALA:HB2	1:O:113:LEU:HD23	1.93	0.49
2:P:546:PRO:HD3	2:P:584:THR:O	2.11	0.49
2:B:22:GLU:HG2	2:B:47:ILE:CD1	2.42	0.49
2:B:289:PHE:N	2:B:290:PRO:HD2	2.27	0.49
1:C:44:LEU:O	1:C:44:LEU:HD12	2.12	0.49
2:D:296:ARG:NE	1:G:37:CYS:SG	2.85	0.49
2:F:176:PHE:CZ	2:F:204:PHE:CZ	3.01	0.49
2:H:85:ARG:HB3	2:H:85:ARG:CZ	2.41	0.49
1:I:44:LEU:O	1:I:44:LEU:HD12	2.12	0.49
2:J:365:VAL:CG2	2:J:387:VAL:HA	2.41	0.49
2:J:22:GLU:OE1	2:J:43:ARG:NH2	2.45	0.49
2:L:85:ARG:NH2	4:L:1100:7JA:O14	2.40	0.49
2:L:545:ILE:HG22	2:L:546:PRO:N	2.27	0.49
2:N:233:LEU:O	2:N:236:VAL:HG23	2.12	0.49
2:N:547:SER:HB3	2:N:564:HIS:CB	2.42	0.49
2:N:78:LEU:HD12	2:N:79:LYS:H	1.77	0.49
1:O:48:THR:HG22	1:O:51:ILE:CB	2.40	0.49
1:A:108:LEU:HD12	1:A:110:ILE:HD11	1.95	0.49
1:A:153:ARG:NH2	2:B:539:TYR:CE1	2.81	0.49
2:D:357:GLY:HA2	2:D:415:ARG:NH2	2.25	0.49
2:H:277:LEU:O	2:H:278:SER:C	2.51	0.49
2:H:385:VAL:HG13	2:H:387:VAL:HG23	1.94	0.49
2:N:22:GLU:HG2	2:N:47:ILE:HD13	1.93	0.49
2:N:519:TRP:CH2	2:N:567:HIS:CG	3.00	0.49
2:D:176:PHE:CZ	2:D:204:PHE:CZ	3.00	0.49
2:D:533:MET:HE3	2:D:588:LEU:HD13	1.93	0.49
2:F:85:ARG:NH2	4:F:1100:7JA:O14	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:365:VAL:CG2	2:F:387:VAL:HA	2.41	0.49
2:H:100:VAL:HG11	2:H:124:VAL:HG22	1.94	0.49
1:G:137:PHE:CD1	2:H:17:VAL:HG13	2.48	0.49
2:H:298:LEU:HD22	2:H:300:LEU:HG	1.94	0.49
2:H:543:GLU:C	2:H:544:LEU:HD23	2.32	0.49
1:K:12:ASP:OD2	1:K:49:SER:HB2	2.11	0.49
2:P:199:PHE:CZ	2:P:227:VAL:HG22	2.47	0.49
1:A:44:LEU:HD12	1:A:44:LEU:O	2.13	0.49
2:H:176:PHE:HZ	2:H:204:PHE:CZ	2.30	0.49
2:H:64:THR:O	2:H:65:PRO:C	2.47	0.49
2:P:168:THR:HB	2:P:196:VAL:CG1	2.17	0.49
2:B:301:LEU:HD23	2:B:324:GLU:HB3	1.94	0.49
2:B:327:ASN:HD22	2:B:328:VAL:N	2.11	0.49
2:H:153:THR:CG2	2:H:178:GLU:HA	2.41	0.49
2:H:390:ILE:HD11	2:H:410:LEU:HD11	1.94	0.49
2:H:428:VAL:O	2:H:432:LEU:HG	2.13	0.49
2:J:133:ALA:HB2	2:J:159:ILE:HG22	1.94	0.49
2:L:161:THR:HG22	2:L:186:GLU:HG2	1.93	0.49
2:L:311:CYS:O	2:L:315:GLN:HB2	2.13	0.49
2:L:80:LEU:O	2:L:122:MET:HE2	2.12	0.49
2:N:22:GLU:HG2	2:N:47:ILE:CD1	2.43	0.49
2:N:275:LEU:HD11	2:N:288:LEU:CD2	2.43	0.49
2:N:533:MET:CE	2:N:588:LEU:HD13	2.42	0.49
2:B:422:LEU:O	2:B:423:PRO:C	2.51	0.49
2:D:419:ILE:CD1	2:D:446:ARG:HH12	2.24	0.49
2:F:121:ARG:HH22	5:F:1103:PO4:P	2.36	0.49
2:H:373:LEU:C	2:H:373:LEU:HD12	2.32	0.49
2:H:395:LEU:N	2:H:395:LEU:HD22	2.28	0.49
1:I:159:PHE:O	1:I:160:GLU:CB	2.59	0.49
2:J:253:LEU:HD12	2:J:280:MET:HB2	1.93	0.49
2:J:337:LEU:HD12	2:J:341:CYS:SG	2.53	0.49
2:D:275:LEU:HD11	2:D:288:LEU:HD21	1.94	0.49
2:H:478:GLU:O	2:H:482:GLU:HG2	2.13	0.49
2:L:542:ILE:HD11	2:L:588:LEU:CD1	2.31	0.49
1:M:52:LEU:O	1:M:56:ILE:HG13	2.12	0.49
2:N:124:VAL:O	2:N:151:PHE:HB3	2.12	0.49
2:N:116:SER:CB	2:N:142:THR:HG23	2.32	0.49
1:A:46:ASN:HB2	1:A:107:TYR:CZ	2.47	0.49
2:D:199:PHE:CE1	2:D:227:VAL:HG22	2.48	0.49
2:D:444:TYR:HA	2:D:471:GLY:CA	2.31	0.49
1:G:102:ILE:HG21	2:H:20:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:386:TYR:CD2	2:H:413:LEU:HD21	2.48	0.49
2:H:65:PRO:HA	2:H:103:TRP:CZ3	2.48	0.49
2:D:311:CYS:O	2:D:315:GLN:HB2	2.13	0.49
2:F:233:LEU:O	2:F:236:VAL:HG23	2.13	0.49
2:F:367:GLN:HB3	2:F:391:THR:HG22	1.95	0.49
2:F:399:GLY:O	2:F:434:GLY:HA3	2.13	0.49
2:H:170:LEU:HD23	2:H:170:LEU:C	2.33	0.49
1:I:160:GLU:CG	2:J:31:PRO:HB3	2.43	0.49
2:L:156:LEU:O	2:L:160:VAL:HG22	2.13	0.49
2:N:40:VAL:O	2:N:41:CYS:HB3	2.13	0.49
2:B:275:LEU:HD11	2:B:288:LEU:CD2	2.42	0.48
1:C:30:ALA:C	1:C:32:MET:H	2.16	0.48
2:F:519:TRP:CZ3	2:F:567:HIS:ND1	2.81	0.48
2:H:119:PHE:O	2:H:146:ASP:HB3	2.13	0.48
2:H:331:ASP:OD2	2:H:366:SER:CB	2.59	0.48
2:H:465:VAL:HG11	2:H:468:MET:HG2	1.95	0.48
2:J:542:ILE:CG1	2:J:588:LEU:HB2	2.43	0.48
2:N:65:PRO:HG3	2:N:103:TRP:CE2	2.48	0.48
1:O:137:PHE:CD1	2:P:17:VAL:HG21	2.47	0.48
2:P:152:THR:HG22	2:P:177:SER:HB2	1.95	0.48
2:P:171:MET:O	2:P:174:SER:HB2	2.12	0.48
2:P:22:GLU:HG2	2:P:47:ILE:HD13	1.94	0.48
2:D:57:MET:HE3	2:D:62:THR:HG22	1.95	0.48
2:F:519:TRP:NE1	4:F:1100:7JA:C01	2.65	0.48
2:H:292:ALA:HA	2:H:295:ILE:HG12	1.95	0.48
2:H:542:ILE:HG12	2:H:588:LEU:HB2	1.92	0.48
2:L:347:LEU:HD21	2:L:349:ILE:HD11	1.94	0.48
1:K:158:ALA:HA	2:L:62:THR:CG2	2.43	0.48
2:P:80:LEU:O	2:P:122:MET:HE2	2.13	0.48
2:B:297:LYS:HG3	2:B:322:VAL:HB	1.95	0.48
2:D:542:ILE:CD1	2:D:588:LEU:HD12	2.38	0.48
2:F:327:ASN:HD22	2:F:328:VAL:N	2.11	0.48
2:N:103:TRP:O	2:N:107:ILE:HG13	2.13	0.48
2:N:392:ASN:HD21	2:N:424:LEU:HA	1.78	0.48
2:N:432:LEU:CD1	2:N:458:ILE:HA	2.44	0.48
2:B:20:VAL:O	2:B:24:VAL:HG23	2.13	0.48
2:B:365:VAL:CG2	2:B:387:VAL:HA	2.41	0.48
1:C:134:ARG:HB2	1:C:139:ILE:O	2.14	0.48
2:D:211:ASP:O	2:D:215:ILE:HG13	2.13	0.48
2:D:247:GLU:HA	2:D:274:ARG:O	2.14	0.48
2:D:280:MET:O	2:D:280:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:465:VAL:HG11	2:J:468:MET:HG3	1.95	0.48
1:K:128:LYS:HB2	1:K:133:ILE:CD1	2.44	0.48
1:E:35:ASP:HB2	2:L:296:ARG:HH22	1.79	0.48
2:L:365:VAL:CG2	2:L:387:VAL:HA	2.43	0.48
1:M:160:GLU:CG	2:N:31:PRO:HB3	2.43	0.48
2:N:422:LEU:HB3	2:N:423:PRO:HD3	1.94	0.48
1:O:12:ASP:OD2	1:O:49:SER:HB2	2.13	0.48
2:P:492:LYS:HE3	2:P:517:TYR:CE2	2.48	0.48
1:A:148:GLU:HG2	1:A:152:ARG:NH1	2.27	0.48
2:D:255:GLU:O	2:D:255:GLU:HG3	2.12	0.48
2:D:296:ARG:CZ	1:G:37:CYS:SG	3.01	0.48
2:D:519:TRP:CH2	2:D:567:HIS:CG	3.01	0.48
2:F:315:GLN:HG2	2:F:340:TYR:CE1	2.49	0.48
1:G:30:ALA:C	1:G:32:MET:H	2.17	0.48
1:I:134:ARG:HH11	2:J:40:VAL:HA	1.78	0.48
2:J:396:GLU:O	2:J:400:THR:HB	2.12	0.48
1:K:141:ASN:OD1	1:K:141:ASN:C	2.52	0.48
2:L:308:GLU:O	2:L:312:THR:HG23	2.13	0.48
2:L:396:GLU:HG2	2:L:430:SER:OG	2.13	0.48
2:L:521:GLN:HG3	2:L:567:HIS:CD2	2.48	0.48
1:M:46:ASN:HB2	1:M:107:TYR:CZ	2.48	0.48
2:N:422:LEU:O	2:N:423:PRO:C	2.50	0.48
2:P:231:GLU:HG2	2:P:254:ASN:ND2	2.28	0.48
4:B:1100:7JA:H04	4:B:1100:7JA:H12A	1.69	0.48
2:B:197:LEU:O	2:B:225:VAL:HA	2.14	0.48
2:H:343:GLN:N	2:H:343:GLN:CD	2.67	0.48
2:H:392:ASN:ND2	2:H:422:LEU:HD13	2.28	0.48
2:L:297:LYS:HE3	2:L:297:LYS:HB2	1.66	0.48
2:N:503:ARG:HB3	2:N:503:ARG:NH1	2.29	0.48
2:F:235:LEU:O	2:F:238:PHE:HB3	2.13	0.48
1:G:129:THR:OG1	1:G:132:GLU:HG3	2.14	0.48
2:H:442:ALA:CB	4:H:1100:7JA:HD1	2.25	0.48
2:H:412:LEU:HD13	2:H:446:ARG:NH2	2.28	0.48
2:N:542:ILE:CG1	2:N:588:LEU:HB2	2.44	0.48
2:P:233:LEU:O	2:P:236:VAL:HG23	2.13	0.48
2:B:133:ALA:HB2	2:B:159:ILE:HG22	1.96	0.48
2:B:396:GLU:HG2	2:B:430:SER:OG	2.14	0.48
2:D:40:VAL:O	2:D:41:CYS:HB3	2.14	0.48
2:F:311:CYS:O	2:F:315:GLN:HB2	2.14	0.48
2:F:465:VAL:HG11	2:F:468:MET:HG3	1.96	0.48
2:H:356:GLN:O	2:H:357:GLY:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:176:PHE:CZ	2:J:204:PHE:CZ	3.01	0.48
2:N:519:TRP:CZ3	2:N:567:HIS:CG	3.01	0.48
1:O:124:MET:O	1:O:128:LYS:HE2	2.14	0.48
2:P:465:VAL:HG11	2:P:468:MET:HG3	1.96	0.48
2:D:190:HIS:HB3	2:H:112:ARG:HD2	1.94	0.48
2:D:248:PHE:CD2	2:D:248:PHE:C	2.86	0.48
2:D:20:VAL:O	2:D:24:VAL:HG23	2.13	0.48
2:D:492:LYS:HG3	2:D:517:TYR:CD2	2.49	0.48
1:E:134:ARG:HB2	1:E:139:ILE:O	2.12	0.48
2:F:247:GLU:HA	2:F:274:ARG:O	2.14	0.48
2:J:80:LEU:HB2	2:J:122:MET:HE2	1.91	0.48
2:L:519:TRP:CH2	2:L:567:HIS:CG	3.02	0.48
2:N:492:LYS:HG3	2:N:517:TYR:CD2	2.49	0.48
2:P:321:GLU:HA	2:P:344:LEU:HA	1.94	0.48
2:P:422:LEU:O	2:P:423:PRO:C	2.51	0.48
2:P:46:LYS:HB2	2:P:46:LYS:HE3	1.49	0.48
2:B:156:LEU:O	2:B:160:VAL:HG22	2.14	0.48
1:K:114:LEU:C	1:K:116:LEU:H	2.16	0.48
2:P:328:VAL:CG2	2:P:359:GLU:HB2	2.43	0.48
2:P:546:PRO:HG2	2:P:584:THR:CB	2.37	0.48
1:A:30:ALA:C	1:A:32:MET:H	2.17	0.47
2:B:519:TRP:CH2	2:B:567:HIS:CG	3.02	0.47
1:C:28:THR:O	1:C:32:MET:HE2	2.13	0.47
2:F:351:ARG:HD3	2:F:413:LEU:HD11	1.95	0.47
1:G:10:SER:OG	1:G:11:SER:N	2.47	0.47
2:H:395:LEU:HD23	2:H:395:LEU:H	1.79	0.47
2:H:71:ARG:HG2	2:H:72:PHE:CD1	2.49	0.47
2:J:248:PHE:CD2	2:J:248:PHE:C	2.87	0.47
2:J:285:MET:N	2:J:286:PRO:CD	2.77	0.47
2:J:22:GLU:HG2	2:J:47:ILE:HD13	1.96	0.47
2:L:171:MET:O	2:L:174:SER:HB2	2.13	0.47
2:L:419:ILE:CD1	2:L:446:ARG:HH12	2.27	0.47
1:M:141:ASN:C	1:M:141:ASN:OD1	2.51	0.47
2:N:542:ILE:HG13	2:N:588:LEU:HB2	1.95	0.47
2:P:289:PHE:N	2:P:290:PRO:CD	2.77	0.47
2:P:503:ARG:HB3	2:P:503:ARG:NH1	2.28	0.47
4:F:1100:7JA:OXT	4:F:1100:7JA:CG2	2.54	0.47
2:F:275:LEU:HD11	2:F:288:LEU:CD2	2.44	0.47
2:H:101:THR:CB	2:H:102:PRO:CD	2.91	0.47
2:H:121:ARG:HA	2:H:147:LYS:O	2.13	0.47
2:H:391:THR:O	2:H:392:ASN:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:THR:O	1:I:32:MET:HE2	2.14	0.47
4:J:1100:7JA:OXT	4:J:1100:7JA:CG2	2.56	0.47
2:J:143:LEU:CD2	2:J:159:ILE:HD13	2.44	0.47
2:J:152:THR:HG22	2:J:177:SER:HB2	1.96	0.47
1:K:148:GLU:HG2	1:K:152:ARG:HH12	1.79	0.47
1:O:28:THR:O	1:O:32:MET:HE2	2.13	0.47
2:F:197:LEU:O	2:F:225:VAL:HA	2.14	0.47
2:F:289:PHE:N	2:F:290:PRO:HD2	2.30	0.47
2:N:389:ASP:OD2	2:N:419:ILE:HG23	2.14	0.47
2:D:124:VAL:O	2:D:151:PHE:HB3	2.15	0.47
2:F:157:LEU:O	2:F:161:THR:HG23	2.14	0.47
1:G:82:ASP:O	1:G:85:ALA:HB3	2.14	0.47
2:H:386:TYR:HB3	2:H:413:LEU:HD21	1.97	0.47
1:M:134:ARG:NE	1:M:141:ASN:HB2	2.30	0.47
2:N:153:THR:HG23	2:N:178:GLU:HA	1.95	0.47
3:Q:212:PHE:CD2	3:Q:213:LEU:HD23	2.48	0.47
2:B:297:LYS:HB2	2:B:297:LYS:HE3	1.57	0.47
1:C:124:MET:O	1:C:128:LYS:HE2	2.14	0.47
2:H:153:THR:HG23	2:H:177:SER:O	2.14	0.47
2:H:201:MET:HG3	2:H:302:TYR:CD1	2.49	0.47
2:H:59:LEU:HD22	2:H:61:TYR:HB2	1.96	0.47
2:J:289:PHE:N	2:J:290:PRO:CD	2.76	0.47
2:N:297:LYS:HB2	2:N:297:LYS:HE3	1.68	0.47
2:N:328:VAL:CG2	2:N:359:GLU:HB2	2.44	0.47
1:A:129:THR:O	1:A:133:ILE:HG12	2.14	0.47
1:C:153:ARG:NH2	2:D:539:TYR:CE1	2.83	0.47
2:D:289:PHE:N	2:D:290:PRO:HD2	2.29	0.47
2:F:443:PHE:HE2	2:F:445:LEU:HD11	1.75	0.47
2:H:512:LEU:HA	2:H:513:PRO:HD3	1.64	0.47
2:J:221:SER:O	2:J:223:VAL:HG23	2.15	0.47
1:K:153:ARG:NH2	2:L:539:TYR:CE1	2.83	0.47
2:L:46:LYS:HE3	2:L:46:LYS:HB2	1.53	0.47
2:N:468:MET:CE	2:N:470:LEU:HD11	2.43	0.47
2:N:55:VAL:CG2	2:N:75:LEU:HD21	2.41	0.47
2:P:289:PHE:N	2:P:290:PRO:HD2	2.28	0.47
2:P:366:SER:HB2	2:P:367:GLN:OE1	2.15	0.47
1:C:148:GLU:HG2	1:C:152:ARG:NH1	2.29	0.47
2:D:275:LEU:HD11	2:D:288:LEU:CD2	2.44	0.47
2:H:392:ASN:HD22	2:H:392:ASN:H	1.62	0.47
2:J:444:TYR:HA	2:J:471:GLY:CA	2.36	0.47
1:M:28:THR:O	1:M:32:MET:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:191:ASN:ND2	2:N:194:LEU:HB2	2.30	0.47
2:P:329:ILE:O	2:P:333:GLY:HA3	2.14	0.47
2:B:46:LYS:HB2	2:B:46:LYS:HE3	1.47	0.47
1:C:48:THR:HG22	1:C:51:ILE:CB	2.44	0.47
2:D:285:MET:N	2:D:286:PRO:CD	2.78	0.47
2:F:308:GLU:O	2:F:312:THR:HG23	2.14	0.47
2:H:492:LYS:HZ1	2:H:516:ARG:HH11	1.59	0.47
2:J:83:LYS:HA	2:J:96:TRP:CZ3	2.49	0.47
2:F:112:ARG:CG	2:L:164:ARG:HD2	2.42	0.47
2:N:512:LEU:HA	2:N:513:PRO:HD2	1.77	0.47
1:O:46:ASN:HB2	1:O:107:TYR:CZ	2.50	0.47
2:P:161:THR:HG22	2:P:186:GLU:HG2	1.96	0.47
2:P:227:VAL:HG13	2:P:228:GLY:H	1.79	0.47
4:B:1100:7JA:O	4:B:1100:7JA:HG2A	2.10	0.47
2:D:96:TRP:O	2:D:578:ARG:NH2	2.39	0.47
2:F:57:MET:HE3	2:F:62:THR:HG22	1.96	0.47
2:H:390:ILE:CD1	2:H:410:LEU:HD11	2.45	0.47
2:H:442:ALA:CB	4:H:1100:7JA:H28	2.44	0.47
2:H:85:ARG:O	2:H:88:MET:HG2	2.15	0.47
1:I:141:ASN:C	1:I:141:ASN:OD1	2.52	0.47
2:L:78:LEU:HD21	2:L:80:LEU:HD21	1.96	0.47
1:M:153:ARG:CG	1:M:157:TRP:CZ3	2.98	0.47
2:P:101:THR:OG1	2:P:102:PRO:HD3	2.15	0.47
2:P:22:GLU:HG2	2:P:47:ILE:CD1	2.45	0.47
2:P:286:PRO:CA	2:P:289:PHE:CE2	2.92	0.47
2:F:503:ARG:HB3	2:F:503:ARG:NH1	2.29	0.47
2:H:286:PRO:C	2:H:288:LEU:N	2.69	0.47
2:H:423:PRO:HA	2:H:449:GLY:O	2.15	0.47
2:J:270:ARG:O	1:M:46:ASN:OD1	2.33	0.47
2:L:248:PHE:C	2:L:248:PHE:CD2	2.88	0.47
2:L:492:LYS:HE3	2:L:517:TYR:CE2	2.50	0.47
2:B:101:THR:OG1	2:B:102:PRO:HD3	2.15	0.47
2:B:199:PHE:CE1	2:B:227:VAL:HG22	2.49	0.47
2:B:465:VAL:HG11	2:B:468:MET:HG3	1.97	0.47
1:C:113:LEU:O	1:C:117:THR:CG2	2.63	0.47
2:F:103:TRP:O	2:F:107:ILE:HG13	2.15	0.47
1:G:134:ARG:HD3	2:H:40:VAL:O	2.15	0.47
2:H:136:ARG:HG3	2:H:136:ARG:NH1	2.30	0.47
2:H:185:HIS:O	2:H:188:ALA:HB3	2.15	0.47
2:H:95:ASN:HD22	2:H:95:ASN:N	2.12	0.47
1:K:114:LEU:C	1:K:116:LEU:N	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:546:PRO:HG2	2:L:584:THR:CB	2.36	0.47
2:N:337:LEU:HD12	2:N:341:CYS:SG	2.55	0.47
2:P:419:ILE:CD1	2:P:446:ARG:HH12	2.26	0.47
2:P:519:TRP:CH2	2:P:567:HIS:CE1	2.99	0.47
2:B:492:LYS:HG3	2:B:517:TYR:CD2	2.50	0.46
2:B:519:TRP:CH2	2:B:567:HIS:CE1	2.99	0.46
1:C:58:TYR:CD2	1:C:113:LEU:HD13	2.50	0.46
1:E:113:LEU:O	1:E:113:LEU:CG	2.63	0.46
2:L:422:LEU:O	2:L:423:PRO:C	2.53	0.46
2:P:545:ILE:HG22	2:P:546:PRO:N	2.30	0.46
2:D:190:HIS:HE1	2:H:110:ASN:HA	1.81	0.46
2:D:289:PHE:N	2:D:290:PRO:CD	2.78	0.46
2:F:101:THR:OG1	2:F:102:PRO:HD3	2.15	0.46
1:G:105:ALA:HB2	1:G:113:LEU:HD23	1.97	0.46
1:G:12:ASP:OD2	1:G:49:SER:HB2	2.14	0.46
1:G:83:LEU:HD23	1:G:83:LEU:HA	1.77	0.46
1:I:44:LEU:HA	1:I:45:PRO:HD3	1.71	0.46
2:N:248:PHE:C	2:N:248:PHE:CD2	2.88	0.46
2:N:367:GLN:HG2	2:N:391:THR:HB	1.96	0.46
2:P:285:MET:N	2:P:286:PRO:CD	2.78	0.46
2:P:347:LEU:HD21	2:P:349:ILE:HD11	1.95	0.46
2:H:476:SER:C	2:H:478:GLU:N	2.67	0.46
2:H:519:TRP:HH2	2:H:567:HIS:ND1	2.00	0.46
2:H:59:LEU:CD2	2:H:61:TYR:HB2	2.45	0.46
2:L:546:PRO:HD3	2:L:584:THR:O	2.14	0.46
1:M:128:LYS:HB2	1:M:133:ILE:HD11	1.97	0.46
1:M:134:ARG:HH11	2:N:40:VAL:HA	1.80	0.46
2:P:477:ASP:OD1	2:P:477:ASP:N	2.48	0.46
2:P:492:LYS:HG3	2:P:517:TYR:CD2	2.50	0.46
1:A:128:LYS:HB2	1:A:133:ILE:CD1	2.46	0.46
1:I:12:ASP:OD2	1:I:49:SER:HB2	2.16	0.46
1:M:102:ILE:HB	2:N:20:VAL:CG2	2.46	0.46
1:A:160:GLU:CG	2:B:31:PRO:HB3	2.45	0.46
2:B:321:GLU:HA	2:B:344:LEU:HA	1.96	0.46
2:D:156:LEU:O	2:D:160:VAL:HG22	2.15	0.46
2:H:266:LEU:CD1	2:H:267:VAL:H	2.26	0.46
1:I:135:THR:HG22	1:I:136:THR:N	2.31	0.46
2:J:321:GLU:HA	2:J:344:LEU:HA	1.97	0.46
2:J:54:HIS:CE1	2:J:56:THR:OG1	2.66	0.46
2:L:321:GLU:HA	2:L:344:LEU:HA	1.97	0.46
1:M:158:ALA:HA	2:N:62:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:GLU:O	2:B:312:THR:HG23	2.16	0.46
1:C:93:ILE:CD1	1:C:97:THR:HG22	2.42	0.46
2:D:367:GLN:HB3	2:D:391:THR:HG22	1.98	0.46
1:C:158:ALA:HA	2:D:62:THR:CG2	2.45	0.46
2:F:124:VAL:O	2:F:151:PHE:HB3	2.16	0.46
2:F:444:TYR:HA	2:F:471:GLY:CA	2.33	0.46
2:F:55:VAL:CG2	2:F:75:LEU:HD21	2.45	0.46
2:H:347:LEU:HD12	2:H:347:LEU:C	2.33	0.46
2:H:39:LEU:HA	2:H:39:LEU:HD23	1.56	0.46
2:L:387:VAL:HG22	2:L:389:ASP:H	1.79	0.46
4:N:1100:7JA:H05	4:N:1100:7JA:H27	1.74	0.46
2:N:419:ILE:CD1	2:N:446:ARG:HH12	2.29	0.46
4:P:1100:7JA:CG2	4:P:1100:7JA:OXT	2.58	0.46
2:B:235:LEU:O	2:B:238:PHE:HB3	2.16	0.46
1:A:158:ALA:HA	2:B:62:THR:CG2	2.46	0.46
2:H:278:SER:C	2:H:280:MET:H	2.19	0.46
2:J:472:TYR:OH	3:U:201:LEU:HB2	2.16	0.46
2:L:399:GLY:O	2:L:434:GLY:HA3	2.16	0.46
2:D:103:TRP:O	2:D:107:ILE:HG13	2.14	0.46
2:D:465:VAL:HG11	2:D:468:MET:HG3	1.98	0.46
2:F:519:TRP:CH2	2:F:567:HIS:CE1	3.03	0.46
2:F:83:LYS:HA	2:F:96:TRP:CZ3	2.51	0.46
2:D:296:ARG:NH1	1:G:35:ASP:OD1	2.41	0.46
2:H:168:THR:HB	2:H:196:VAL:CG1	2.45	0.46
2:H:494:GLU:HA	2:H:519:TRP:O	2.15	0.46
2:H:533:MET:O	2:H:535:MET:N	2.46	0.46
1:I:134:ARG:NE	1:I:141:ASN:HB2	2.31	0.46
1:K:148:GLU:HG2	1:K:152:ARG:NH1	2.31	0.46
1:K:30:ALA:C	1:K:32:MET:H	2.19	0.46
2:L:22:GLU:HG2	2:L:47:ILE:CD1	2.45	0.46
2:P:153:THR:HG23	2:P:178:GLU:HA	1.97	0.46
2:P:226:LYS:HA	2:P:249:CYS:O	2.15	0.46
3:V:201:LEU:HD23	3:V:201:LEU:HA	1.72	0.46
2:D:191:ASN:ND2	2:D:194:LEU:HB2	2.30	0.46
2:H:108:SER:OG	2:H:135:ALA:HB2	2.16	0.46
2:H:366:SER:OG	2:H:368:ARG:HG2	2.16	0.46
2:H:59:LEU:CD2	2:H:61:TYR:H	2.29	0.46
1:M:134:ARG:HB2	1:M:139:ILE:O	2.15	0.46
2:P:194:LEU:HD12	2:P:194:LEU:HA	1.81	0.46
2:P:297:LYS:HE3	2:P:297:LYS:HB2	1.68	0.46
2:P:332:ARG:O	2:P:336:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:40:VAL:O	2:P:41:CYS:HB3	2.16	0.46
2:P:542:ILE:CD1	2:P:588:LEU:HD12	2.36	0.46
3:S:201:LEU:HD23	3:S:201:LEU:HA	1.61	0.46
1:E:160:GLU:CG	2:F:31:PRO:HB3	2.45	0.46
2:F:564:HIS:HA	2:F:565:PRO:HD2	1.76	0.46
2:H:94:GLU:CG	2:H:95:ASN:H	2.29	0.46
2:J:329:ILE:O	2:J:333:GLY:HA3	2.16	0.46
2:J:542:ILE:CD1	2:J:588:LEU:HD12	2.36	0.46
1:K:134:ARG:HB2	1:K:139:ILE:O	2.16	0.46
1:K:160:GLU:CG	2:L:31:PRO:HB3	2.46	0.46
2:N:443:PHE:HE2	2:N:445:LEU:HD11	1.80	0.46
2:N:519:TRP:CZ3	2:N:567:HIS:HB3	2.51	0.46
2:N:519:TRP:CH2	2:N:567:HIS:CE1	3.02	0.46
1:O:42:VAL:HA	1:O:43:PRO:HD3	1.82	0.46
2:P:432:LEU:CD1	2:P:458:ILE:HA	2.46	0.46
2:B:419:ILE:HD11	2:B:446:ARG:NH2	2.27	0.45
2:H:317:CYS:O	2:H:320:LEU:HB2	2.16	0.45
2:H:327:ASN:HA	2:H:349:ILE:CG2	2.46	0.45
2:J:20:VAL:O	2:J:24:VAL:HG23	2.16	0.45
2:L:285:MET:N	2:L:286:PRO:CD	2.79	0.45
2:N:338:ALA:O	2:N:376:GLY:HA3	2.16	0.45
1:O:30:ALA:C	1:O:32:MET:H	2.20	0.45
2:P:211:ASP:HA	2:P:214:THR:CG2	2.43	0.45
2:P:275:LEU:HD11	2:P:288:LEU:CD2	2.46	0.45
2:L:172:GLU:HG3	2:L:200:TYR:HB3	1.96	0.45
1:A:102:ILE:HG12	1:A:117:THR:OG1	2.16	0.45
2:B:310:HIS:HE1	2:B:325:THR:OG1	1.98	0.45
2:B:431:LEU:CD1	2:B:435:CYS:SG	3.04	0.45
2:D:133:ALA:HB2	2:D:159:ILE:HG22	1.98	0.45
1:E:130:PRO:O	1:E:134:ARG:HG2	2.16	0.45
2:F:255:GLU:O	2:F:255:GLU:HG3	2.16	0.45
2:H:351:ARG:HG3	2:H:359:GLU:HB3	1.97	0.45
2:H:375:GLN:HG2	2:H:401:TYR:CE1	2.51	0.45
2:J:164:ARG:HE	2:N:112:ARG:HG2	1.69	0.45
2:J:495:MET:O	2:J:520:VAL:HA	2.16	0.45
2:L:194:LEU:HD12	2:L:194:LEU:HA	1.74	0.45
1:M:103:LEU:HD11	2:N:19:ASP:HB3	1.98	0.45
2:N:20:VAL:O	2:N:24:VAL:HG23	2.17	0.45
2:P:159:ILE:HD11	2:P:169:LEU:HD13	1.99	0.45
3:X:201:LEU:HD23	3:X:201:LEU:HA	1.69	0.45
2:D:191:ASN:ND2	2:D:194:LEU:H	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:GLU:HA	2:D:344:LEU:HA	1.98	0.45
2:F:168:THR:HB	2:F:196:VAL:CG1	2.20	0.45
2:F:321:GLU:HA	2:F:344:LEU:HA	1.99	0.45
1:G:137:PHE:CD1	2:H:17:VAL:CG1	3.00	0.45
2:H:16:THR:O	2:H:17:VAL:C	2.54	0.45
2:H:314:ILE:HG22	2:H:341:CYS:SG	2.56	0.45
2:H:327:ASN:HD22	2:H:364:LEU:CD2	2.30	0.45
2:J:298:LEU:HD12	2:J:298:LEU:HA	1.67	0.45
2:J:311:CYS:O	2:J:315:GLN:HB2	2.16	0.45
1:K:134:ARG:NE	1:K:141:ASN:HB2	2.31	0.45
2:L:22:GLU:OE1	2:L:43:ARG:NH2	2.49	0.45
2:L:275:LEU:HD11	2:L:288:LEU:HD21	1.97	0.45
2:L:367:GLN:HG2	2:L:391:THR:HB	1.98	0.45
1:K:158:ALA:CB	2:L:62:THR:HG23	2.47	0.45
2:N:310:HIS:HE1	2:N:325:THR:OG1	2.00	0.45
2:N:451:THR:HA	2:N:475:GLU:HG3	1.98	0.45
3:R:201:LEU:HD23	3:R:201:LEU:HA	1.74	0.45
2:B:503:ARG:HB3	2:B:503:ARG:NH1	2.31	0.45
2:D:101:THR:OG1	2:D:102:PRO:HD3	2.17	0.45
2:D:194:LEU:HA	2:D:194:LEU:HD12	1.80	0.45
2:D:297:LYS:HG3	2:D:322:VAL:HB	1.98	0.45
2:D:351:ARG:HG3	2:D:351:ARG:O	2.16	0.45
2:F:20:VAL:O	2:F:24:VAL:HG23	2.17	0.45
2:F:329:ILE:O	2:F:333:GLY:HA3	2.17	0.45
2:H:230:PHE:CD1	2:H:235:LEU:HD21	2.39	0.45
2:P:54:HIS:CE1	2:P:56:THR:OG1	2.66	0.45
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.84	0.45
2:B:114:LEU:O	2:B:136:ARG:NH1	2.48	0.45
2:B:545:ILE:HA	2:B:546:PRO:HD3	1.76	0.45
2:B:546:PRO:HG2	2:B:584:THR:CB	2.42	0.45
2:D:22:GLU:OE1	2:D:43:ARG:NH2	2.49	0.45
2:D:329:ILE:O	2:D:333:GLY:HA3	2.17	0.45
2:F:240:LYS:CG	2:F:267:VAL:HG21	2.44	0.45
2:F:387:VAL:HG22	2:F:389:ASP:H	1.80	0.45
2:H:32:LYS:HA	2:H:32:LYS:HD3	1.49	0.45
2:J:399:GLY:O	2:J:434:GLY:HA3	2.17	0.45
2:J:519:TRP:CH2	2:J:567:HIS:CG	3.04	0.45
2:J:54:HIS:CD2	2:J:77:SER:OG	2.69	0.45
1:K:44:LEU:HD12	1:K:44:LEU:O	2.17	0.45
2:L:54:HIS:CE1	2:L:56:THR:OG1	2.69	0.45
2:N:404:ASN:HA	2:N:437:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:65:PRO:HA	2:N:103:TRP:CZ3	2.52	0.45
1:O:105:ALA:HB3	1:O:114:LEU:HD13	1.98	0.45
2:P:95:ASN:O	2:P:582:PRO:HG3	2.17	0.45
2:P:63:ALA:HB1	2:P:67:ARG:HD2	1.99	0.45
2:D:546:PRO:HG2	2:D:584:THR:CB	2.40	0.45
4:F:1100:7JA:OXT	4:F:1100:7JA:HG2A	2.13	0.45
2:J:199:PHE:CZ	2:J:227:VAL:HG22	2.52	0.45
2:J:419:ILE:O	2:J:420:THR:C	2.55	0.45
1:I:153:ARG:NH2	2:J:539:TYR:CE1	2.85	0.45
2:L:305:LEU:H	2:L:305:LEU:HD22	1.80	0.45
1:M:112:ASN:O	1:M:114:LEU:N	2.46	0.45
2:N:343:GLN:O	2:N:345:LYS:HG2	2.17	0.45
2:P:255:GLU:O	2:P:255:GLU:HG3	2.16	0.45
2:P:512:LEU:HA	2:P:513:PRO:HD2	1.76	0.45
3:R:212:PHE:CD2	3:R:213:LEU:HD23	2.52	0.45
1:E:128:LYS:HB2	1:E:133:ILE:HD11	1.99	0.45
4:F:1100:7JA:H05	4:F:1100:7JA:H27	1.65	0.45
1:E:137:PHE:CD1	2:F:17:VAL:HG21	2.52	0.45
2:H:100:VAL:HG21	2:H:119:PHE:CZ	2.51	0.45
2:H:455:LEU:HA	2:H:455:LEU:HD23	1.66	0.45
4:J:1100:7JA:HG2A	4:J:1100:7JA:OXT	2.12	0.45
1:K:124:MET:O	1:K:128:LYS:HE2	2.16	0.45
2:L:80:LEU:HD12	2:L:122:MET:HE1	1.97	0.45
2:N:199:PHE:CZ	2:N:227:VAL:HG22	2.52	0.45
2:N:247:GLU:HA	2:N:274:ARG:O	2.16	0.45
2:N:398:ILE:CG2	2:N:402:LEU:HD11	2.45	0.45
2:B:245:LEU:HA	2:B:245:LEU:HD12	1.80	0.45
1:A:134:ARG:NH1	2:B:40:VAL:HA	2.31	0.45
2:D:419:ILE:HD11	2:D:446:ARG:NH2	2.25	0.45
1:E:91:MET:HG3	1:E:116:LEU:HD11	1.98	0.45
2:F:153:THR:HG23	2:F:178:GLU:HA	1.99	0.45
2:F:392:ASN:HD21	2:F:424:LEU:HA	1.82	0.45
2:F:545:ILE:HG22	2:F:546:PRO:N	2.32	0.45
2:H:100:VAL:HG23	2:H:122:MET:HE2	1.98	0.45
2:H:371:ILE:HG22	2:H:375:GLN:NE2	2.20	0.45
1:I:128:LYS:HB2	1:I:133:ILE:HD11	1.99	0.45
2:J:80:LEU:O	2:J:122:MET:HE2	2.16	0.45
1:K:153:ARG:HG2	1:K:157:TRP:CZ3	2.52	0.45
2:N:301:LEU:CD2	2:N:324:GLU:HB3	2.46	0.45
2:N:91:LEU:O	2:N:567:HIS:HE1	2.00	0.45
1:A:8:LEU:HD23	1:A:42:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:LYS:HE3	2:F:46:LYS:HB2	1.56	0.45
2:H:477:ASP:HB3	2:H:504:ALA:CB	2.47	0.45
2:J:275:LEU:HD11	2:J:288:LEU:CD2	2.46	0.45
2:J:37:ALA:O	2:J:40:VAL:HG13	2.17	0.45
1:M:30:ALA:C	1:M:32:MET:H	2.21	0.45
1:O:134:ARG:HB2	1:O:139:ILE:O	2.17	0.45
1:O:160:GLU:CG	2:P:31:PRO:HB3	2.47	0.45
2:P:431:LEU:CD1	2:P:435:CYS:SG	3.05	0.45
2:D:172:GLU:HG3	2:D:200:TYR:HB3	1.99	0.44
2:D:429:ARG:HG2	2:D:433:ILE:HD11	1.99	0.44
2:H:314:ILE:C	2:H:316:LYS:H	2.18	0.44
2:H:310:HIS:NE2	2:H:328:VAL:HG23	2.31	0.44
2:H:410:LEU:HD13	2:H:411:VAL:N	2.32	0.44
1:I:134:ARG:HB2	1:I:139:ILE:O	2.17	0.44
1:I:158:ALA:CB	2:J:62:THR:HG23	2.47	0.44
1:M:99:PHE:HZ	2:N:17:VAL:HG22	1.82	0.44
1:O:141:ASN:OD1	1:O:141:ASN:C	2.55	0.44
2:P:301:LEU:CD2	2:P:324:GLU:HB3	2.47	0.44
2:P:405:LEU:HA	2:P:405:LEU:HD23	1.80	0.44
2:B:419:ILE:CD1	2:B:446:ARG:HH12	2.27	0.44
2:H:142:THR:HA	2:H:168:THR:O	2.17	0.44
2:H:156:LEU:HD11	2:H:171:MET:HE3	2.00	0.44
2:H:161:THR:HG22	2:H:186:GLU:HG2	1.99	0.44
1:M:111:LYS:O	1:M:114:LEU:CB	2.65	0.44
2:N:469:LEU:HA	2:N:494:GLU:O	2.17	0.44
2:P:101:THR:CG2	2:P:128:ASP:OD1	2.55	0.44
2:B:389:ASP:OD2	2:B:419:ILE:HG23	2.17	0.44
2:F:301:LEU:CD2	2:F:324:GLU:HB3	2.48	0.44
2:H:366:SER:O	2:H:369:GLY:N	2.49	0.44
2:J:22:GLU:HG2	2:J:47:ILE:CD1	2.46	0.44
2:J:432:LEU:CD1	2:J:458:ILE:HA	2.48	0.44
2:J:519:TRP:CH2	2:J:567:HIS:CE1	3.00	0.44
1:K:28:THR:O	1:K:32:MET:HE2	2.18	0.44
2:L:101:THR:OG1	2:L:102:PRO:HD3	2.17	0.44
2:L:532:LEU:HA	2:L:532:LEU:HD23	1.75	0.44
2:J:164:ARG:NE	2:N:112:ARG:HG3	2.14	0.44
2:N:227:VAL:CG1	2:N:228:GLY:N	2.81	0.44
1:O:48:THR:HG22	1:O:51:ILE:N	2.22	0.44
2:P:245:LEU:HD12	2:P:245:LEU:HA	1.85	0.44
2:P:532:LEU:HD23	2:P:532:LEU:HA	1.70	0.44
2:P:519:TRP:CH2	2:P:567:HIS:CG	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:VAL:CG2	2:B:359:GLU:HB2	2.45	0.44
2:D:46:LYS:HE3	2:D:46:LYS:HB2	1.51	0.44
2:D:521:GLN:HG3	2:D:567:HIS:HD2	1.82	0.44
1:E:44:LEU:HA	1:E:45:PRO:HD3	1.71	0.44
2:H:117:VAL:HG11	2:H:119:PHE:CZ	2.52	0.44
2:H:64:THR:O	2:H:67:ARG:N	2.47	0.44
2:H:56:THR:CG2	2:H:79:LYS:HD2	2.46	0.44
2:L:199:PHE:CZ	2:L:227:VAL:HG22	2.52	0.44
1:M:154:GLU:OE1	2:N:67:ARG:NH1	2.51	0.44
2:N:34:ARG:NH1	2:N:48:ASP:OD1	2.50	0.44
2:F:366:SER:HB2	2:F:367:GLN:OE1	2.17	0.44
1:E:153:ARG:NH2	2:F:539:TYR:CE1	2.85	0.44
2:H:409:ARG:CB	4:H:1100:7JA:HD1	2.48	0.44
2:H:121:ARG:NH2	5:H:1103:PO4:O4	2.49	0.44
2:H:320:LEU:HA	2:H:320:LEU:HD12	1.71	0.44
2:H:495:MET:HB2	2:H:520:VAL:HG22	1.99	0.44
2:H:506:ALA:HB1	2:H:535:MET:HB2	1.99	0.44
2:H:71:ARG:HG2	2:H:72:PHE:CE1	2.52	0.44
2:J:431:LEU:CD1	2:J:435:CYS:SG	3.05	0.44
2:L:441:PHE:O	2:L:468:MET:HA	2.18	0.44
1:M:130:PRO:O	1:M:134:ARG:HG2	2.17	0.44
2:N:101:THR:N	2:N:102:PRO:CD	2.81	0.44
2:N:351:ARG:HB3	2:N:386:TYR:CG	2.52	0.44
2:P:443:PHE:HE2	2:P:445:LEU:HD11	1.82	0.44
1:A:105:ALA:HB2	1:A:113:LEU:HD23	1.99	0.44
2:B:172:GLU:HG3	2:B:200:TYR:HB3	1.98	0.44
2:B:247:GLU:HA	2:B:274:ARG:O	2.17	0.44
2:B:519:TRP:CZ3	2:B:567:HIS:CG	3.06	0.44
1:C:46:ASN:HB2	1:C:107:TYR:CZ	2.53	0.44
2:D:308:GLU:O	2:D:312:THR:HG23	2.18	0.44
1:G:125:ILE:HG23	1:G:133:ILE:CD1	2.48	0.44
2:H:211:ASP:HA	2:H:214:THR:HG23	1.99	0.44
2:H:390:ILE:HD13	2:H:390:ILE:N	2.32	0.44
2:H:392:ASN:H	2:H:392:ASN:ND2	2.15	0.44
2:H:424:LEU:O	2:H:427:GLY:N	2.50	0.44
2:H:75:LEU:HA	2:H:75:LEU:HD23	1.60	0.44
2:J:117:VAL:HG11	2:J:119:PHE:CZ	2.52	0.44
2:L:444:TYR:HA	2:L:471:GLY:CA	2.37	0.44
2:L:519:TRP:CZ3	2:L:567:HIS:CG	3.06	0.44
2:L:578:ARG:HG3	2:L:578:ARG:H	1.46	0.44
2:N:315:GLN:HG2	2:N:340:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:125:ILE:HG23	1:O:133:ILE:CD1	2.42	0.44
4:P:1100:7JA:H05	4:P:1100:7JA:H27	1.67	0.44
2:P:495:MET:O	2:P:520:VAL:HA	2.16	0.44
2:P:519:TRP:CZ3	2:P:567:HIS:CG	3.05	0.44
2:P:83:LYS:HA	2:P:84:PRO:HD3	1.88	0.44
1:E:158:ALA:HA	2:F:62:THR:CG2	2.48	0.44
2:F:492:LYS:HG3	2:F:517:TYR:CD2	2.53	0.44
2:H:121:ARG:NH2	5:H:1103:PO4:P	2.91	0.44
2:D:165:LYS:NZ	2:H:139:ASP:OD1	2.46	0.44
2:H:424:LEU:N	2:H:449:GLY:O	2.47	0.44
2:H:96:TRP:O	2:H:578:ARG:NH2	2.51	0.44
2:J:546:PRO:HD3	2:J:584:THR:O	2.18	0.44
2:P:191:ASN:HD21	2:P:194:LEU:N	2.09	0.44
2:P:456:SER:HB2	2:P:482:GLU:HB3	1.97	0.44
2:P:533:MET:HE3	2:P:588:LEU:HB3	2.00	0.44
3:R:201:LEU:HA	3:R:202:PRO:HD3	1.83	0.44
3:W:201:LEU:HA	3:W:201:LEU:HD23	1.68	0.44
2:B:22:GLU:OE1	2:B:43:ARG:NH2	2.51	0.44
1:C:134:ARG:NE	1:C:141:ASN:HB2	2.33	0.44
2:F:311:CYS:CB	2:F:336:VAL:HG21	2.45	0.44
2:F:429:ARG:HG2	2:F:433:ILE:HD11	2.00	0.44
1:G:147:GLU:O	1:G:148:GLU:C	2.54	0.44
2:J:46:LYS:HE3	2:J:46:LYS:HB2	1.50	0.44
2:L:545:ILE:HA	2:L:546:PRO:HD3	1.74	0.44
1:M:99:PHE:CD2	2:N:16:THR:CA	3.00	0.44
2:N:441:PHE:O	2:N:468:MET:HA	2.17	0.44
1:E:12:ASP:OD2	1:E:49:SER:HB2	2.17	0.44
2:F:343:GLN:O	2:F:345:LYS:HG2	2.18	0.44
2:F:405:LEU:HD23	2:F:405:LEU:HA	1.77	0.44
1:G:152:ARG:O	1:G:153:ARG:C	2.56	0.44
2:H:255:GLU:HB3	2:H:263:TYR:HE1	1.83	0.44
2:L:320:LEU:HD21	2:L:323:LEU:HB2	1.99	0.44
1:A:125:ILE:HG23	1:A:133:ILE:CD1	2.45	0.43
2:B:285:MET:N	2:B:286:PRO:CD	2.81	0.43
2:B:542:ILE:HD11	2:B:588:LEU:CD1	2.37	0.43
1:C:8:LEU:HD23	1:C:42:VAL:HG13	1.99	0.43
2:H:124:VAL:CG1	2:H:129:LEU:HD13	2.48	0.43
2:H:140:LEU:HD23	2:H:163:CYS:SG	2.58	0.43
2:H:206:LYS:HE3	2:H:206:LYS:HB2	1.81	0.43
2:H:314:ILE:O	2:H:316:LYS:N	2.51	0.43
2:J:80:LEU:HD12	2:J:122:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:103:TRP:O	2:L:107:ILE:HG13	2.18	0.43
2:L:138:ASP:OD2	2:L:164:ARG:HG3	2.18	0.43
2:L:310:HIS:HE1	2:L:325:THR:OG1	2.00	0.43
2:L:328:VAL:CG2	2:L:359:GLU:HB2	2.43	0.43
2:L:519:TRP:CH2	2:L:567:HIS:CE1	3.02	0.43
2:N:37:ALA:O	2:N:40:VAL:HG13	2.18	0.43
2:P:451:THR:HB	2:P:475:GLU:OE2	2.18	0.43
2:B:101:THR:HG22	2:B:128:ASP:CG	2.37	0.43
2:B:83:LYS:O	2:B:121:ARG:HD2	2.19	0.43
2:B:546:PRO:HD3	2:B:584:THR:O	2.18	0.43
2:D:22:GLU:HG2	2:D:47:ILE:HD13	2.01	0.43
2:D:297:LYS:HB2	2:D:297:LYS:HE3	1.67	0.43
2:D:348:ARG:HH22	4:D:1100:7JA:C	2.32	0.43
2:F:199:PHE:CZ	2:F:227:VAL:HG22	2.53	0.43
2:F:432:LEU:CD1	2:F:458:ILE:HA	2.48	0.43
2:F:519:TRP:CH2	2:F:567:HIS:CG	3.06	0.43
2:H:225:VAL:HG23	2:H:225:VAL:O	2.17	0.43
2:H:328:VAL:CG1	2:H:359:GLU:HG2	2.40	0.43
1:I:6:ILE:HG22	1:I:7:VAL:N	2.33	0.43
1:M:137:PHE:CD1	2:N:17:VAL:HG21	2.52	0.43
1:O:128:LYS:HB2	1:O:133:ILE:HD11	1.99	0.43
2:P:235:LEU:O	2:P:238:PHE:HB3	2.17	0.43
2:B:477:ASP:N	2:B:477:ASP:OD1	2.50	0.43
1:C:13:GLY:HA3	1:K:9:LYS:NZ	2.32	0.43
2:D:519:TRP:CZ3	2:D:567:HIS:CG	3.06	0.43
2:D:546:PRO:HD3	2:D:584:THR:O	2.17	0.43
2:H:351:ARG:HH11	2:H:360:ASP:HA	1.83	0.43
2:H:542:ILE:HD13	2:H:544:LEU:HD21	2.00	0.43
2:J:490:LEU:HD23	2:J:490:LEU:HA	1.86	0.43
2:L:211:ASP:HA	2:L:214:THR:CG2	2.47	0.43
1:M:6:ILE:HG22	1:M:7:VAL:N	2.33	0.43
2:N:482:GLU:O	2:N:485:ARG:HG2	2.18	0.43
2:N:545:ILE:HG23	2:N:546:PRO:HD2	2.01	0.43
2:B:546:PRO:HB2	2:B:547:SER:H	1.60	0.43
2:D:398:ILE:CG2	2:D:402:LEU:HD11	2.43	0.43
2:F:297:LYS:HE2	2:F:322:VAL:CG2	2.48	0.43
2:F:422:LEU:O	2:F:424:LEU:HG	2.18	0.43
1:G:142:ASP:N	1:G:142:ASP:OD2	2.51	0.43
2:H:491:GLN:HA	2:H:515:LEU:HA	1.99	0.43
1:I:30:ALA:C	1:I:32:MET:H	2.22	0.43
2:L:114:LEU:HD12	2:L:114:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:297:LYS:HE2	2:L:322:VAL:CG2	2.48	0.43
1:M:8:LEU:HD23	1:M:42:VAL:HG13	2.00	0.43
2:N:419:ILE:O	2:N:420:THR:C	2.57	0.43
1:O:108:LEU:HD12	1:O:110:ILE:HD11	2.00	0.43
2:P:114:LEU:O	2:P:136:ARG:NH1	2.49	0.43
2:P:285:MET:HB3	2:P:286:PRO:HD3	2.00	0.43
3:U:212:PHE:CD2	3:U:213:LEU:HD23	2.53	0.43
2:D:503:ARG:NH1	2:D:503:ARG:HB3	2.34	0.43
2:D:78:LEU:HD12	2:D:79:LYS:H	1.83	0.43
2:F:101:THR:N	2:F:102:PRO:CD	2.82	0.43
4:H:1100:7JA:H12	4:H:1100:7JA:H05A	1.84	0.43
2:H:328:VAL:CG1	2:H:359:GLU:CG	2.96	0.43
2:H:364:LEU:HD13	2:H:388:SER:CB	2.49	0.43
1:I:42:VAL:O	1:I:42:VAL:HG22	2.18	0.43
2:J:503:ARG:HB3	2:J:503:ARG:NH1	2.34	0.43
2:L:247:GLU:HA	2:L:274:ARG:O	2.18	0.43
2:N:194:LEU:HD12	2:N:194:LEU:HA	1.73	0.43
2:N:298:LEU:HD12	2:N:298:LEU:HA	1.70	0.43
2:D:521:GLN:HG3	2:D:567:HIS:CD2	2.53	0.43
1:E:46:ASN:HB2	1:E:107:TYR:CZ	2.54	0.43
1:G:148:GLU:HG2	1:G:152:ARG:NH1	2.33	0.43
1:G:46:ASN:HB2	1:G:107:TYR:CZ	2.53	0.43
2:J:398:ILE:CG2	2:J:402:LEU:HD11	2.43	0.43
2:J:512:LEU:HA	2:J:513:PRO:HD2	1.73	0.43
2:L:85:ARG:NH1	5:L:1101:PO4:O3	2.51	0.43
2:L:405:LEU:HA	2:L:405:LEU:HD23	1.84	0.43
1:O:10:SER:OG	1:O:11:SER:N	2.51	0.43
1:O:158:ALA:HA	2:P:62:THR:CG2	2.46	0.43
2:P:315:GLN:HG2	2:P:340:TYR:CE1	2.54	0.43
2:P:453:LEU:HD11	2:P:457:TYR:OH	2.18	0.43
2:B:404:ASN:HA	2:B:437:LYS:HD2	2.01	0.43
2:B:451:THR:HA	2:B:475:GLU:HG3	2.00	0.43
2:D:187:LEU:HD23	2:D:187:LEU:HA	1.85	0.43
2:D:578:ARG:H	2:D:578:ARG:HG3	1.48	0.43
1:E:91:MET:HG2	1:E:116:LEU:HD21	2.00	0.43
2:F:409:ARG:HB3	4:F:1100:7JA:HG1	2.01	0.43
2:H:207:ILE:HD12	2:H:230:PHE:HZ	1.84	0.43
2:H:213:GLU:OE2	2:H:237:GLY:HA3	2.18	0.43
2:H:233:LEU:HD11	2:H:262:LYS:HD3	2.01	0.43
2:H:385:VAL:HG13	2:H:387:VAL:CG2	2.48	0.43
2:H:96:TRP:HA	2:H:582:PRO:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:120:ARG:HD2	2:J:146:ASP:OD2	2.18	0.43
1:I:126:LYS:HZ1	2:J:29:THR:H	1.67	0.43
2:J:315:GLN:HG2	2:J:340:TYR:CE1	2.54	0.43
2:J:411:VAL:HG22	2:J:444:TYR:HB3	1.99	0.43
2:J:547:SER:CB	2:J:564:HIS:CB	2.96	0.43
2:L:114:LEU:O	2:L:136:ARG:NH1	2.50	0.43
2:L:297:LYS:HG3	2:L:322:VAL:HB	2.01	0.43
2:L:429:ARG:HG2	2:L:433:ILE:HD11	2.01	0.43
2:N:83:LYS:HA	2:N:84:PRO:HD3	1.88	0.43
2:P:563:GLU:O	2:P:563:GLU:CG	2.66	0.43
1:A:124:MET:O	1:A:128:LYS:HE2	2.18	0.43
2:B:85:ARG:NH2	4:B:1100:7JA:O14	2.45	0.43
2:D:431:LEU:C	2:D:431:LEU:CD1	2.82	0.43
2:D:547:SER:CB	2:D:564:HIS:CB	2.97	0.43
2:F:107:ILE:HG12	2:F:111:LEU:HD12	2.00	0.43
2:F:112:ARG:HG2	2:L:164:ARG:CD	2.43	0.43
2:H:227:VAL:O	2:H:250:GLY:HA3	2.19	0.43
2:J:191:ASN:HD21	2:J:194:LEU:N	2.12	0.43
2:J:344:LEU:HD23	2:J:380:LEU:HD21	2.00	0.43
2:L:20:VAL:O	2:L:24:VAL:HG23	2.19	0.43
2:L:389:ASP:OD2	2:L:419:ILE:HG23	2.18	0.43
2:L:419:ILE:HD11	2:L:446:ARG:NH2	2.29	0.43
2:L:78:LEU:HD12	2:L:79:LYS:H	1.84	0.43
2:N:311:CYS:CB	2:N:336:VAL:HG21	2.48	0.43
1:O:153:ARG:CG	1:O:157:TRP:CZ3	3.02	0.43
2:P:339:GLN:HA	2:P:342:LYS:HE2	2.00	0.43
2:P:52:ARG:HH11	2:P:52:ARG:HD3	1.70	0.43
2:B:65:PRO:HG3	2:B:103:TRP:CE2	2.54	0.43
2:F:114:LEU:HD12	2:F:114:LEU:HA	1.79	0.43
2:F:211:ASP:HA	2:F:214:THR:CG2	2.48	0.43
2:H:121:ARG:HH22	5:H:1103:PO4:P	2.41	0.43
2:H:100:VAL:HG21	2:H:119:PHE:CE1	2.53	0.43
2:H:495:MET:HE2	2:H:520:VAL:HG22	2.00	0.43
2:J:297:LYS:HG3	2:J:322:VAL:HB	2.00	0.43
2:J:492:LYS:HG3	2:J:517:TYR:CD2	2.54	0.43
2:N:365:VAL:CG2	2:N:387:VAL:HA	2.46	0.43
1:O:135:THR:HG22	1:O:136:THR:N	2.33	0.43
2:P:419:ILE:O	2:P:420:THR:C	2.57	0.43
2:P:304:LEU:HD11	3:X:216:ARG:HG3	2.00	0.43
2:B:143:LEU:CD2	2:B:159:ILE:HD13	2.47	0.43
2:B:367:GLN:HG2	2:B:391:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLU:CG	2:D:31:PRO:HB3	2.49	0.43
2:D:328:VAL:CG2	2:D:359:GLU:HB2	2.44	0.43
2:H:467:TRP:CZ3	2:H:494:GLU:OE1	2.72	0.43
2:H:542:ILE:HG13	2:H:588:LEU:HB2	1.97	0.43
1:I:102:ILE:HG12	1:I:117:THR:HB	2.01	0.43
1:K:126:LYS:HZ1	2:L:29:THR:H	1.67	0.43
2:L:451:THR:HA	2:L:475:GLU:HG3	2.00	0.43
1:M:26:SER:OG	1:M:108:LEU:HB3	2.19	0.43
2:N:542:ILE:CD1	2:N:588:LEU:HD12	2.39	0.43
2:B:441:PHE:O	2:B:468:MET:HA	2.19	0.42
1:C:19:GLU:OE1	1:C:19:GLU:N	2.49	0.42
2:D:495:MET:O	2:D:520:VAL:HA	2.19	0.42
2:F:245:LEU:HD12	2:F:245:LEU:HA	1.79	0.42
1:G:149:GLU:OE1	1:G:153:ARG:NE	2.52	0.42
2:H:43:ARG:NH2	2:H:47:ILE:HD11	2.34	0.42
2:H:487:CYS:N	2:H:488:PRO:CD	2.82	0.42
2:L:432:LEU:CD1	2:L:458:ILE:HA	2.49	0.42
2:L:443:PHE:HE2	2:L:445:LEU:HD11	1.80	0.42
2:L:468:MET:CE	2:L:470:LEU:HD11	2.49	0.42
2:N:161:THR:HG22	2:N:186:GLU:HG2	2.00	0.42
2:P:17:VAL:O	2:P:20:VAL:HG12	2.19	0.42
2:P:545:ILE:HA	2:P:546:PRO:HD3	1.76	0.42
1:A:134:ARG:HB2	1:A:139:ILE:O	2.19	0.42
1:C:12:ASP:O	1:K:40:ASN:HB2	2.19	0.42
2:F:289:PHE:N	2:F:290:PRO:CD	2.81	0.42
2:F:563:GLU:O	2:F:563:GLU:CG	2.67	0.42
2:H:198:ASN:O	2:H:198:ASN:OD1	2.38	0.42
2:H:289:PHE:N	2:H:290:PRO:HD2	2.34	0.42
2:H:440:ARG:HB3	2:H:467:TRP:CD1	2.54	0.42
2:H:94:GLU:CG	2:H:95:ASN:N	2.82	0.42
2:J:58:ALA:O	2:J:81:LYS:HB2	2.19	0.42
2:L:168:THR:HB	2:L:196:VAL:CG1	2.16	0.42
2:L:233:LEU:HA	2:L:233:LEU:HD23	1.88	0.42
2:N:453:LEU:HD11	2:N:457:TYR:OH	2.19	0.42
2:N:564:HIS:HA	2:N:565:PRO:HD2	1.76	0.42
2:P:297:LYS:HG3	2:P:322:VAL:HB	1.99	0.42
3:Q:201:LEU:HA	3:Q:202:PRO:HD3	1.81	0.42
2:D:453:LEU:HD11	2:D:457:TYR:OH	2.19	0.42
1:E:134:ARG:NH1	2:F:40:VAL:HA	2.34	0.42
2:F:298:LEU:HB2	2:F:320:LEU:HD11	2.02	0.42
2:F:32:LYS:HD2	2:F:32:LYS:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:537:ARG:HB3	2:H:538:PRO:CD	2.49	0.42
2:H:542:ILE:HD12	2:H:543:GLU:CA	2.49	0.42
2:H:92:ILE:CG2	2:H:93:PRO:O	2.68	0.42
2:J:247:GLU:HA	2:J:274:ARG:O	2.20	0.42
2:J:96:TRP:O	2:J:578:ARG:NH2	2.45	0.42
2:L:191:ASN:ND2	2:L:194:LEU:HB2	2.35	0.42
2:P:37:ALA:O	2:P:40:VAL:HG13	2.20	0.42
2:B:248:PHE:C	2:B:248:PHE:CD2	2.92	0.42
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.77	0.42
1:C:12:ASP:O	1:K:40:ASN:HB3	2.19	0.42
2:D:101:THR:CG2	2:D:128:ASP:OD1	2.55	0.42
1:C:99:PHE:CZ	2:D:17:VAL:HG22	2.55	0.42
2:F:191:ASN:ND2	2:F:194:LEU:HB2	2.34	0.42
2:F:422:LEU:O	2:F:423:PRO:C	2.57	0.42
2:F:578:ARG:HG3	2:F:578:ARG:H	1.48	0.42
2:H:200:TYR:C	2:H:200:TYR:CD1	2.90	0.42
2:H:21:ILE:HG23	2:H:47:ILE:HD13	2.02	0.42
2:H:502:GLU:CD	2:H:526:SER:HB2	2.40	0.42
2:J:194:LEU:HA	2:J:194:LEU:HD12	1.74	0.42
1:K:8:LEU:HD23	1:K:42:VAL:HG13	2.00	0.42
2:N:335:GLU:O	2:N:338:ALA:HB3	2.20	0.42
1:O:82:ASP:O	1:O:85:ALA:HB3	2.19	0.42
2:P:386:TYR:HE1	4:P:1100:7JA:HG2	1.72	0.42
2:P:451:THR:HA	2:P:475:GLU:HG3	2.02	0.42
1:A:160:GLU:HG3	2:B:31:PRO:HB3	2.01	0.42
2:B:419:ILE:O	2:B:420:THR:C	2.57	0.42
1:E:10:SER:OG	1:E:11:SER:N	2.50	0.42
2:F:187:LEU:HD23	2:F:187:LEU:HA	1.83	0.42
2:F:188:ALA:HA	2:F:215:ILE:HG12	2.02	0.42
2:F:431:LEU:CD1	2:F:435:CYS:SG	3.08	0.42
2:F:490:LEU:HD23	2:F:490:LEU:HA	1.89	0.42
2:F:96:TRP:O	2:F:578:ARG:NH2	2.45	0.42
2:H:409:ARG:CB	4:H:1100:7JA:H29	2.35	0.42
2:J:101:THR:CG2	2:J:128:ASP:OD1	2.59	0.42
2:J:387:VAL:HG22	2:J:389:ASP:H	1.84	0.42
2:J:419:ILE:HD11	2:J:446:ARG:NH2	2.25	0.42
1:M:114:LEU:C	1:M:116:LEU:N	2.72	0.42
1:M:100:GLU:CG	2:N:15:ALA:HB2	2.48	0.42
2:N:297:LYS:HE2	2:N:322:VAL:CG2	2.49	0.42
3:X:201:LEU:HA	3:X:202:PRO:HD3	1.83	0.42
1:A:63:VAL:C	1:A:65:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:343:GLN:O	2:D:345:LYS:HG2	2.20	0.42
2:H:345:LYS:NZ	2:H:345:LYS:HB3	2.35	0.42
2:H:87:ALA:C	2:H:89:PHE:H	2.23	0.42
2:J:366:SER:HB2	2:J:367:GLN:OE1	2.19	0.42
2:N:289:PHE:HB2	2:N:290:PRO:HD3	2.02	0.42
1:O:44:LEU:HA	1:O:45:PRO:HD3	1.77	0.42
2:P:466:ARG:HG2	2:P:491:GLN:OE1	2.19	0.42
2:B:226:LYS:HA	2:B:249:CYS:O	2.20	0.42
2:B:22:GLU:HG2	2:B:47:ILE:HD13	2.00	0.42
1:C:141:ASN:OD1	1:C:141:ASN:C	2.58	0.42
2:F:532:LEU:HA	2:F:532:LEU:HD23	1.70	0.42
1:G:160:GLU:HB3	2:H:31:PRO:HB3	2.02	0.42
2:H:107:ILE:HA	2:H:111:LEU:HB2	2.02	0.42
2:H:302:TYR:N	2:H:302:TYR:CD2	2.83	0.42
2:H:343:GLN:N	2:H:343:GLN:NE2	2.67	0.42
2:J:101:THR:N	2:J:102:PRO:CD	2.82	0.42
2:J:335:GLU:O	2:J:338:ALA:HB3	2.20	0.42
2:L:22:GLU:HG2	2:L:47:ILE:HD13	2.01	0.42
2:L:235:LEU:O	2:L:238:PHE:HB3	2.19	0.42
4:N:1100:7JA:H10	4:N:1100:7JA:HN	1.85	0.42
2:N:235:LEU:O	2:N:238:PHE:HB3	2.19	0.42
2:N:285:MET:N	2:N:286:PRO:CD	2.82	0.42
2:P:298:LEU:HA	2:P:298:LEU:HD12	1.87	0.42
2:B:329:ILE:O	2:B:333:GLY:HA3	2.19	0.42
2:B:419:ILE:HD12	2:B:419:ILE:N	2.35	0.42
2:D:152:THR:HG22	2:D:177:SER:HB2	2.02	0.42
2:D:411:VAL:HG22	2:D:444:TYR:CB	2.49	0.42
2:F:114:LEU:O	2:F:136:ARG:NH1	2.52	0.42
2:F:285:MET:N	2:F:286:PRO:CD	2.81	0.42
1:G:42:VAL:O	1:G:42:VAL:HG22	2.20	0.42
2:H:172:GLU:O	2:H:202:THR:CG2	2.68	0.42
2:H:364:LEU:O	2:H:365:VAL:HG13	2.20	0.42
2:H:510:THR:HG22	2:H:511:LYS:N	2.35	0.42
2:J:328:VAL:CG2	2:J:359:GLU:HB2	2.44	0.42
1:M:102:ILE:CB	2:N:20:VAL:HG21	2.50	0.42
2:N:54:HIS:CD2	2:N:77:SER:OG	2.71	0.42
3:X:212:PHE:CD2	3:X:213:LEU:HD23	2.55	0.42
1:A:6:ILE:HG22	1:A:7:VAL:N	2.35	0.42
2:B:305:LEU:HD22	2:B:305:LEU:H	1.85	0.42
2:B:366:SER:HB2	2:B:367:GLN:OE1	2.19	0.42
2:B:545:ILE:HG23	2:B:546:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:LEU:O	2:D:424:LEU:HG	2.20	0.42
2:F:542:ILE:HD11	2:F:588:LEU:CD1	2.36	0.42
1:I:10:SER:OG	1:I:11:SER:N	2.52	0.42
1:I:111:LYS:O	1:I:115:ASP:HB2	2.19	0.42
2:J:161:THR:HG22	2:J:186:GLU:HG2	2.02	0.42
1:K:83:LEU:HD23	1:K:83:LEU:HA	1.81	0.42
2:L:367:GLN:HB3	2:L:391:THR:HG22	2.01	0.42
2:L:419:ILE:O	2:L:420:THR:C	2.58	0.42
2:L:492:LYS:HG3	2:L:517:TYR:CD2	2.55	0.42
1:A:93:ILE:CD1	1:A:97:THR:HG22	2.42	0.42
2:B:30:ASP:HA	2:B:31:PRO:HD3	1.90	0.42
2:B:387:VAL:HG22	2:B:389:ASP:H	1.84	0.42
2:B:547:SER:CB	2:B:564:HIS:CB	2.97	0.42
2:D:226:LYS:HA	2:D:249:CYS:O	2.19	0.42
2:F:159:ILE:HD11	2:F:169:LEU:HD13	2.02	0.42
2:F:419:ILE:HD11	2:F:446:ARG:NH2	2.27	0.42
1:I:153:ARG:CG	1:I:157:TRP:CZ3	3.01	0.42
1:I:48:THR:HG22	1:I:51:ILE:CB	2.50	0.42
2:J:405:LEU:HA	2:J:405:LEU:HD23	1.74	0.42
1:M:102:ILE:HB	2:N:20:VAL:HG21	2.02	0.42
2:N:63:ALA:HB1	2:N:67:ARG:HD2	2.02	0.42
3:S:212:PHE:CD2	3:S:213:LEU:HD23	2.55	0.42
3:W:212:PHE:CD2	3:W:213:LEU:HD23	2.55	0.42
2:B:482:GLU:O	2:B:485:ARG:HG2	2.20	0.41
2:B:490:LEU:HA	2:B:490:LEU:HD23	1.85	0.41
1:C:126:LYS:HZ3	2:D:29:THR:H	1.67	0.41
2:D:315:GLN:HG2	2:D:340:TYR:CE1	2.55	0.41
2:D:83:LYS:HA	2:D:96:TRP:CZ3	2.55	0.41
1:E:8:LEU:HD23	1:E:42:VAL:HG13	2.02	0.41
2:H:114:LEU:O	2:H:136:ARG:NH1	2.53	0.41
2:H:123:ILE:HG21	2:H:123:ILE:HD13	1.88	0.41
2:H:227:VAL:HG22	2:H:228:GLY:H	1.85	0.41
2:J:532:LEU:HA	2:J:532:LEU:HD23	1.75	0.41
2:J:91:LEU:O	2:J:567:HIS:HE1	2.03	0.41
1:K:160:GLU:HG3	2:L:31:PRO:HB3	2.02	0.41
4:L:1100:7JA:OXT	4:L:1100:7JA:HG2A	2.11	0.41
2:L:30:ASP:HA	2:L:31:PRO:HD3	1.93	0.41
2:N:221:SER:O	2:N:223:VAL:HG23	2.19	0.41
2:N:405:LEU:HA	2:N:405:LEU:HD23	1.80	0.41
2:P:20:VAL:O	2:P:24:VAL:HG23	2.20	0.41
2:P:392:ASN:HD21	2:P:424:LEU:HA	1.85	0.41

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PRO:O	1:A:134:ARG:HG2	2.21	0.41
2:B:63:ALA:HB1	2:B:67:ARG:HD2	2.02	0.41
2:H:409:ARG:HD2	4:H:1100:7JA:H29	2.02	0.41
2:H:152:THR:HB	2:H:177:SER:HB2	2.02	0.41
2:H:255:GLU:HB3	2:H:263:TYR:CE1	2.55	0.41
2:H:314:ILE:HG12	2:H:314:ILE:H	1.51	0.41
1:I:154:GLU:OE1	2:J:67:ARG:NH1	2.53	0.41
2:J:456:SER:HB2	2:J:482:GLU:HB3	2.01	0.41
2:L:305:LEU:CD2	2:L:305:LEU:H	2.33	0.41
2:L:411:VAL:HG22	2:L:444:TYR:HB3	2.02	0.41
2:N:222:LEU:HD12	2:N:222:LEU:HA	1.85	0.41
1:E:42:VAL:HA	1:E:43:PRO:HD3	1.84	0.41
2:F:419:ILE:O	2:F:420:THR:C	2.58	0.41
2:H:347:LEU:HD11	2:H:349:ILE:CG1	2.48	0.41
2:H:492:LYS:HZ1	2:H:516:ARG:NH1	2.18	0.41
2:H:83:LYS:HA	2:H:84:PRO:HD3	1.88	0.41
1:K:58:TYR:CD2	1:K:113:LEU:HD13	2.55	0.41
1:M:134:ARG:NH2	1:M:141:ASN:HD22	2.18	0.41
1:O:44:LEU:HD12	1:O:44:LEU:O	2.20	0.41
2:P:107:ILE:HG12	2:P:111:LEU:HD12	2.02	0.41
2:P:436:LYS:HB3	2:P:436:LYS:HE2	1.89	0.41
2:P:546:PRO:HB2	2:P:547:SER:H	1.63	0.41
2:B:80:LEU:HB2	2:B:122:MET:HE2	1.97	0.41
1:C:115:ASP:HA	2:D:27:TYR:HE2	1.85	0.41
1:C:58:TYR:CE1	1:C:62:HIS:CE1	3.09	0.41
2:D:304:LEU:HD12	2:D:304:LEU:HA	1.91	0.41
2:D:443:PHE:HE2	2:D:445:LEU:HD11	1.80	0.41
1:E:134:ARG:NE	1:E:141:ASN:HB2	2.34	0.41
1:E:158:ALA:CB	2:F:62:THR:HG23	2.51	0.41
1:E:51:ILE:HD13	1:E:51:ILE:HA	1.91	0.41
2:F:120:ARG:NH2	5:F:1103:PO4:O4	2.53	0.41
2:F:91:LEU:O	2:F:567:HIS:HE1	2.03	0.41
2:H:442:ALA:HB1	4:H:1100:7JA:H28	2.02	0.41
2:H:481:MET:O	2:H:482:GLU:C	2.57	0.41
2:H:587:VAL:HG12	2:H:589:LYS:HD3	2.02	0.41
4:J:1100:7JA:H27	4:J:1100:7JA:H05	1.65	0.41
2:J:386:TYR:HE1	4:J:1100:7JA:HG2	1.73	0.41
2:J:209:PRO:HD3	2:J:230:PHE:CE2	2.56	0.41
2:N:289:PHE:N	2:N:290:PRO:CD	2.82	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.80	0.41
2:B:91:LEU:O	2:B:567:HIS:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:ARG:NH2	5:D:1103:PO4:O4	2.54	0.41
2:D:314:ILE:H	2:D:314:ILE:HG12	1.65	0.41
2:D:327:ASN:HD22	2:D:328:VAL:N	2.19	0.41
1:I:13:GLY:O	1:I:14:GLU:HG2	2.20	0.41
2:J:527:MET:O	2:J:528:THR:C	2.59	0.41
2:J:564:HIS:HA	2:J:565:PRO:HD2	1.80	0.41
2:L:120:ARG:HD2	2:L:146:ASP:OD2	2.20	0.41
2:L:466:ARG:HG2	2:L:491:GLN:OE1	2.21	0.41
2:L:456:SER:HB2	2:L:482:GLU:HB3	2.01	0.41
2:N:120:ARG:HD2	2:N:146:ASP:OD2	2.20	0.41
1:O:134:ARG:NE	1:O:141:ASN:HB2	2.36	0.41
3:V:212:PHE:CD2	3:V:213:LEU:HD23	2.56	0.41
2:B:453:LEU:HD11	2:B:457:TYR:OH	2.21	0.41
2:B:80:LEU:HD12	2:B:122:MET:HE1	2.03	0.41
1:C:44:LEU:HA	1:C:45:PRO:HD3	1.76	0.41
2:D:83:LYS:O	2:D:121:ARG:HD2	2.21	0.41
2:D:419:ILE:O	2:D:420:THR:C	2.59	0.41
2:D:80:LEU:HB2	2:D:122:MET:HE1	1.95	0.41
2:F:298:LEU:HD12	2:F:298:LEU:HA	1.73	0.41
2:F:451:THR:HA	2:F:475:GLU:HG3	2.03	0.41
2:H:289:PHE:O	2:H:290:PRO:C	2.58	0.41
2:H:300:LEU:HD23	2:H:300:LEU:HA	1.89	0.41
1:I:137:PHE:CD1	2:J:17:VAL:HG21	2.55	0.41
2:J:157:LEU:O	2:J:161:THR:HG23	2.20	0.41
2:J:211:ASP:HA	2:J:214:THR:CG2	2.47	0.41
2:J:298:LEU:HB2	2:J:320:LEU:HD11	2.01	0.41
2:J:55:VAL:HG12	2:J:56:THR:N	2.36	0.41
2:P:367:GLN:HG2	2:P:391:THR:HB	2.03	0.41
3:Q:201:LEU:HA	3:Q:201:LEU:HD23	1.74	0.41
1:A:19:GLU:OE1	1:A:19:GLU:N	2.52	0.41
1:A:98:LEU:HD21	1:A:120:THR:CG2	2.48	0.41
2:B:55:VAL:CG2	2:B:75:LEU:HD21	2.46	0.41
2:D:389:ASP:OD2	2:D:419:ILE:HG23	2.21	0.41
2:D:532:LEU:HA	2:D:532:LEU:HD23	1.74	0.41
2:F:347:LEU:HD21	2:F:349:ILE:HD11	2.02	0.41
2:H:431:LEU:CD2	2:H:432:LEU:HD23	2.48	0.41
2:H:71:ARG:C	2:H:73:PRO:HD3	2.41	0.41
2:J:367:GLN:HG2	2:J:391:THR:HB	2.03	0.41
2:J:57:MET:CE	2:J:62:THR:HG22	2.50	0.41
2:L:335:GLU:O	2:L:338:ALA:HB3	2.21	0.41
2:L:419:ILE:HD12	2:L:419:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:527:MET:O	2:L:528:THR:C	2.58	0.41
1:M:128:LYS:HB2	1:M:133:ILE:HD13	2.02	0.41
2:N:386:TYR:OH	4:N:1100:7JA:HG2B	2.21	0.41
1:O:101:LEU:HA	1:O:101:LEU:HD23	1.92	0.41
1:A:26:SER:OG	1:A:108:LEU:HB3	2.20	0.41
2:D:366:SER:HB2	2:D:367:GLN:OE1	2.21	0.41
1:E:105:ALA:CB	1:E:114:LEU:HD13	2.50	0.41
2:F:297:LYS:HE3	2:F:297:LYS:HB2	1.67	0.41
2:F:519:TRP:CZ3	2:F:567:HIS:CG	3.09	0.41
2:F:545:ILE:HA	2:F:546:PRO:HD3	1.79	0.41
1:G:44:LEU:O	1:G:44:LEU:HD12	2.20	0.41
2:H:266:LEU:HA	2:H:266:LEU:HD22	1.89	0.41
2:H:425:ASP:OD1	2:H:454:GLY:HA3	2.21	0.41
2:H:511:LYS:HB2	2:H:511:LYS:HE2	1.91	0.41
1:I:34:GLU:C	1:I:36:ASP:H	2.24	0.41
2:L:152:THR:HG22	2:L:177:SER:HB2	2.04	0.41
2:L:211:ASP:O	2:L:215:ILE:HG13	2.21	0.41
1:M:99:PHE:CB	2:N:15:ALA:HB1	2.51	0.41
4:N:1100:7JA:OXT	4:N:1100:7JA:CG2	2.66	0.41
2:N:422:LEU:O	2:N:424:LEU:HG	2.21	0.41
2:N:465:VAL:CG1	2:N:468:MET:HG3	2.50	0.41
2:P:55:VAL:CG2	2:P:75:LEU:HD21	2.42	0.41
2:B:191:ASN:HD21	2:B:194:LEU:N	2.11	0.40
2:B:546:PRO:O	2:B:547:SER:CB	2.70	0.40
2:D:311:CYS:CB	2:D:336:VAL:HG21	2.47	0.40
2:D:367:GLN:HG2	2:D:391:THR:HB	2.03	0.40
2:D:564:HIS:HA	2:D:565:PRO:HD2	1.77	0.40
2:F:289:PHE:HB2	2:F:290:PRO:HD3	2.03	0.40
2:H:220:ARG:HA	2:H:220:ARG:NE	2.36	0.40
2:H:490:LEU:HA	2:H:490:LEU:HD23	1.85	0.40
2:H:544:LEU:HD23	2:H:544:LEU:N	2.36	0.40
1:K:144:THR:OG1	1:K:147:GLU:HG3	2.22	0.40
2:L:153:THR:HG23	2:L:178:GLU:HA	2.02	0.40
2:L:55:VAL:CG2	2:L:75:LEU:HD21	2.49	0.40
2:N:545:ILE:HA	2:N:546:PRO:HD3	1.78	0.40
1:O:83:LEU:HD23	1:O:83:LEU:HA	1.80	0.40
2:B:190:HIS:HE1	2:P:110:ASN:HA	1.86	0.40
2:P:247:GLU:HA	2:P:274:ARG:O	2.20	0.40
3:U:201:LEU:HA	3:U:201:LEU:HD23	1.69	0.40
2:B:532:LEU:HA	2:B:532:LEU:HD23	1.76	0.40
2:D:153:THR:HG23	2:D:178:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:TYR:O	2:H:304:LEU:HB2	2.22	0.40
2:H:432:LEU:HD11	2:H:458:ILE:CD1	2.52	0.40
2:J:348:ARG:HH22	4:J:1100:7JA:C	2.35	0.40
2:J:75:LEU:HA	2:J:75:LEU:HD23	1.87	0.40
2:L:191:ASN:ND2	2:L:194:LEU:H	2.16	0.40
2:L:301:LEU:CD2	2:L:324:GLU:HB3	2.52	0.40
2:L:533:MET:HE3	2:L:588:LEU:HB3	2.01	0.40
1:M:99:PHE:HD2	2:N:15:ALA:C	2.20	0.40
2:N:107:ILE:HA	2:N:111:LEU:HB2	2.03	0.40
2:P:65:PRO:HG3	2:P:103:TRP:CE2	2.56	0.40
2:P:58:ALA:O	2:P:81:LYS:HB2	2.22	0.40
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.92	0.40
2:B:512:LEU:HA	2:B:513:PRO:HD2	1.78	0.40
1:C:158:ALA:CB	2:D:62:THR:HG23	2.51	0.40
2:D:227:VAL:HG13	2:D:228:GLY:H	1.83	0.40
2:D:267:VAL:HG23	2:D:267:VAL:O	2.22	0.40
2:D:298:LEU:HD12	2:D:298:LEU:HA	1.72	0.40
2:D:563:GLU:CG	2:D:563:GLU:O	2.65	0.40
2:D:75:LEU:HA	2:D:75:LEU:HD23	1.85	0.40
1:E:83:LEU:HD23	1:E:83:LEU:HA	1.82	0.40
2:H:348:ARG:HG3	2:H:384:ALA:HB3	2.03	0.40
2:H:454:GLY:O	2:H:457:TYR:HB2	2.20	0.40
2:H:461:TYR:C	2:H:463:PRO:HD3	2.41	0.40
2:H:487:CYS:HB3	2:H:490:LEU:HB2	2.03	0.40
2:H:59:LEU:O	2:H:62:THR:HB	2.21	0.40
1:I:125:ILE:HG23	1:I:133:ILE:CD1	2.42	0.40
2:J:233:LEU:HA	2:J:233:LEU:HD23	1.82	0.40
2:P:429:ARG:HG2	2:P:433:ILE:HD11	2.04	0.40
2:P:564:HIS:HA	2:P:565:PRO:HD2	1.78	0.40
2:B:311:CYS:O	2:B:315:GLN:HB2	2.21	0.40
1:C:102:ILE:HG21	2:D:20:VAL:HG22	2.02	0.40
1:C:134:ARG:NH2	1:C:141:ASN:HD22	2.19	0.40
2:D:399:GLY:O	2:D:434:GLY:HA3	2.22	0.40
2:D:65:PRO:HA	2:D:103:TRP:CZ3	2.57	0.40
2:F:285:MET:HB3	2:F:286:PRO:HD3	2.03	0.40
2:F:431:LEU:CD1	2:F:431:LEU:C	2.89	0.40
2:F:468:MET:HE1	2:F:483:PHE:CE1	2.55	0.40
2:H:259:MET:C	2:H:261:GLU:N	2.72	0.40
2:H:482:GLU:HG2	2:H:482:GLU:H	1.60	0.40
2:H:492:LYS:NZ	2:H:516:ARG:HD2	2.35	0.40
2:H:501:SER:HB2	2:H:503:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:517:TYR:CE1	2:H:569:LEU:HD11	2.57	0.40
2:L:275:LEU:HD11	2:L:288:LEU:CD2	2.51	0.40
2:L:547:SER:CB	2:L:564:HIS:CB	2.99	0.40
3:U:201:LEU:HA	3:U:202:PRO:HD3	1.80	0.40
2:B:119:PHE:CD1	2:B:122:MET:HE3	2.57	0.40
2:B:211:ASP:O	2:B:215:ILE:HG13	2.21	0.40
2:B:436:LYS:HE2	2:B:436:LYS:HB3	1.96	0.40
2:B:456:SER:HB2	2:B:482:GLU:HB3	2.03	0.40
1:C:83:LEU:HA	1:C:83:LEU:HD23	1.84	0.40
2:F:85:ARG:NH1	5:F:1101:PO4:O3	2.54	0.40
2:F:329:ILE:HG23	2:F:330:GLY:N	2.36	0.40
2:F:441:PHE:O	2:F:468:MET:HA	2.22	0.40
2:F:469:LEU:HA	2:F:494:GLU:O	2.22	0.40
1:G:6:ILE:HG22	1:G:7:VAL:N	2.36	0.40
4:H:1100:7JA:H12A	4:H:1100:7JA:C04	2.50	0.40
2:H:21:ILE:C	2:H:23:GLN:N	2.75	0.40
2:H:306:GLU:OE2	2:H:307:THR:HG22	2.21	0.40
2:H:363:GLY:O	2:H:364:LEU:C	2.60	0.40
2:J:114:LEU:HA	2:J:114:LEU:HD12	1.72	0.40
2:L:245:LEU:HD12	2:L:245:LEU:HA	1.80	0.40
2:L:298:LEU:HA	2:L:298:LEU:HD12	1.82	0.40
2:L:367:GLN:NE2	2:L:389:ASP:OD1	2.53	0.40
1:K:134:ARG:NH1	2:L:40:VAL:HA	2.35	0.40
2:L:588:LEU:HA	2:L:588:LEU:HD23	1.97	0.40
2:L:96:TRP:O	2:L:578:ARG:NH2	2.44	0.40
2:N:366:SER:HB2	2:N:367:GLN:OE1	2.21	0.40
2:P:120:ARG:NH2	5:P:1103:PO4:O4	2.52	0.40
2:P:329:ILE:HG23	2:P:330:GLY:N	2.35	0.40
2:P:422:LEU:O	2:P:424:LEU:HG	2.21	0.40
2:P:404:ASN:HA	2:P:437:LYS:HD2	2.02	0.40
2:P:578:ARG:HG3	2:P:578:ARG:H	1.41	0.40

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

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

5.3 Torsion angles (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%)	22 (16%)	3 (2%)	7	34
1	C	140/160 (88%)	113 (81%)	23 (16%)	4 (3%)	4	26
1	E	140/160 (88%)	114 (81%)	23 (16%)	3 (2%)	7	34
1	G	140/160 (88%)	114 (81%)	22 (16%)	4 (3%)	4	26
1	I	140/160 (88%)	117 (84%)	20 (14%)	3 (2%)	7	34
1	K	140/160 (88%)	117 (84%)	19 (14%)	4 (3%)	4	26
1	M	140/160 (88%)	110 (79%)	27 (19%)	3 (2%)	7	34
1	O	140/160 (88%)	112 (80%)	25 (18%)	3 (2%)	7	34
2	B	564/592 (95%)	500 (89%)	57 (10%)	7 (1%)	13	48
2	D	564/592 (95%)	504 (89%)	53 (9%)	7 (1%)	13	48
2	F	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	13	48
2	H	558/592 (94%)	430 (77%)	98 (18%)	30 (5%)	2	13
2	J	564/592 (95%)	504 (89%)	52 (9%)	8 (1%)	11	44
2	L	564/592 (95%)	503 (89%)	54 (10%)	7 (1%)	13	48
2	N	564/592 (95%)	504 (89%)	51 (9%)	9 (2%)	9	41
2	P	564/592 (95%)	500 (89%)	56 (10%)	8 (1%)	11	44
3	Q	16/21 (76%)	16 (100%)	0	0	100	100
3	R	16/21 (76%)	16 (100%)	0	0	100	100
3	S	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	U	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	V	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	W	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	X	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
All	All	5738/6163 (93%)	4969 (87%)	659 (12%)	110 (2%)	8	37

All (110) Ramachandran outliers are listed below:

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

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

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

5.3.2 Protein sidechains (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%)	113 (89%)	14 (11%)	6 24
1	C	127/137 (93%)	113 (89%)	14 (11%)	6 24
1	E	127/137 (93%)	113 (89%)	14 (11%)	6 24
1	G	127/137 (93%)	115 (91%)	12 (9%)	8 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	127/137 (93%)	113 (89%)	14 (11%)	6 24
1	K	127/137 (93%)	116 (91%)	11 (9%)	10 35
1	M	127/137 (93%)	112 (88%)	15 (12%)	5 22
1	O	127/137 (93%)	115 (91%)	12 (9%)	8 31
2	B	500/523 (96%)	436 (87%)	64 (13%)	4 18
2	D	500/523 (96%)	431 (86%)	69 (14%)	3 16
2	F	500/523 (96%)	435 (87%)	65 (13%)	4 18
2	H	494/523 (94%)	395 (80%)	99 (20%)	1 6
2	J	500/523 (96%)	436 (87%)	64 (13%)	4 18
2	L	500/523 (96%)	439 (88%)	61 (12%)	5 20
2	N	500/523 (96%)	437 (87%)	63 (13%)	4 19
2	P	500/523 (96%)	436 (87%)	64 (13%)	4 18
3	Q	16/19 (84%)	15 (94%)	1 (6%)	18 50
3	R	16/19 (84%)	15 (94%)	1 (6%)	18 50
3	S	16/19 (84%)	15 (94%)	1 (6%)	18 50
3	U	16/19 (84%)	15 (94%)	1 (6%)	18 50
3	V	16/19 (84%)	15 (94%)	1 (6%)	18 50
3	W	16/19 (84%)	15 (94%)	1 (6%)	18 50
3	X	16/19 (84%)	15 (94%)	1 (6%)	18 50
All	All	5122/5413 (95%)	4460 (87%)	662 (13%)	4 18

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA

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 monosaccharides 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	1101	-	4,4,4	4.05	4 (100%)	6,6,6	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	7JA	L	1100	-	20,23,23	1.43	3 (15%)	20,30,30	2.05	3 (15%)
5	PO4	D	1102	-	4,4,4	4.19	4 (100%)	6,6,6	0.26	0
5	PO4	B	1104	-	4,4,4	4.30	4 (100%)	6,6,6	0.99	0
4	7JA	B	1100	-	20,23,23	1.58	3 (15%)	20,30,30	2.34	6 (30%)
4	7JA	F	1100	-	20,23,23	1.53	3 (15%)	20,30,30	2.25	4 (20%)
5	PO4	B	1101	-	4,4,4	4.29	4 (100%)	6,6,6	0.66	0
4	7JA	H	1100	-	20,23,23	1.46	3 (15%)	20,30,30	2.19	7 (35%)
5	PO4	H	1102	-	4,4,4	4.41	4 (100%)	6,6,6	0.62	0
4	7JA	N	1100	-	20,23,23	1.45	3 (15%)	20,30,30	2.31	5 (25%)
5	PO4	B	1102	-	4,4,4	4.20	4 (100%)	6,6,6	0.66	0
5	PO4	J	1101	-	4,4,4	4.14	4 (100%)	6,6,6	0.90	0
4	7JA	P	1100	-	20,23,23	1.50	3 (15%)	20,30,30	2.18	5 (25%)
5	PO4	J	1102	-	4,4,4	4.41	4 (100%)	6,6,6	0.41	0
5	PO4	N	1104	-	4,4,4	4.40	3 (75%)	6,6,6	0.95	0
5	PO4	H	1103	-	4,4,4	4.23	4 (100%)	6,6,6	0.64	0
5	PO4	J	1103	-	4,4,4	4.23	4 (100%)	6,6,6	0.75	0
5	PO4	J	1104	-	4,4,4	4.22	4 (100%)	6,6,6	0.77	0
5	PO4	H	1101	-	4,4,4	4.40	4 (100%)	6,6,6	1.00	1 (16%)
5	PO4	N	1102	-	4,4,4	4.41	4 (100%)	6,6,6	0.72	0
5	PO4	F	1104	-	4,4,4	4.18	4 (100%)	6,6,6	1.27	0
5	PO4	P	1101	-	4,4,4	4.31	4 (100%)	6,6,6	0.68	0
5	PO4	B	1103	-	4,4,4	3.99	4 (100%)	6,6,6	0.71	0
5	PO4	D	1104	-	4,4,4	4.20	3 (75%)	6,6,6	1.09	0
5	PO4	F	1101	-	4,4,4	4.24	4 (100%)	6,6,6	1.63	2 (33%)
5	PO4	L	1104	-	4,4,4	4.20	4 (100%)	6,6,6	0.77	0
5	PO4	L	1103	-	4,4,4	4.30	4 (100%)	6,6,6	0.60	0
5	PO4	P	1102	-	4,4,4	4.34	4 (100%)	6,6,6	0.46	0
5	PO4	F	1102	-	4,4,4	4.45	4 (100%)	6,6,6	0.36	0
5	PO4	D	1103	-	4,4,4	4.10	4 (100%)	6,6,6	0.87	0
5	PO4	P	1103	-	4,4,4	4.31	3 (75%)	6,6,6	0.92	0
5	PO4	F	1103	-	4,4,4	4.07	4 (100%)	6,6,6	0.70	0
5	PO4	L	1102	-	4,4,4	4.32	4 (100%)	6,6,6	0.30	0
5	PO4	N	1103	-	4,4,4	4.18	4 (100%)	6,6,6	1.12	0
5	PO4	H	1104	-	4,4,4	4.28	4 (100%)	6,6,6	1.85	1 (16%)
5	PO4	D	1101	-	4,4,4	4.10	4 (100%)	6,6,6	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	7JA	D	1100	-	20,23,23	1.49	3 (15%)	20,30,30	2.23	5 (25%)
4	7JA	J	1100	-	20,23,23	1.48	3 (15%)	20,30,30	2.29	6 (30%)
5	PO4	P	1104	-	4,4,4	4.27	4 (100%)	6,6,6	1.01	0
5	PO4	N	1101	-	4,4,4	4.14	4 (100%)	6,6,6	1.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	7JA	N	1100	-	-	5/19/36/36	0/1/1/1
4	7JA	L	1100	-	-	5/19/36/36	0/1/1/1
4	7JA	P	1100	-	-	7/19/36/36	0/1/1/1
4	7JA	B	1100	-	-	5/19/36/36	0/1/1/1
4	7JA	F	1100	-	-	7/19/36/36	0/1/1/1
4	7JA	D	1100	-	-	7/19/36/36	0/1/1/1
4	7JA	J	1100	-	-	4/19/36/36	0/1/1/1
4	7JA	H	1100	-	-	12/19/36/36	0/1/1/1

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1102	PO4	P-O1	6.86	1.67	1.50
5	P	1103	PO4	P-O1	6.79	1.66	1.50
5	J	1104	PO4	P-O1	6.76	1.66	1.50
5	P	1104	PO4	P-O1	6.71	1.66	1.50
5	H	1102	PO4	P-O1	6.64	1.66	1.50
5	N	1102	PO4	P-O1	6.59	1.66	1.50
5	J	1102	PO4	P-O1	6.58	1.66	1.50
5	N	1104	PO4	P-O1	6.52	1.66	1.50
5	L	1103	PO4	P-O1	6.50	1.66	1.50
5	D	1104	PO4	P-O1	6.42	1.65	1.50
5	J	1103	PO4	P-O1	6.40	1.65	1.50
5	P	1101	PO4	P-O1	6.40	1.65	1.50
5	B	1104	PO4	P-O1	6.34	1.65	1.50
5	D	1102	PO4	P-O1	6.29	1.65	1.50
5	L	1102	PO4	P-O1	6.29	1.65	1.50
5	P	1102	PO4	P-O1	6.27	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1102	PO4	P-O1	6.26	1.65	1.50
5	B	1101	PO4	P-O1	6.26	1.65	1.50
5	N	1103	PO4	P-O1	6.25	1.65	1.50
5	L	1104	PO4	P-O1	6.20	1.65	1.50
5	F	1103	PO4	P-O1	6.17	1.65	1.50
5	F	1104	PO4	P-O1	6.14	1.65	1.50
5	H	1104	PO4	P-O1	6.12	1.65	1.50
5	F	1101	PO4	P-O1	6.11	1.65	1.50
5	H	1103	PO4	P-O1	6.09	1.65	1.50
5	H	1101	PO4	P-O1	6.05	1.65	1.50
5	D	1103	PO4	P-O1	6.03	1.65	1.50
5	J	1101	PO4	P-O1	6.00	1.65	1.50
5	L	1101	PO4	P-O1	5.93	1.64	1.50
5	N	1101	PO4	P-O1	5.86	1.64	1.50
5	B	1103	PO4	P-O1	5.86	1.64	1.50
5	D	1101	PO4	P-O1	5.78	1.64	1.50
4	B	1100	7JA	C13-N	5.31	1.45	1.34
4	J	1100	7JA	C13-N	5.12	1.45	1.34
4	F	1100	7JA	C13-N	5.12	1.45	1.34
4	P	1100	7JA	C13-N	5.09	1.44	1.34
4	L	1100	7JA	C13-N	4.85	1.44	1.34
4	D	1100	7JA	C13-N	4.62	1.43	1.34
4	N	1100	7JA	C13-N	4.56	1.43	1.34
4	H	1100	7JA	C13-N	4.55	1.43	1.34
5	H	1101	PO4	P-O4	4.26	1.67	1.54
5	N	1101	PO4	P-O3	4.23	1.67	1.54
5	H	1104	PO4	P-O3	4.16	1.67	1.54
5	L	1103	PO4	P-O3	4.13	1.67	1.54
5	N	1102	PO4	P-O4	4.05	1.66	1.54
5	N	1104	PO4	P-O4	4.02	1.66	1.54
5	F	1104	PO4	P-O3	3.96	1.66	1.54
5	B	1101	PO4	P-O3	3.93	1.66	1.54
5	H	1102	PO4	P-O4	3.90	1.66	1.54
5	J	1102	PO4	P-O3	3.89	1.66	1.54
5	P	1102	PO4	P-O3	3.89	1.66	1.54
5	N	1104	PO4	P-O3	3.88	1.66	1.54
5	P	1101	PO4	P-O4	3.85	1.66	1.54
5	D	1102	PO4	P-O4	3.84	1.66	1.54
5	P	1102	PO4	P-O4	3.83	1.66	1.54
5	H	1101	PO4	P-O3	3.81	1.66	1.54
5	L	1102	PO4	P-O3	3.80	1.66	1.54
5	B	1104	PO4	P-O4	3.80	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1101	PO4	P-O3	3.79	1.66	1.54
5	B	1104	PO4	P-O3	3.77	1.65	1.54
5	L	1104	PO4	P-O4	3.76	1.65	1.54
5	H	1103	PO4	P-O4	3.75	1.65	1.54
5	N	1102	PO4	P-O3	3.74	1.65	1.54
5	N	1103	PO4	P-O4	3.72	1.65	1.54
5	B	1102	PO4	P-O4	3.72	1.65	1.54
5	H	1103	PO4	P-O3	3.68	1.65	1.54
5	J	1101	PO4	P-O4	3.67	1.65	1.54
5	H	1102	PO4	P-O3	3.67	1.65	1.54
5	H	1104	PO4	P-O4	3.67	1.65	1.54
5	F	1102	PO4	P-O4	3.66	1.65	1.54
5	D	1104	PO4	P-O3	3.66	1.65	1.54
5	F	1101	PO4	P-O3	3.65	1.65	1.54
5	L	1104	PO4	P-O3	3.65	1.65	1.54
5	J	1103	PO4	P-O4	3.64	1.65	1.54
5	L	1102	PO4	P-O4	3.63	1.65	1.54
5	D	1103	PO4	P-O3	3.61	1.65	1.54
5	J	1102	PO4	P-O4	3.61	1.65	1.54
5	L	1101	PO4	P-O3	3.61	1.65	1.54
5	P	1101	PO4	P-O3	3.60	1.65	1.54
5	D	1101	PO4	P-O4	3.59	1.65	1.54
5	D	1101	PO4	P-O3	3.59	1.65	1.54
5	P	1104	PO4	P-O4	3.56	1.65	1.54
5	D	1104	PO4	P-O4	3.53	1.65	1.54
5	P	1103	PO4	P-O4	3.51	1.65	1.54
5	N	1101	PO4	P-O4	3.50	1.65	1.54
5	P	1103	PO4	P-O3	3.45	1.65	1.54
5	F	1103	PO4	P-O3	3.37	1.64	1.54
5	B	1103	PO4	P-O3	3.36	1.64	1.54
5	P	1104	PO4	P-O3	3.33	1.64	1.54
5	N	1103	PO4	P-O3	3.33	1.64	1.54
5	F	1101	PO4	P-O2	-3.30	1.44	1.54
5	J	1103	PO4	P-O3	3.28	1.64	1.54
5	F	1101	PO4	P-O4	3.24	1.64	1.54
5	F	1102	PO4	P-O3	3.23	1.64	1.54
5	F	1104	PO4	P-O4	3.22	1.64	1.54
5	J	1104	PO4	P-O4	3.21	1.64	1.54
5	B	1103	PO4	P-O4	3.20	1.64	1.54
5	B	1101	PO4	P-O2	-3.18	1.45	1.54
5	L	1101	PO4	P-O4	3.16	1.64	1.54
5	F	1103	PO4	P-O4	3.11	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1102	PO4	P-O3	3.10	1.63	1.54
5	J	1104	PO4	P-O3	3.09	1.63	1.54
5	B	1102	PO4	P-O3	3.08	1.63	1.54
5	D	1103	PO4	P-O4	3.01	1.63	1.54
5	D	1103	PO4	P-O2	-2.98	1.45	1.54
5	B	1101	PO4	P-O4	2.97	1.63	1.54
5	L	1103	PO4	P-O4	2.96	1.63	1.54
4	F	1100	7JA	O14-C13	-2.88	1.17	1.23
5	F	1102	PO4	P-O2	-2.86	1.46	1.54
5	H	1101	PO4	P-O2	-2.86	1.46	1.54
5	B	1103	PO4	P-O2	-2.82	1.46	1.54
4	D	1100	7JA	O14-C13	-2.81	1.17	1.23
5	B	1102	PO4	P-O2	-2.81	1.46	1.54
5	D	1101	PO4	P-O2	-2.81	1.46	1.54
4	B	1100	7JA	O08-C07	-2.76	1.17	1.21
5	L	1101	PO4	P-O2	-2.74	1.46	1.54
5	L	1102	PO4	P-O2	-2.74	1.46	1.54
4	N	1100	7JA	C09-C07	2.69	1.55	1.51
5	F	1103	PO4	P-O2	-2.69	1.46	1.54
5	H	1103	PO4	P-O2	-2.63	1.46	1.54
5	J	1103	PO4	P-O2	-2.60	1.46	1.54
4	H	1100	7JA	C09-C07	2.59	1.55	1.51
4	B	1100	7JA	O14-C13	-2.58	1.18	1.23
4	H	1100	7JA	O14-C13	-2.56	1.18	1.23
5	J	1102	PO4	P-O2	-2.52	1.47	1.54
4	N	1100	7JA	O14-C13	-2.49	1.18	1.23
5	F	1104	PO4	P-O2	-2.49	1.47	1.54
5	P	1102	PO4	P-O2	-2.49	1.47	1.54
5	L	1103	PO4	P-O2	-2.47	1.47	1.54
5	D	1102	PO4	P-O2	-2.47	1.47	1.54
4	P	1100	7JA	C09-C07	2.46	1.55	1.51
4	F	1100	7JA	O08-C07	-2.45	1.17	1.21
5	N	1103	PO4	P-O2	-2.42	1.47	1.54
4	L	1100	7JA	O14-C13	-2.37	1.18	1.23
5	J	1104	PO4	P-O2	-2.35	1.47	1.54
4	J	1100	7JA	O14-C13	-2.34	1.18	1.23
5	P	1101	PO4	P-O2	-2.33	1.47	1.54
5	H	1102	PO4	P-O2	-2.27	1.47	1.54
5	B	1104	PO4	P-O2	-2.25	1.47	1.54
4	J	1100	7JA	O08-C07	-2.25	1.17	1.21
5	H	1104	PO4	P-O2	-2.24	1.47	1.54
4	P	1100	7JA	O14-C13	-2.18	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1104	PO4	P-O2	-2.18	1.48	1.54
4	D	1100	7JA	O08-C07	-2.16	1.18	1.21
5	J	1101	PO4	P-O2	-2.15	1.48	1.54
4	L	1100	7JA	C09-C07	2.05	1.54	1.51
5	N	1101	PO4	P-O2	-2.03	1.48	1.54
5	N	1102	PO4	P-O2	-2.00	1.48	1.54
5	P	1104	PO4	P-O2	-2.00	1.48	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	1100	7JA	CB-CA-N	-6.27	98.25	111.34
4	J	1100	7JA	CB-CA-N	-5.70	99.44	111.34
4	D	1100	7JA	CB-CA-N	-5.69	99.46	111.34
4	B	1100	7JA	CB-CA-N	-5.67	99.51	111.34
4	P	1100	7JA	C11-C12-C13	5.57	121.07	112.88
4	J	1100	7JA	C11-C12-C13	5.56	121.05	112.88
4	F	1100	7JA	CB-CA-N	-5.50	99.86	111.34
4	F	1100	7JA	C11-C12-C13	5.45	120.88	112.88
4	B	1100	7JA	C11-C12-C13	5.26	120.61	112.88
4	D	1100	7JA	C11-C12-C13	5.25	120.59	112.88
4	H	1100	7JA	C11-C12-C13	5.23	120.56	112.88
4	P	1100	7JA	CB-CA-N	-5.20	100.48	111.34
4	L	1100	7JA	C11-C12-C13	5.18	120.50	112.88
4	N	1100	7JA	C11-C12-C13	5.16	120.46	112.88
4	L	1100	7JA	CB-CA-N	-5.04	100.81	111.34
4	N	1100	7JA	C06-C05-C04	3.92	121.10	112.94
4	F	1100	7JA	O14-C13-C12	-3.89	115.80	121.50
4	H	1100	7JA	CB-CA-N	-3.83	103.36	111.34
4	J	1100	7JA	C06-C05-C04	3.76	120.78	112.94
4	D	1100	7JA	C06-C05-C04	3.65	120.55	112.94
5	H	1104	PO4	O3-P-O2	3.62	119.59	107.97
4	B	1100	7JA	O14-C13-C12	-3.54	116.31	121.50
4	L	1100	7JA	C06-C05-C04	3.47	120.16	112.94
4	B	1100	7JA	C06-C05-C04	3.37	119.96	112.94
4	P	1100	7JA	C06-C05-C04	3.20	119.60	112.94
4	H	1100	7JA	O14-C13-N	-3.14	117.66	122.95
4	H	1100	7JA	C10-C11-C06	2.94	107.58	103.34
4	H	1100	7JA	CG1-CB-CA	-2.93	103.89	111.17
4	N	1100	7JA	C10-C11-C12	-2.92	107.98	113.41
4	B	1100	7JA	C10-C09-C07	-2.91	102.50	105.42
4	F	1100	7JA	C06-C05-C04	2.84	118.86	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	1100	7JA	C10-C11-C12	-2.69	108.40	113.41
4	D	1100	7JA	CG2-CB-CA	-2.61	104.60	111.03
4	D	1100	7JA	O14-C13-C12	-2.58	117.72	121.50
4	P	1100	7JA	O14-C13-C12	-2.56	117.75	121.50
4	H	1100	7JA	C06-C05-C04	2.43	118.00	112.94
4	B	1100	7JA	C10-C11-C12	-2.40	108.94	113.41
4	J	1100	7JA	O14-C13-C12	-2.36	118.04	121.50
5	F	1101	PO4	O3-P-O2	2.31	115.39	107.97
4	J	1100	7JA	C10-C11-C12	-2.23	109.25	113.41
5	H	1101	PO4	O4-P-O3	2.21	115.05	107.97
4	N	1100	7JA	O14-C13-C12	-2.12	118.39	121.50
4	J	1100	7JA	CG2-CB-CA	-2.10	105.84	111.03
5	F	1101	PO4	O4-P-O3	2.06	114.60	107.97
4	H	1100	7JA	O08-C07-C06	-2.00	123.00	125.58

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1100	7JA	C11-C12-C13-N
4	L	1100	7JA	C11-C12-C13-O14
4	B	1100	7JA	C11-C12-C13-N
4	B	1100	7JA	C11-C12-C13-O14
4	F	1100	7JA	C11-C12-C13-N
4	F	1100	7JA	C11-C12-C13-O14
4	H	1100	7JA	N-CA-CB-CG2
4	H	1100	7JA	C01-C02-C03-C04
4	H	1100	7JA	C11-C12-C13-O14
4	N	1100	7JA	C11-C12-C13-N
4	N	1100	7JA	C11-C12-C13-O14
4	P	1100	7JA	C11-C12-C13-N
4	P	1100	7JA	C11-C12-C13-O14
4	D	1100	7JA	C11-C12-C13-N
4	D	1100	7JA	C11-C12-C13-O14
4	J	1100	7JA	C11-C12-C13-N
4	J	1100	7JA	C11-C12-C13-O14
4	H	1100	7JA	CA-CB-CG1-CD1
4	H	1100	7JA	C11-C12-C13-N
4	L	1100	7JA	C-CA-N-C13
4	B	1100	7JA	C-CA-N-C13
4	F	1100	7JA	C-CA-N-C13
4	N	1100	7JA	C-CA-N-C13

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Mol	Chain	Res	Type	Atoms
4	P	1100	7JA	C-CA-N-C13
4	D	1100	7JA	C-CA-N-C13
4	J	1100	7JA	C-CA-N-C13
4	H	1100	7JA	CG2-CB-CG1-CD1
4	H	1100	7JA	N-CA-CB-CG1
4	H	1100	7JA	C-CA-CB-CG2
4	L	1100	7JA	C04-C05-C06-C11
4	H	1100	7JA	C04-C05-C06-C07
4	P	1100	7JA	N-CA-CB-CG2
4	B	1100	7JA	C01-C02-C03-C04
4	N	1100	7JA	C01-C02-C03-C04
4	P	1100	7JA	C01-C02-C03-C04
4	H	1100	7JA	C12-C13-N-CA
4	F	1100	7JA	C04-C05-C06-C11
4	H	1100	7JA	C04-C05-C06-C11
4	P	1100	7JA	C04-C05-C06-C11
4	D	1100	7JA	C04-C05-C06-C11
4	J	1100	7JA	C04-C05-C06-C11
4	H	1100	7JA	C-CA-CB-CG1
4	B	1100	7JA	C-CA-CB-CG2
4	F	1100	7JA	C-CA-CB-CG2
4	P	1100	7JA	C-CA-CB-CG2
4	D	1100	7JA	C-CA-CB-CG2
4	F	1100	7JA	N-CA-CB-CG2
4	L	1100	7JA	C01-C02-C03-C04
4	F	1100	7JA	C01-C02-C03-C04
4	D	1100	7JA	C01-C02-C03-C04
4	D	1100	7JA	N-CA-CB-CG2
4	N	1100	7JA	C02-C03-C04-C05

There are no ring outliers.

18 monomers are involved in 158 short contacts:

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

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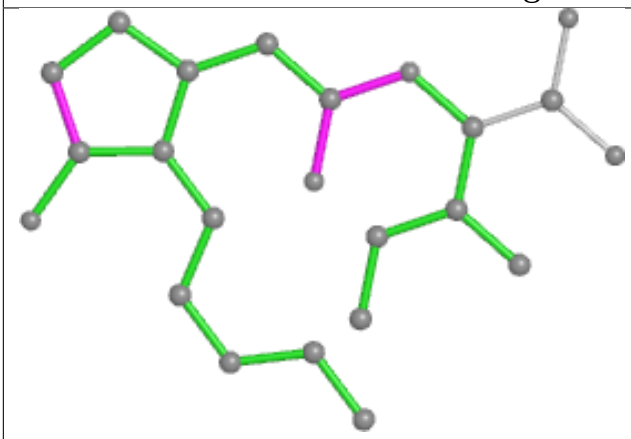
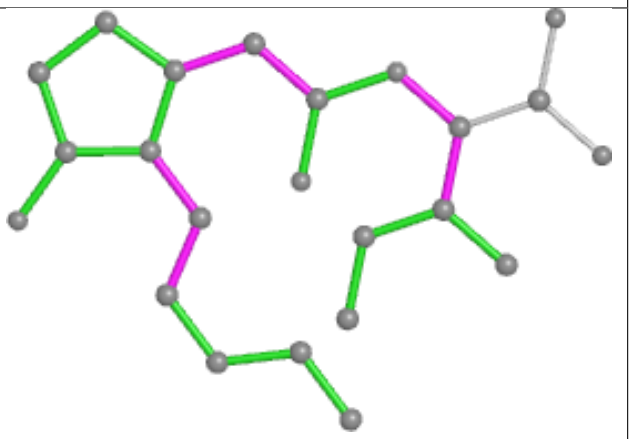
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1103	PO4	2	0
5	B	1103	PO4	2	0
5	F	1101	PO4	1	0
5	L	1103	PO4	2	0
5	D	1103	PO4	3	0
5	P	1103	PO4	3	0
5	F	1103	PO4	3	0
5	N	1103	PO4	2	0
4	D	1100	7JA	15	0
4	J	1100	7JA	17	0

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.

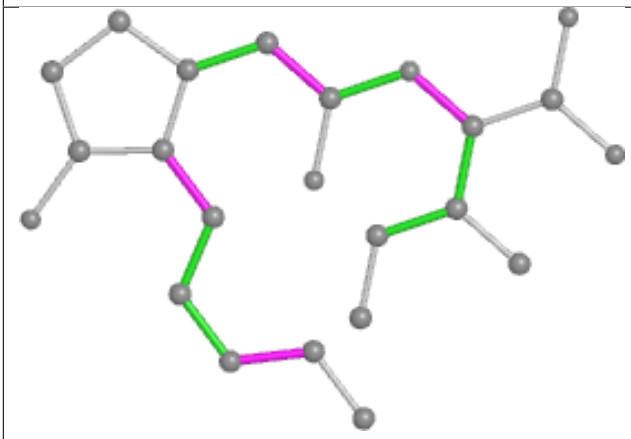
Ligand 7JA L 1100



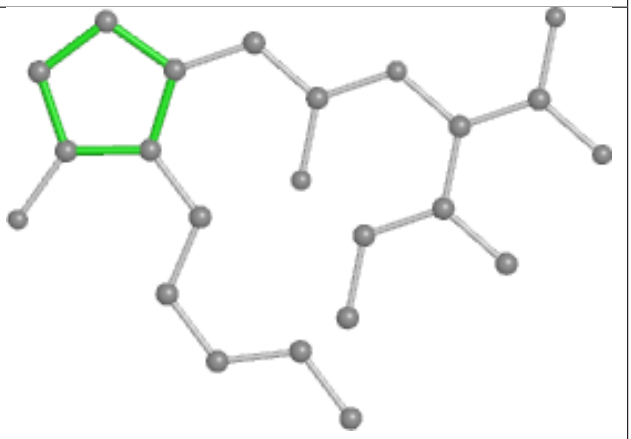
Bond lengths



Bond angles

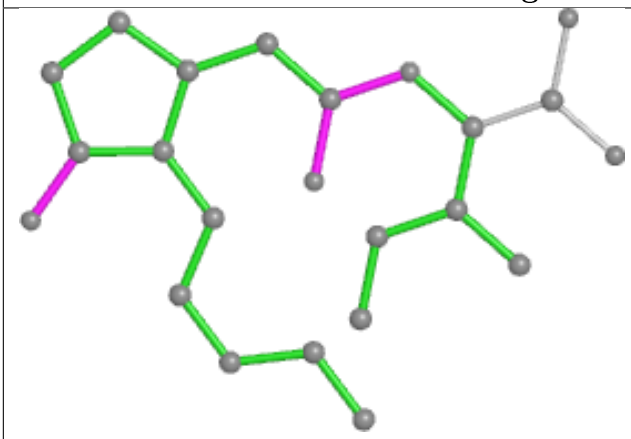


Torsions

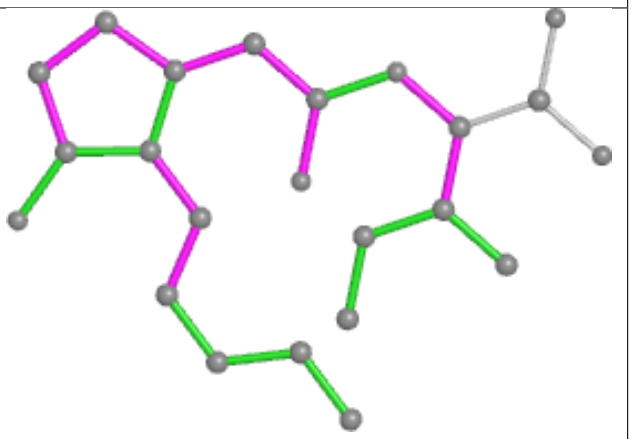


Rings

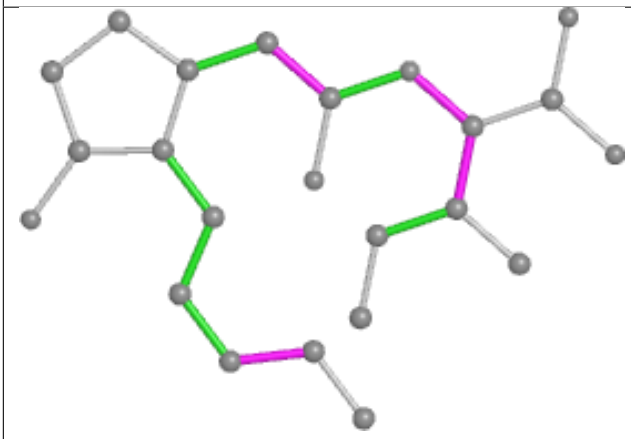
Ligand 7JA B 1100



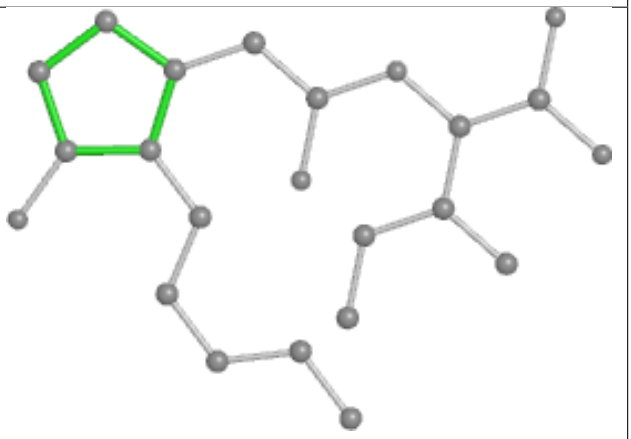
Bond lengths



Bond angles

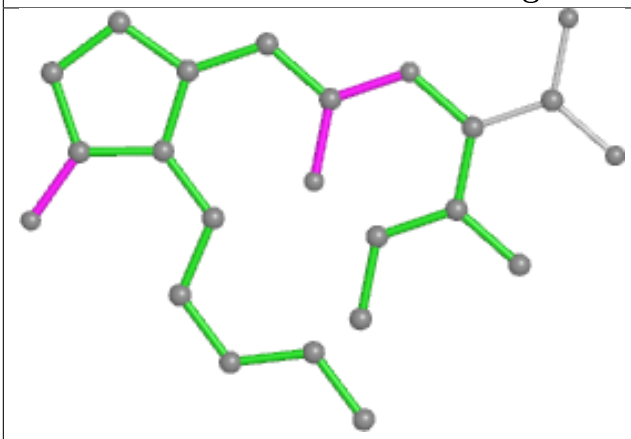


Torsions

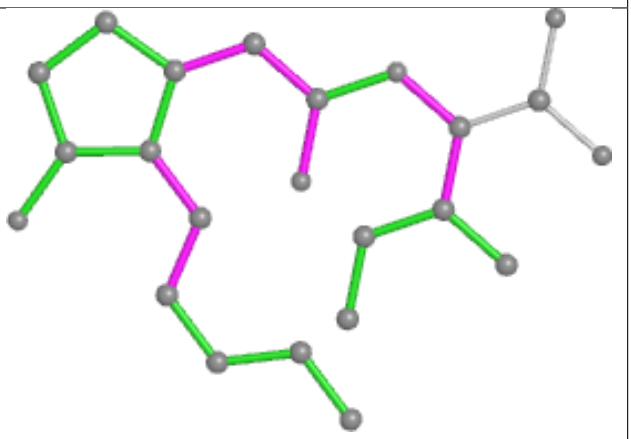


Rings

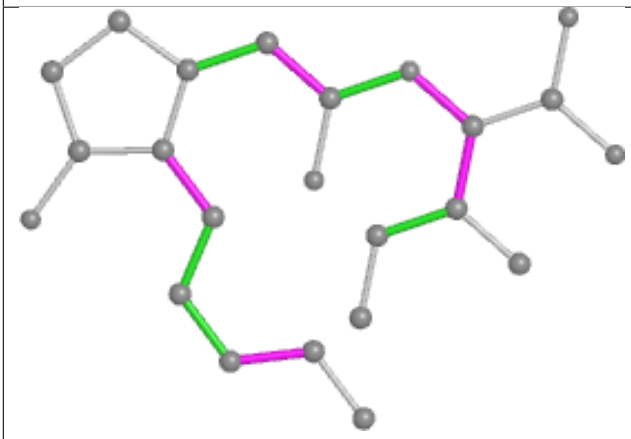
Ligand 7JA F 1100



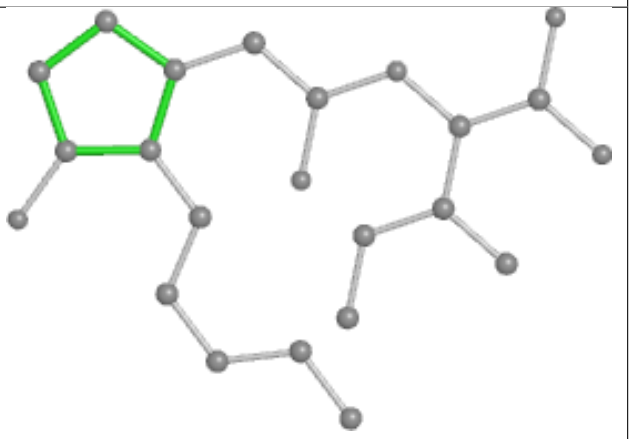
Bond lengths



Bond angles

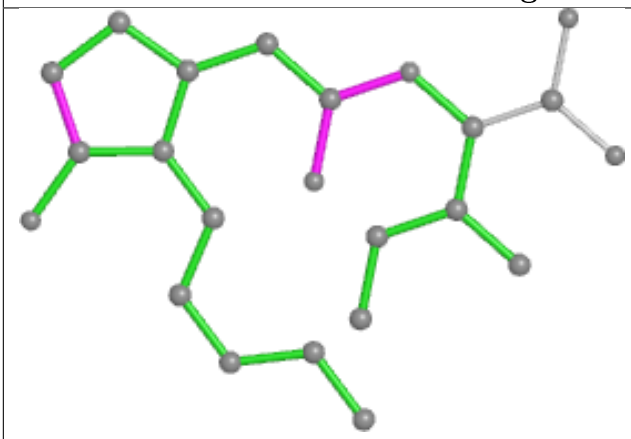


Torsions

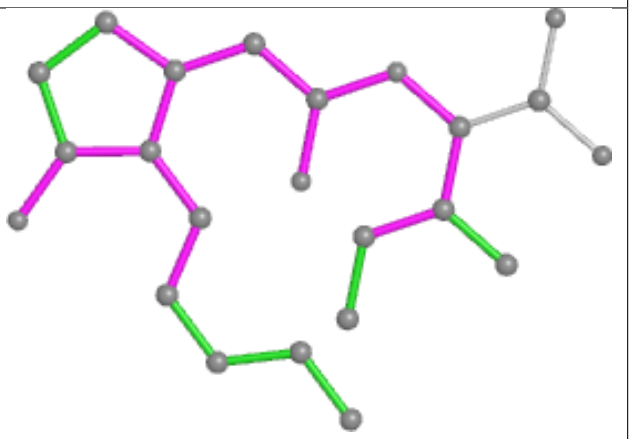


Rings

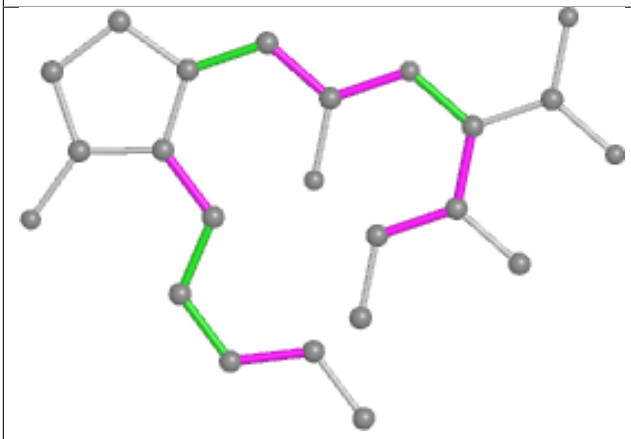
Ligand 7JA H 1100



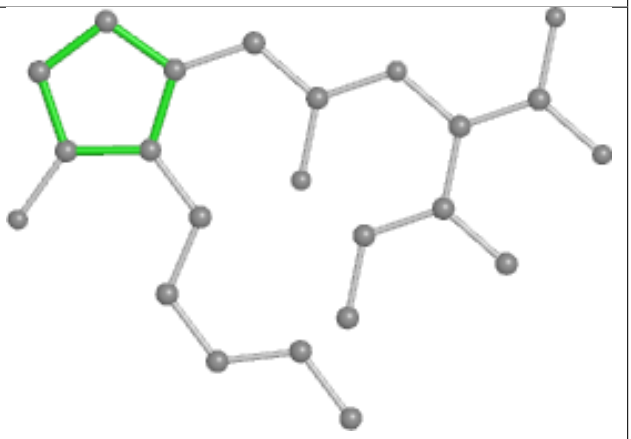
Bond lengths



Bond angles

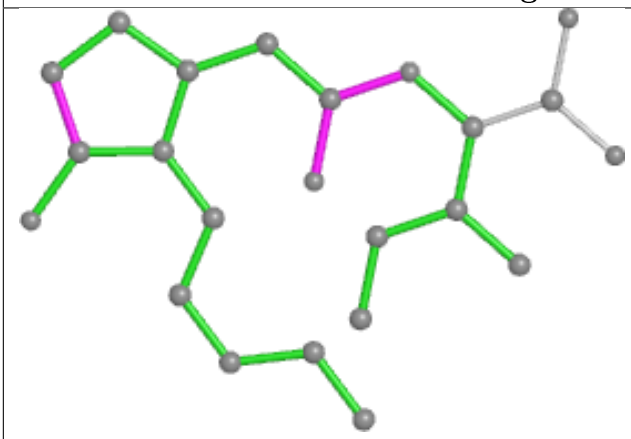


Torsions

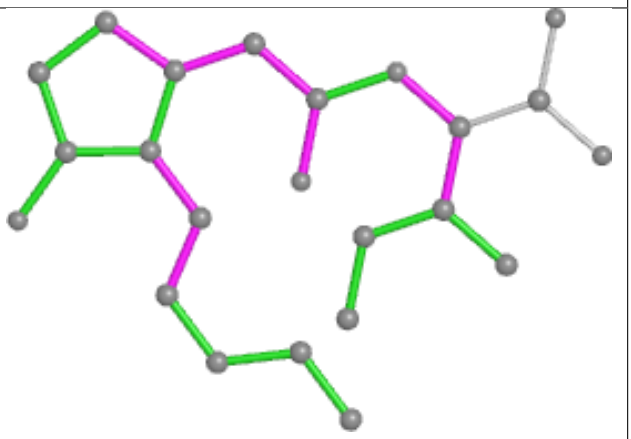


Rings

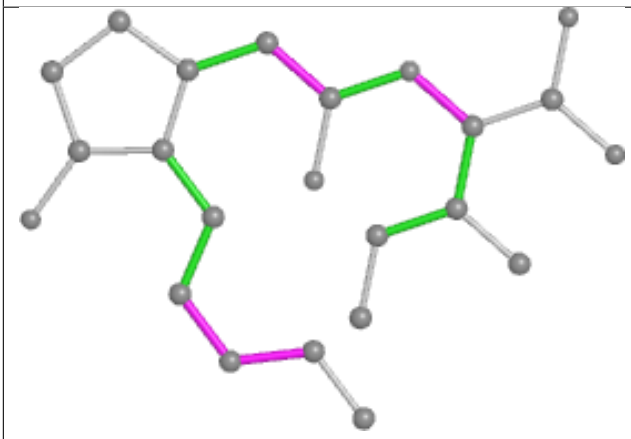
Ligand 7JA N 1100



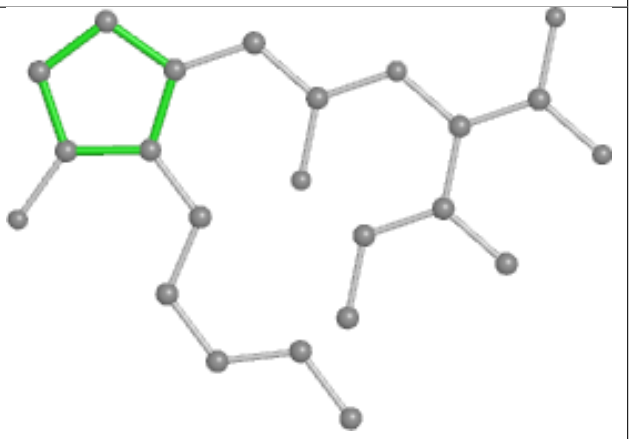
Bond lengths



Bond angles

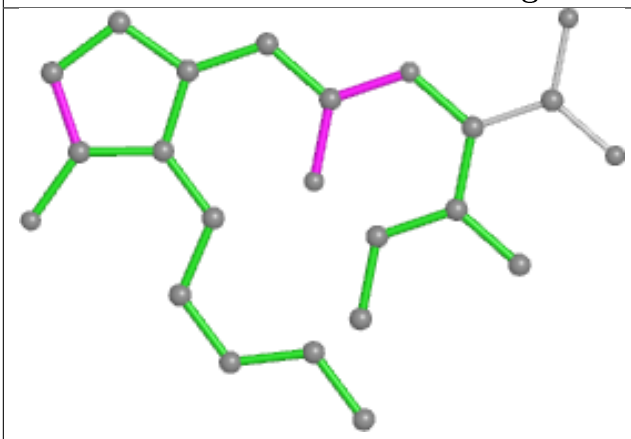


Torsions

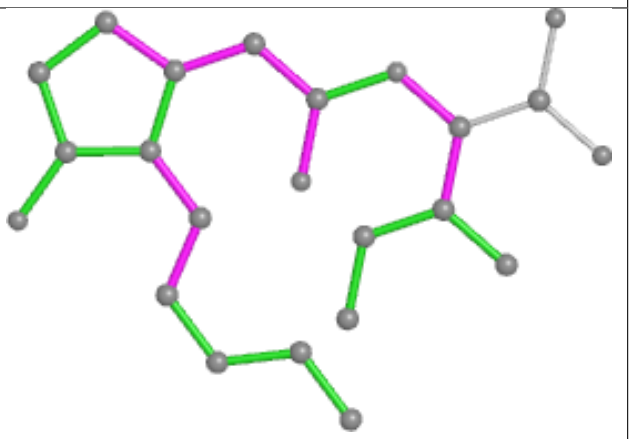


Rings

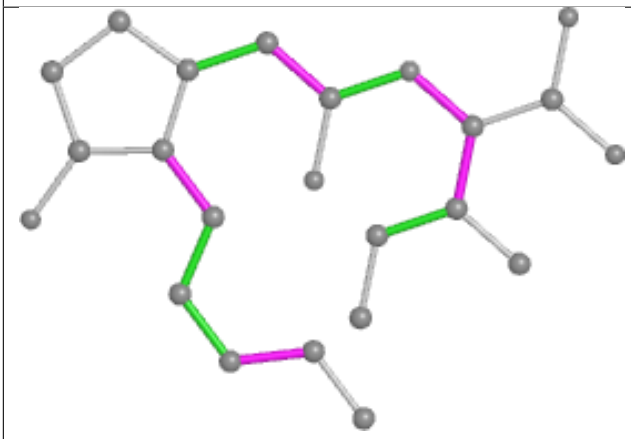
Ligand 7JA P 1100



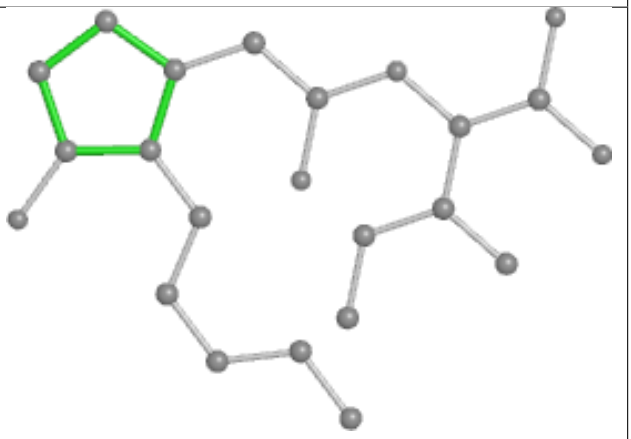
Bond lengths



Bond angles

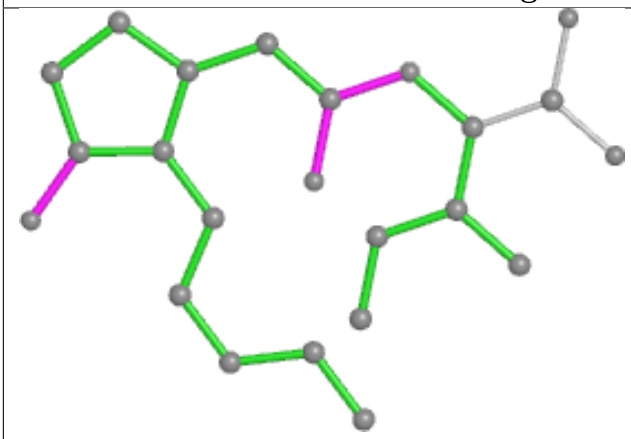


Torsions

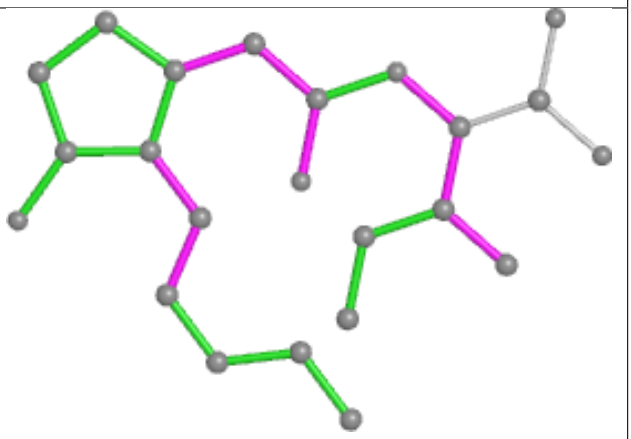


Rings

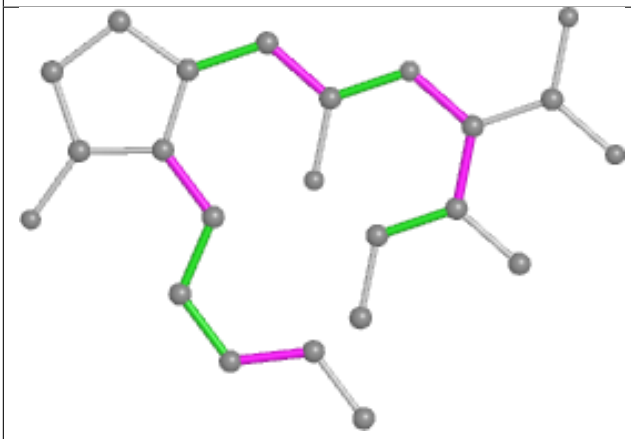
Ligand 7JA D 1100



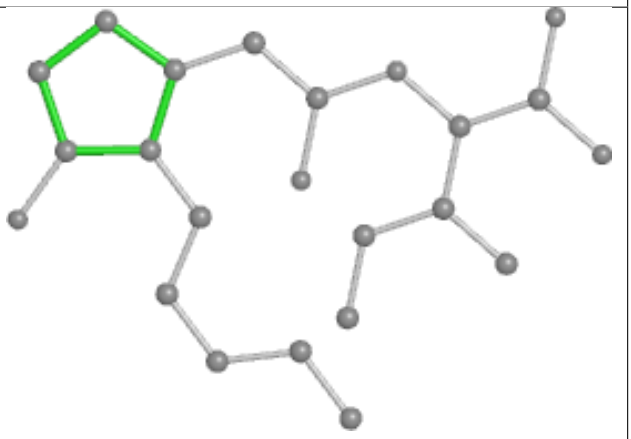
Bond lengths



Bond angles

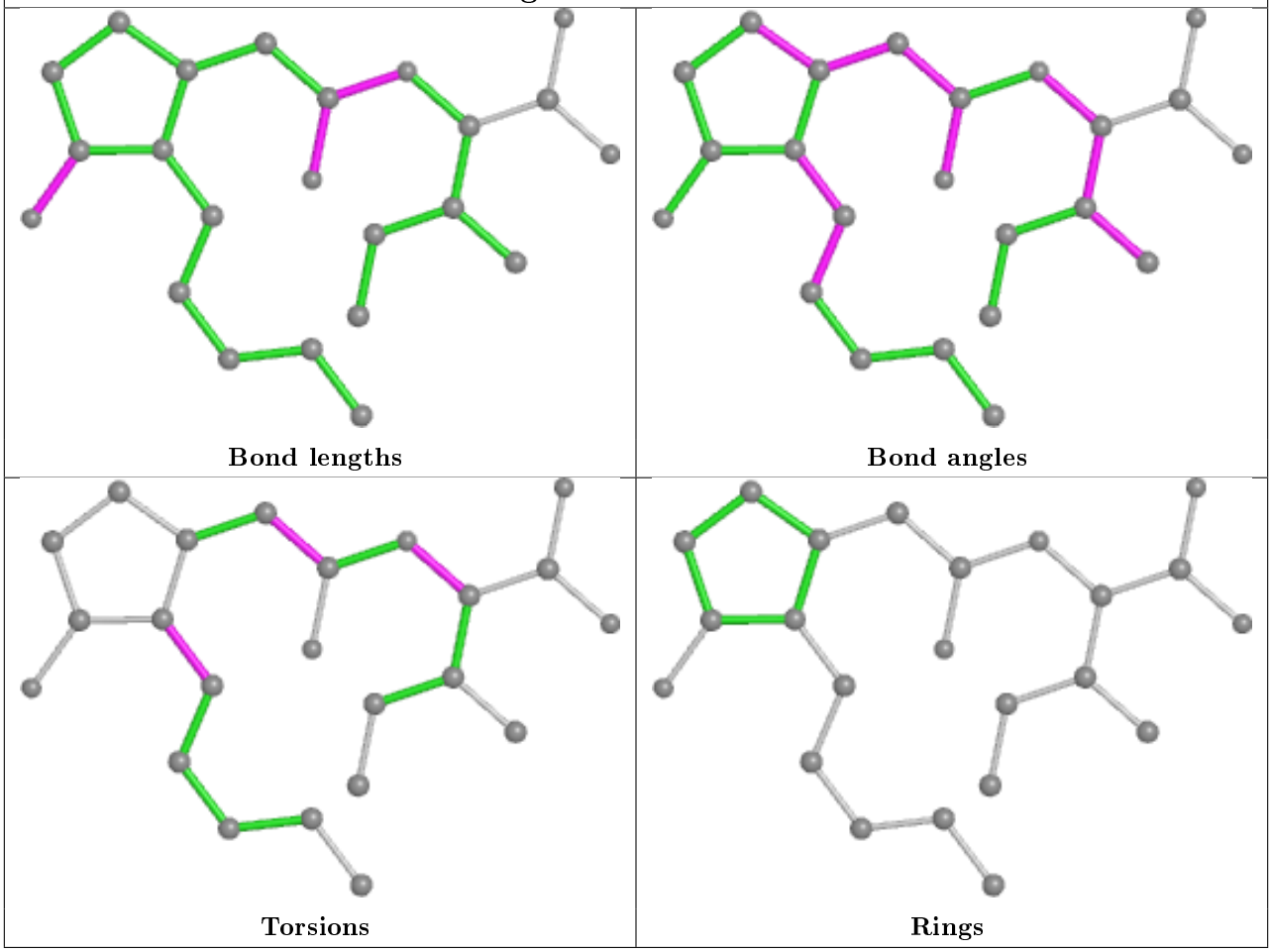


Torsions



Rings

Ligand 7JA J 1100



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%)	0.27	4 (2%) 53 37	38, 87, 141, 157	0
1	C	144/160 (90%)	0.53	8 (5%) 24 13	40, 90, 140, 159	0
1	E	144/160 (90%)	0.04	0 100 100	41, 85, 136, 157	0
1	G	144/160 (90%)	-0.09	0 100 100	37, 81, 136, 156	0
1	I	144/160 (90%)	0.34	8 (5%) 24 13	43, 88, 138, 160	0
1	K	144/160 (90%)	0.44	10 (6%) 16 9	43, 89, 140, 158	0
1	M	144/160 (90%)	0.60	18 (12%) 3 2	45, 89, 139, 163	0
1	O	144/160 (90%)	0.61	16 (11%) 5 3	43, 88, 138, 159	0
2	B	568/592 (95%)	-0.22	10 (1%) 68 55	31, 60, 122, 191	0
2	D	568/592 (95%)	-0.19	11 (1%) 66 53	33, 61, 124, 190	0
2	F	568/592 (95%)	-0.24	18 (3%) 47 31	32, 63, 125, 191	0
2	H	562/592 (94%)	-0.47	6 (1%) 80 69	29, 57, 106, 169	0
2	J	568/592 (95%)	-0.31	13 (2%) 60 46	33, 64, 124, 194	0
2	L	568/592 (95%)	-0.30	10 (1%) 68 55	33, 64, 125, 192	0
2	N	568/592 (95%)	0.08	27 (4%) 30 17	33, 69, 126, 194	0
2	P	568/592 (95%)	-0.18	19 (3%) 46 30	34, 68, 126, 192	0
3	Q	18/21 (85%)	-0.13	0 100 100	61, 77, 108, 128	0
3	R	18/21 (85%)	-0.11	1 (5%) 24 13	63, 78, 108, 131	0
3	S	18/21 (85%)	-0.28	0 100 100	64, 78, 109, 129	0
3	U	18/21 (85%)	-0.32	0 100 100	60, 80, 109, 130	0
3	V	18/21 (85%)	-0.18	1 (5%) 24 13	61, 81, 108, 132	0
3	W	18/21 (85%)	0.11	1 (5%) 24 13	66, 83, 110, 132	0
3	X	18/21 (85%)	-0.22	1 (5%) 24 13	65, 81, 109, 131	0
All	All	5816/6163 (94%)	-0.11	182 (3%) 49 32	29, 68, 128, 194	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	592	ILE	9.3
2	N	12	SER	8.6
2	P	12	SER	7.9
2	L	359	GLU	7.5
2	F	547	SER	7.0
2	D	360	ASP	7.0
2	D	12	SER	6.9
2	N	590	GLU	6.4
2	N	591	PRO	6.4
3	W	200	GLU	6.1
2	F	592	ILE	6.1
2	L	360	ASP	6.0
1	O	80	ASP	5.2
1	K	13	GLY	5.1
2	J	360	ASP	5.0
1	A	21	ALA	5.0
2	N	360	ASP	5.0
2	B	360	ASP	5.0
2	L	592	ILE	4.9
1	M	115	ASP	4.9
2	P	362	GLU	4.9
2	B	549	ARG	4.8
2	N	15	ALA	4.8
1	M	80	ASP	4.8
2	B	356	GLN	4.7
2	F	591	PRO	4.7
2	F	548	ARG	4.6
2	B	358	MET	4.6
2	J	12	SER	4.4
2	D	592	ILE	4.4
2	F	356	GLN	4.2
2	N	361	GLU	4.2
2	P	547	SER	4.1
2	N	359	GLU	4.1
2	L	362	GLU	4.0
2	D	361	GLU	4.0
1	C	115	ASP	3.9
2	H	353	ALA	3.9
2	J	592	ILE	3.9
1	C	13	GLY	3.9
2	F	546	PRO	3.9
2	P	592	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	356	GLN	3.7
2	F	590	GLU	3.7
2	P	546	PRO	3.7
2	J	362	GLU	3.6
2	N	358	MET	3.6
2	N	354	ASP	3.6
3	V	200	GLU	3.6
2	P	548	ARG	3.6
1	M	17	GLU	3.6
2	N	355	GLU	3.5
2	F	549	ARG	3.5
2	B	359	GLU	3.4
3	X	200	GLU	3.4
2	J	549	ARG	3.4
2	N	357	GLY	3.4
2	N	13	CYS	3.4
2	P	591	PRO	3.3
2	D	358	MET	3.3
1	M	21	ALA	3.3
2	B	527	MET	3.2
2	P	360	ASP	3.2
2	J	548	ARG	3.2
1	C	7	VAL	3.2
2	N	362	GLU	3.2
2	B	592	ILE	3.2
2	F	12	SER	3.1
2	N	548	ARG	3.1
1	M	116	LEU	3.1
2	P	356	GLN	3.1
1	O	56	ILE	3.1
1	K	7	VAL	3.0
2	F	358	MET	3.0
1	C	20	GLU	3.0
1	O	84	LYS	3.0
2	F	355	GLU	3.0
1	K	6	ILE	3.0
2	F	359	GLU	3.0
2	D	549	ARG	3.0
1	K	20	GLU	3.0
2	D	418	ARG	2.9
2	H	362	GLU	2.9
1	O	91	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	63	VAL	2.9
1	K	17	GLU	2.9
1	O	115	ASP	2.9
2	B	355	GLU	2.9
2	H	12	SER	2.9
1	M	84	LYS	2.9
1	O	52	LEU	2.8
1	I	38	VAL	2.7
2	P	549	ARG	2.7
1	M	6	ILE	2.7
1	O	89	ASP	2.7
2	N	527	MET	2.7
1	I	20	GLU	2.7
2	J	359	GLU	2.6
2	N	588	LEU	2.6
1	K	15	SER	2.6
1	M	35	ASP	2.6
2	N	356	GLN	2.6
1	K	67	ALA	2.6
1	I	47	VAL	2.6
3	R	200	GLU	2.5
1	K	63	VAL	2.5
2	D	548	ARG	2.5
1	A	20	GLU	2.5
2	J	591	PRO	2.5
2	P	590	GLU	2.5
2	N	363	GLY	2.5
2	N	314	ILE	2.5
2	D	22	GLU	2.5
1	I	39	ASP	2.5
2	F	361	GLU	2.4
2	P	418	ARG	2.4
2	P	359	GLU	2.4
1	M	87	ASP	2.4
2	F	360	ASP	2.4
2	B	548	ARG	2.4
2	N	547	SER	2.4
1	I	37	CYS	2.4
1	M	38	VAL	2.4
2	L	548	ARG	2.3
1	O	58	TYR	2.3
2	J	361	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	355	GLU	2.3
1	M	81	ASP	2.3
2	H	527	MET	2.3
1	I	42	VAL	2.3
1	M	90	PHE	2.3
1	C	66	ALA	2.3
2	J	355	GLU	2.3
1	A	124	MET	2.3
1	M	82	ASP	2.3
1	O	19	GLU	2.3
2	F	527	MET	2.3
2	D	357	GLY	2.3
2	L	258	GLY	2.3
2	F	354	ASP	2.3
2	N	402	LEU	2.2
2	P	361	GLU	2.2
1	O	22	VAL	2.2
2	P	370	LEU	2.2
1	A	59	CYS	2.2
1	I	84	LYS	2.2
2	L	591	PRO	2.2
2	J	547	SER	2.2
1	C	118	CYS	2.2
1	I	6	ILE	2.2
2	N	546	PRO	2.2
2	N	398	ILE	2.2
2	P	255	GLU	2.2
2	P	527	MET	2.2
2	F	357	GLY	2.2
2	L	12	SER	2.2
2	N	383	MET	2.2
2	F	258	GLY	2.1
2	J	356	GLN	2.1
1	M	16	PHE	2.1
1	K	22	VAL	2.1
1	O	16	PHE	2.1
2	J	415	ARG	2.1
1	O	55	VAL	2.1
2	P	589	LYS	2.1
2	H	359	GLU	2.1
2	N	428	VAL	2.1
1	K	114	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	91	MET	2.1
2	N	589	LYS	2.1
1	M	119	GLN	2.1
2	H	355	GLU	2.1
2	B	564	HIS	2.1
1	C	40	ASN	2.1
2	D	362	GLU	2.1
1	O	88	ALA	2.0
1	M	145	PRO	2.0
2	P	315	GLN	2.0
1	O	93	ILE	2.0
1	C	119	GLN	2.0
1	O	117	THR	2.0
1	M	83	LEU	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 monosaccharides 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	1102	5/5	0.90	0.18	72,73,108,121	0
5	PO4	B	1102	5/5	0.91	0.23	49,75,81,91	0
5	PO4	N	1102	5/5	0.91	0.26	64,78,83,116	0
5	PO4	D	1104	5/5	0.91	0.21	49,60,85,91	0
5	PO4	L	1104	5/5	0.91	0.21	52,60,91,94	0
5	PO4	N	1104	5/5	0.92	0.29	56,57,89,100	0
5	PO4	P	1103	5/5	0.93	0.21	47,55,70,76	0
5	PO4	D	1102	5/5	0.93	0.22	55,73,86,95	0
5	PO4	J	1104	5/5	0.93	0.22	57,60,82,86	0

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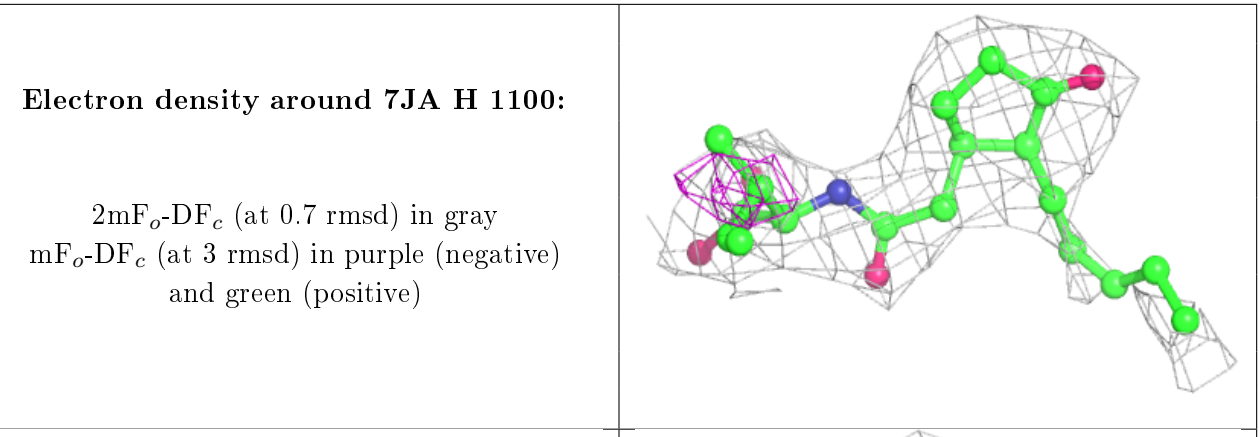
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	H	1104	5/5	0.93	0.23	57,64,69,95	0
4	7JA	H	1100	23/23	0.94	0.30	38,62,77,81	0
5	PO4	B	1104	5/5	0.94	0.16	47,63,91,96	0
4	7JA	N	1100	23/23	0.94	0.23	49,61,73,86	0
5	PO4	H	1101	5/5	0.94	0.18	65,80,94,96	0
5	PO4	P	1104	5/5	0.94	0.22	50,58,89,93	0
5	PO4	N	1101	5/5	0.94	0.22	42,48,74,75	0
4	7JA	L	1100	23/23	0.95	0.23	42,58,72,86	0
4	7JA	F	1100	23/23	0.95	0.27	42,56,70,88	0
5	PO4	F	1102	5/5	0.95	0.20	56,74,78,96	0
5	PO4	P	1102	5/5	0.95	0.18	63,72,83,106	0
4	7JA	B	1100	23/23	0.95	0.27	34,55,70,87	0
4	7JA	P	1100	23/23	0.95	0.25	47,59,73,85	0
5	PO4	F	1104	5/5	0.95	0.20	48,54,80,83	0
5	PO4	J	1102	5/5	0.96	0.24	53,74,83,101	0
4	7JA	J	1100	23/23	0.96	0.24	39,55,72,83	0
5	PO4	H	1103	5/5	0.96	0.16	35,56,67,68	0
5	PO4	L	1102	5/5	0.96	0.30	64,67,83,96	0
5	PO4	F	1103	5/5	0.97	0.25	44,47,48,69	0
5	PO4	L	1103	5/5	0.97	0.24	45,48,58,71	0
5	PO4	N	1103	5/5	0.97	0.22	48,51,62,80	0
5	PO4	B	1101	5/5	0.97	0.20	35,48,61,72	0
4	7JA	D	1100	23/23	0.97	0.24	37,55,68,85	0
5	PO4	J	1101	5/5	0.97	0.20	37,45,66,73	0
5	PO4	L	1101	5/5	0.97	0.27	36,48,65,73	0
5	PO4	J	1103	5/5	0.97	0.23	42,45,52,68	0
5	PO4	P	1101	5/5	0.98	0.24	40,51,70,73	0
5	PO4	B	1103	5/5	0.98	0.24	41,45,51,66	0
5	PO4	D	1103	5/5	0.98	0.23	38,46,52,75	0
5	PO4	F	1101	5/5	0.98	0.22	40,41,55,77	0
5	PO4	D	1101	5/5	0.99	0.21	42,45,58,71	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.

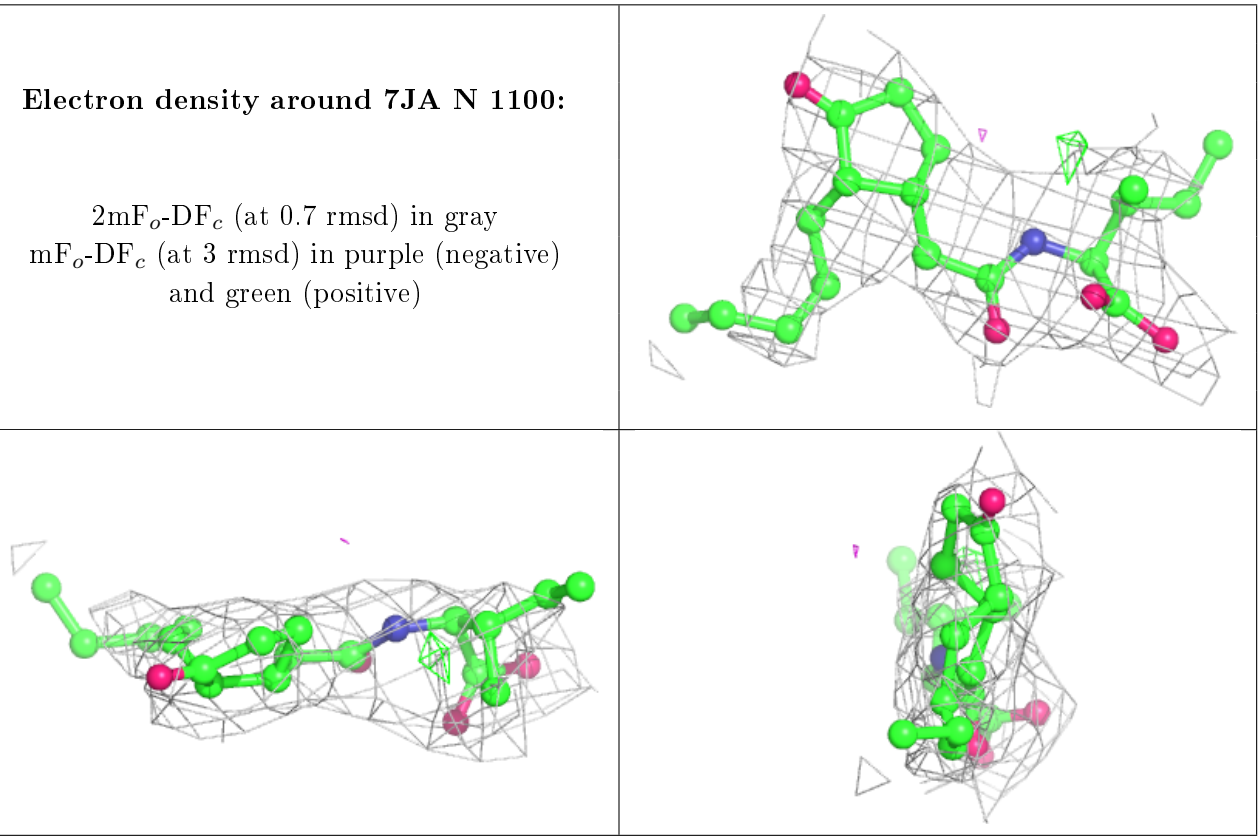
Electron density around 7JA H 1100:

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



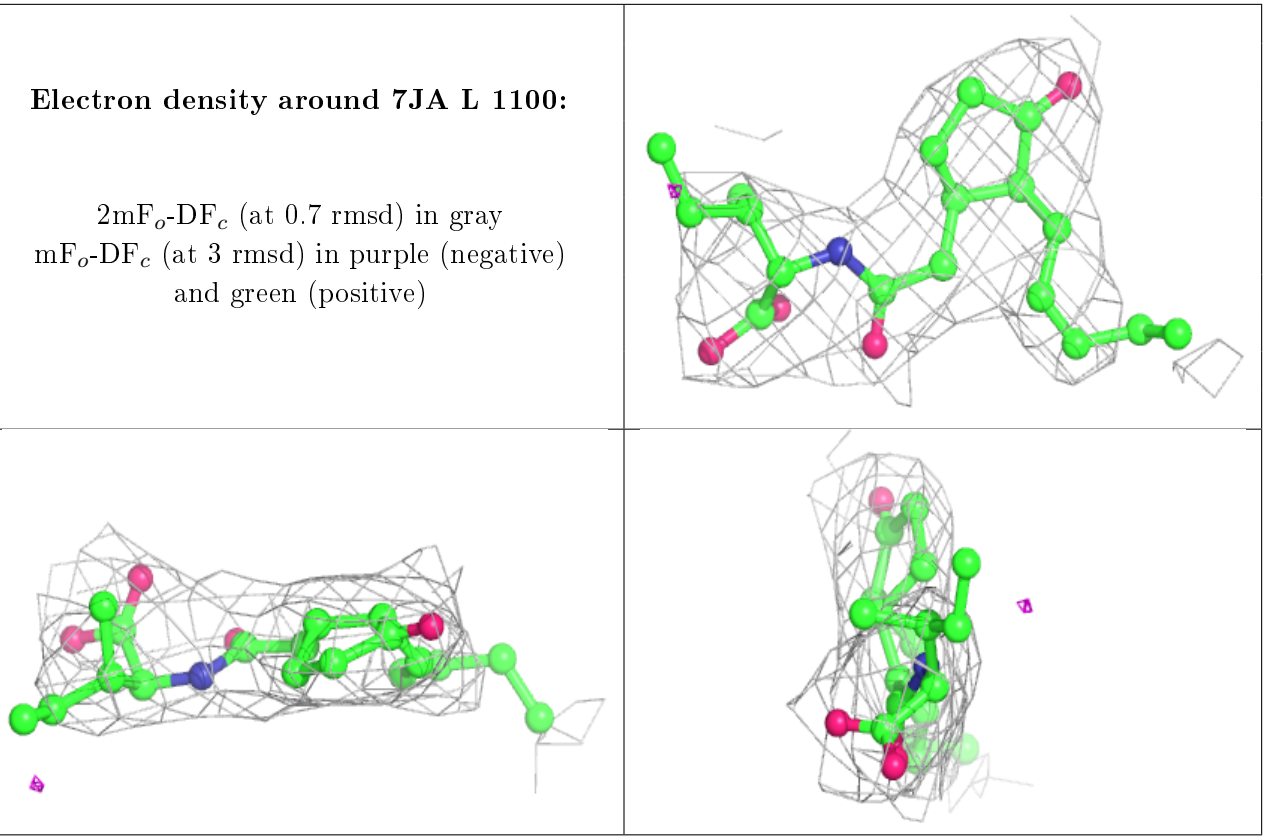
Electron density around 7JA N 1100:

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



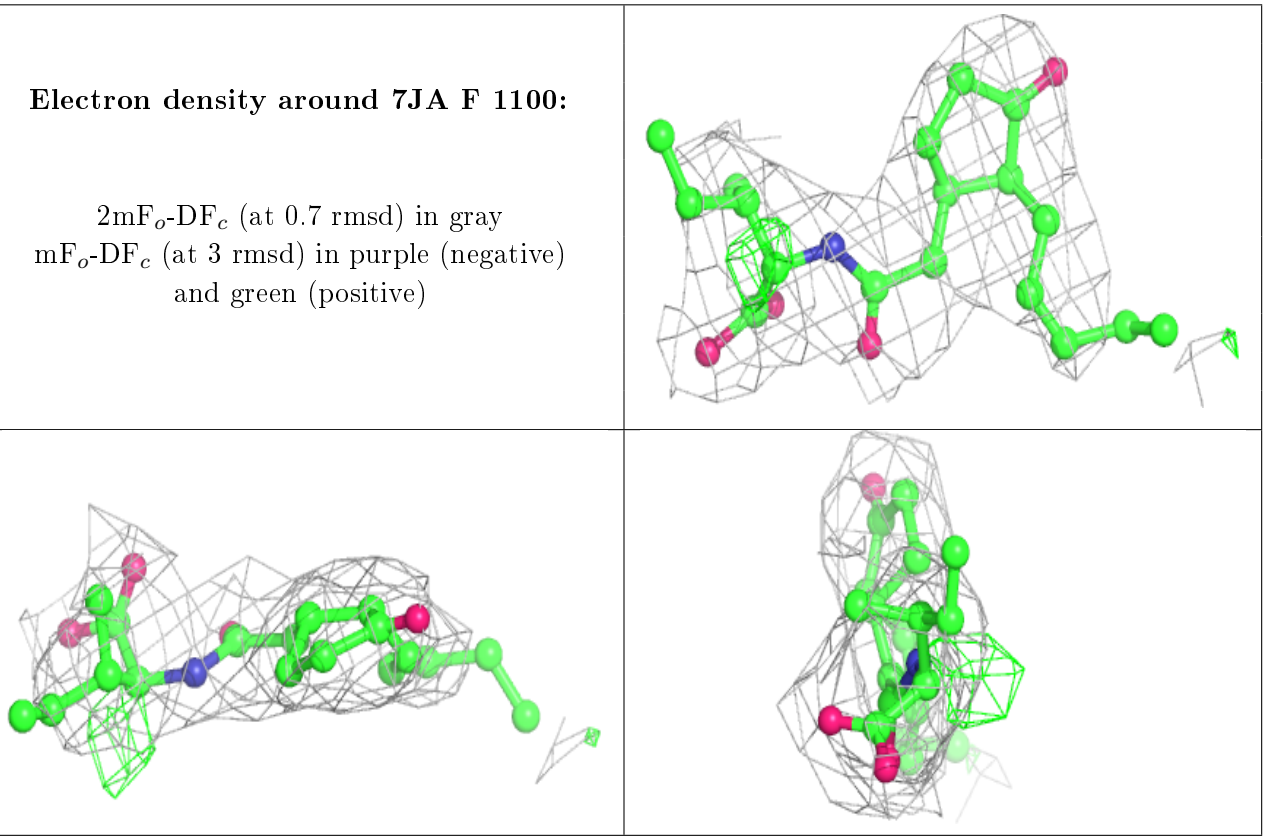
Electron density around 7JA L 1100:

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



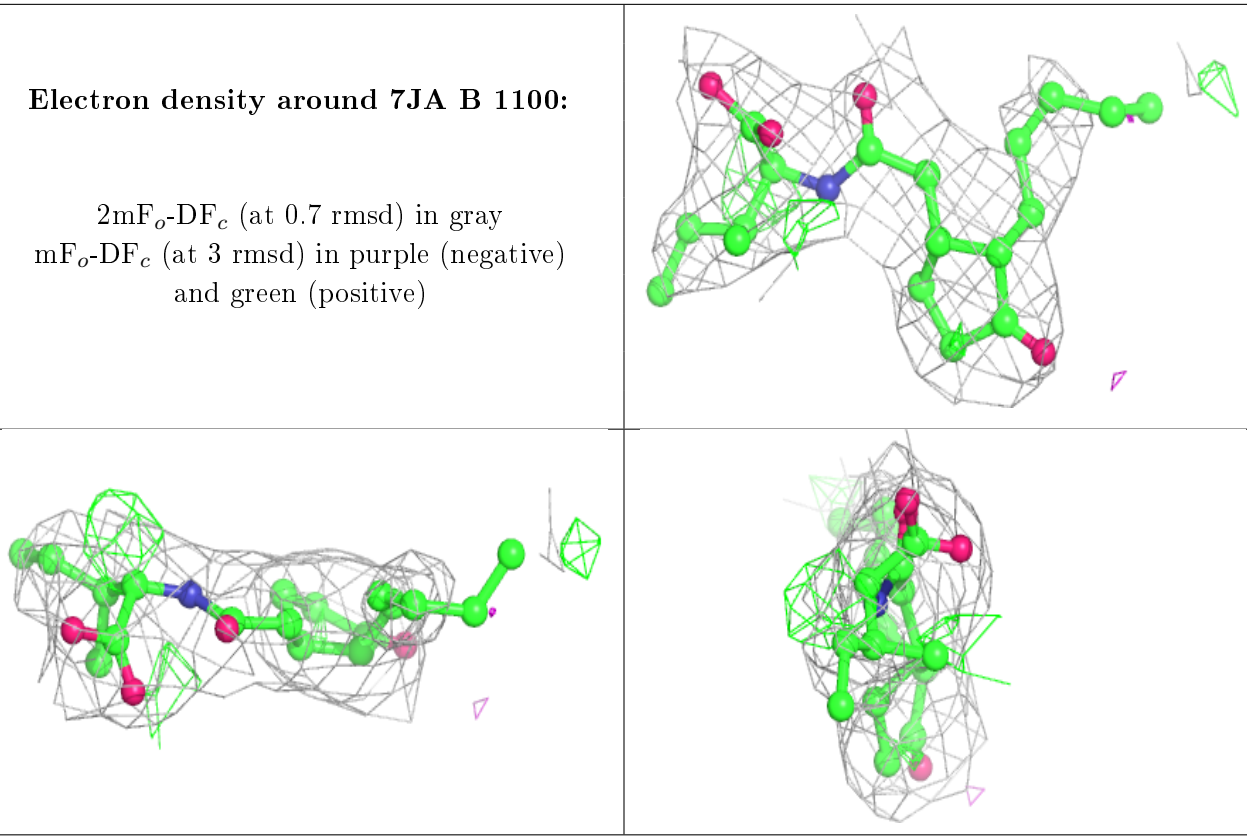
Electron density around 7JA F 1100:

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



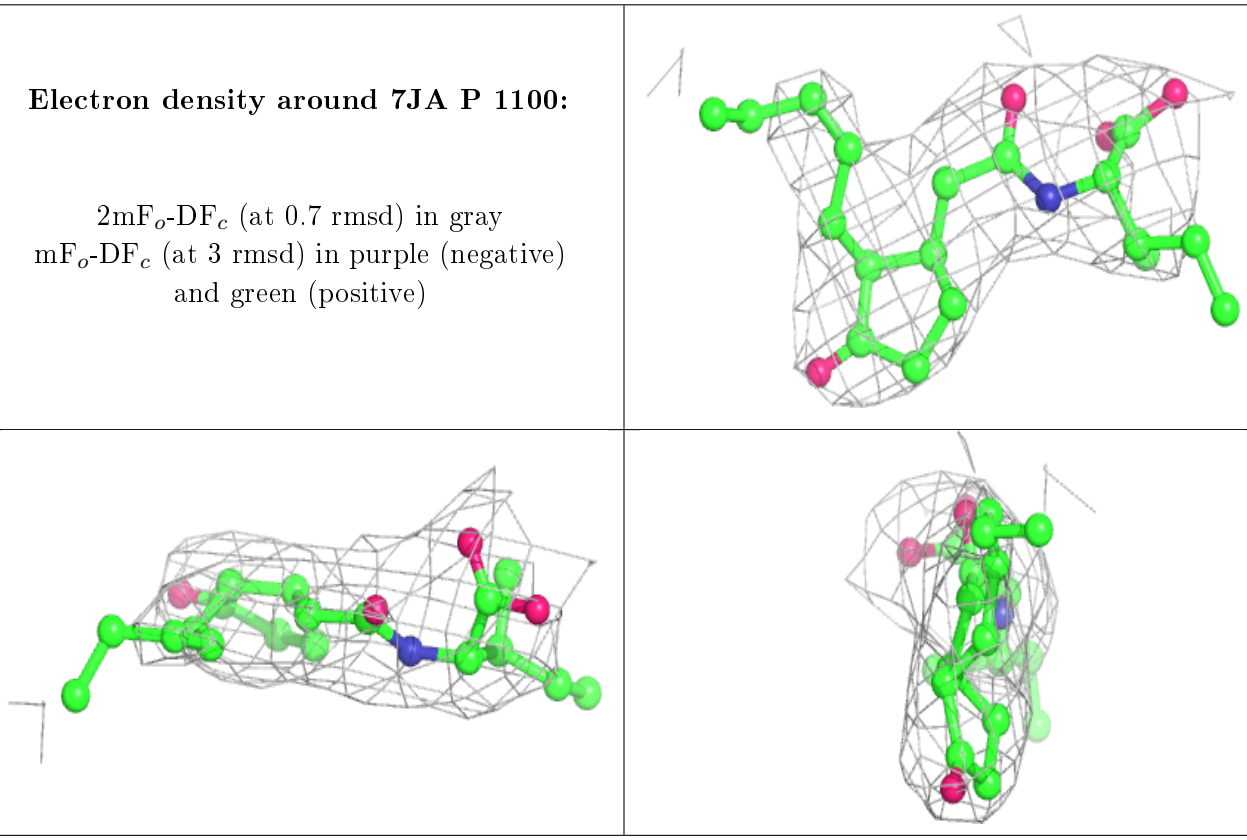
Electron density around 7JA B 1100:

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



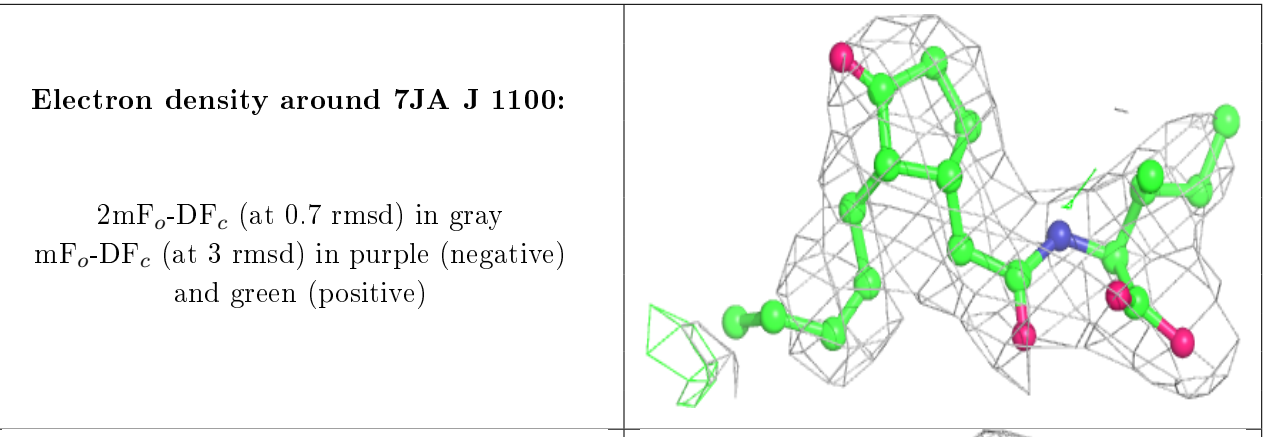
Electron density around 7JA P 1100:

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



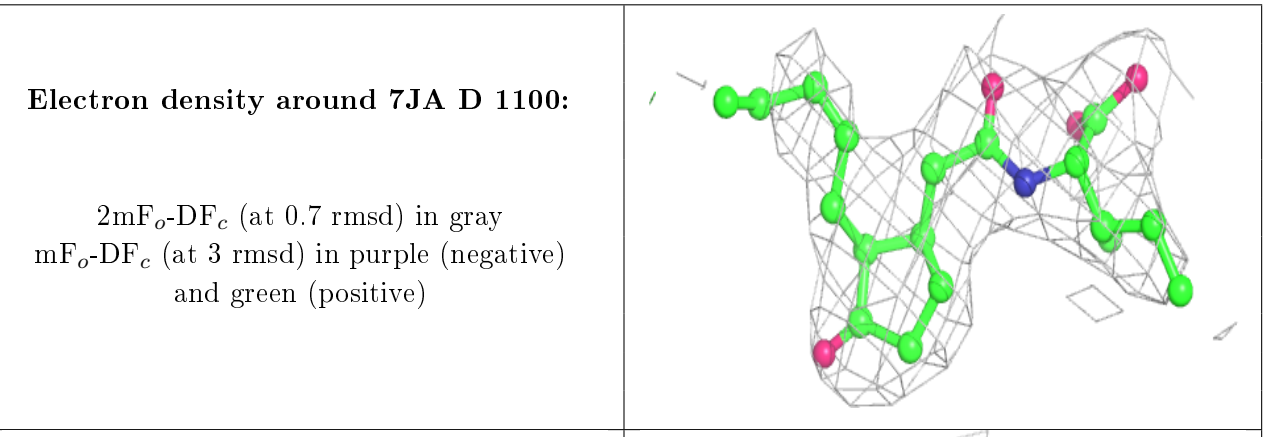
Electron density around 7JA J 1100:

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



Electron density around 7JA D 1100:

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



6.5 Other polymers (i)

There are no such residues in this entry.