Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2024 – 09:30 PM JST

PDB ID	:	8XFV
Title	:	Crystal structure of human Golgi resident glutaminyl cyclase in complex with (Z)-3-((1H-benzo[d]imidazol-5-yl)methylene)-4-(piperidin-4-yloxy)indolin-2-one
Authors	:	Li, G.-B.; Wang, X.-Y.
Deposited on	:	2023-12-14
Resolution	:	3.13 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

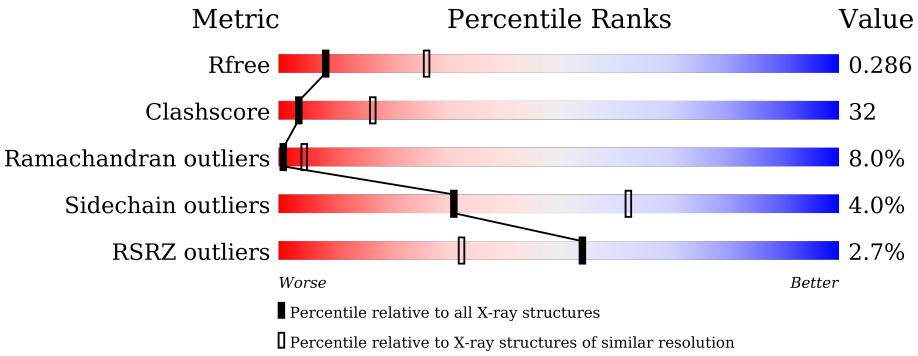
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	313	60% 33% 6%
1	B	313	50% 44%
1	C	313	62% 35%
1	D	313	50% 42% 7%
1	E	313	43% 46% 9%

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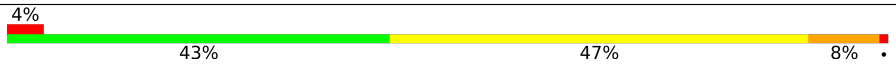
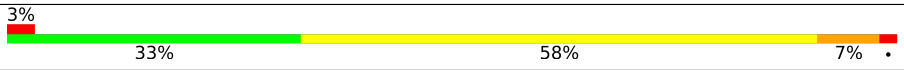
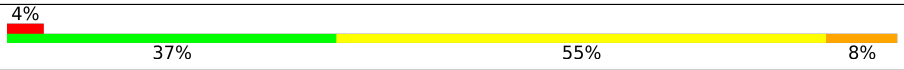
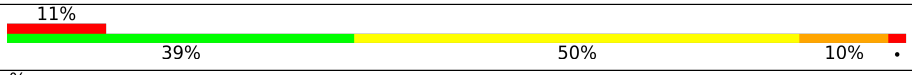
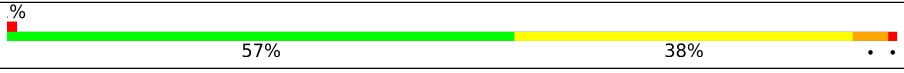
Mol	Chain	Length	Quality of chain
1	F	313	
1	G	313	
1	H	313	
1	I	313	
1	J	313	
1	X	313	

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
3	A1D46	A	402	-	-	-	X
3	A1D46	B	402	-	-	-	X
3	A1D46	F	402	-	-	-	X
3	A1D46	G	402	-	-	-	X
3	A1D46	H	402	-	-	-	X
3	A1D46	J	402	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27523 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 Glutaminyl-peptide cyclotransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	313	Total	C	N	O	S	0	0	0
			2474	1601	436	431	6			
1	A	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	B	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	C	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	D	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	E	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	F	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	G	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	H	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	I	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	J	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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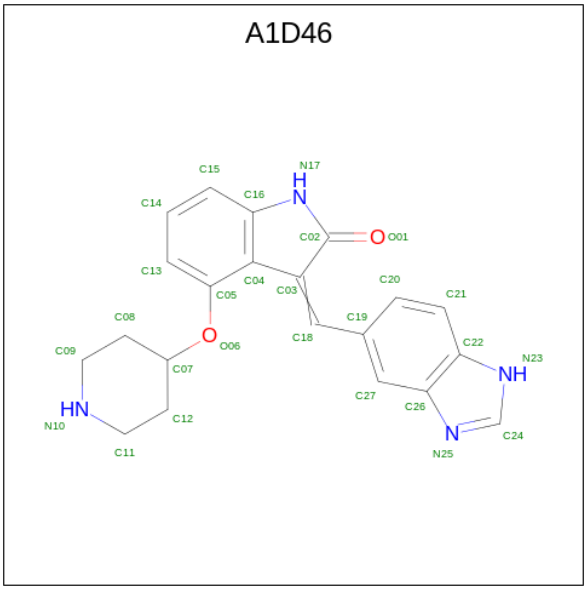
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0

- Molecule 3 is 3-(1 {H}-benzimidazol-5-ylmethylidene)-4-piperidin-4-yloxy-1 {H}-indol-2-one (three-letter code: A1D46) (formula: $C_{21}H_{20}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	1	Total C N O 27 21 4 2	0	0
3	A	1	Total C N O 27 21 4 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			27	21	4	2		
3	C	1	Total	C	N	O	0	0
			27	21	4	2		
3	D	1	Total	C	N	O	0	0
			27	21	4	2		
3	E	1	Total	C	N	O	0	0
			27	21	4	2		
3	F	1	Total	C	N	O	0	0
			27	21	4	2		
3	G	1	Total	C	N	O	0	0
			27	21	4	2		
3	H	1	Total	C	N	O	0	0
			27	21	4	2		
3	I	1	Total	C	N	O	0	0
			27	21	4	2		
3	J	1	Total	C	N	O	0	0
			27	21	4	2		

- Molecule 4 is water.

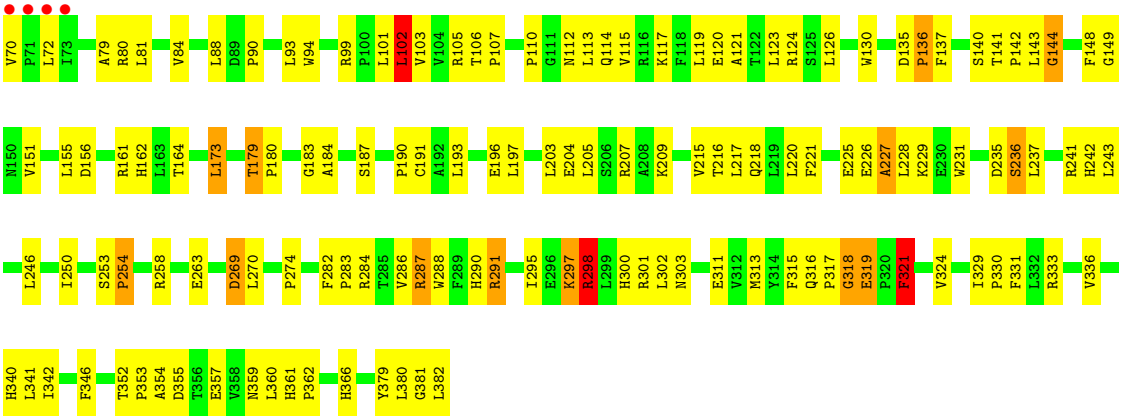
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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

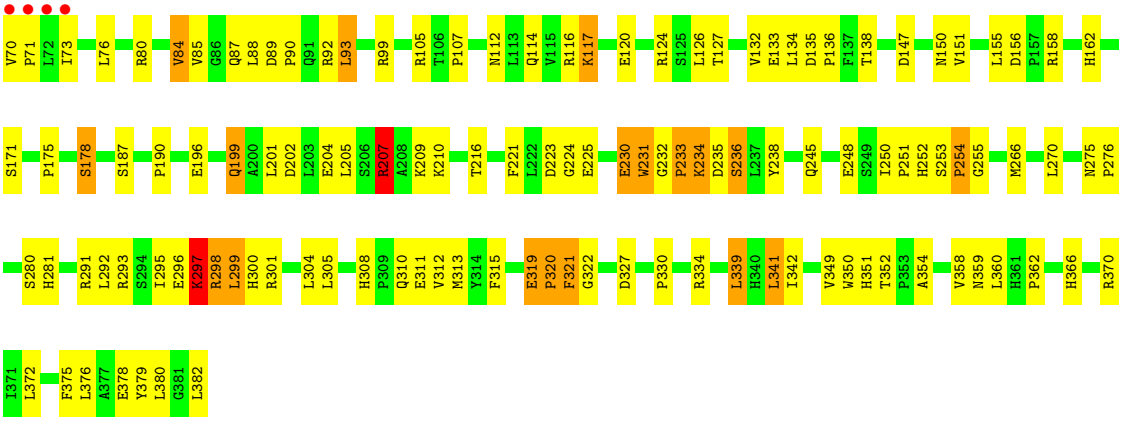
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain X:



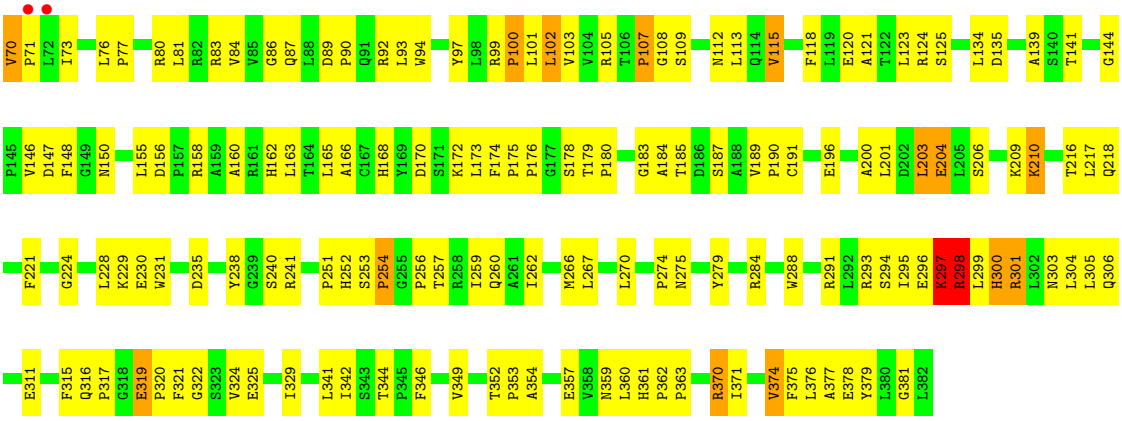
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain A:



• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain B:

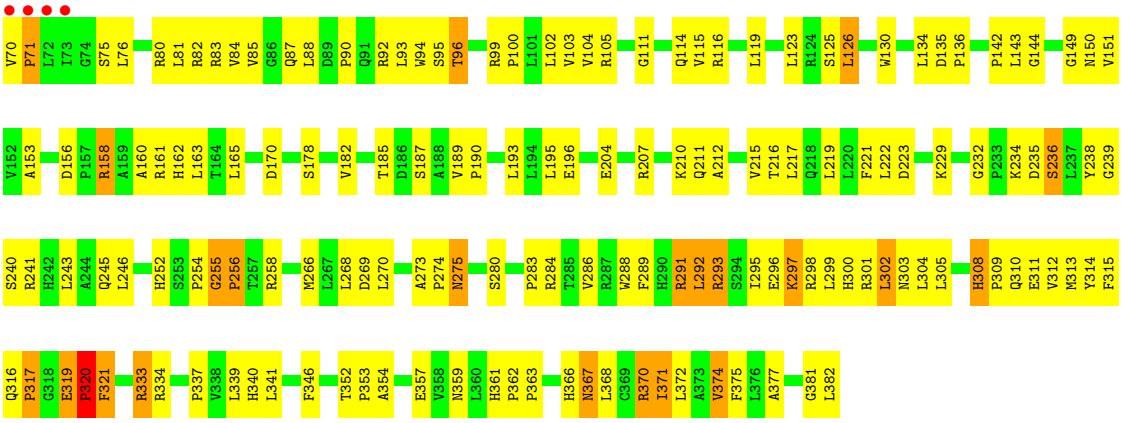


• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain C:

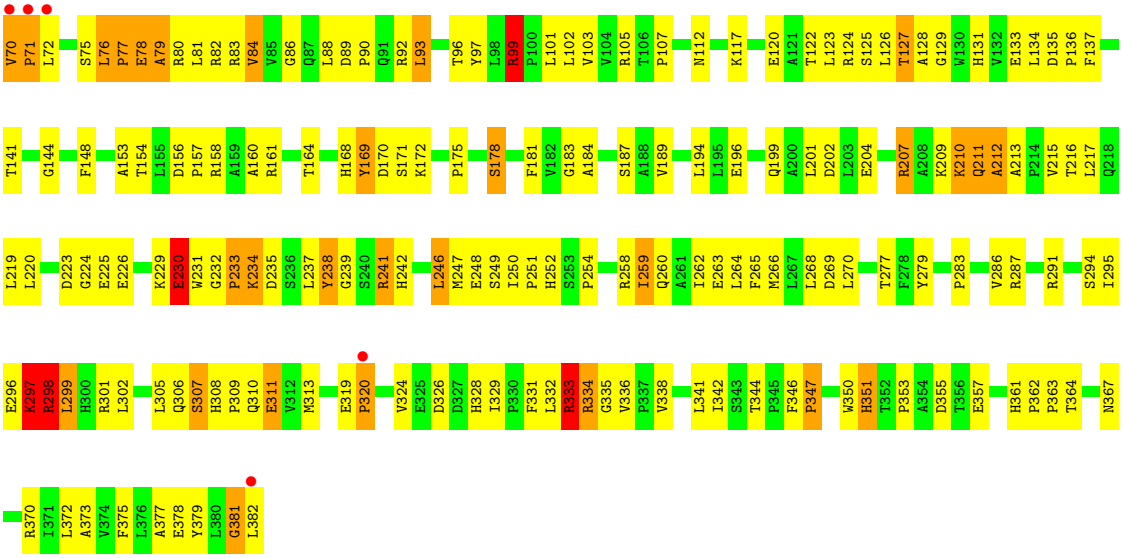
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain D:



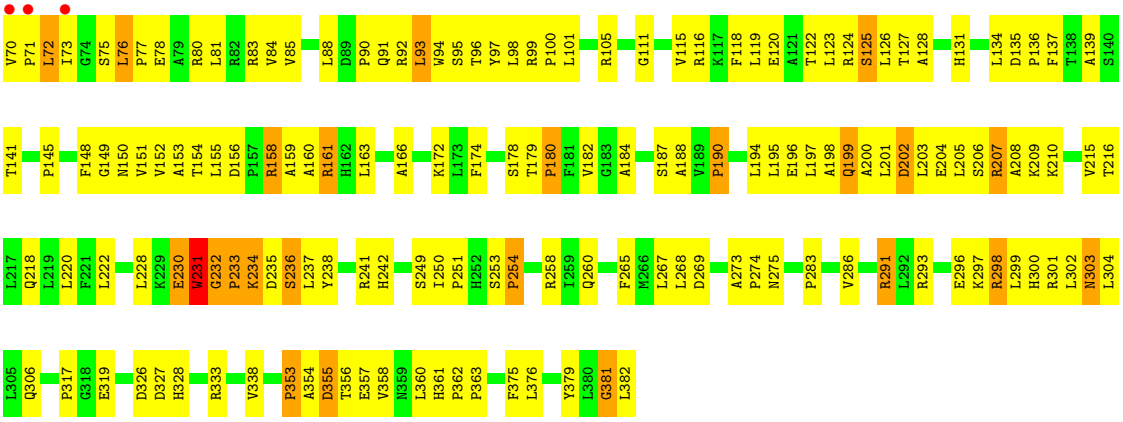
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain E:



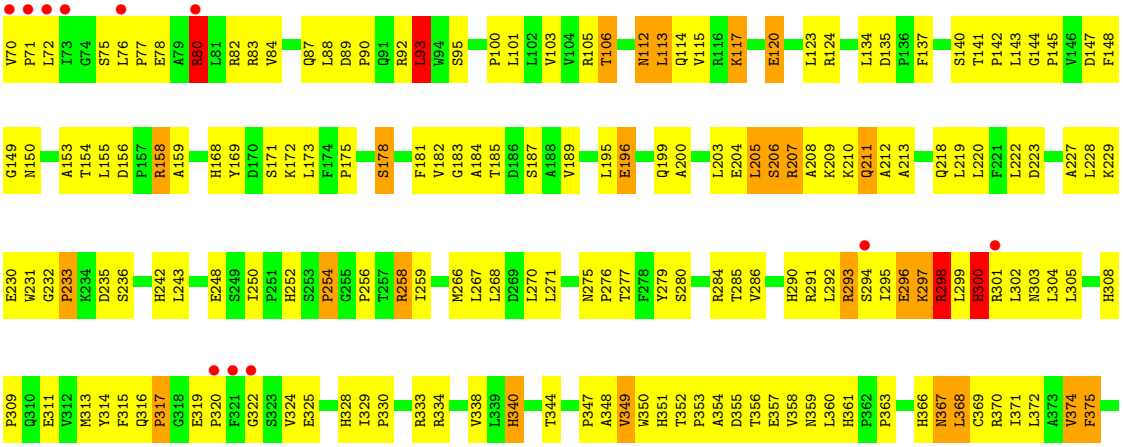
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain F:



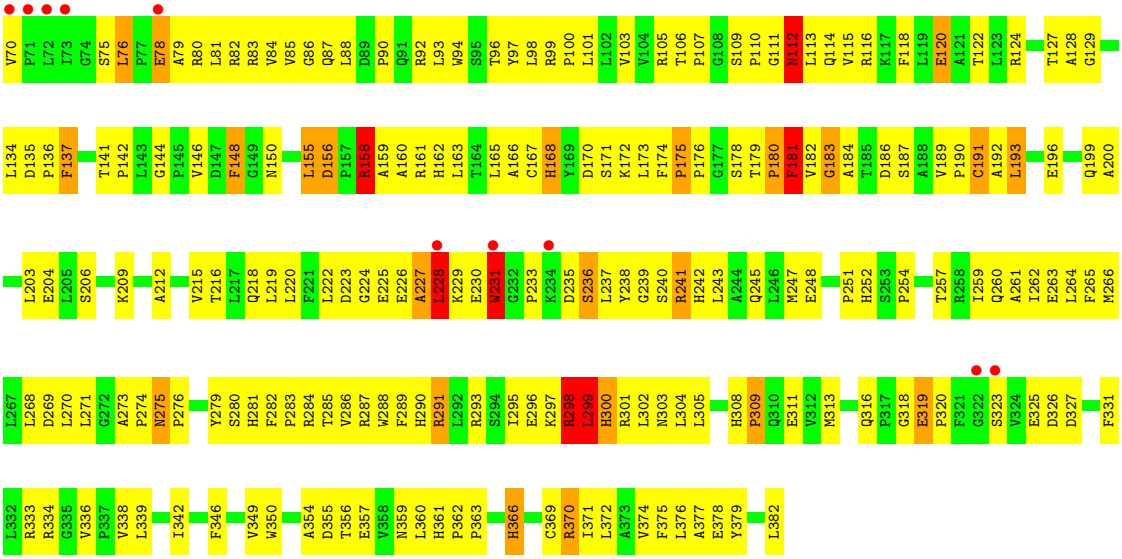
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain G:



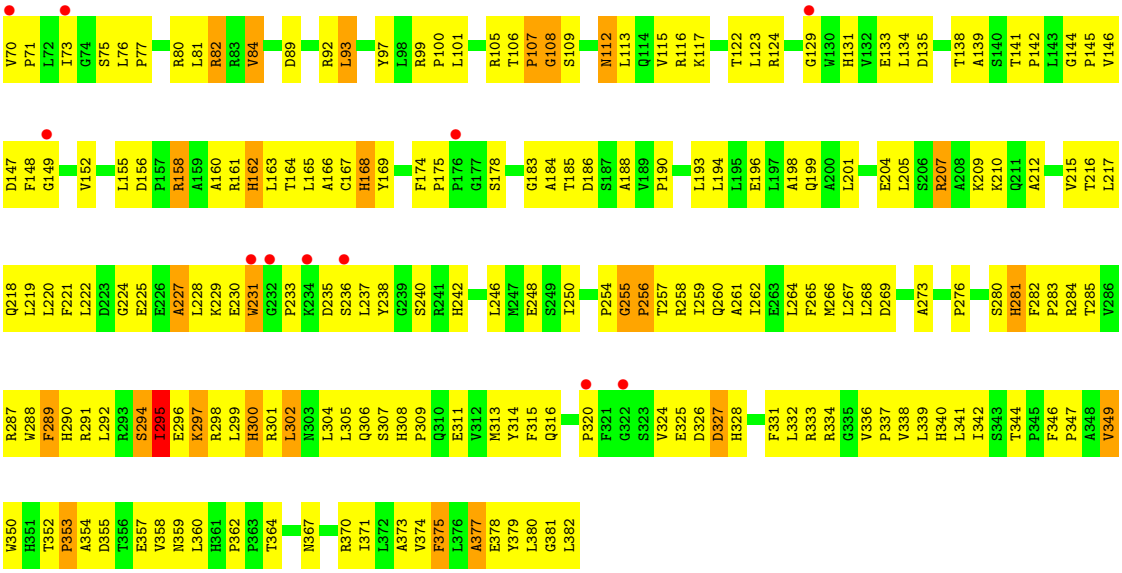
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain H:



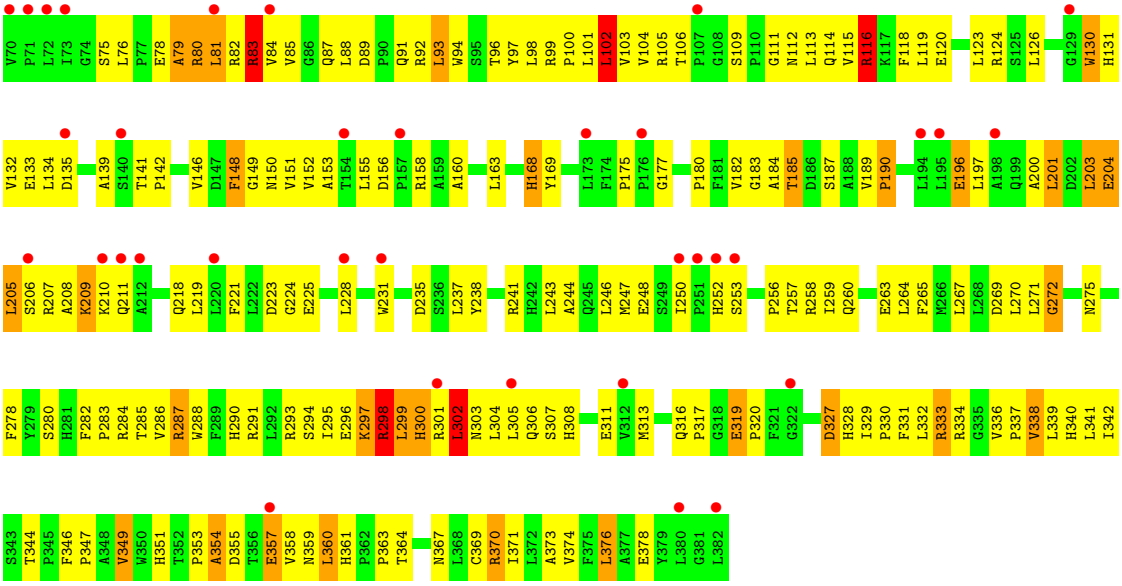
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain I:



• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain J:


V70 P71 L72 I73 G74 S75 L76 P77 E78 A79 R80 L81 R82 R83 V84 V85 G86 Q87 L88 D89 P90 Q91 R92 L93 W94 S95 T96 Y97 L98 R99 P100 L101 L102 V103 V104 R105 T106 P107 G108 S109 P110 G111 N112 L113 Q114 V115 R116 K117 F118 L119 E120 L123 R124 S125 L126 G129 W130 H131
V132 E133 L134 D135 A139 S140 T141 P142 V146 D147 F148 G149 N150 V151 V152 A153 T154 L155 D156 P157 R158 A159 A160 L163 H168 Y169 L173 F174 P175 P176 G177 P180 F181 V182 G183 A184 T185 D186 S187 A188 V189 P190 L194 L195 E196 L197 A198 Q199 A200 L201 D202 L203 E204
L205 S206 R207 A208 K209 K210 Q211 A212 Q218 L219 L220 F221 L222 D223 G224 E225 L228 W231 D235 S236 L237 Y238 R241 H242 L243 A244 Q245 L246 M247 E248 S249 I250 P251 H252 S253 P256 T257 R258 I259 Q260 E263 L264 P265 M266 L267 L268 D269 L270 L271 G272 N275
F278 Y279 S280 H281 F282 P283 R284 T285 V286 R287 W288 F289 H290 R291 L292 R293 S294 I295 E296 K297 R298 L299 H300 R301 L302 N303 L304 L305 Q306 S307 H308 E311 V312 M313 Q316 P317 G318 E319 P320 F321 G322 D327 H328 I329 P330 F331 L332 R333 R334 G335 V336 P337 V338 L339 H340 L341 I342
S343 T344 P345 F346 P347 A348 V349 W350 H351 T352 P353 A354 D355 T356 E357 V358 N359 L360 H361 P362 P363 T364 N367 L368 C369 R370 I371 L372 A373 V374 F375 L376 A377 E378 Y379 L380 G381 L382

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.28Å 109.13Å 159.54Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	42.87 – 3.13 42.87 – 3.13	Depositor EDS
% Data completeness (in resolution range)	95.1 (42.87-3.13) 95.1 (42.87-3.13)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.284 0.207 , 0.286	Depositor DCC
R_{free} test set	1997 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27523	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: A1D46, ZN

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	0.68	1/2550 (0.0%)	0.88	5/3488 (0.1%)
1	B	0.70	2/2550 (0.1%)	0.91	8/3488 (0.2%)
1	C	0.78	2/2550 (0.1%)	1.00	5/3488 (0.1%)
1	D	0.66	1/2550 (0.0%)	0.91	5/3488 (0.1%)
1	E	0.82	5/2550 (0.2%)	0.88	6/3488 (0.2%)
1	F	0.60	1/2550 (0.0%)	0.83	2/3488 (0.1%)
1	G	0.61	2/2550 (0.1%)	0.85	3/3488 (0.1%)
1	H	0.66	2/2550 (0.1%)	0.93	5/3488 (0.1%)
1	I	0.56	1/2550 (0.0%)	0.80	2/3488 (0.1%)
1	J	0.65	2/2550 (0.1%)	0.93	10/3488 (0.3%)
1	X	0.70	3/2550 (0.1%)	0.91	6/3488 (0.2%)
All	All	0.68	22/28050 (0.1%)	0.89	57/38368 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	F	0	1
1	J	0	1
1	X	0	1
All	All	0	5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	333	ARG	CZ-NH2	-15.28	1.13	1.33
1	J	190	PRO	N-CD	-15.24	1.26	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	333	ARG	CZ-NH1	-13.10	1.16	1.33
1	E	333	ARG	NE-CZ	-10.14	1.19	1.33
1	E	333	ARG	CD-NE	-7.21	1.34	1.46
1	D	288	TRP	CB-CG	-6.68	1.38	1.50
1	F	319	GLU	CG-CD	6.64	1.61	1.51
1	H	231	TRP	CB-CG	6.58	1.62	1.50
1	I	231	TRP	CB-CG	6.40	1.61	1.50
1	X	191	CYS	CB-SG	-6.37	1.71	1.82
1	B	288	TRP	CB-CG	-6.29	1.39	1.50
1	J	175	PRO	C-N	6.22	1.46	1.34
1	E	99	ARG	CZ-NH2	-5.99	1.25	1.33
1	H	325	GLU	CG-CD	5.83	1.60	1.51
1	G	80	ARG	CZ-NH2	-5.72	1.25	1.33
1	C	167	CYS	CB-SG	-5.53	1.72	1.81
1	X	288	TRP	CB-CG	-5.49	1.40	1.50
1	A	245	GLN	CG-CD	5.47	1.63	1.51
1	X	321	PHE	CB-CG	5.36	1.60	1.51
1	B	191	CYS	CB-SG	-5.32	1.73	1.81
1	C	325	GLU	CG-CD	5.29	1.59	1.51
1	G	120	GLU	CB-CG	-5.22	1.42	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	333	ARG	NE-CZ-NH1	-14.23	113.19	120.30
1	J	116	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	H	158	ARG	NE-CZ-NH1	-12.29	114.15	120.30
1	D	333	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	C	297	LYS	N-CA-C	-8.78	87.29	111.00
1	J	338	VAL	CG1-CB-CG2	-8.26	97.69	110.90
1	J	298	ARG	C-N-CA	-8.14	101.35	121.70
1	C	302	LEU	CB-CG-CD1	-8.03	97.34	111.00
1	F	93	LEU	CA-CB-CG	7.93	133.53	115.30
1	J	93	LEU	CA-CB-CG	7.60	132.79	115.30
1	G	93	LEU	CA-CB-CG	7.53	132.62	115.30
1	G	293	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	J	116	ARG	CD-NE-CZ	7.00	133.41	123.60
1	B	297	LYS	N-CA-C	6.98	129.84	111.00
1	A	341	LEU	CA-CB-CG	6.82	130.97	115.30
1	I	93	LEU	CA-CB-CG	6.67	130.63	115.30
1	J	81	LEU	CA-CB-CG	6.66	130.61	115.30
1	E	93	LEU	CA-CB-CG	6.60	130.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	333	ARG	CA-CB-CG	6.56	127.84	113.40
1	J	302	LEU	CA-CB-CG	6.53	130.32	115.30
1	X	298	ARG	N-CA-CB	6.45	122.21	110.60
1	X	297	LYS	C-N-CA	6.34	137.56	121.70
1	X	102	LEU	CB-CG-CD2	-6.34	100.23	111.00
1	H	370	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	A	319	GLU	C-N-CD	-6.20	106.96	120.60
1	A	297	LYS	O-C-N	-6.16	112.84	122.70
1	A	297	LYS	C-N-CA	6.16	137.10	121.70
1	C	72	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	341	LEU	CB-CG-CD2	-6.04	100.74	111.00
1	B	70	VAL	CB-CA-C	6.00	122.79	111.40
1	D	372	LEU	CA-CB-CG	5.94	128.97	115.30
1	J	102	LEU	CB-CG-CD1	-5.93	100.91	111.00
1	H	155	LEU	CA-CB-CG	5.92	128.91	115.30
1	E	70	VAL	CB-CA-C	5.87	122.55	111.40
1	E	351	HIS	C-N-CA	5.83	136.27	121.70
1	B	300	HIS	CB-CA-C	5.82	122.03	110.40
1	X	173	LEU	CA-CB-CG	5.58	128.14	115.30
1	E	70	VAL	CA-CB-CG1	5.55	119.23	110.90
1	E	241	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	E	299	LEU	CA-CB-CG	-5.55	102.54	115.30
1	X	88	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	B	298	ARG	N-CA-C	5.47	125.77	111.00
1	B	297	LYS	CB-CA-C	-5.46	99.48	110.40
1	B	81	LEU	CA-CB-CG	-5.44	102.80	115.30
1	X	297	LYS	CA-C-N	5.39	129.05	117.20
1	F	72	LEU	CA-CB-CG	5.37	127.65	115.30
1	I	333	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	230	GLU	C-N-CA	5.33	135.02	121.70
1	G	382	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	320	PRO	N-CA-C	5.27	125.81	112.10
1	C	143	LEU	CA-CB-CG	-5.26	103.20	115.30
1	B	201	LEU	CA-CB-CG	-5.26	103.21	115.30
1	J	83	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	163	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	J	333	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	H	299	LEU	CA-CB-CG	-5.05	103.69	115.30
1	H	228	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	GLU	Peptide
1	E	76	LEU	Peptide
1	F	231	TRP	Peptide
1	J	185	THR	Peptide
1	X	144	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2474	0	2498	102	0
1	B	2474	0	2499	161	0
1	C	2474	0	2499	83	1
1	D	2474	0	2499	124	1
1	E	2474	0	2496	160	0
1	F	2474	0	2499	125	0
1	G	2474	0	2496	211	1
1	H	2474	0	2499	248	0
1	I	2474	0	2494	176	0
1	J	2474	0	2495	288	0
1	X	2474	0	2499	94	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	X	1	0	0	0	0
3	A	27	0	0	1	0
3	B	27	0	0	1	0
3	C	27	0	0	2	0
3	D	27	0	0	1	0
3	E	27	0	0	2	0
3	F	27	0	0	4	0
3	G	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	27	0	0	3	0
3	I	27	0	0	1	0
3	J	27	0	0	0	0
3	X	27	0	0	1	0
4	F	1	0	0	0	0
All	All	27523	0	27473	1738	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 32.

All (1738) 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)
1:J:297:LYS:HE3	1:J:301:ARG:CZ	1.16	1.56
1:J:297:LYS:CE	1:J:301:ARG:CZ	1.87	1.50
1:A:296:GLU:O	1:A:297:LYS:CG	1.64	1.44
1:J:297:LYS:HE3	1:J:301:ARG:NE	1.24	1.43
1:J:155:LEU:CD2	1:J:205:LEU:CD2	1.96	1.43
1:H:297:LYS:CD	1:H:311:GLU:HB3	1.51	1.39
1:J:155:LEU:CD2	1:J:205:LEU:HD22	1.55	1.37
1:J:297:LYS:NZ	1:J:301:ARG:NH1	1.69	1.36
1:J:155:LEU:HD22	1:J:205:LEU:CD2	1.55	1.33
1:J:297:LYS:CD	1:J:301:ARG:HG2	1.60	1.30
1:B:297:LYS:CD	1:B:301:ARG:H	1.45	1.30
1:H:297:LYS:NZ	1:H:301:ARG:HH21	1.32	1.23
1:H:297:LYS:CE	1:H:311:GLU:HB3	1.67	1.23
1:I:296:GLU:O	1:I:298:ARG:N	1.76	1.18
1:E:295:ILE:O	1:E:299:LEU:HD12	1.44	1.16
1:A:296:GLU:O	1:A:297:LYS:HG3	0.99	1.15
1:H:297:LYS:NZ	1:H:301:ARG:NH2	1.92	1.14
1:J:299:LEU:HD12	1:J:305:LEU:HD21	1.21	1.14
1:J:155:LEU:HD21	1:J:205:LEU:HD22	1.21	1.13
1:J:297:LYS:O	1:J:311:GLU:O	1.65	1.13
1:G:297:LYS:HD2	1:G:311:GLU:O	1.47	1.13
1:J:155:LEU:CD2	1:J:205:LEU:HD21	1.69	1.12
1:B:297:LYS:HE2	1:B:301:ARG:HG3	1.21	1.12
1:G:297:LYS:NZ	1:G:311:GLU:HA	1.62	1.12
1:J:297:LYS:HD2	1:J:301:ARG:CG	1.78	1.12
1:B:297:LYS:HB2	1:B:300:HIS:HB3	1.30	1.11
1:J:116:ARG:CZ	1:J:169:TYR:HE1	1.64	1.11
1:I:281:HIS:HE1	1:I:340:HIS:HB3	1.01	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LYS:HE2	1:B:301:ARG:CG	1.81	1.10
1:H:297:LYS:HD3	1:H:311:GLU:HB3	1.10	1.09
1:H:297:LYS:HE2	1:H:311:GLU:HG2	1.33	1.09
1:G:354:ALA:O	1:G:359:ASN:ND2	1.85	1.08
1:H:298:ARG:O	1:H:300:HIS:N	1.88	1.06
1:G:293:ARG:HH12	1:G:317:PRO:HB3	1.15	1.06
1:G:297:LYS:CD	1:G:311:GLU:O	2.04	1.06
1:E:70:VAL:HG13	1:E:298:ARG:HD3	1.11	1.05
1:E:233:PRO:O	1:E:241:ARG:NH1	1.90	1.05
1:G:297:LYS:HD2	1:G:311:GLU:C	1.76	1.04
1:H:297:LYS:HD3	1:H:311:GLU:CB	1.88	1.03
1:J:297:LYS:HZ2	1:J:301:ARG:NH1	1.54	1.03
1:B:297:LYS:CE	1:B:301:ARG:HG3	1.89	1.02
1:I:281:HIS:CE1	1:I:340:HIS:HB3	1.94	1.02
1:E:297:LYS:HA	1:E:299:LEU:N	1.76	1.01
1:H:297:LYS:CD	1:H:311:GLU:CB	2.37	1.01
1:H:297:LYS:HE2	1:H:311:GLU:CG	1.88	1.01
1:B:297:LYS:CE	1:B:301:ARG:CG	2.38	1.00
1:A:291:ARG:NH2	1:A:378:GLU:OE1	1.93	1.00
1:B:297:LYS:HE3	1:B:301:ARG:CA	1.91	1.00
1:H:304:LEU:O	1:H:370:ARG:NH1	1.94	0.99
1:H:297:LYS:HE2	1:H:311:GLU:CB	1.92	0.99
1:H:297:LYS:HZ3	1:H:301:ARG:HH21	1.03	0.99
1:H:297:LYS:NZ	1:H:301:ARG:HE	1.62	0.98
1:X:297:LYS:O	1:X:300:HIS:HB3	1.65	0.97
1:B:70:VAL:HG12	1:B:71:PRO:HD3	1.47	0.97
1:H:297:LYS:HZ1	1:H:301:ARG:NH2	1.59	0.97
1:J:299:LEU:O	1:J:301:ARG:N	1.98	0.97
1:H:297:LYS:CE	1:H:311:GLU:CB	2.42	0.96
1:J:155:LEU:HD22	1:J:205:LEU:HD21	1.28	0.96
1:C:296:GLU:O	1:C:297:LYS:HB2	1.65	0.96
1:I:291:ARG:NH2	1:I:378:GLU:OE1	1.97	0.96
1:B:297:LYS:HD2	1:B:301:ARG:H	1.29	0.96
1:E:298:ARG:HG3	1:E:302:LEU:CD1	1.96	0.95
1:H:297:LYS:HZ2	1:H:301:ARG:NE	1.64	0.95
1:J:297:LYS:HZ1	1:J:301:ARG:NH1	1.46	0.95
1:G:158:ARG:NH2	1:G:209:LYS:O	1.99	0.95
1:A:296:GLU:C	1:A:297:LYS:HG3	1.85	0.95
1:D:92:ARG:O	1:D:96:THR:OG1	1.83	0.95
1:C:291:ARG:O	1:C:295:ILE:HD12	1.66	0.95
1:B:297:LYS:CD	1:B:301:ARG:N	2.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:CG1	1:E:298:ARG:HD3	1.97	0.94
1:B:297:LYS:HD3	1:B:300:HIS:CG	2.02	0.94
1:J:297:LYS:HD2	1:J:301:ARG:HG2	0.97	0.94
1:J:116:ARG:HH22	1:J:223:ASP:CG	1.71	0.94
1:G:297:LYS:HA	1:G:299:LEU:N	1.82	0.94
1:H:297:LYS:NZ	1:H:301:ARG:NE	2.15	0.93
1:E:297:LYS:HA	1:E:298:ARG:C	1.90	0.92
1:B:297:LYS:HG2	1:B:311:GLU:HG3	1.49	0.92
1:H:297:LYS:NZ	1:H:301:ARG:CZ	2.32	0.92
1:J:295:ILE:C	1:J:298:ARG:HB3	1.89	0.92
1:I:295:ILE:HD12	1:I:295:ILE:H	1.33	0.91
1:G:300:HIS:CD2	1:G:311:GLU:HA	2.07	0.90
1:B:73:ILE:O	1:B:291:ARG:NH2	2.05	0.89
1:G:297:LYS:CG	1:G:311:GLU:O	2.19	0.89
1:A:135:ASP:HB3	1:A:150:ASN:HB2	1.53	0.89
1:I:281:HIS:HE1	1:I:340:HIS:CB	1.85	0.89
1:J:224:GLY:HA3	1:J:238:TYR:HB2	1.55	0.89
1:G:359:ASN:OD1	1:J:333:ARG:NH1	2.06	0.88
1:J:297:LYS:CE	1:J:301:ARG:NE	2.19	0.88
1:D:84:VAL:HA	1:D:87:GLN:OE1	1.73	0.88
1:B:297:LYS:CE	1:B:301:ARG:H	1.86	0.88
1:G:299:LEU:O	1:G:302:LEU:N	2.05	0.88
1:G:300:HIS:HD2	1:G:311:GLU:HA	1.34	0.88
1:E:101:LEU:O	1:E:105:ARG:NH1	2.06	0.88
1:H:297:LYS:HZ2	1:H:301:ARG:HE	1.14	0.88
1:J:330:PRO:O	1:J:334:ARG:NH1	2.07	0.87
1:X:161:ARG:HB2	1:X:215:VAL:HG22	1.57	0.87
1:G:70:VAL:HG12	1:G:71:PRO:HD2	1.56	0.87
1:C:155:LEU:O	1:C:209:LYS:NZ	2.08	0.87
1:B:297:LYS:HG2	1:B:300:HIS:HD2	1.38	0.87
1:E:207:ARG:NH2	1:E:210:LYS:HD2	1.90	0.87
1:J:297:LYS:CG	1:J:298:ARG:HA	2.05	0.87
1:X:301:ARG:NH1	1:X:311:GLU:OE1	2.09	0.86
1:H:120:GLU:OE1	1:H:124:ARG:NH1	2.08	0.86
1:I:224:GLY:O	1:I:238:TYR:N	2.09	0.86
1:A:296:GLU:O	1:A:297:LYS:HG2	1.73	0.85
1:B:297:LYS:HD3	1:B:300:HIS:CB	2.06	0.85
1:G:297:LYS:CB	1:G:300:HIS:HB3	2.06	0.85
1:B:297:LYS:HG2	1:B:311:GLU:CG	2.07	0.84
1:G:297:LYS:HG2	1:G:311:GLU:O	1.75	0.84
1:J:296:GLU:HA	1:J:298:ARG:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ARG:O	1:E:302:LEU:HD12	1.77	0.84
1:B:297:LYS:HZ3	1:B:311:GLU:HG3	1.40	0.84
1:F:70:VAL:HG13	1:F:298:ARG:HH11	1.42	0.84
1:J:116:ARG:CZ	1:J:169:TYR:CE1	2.56	0.84
1:G:120:GLU:OE1	1:G:124:ARG:NH1	2.10	0.84
1:H:158:ARG:HD2	1:H:158:ARG:C	1.98	0.84
1:J:257:THR:OG1	1:J:260:GLN:OE1	1.95	0.83
1:H:70:VAL:HG13	1:H:298:ARG:NE	1.93	0.83
1:E:232:GLY:O	1:E:234:LYS:N	2.11	0.83
1:A:304:LEU:O	1:A:370:ARG:NH1	2.12	0.83
1:G:304:LEU:HD12	1:G:370:ARG:HH12	1.42	0.83
1:J:116:ARG:NH2	1:J:169:TYR:HE1	1.77	0.83
1:J:297:LYS:HZ1	1:J:301:ARG:HH12	1.23	0.83
1:F:233:PRO:O	1:F:235:ASP:N	2.12	0.83
1:I:76:LEU:O	1:I:298:ARG:NH2	2.13	0.82
1:H:227:ALA:O	1:H:230:GLU:N	2.11	0.82
1:I:296:GLU:C	1:I:298:ARG:N	2.32	0.82
1:B:297:LYS:HD3	1:B:300:HIS:CD2	2.14	0.82
1:C:233:PRO:O	1:C:235:ASP:N	2.13	0.82
1:I:296:GLU:O	1:I:297:LYS:C	2.17	0.81
1:G:297:LYS:HB3	1:G:300:HIS:CB	2.09	0.81
1:H:227:ALA:O	1:H:229:LYS:N	2.14	0.81
1:J:297:LYS:HZ2	1:J:301:ARG:HH11	1.24	0.81
1:J:133:GLU:HG3	1:J:152:VAL:HB	1.62	0.81
1:J:297:LYS:CE	1:J:301:ARG:NH1	2.25	0.81
1:B:297:LYS:CB	1:B:300:HIS:HB3	2.11	0.81
1:D:354:ALA:O	1:D:359:ASN:ND2	2.13	0.81
1:J:99:ARG:HA	1:J:102:LEU:CD1	2.10	0.80
1:B:187:SER:HB3	1:B:190:PRO:HG2	1.64	0.80
1:H:161:ARG:HH21	1:H:263:GLU:HG3	1.45	0.80
1:J:298:ARG:HD3	1:J:299:LEU:H	1.47	0.80
1:E:70:VAL:HG13	1:E:298:ARG:CD	2.04	0.80
1:H:120:GLU:OE2	1:H:134:LEU:HD12	1.81	0.80
1:G:203:LEU:HA	1:G:206:SER:HB3	1.62	0.80
1:I:227:ALA:HB1	1:I:230:GLU:HA	1.62	0.80
1:B:297:LYS:HD3	1:B:301:ARG:H	1.45	0.80
1:H:118:PHE:O	1:H:122:THR:OG1	1.99	0.80
1:H:297:LYS:HA	1:H:298:ARG:O	1.82	0.80
1:A:266:MET:HE2	1:A:339:LEU:HD22	1.61	0.80
1:E:234:LYS:HD3	1:E:234:LYS:H	1.45	0.80
1:G:297:LYS:CE	1:G:311:GLU:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:LEU:HD22	1:H:136:PRO:HG3	1.64	0.80
1:H:70:VAL:HG13	1:H:298:ARG:HE	1.46	0.79
1:I:82:ARG:HH21	1:I:302:LEU:HD23	1.47	0.79
1:J:116:ARG:NH2	1:J:169:TYR:CE1	2.50	0.79
1:G:135:ASP:HB3	1:G:150:ASN:HB2	1.65	0.79
1:H:76:LEU:HD23	1:H:378:GLU:HG3	1.65	0.79
1:B:297:LYS:HE3	1:B:301:ARG:N	1.96	0.79
1:H:155:LEU:O	1:H:209:LYS:HE3	1.83	0.79
1:J:200:ALA:C	1:J:201:LEU:HD23	2.03	0.79
1:J:296:GLU:HG3	1:J:297:LYS:O	1.80	0.79
1:F:155:LEU:O	1:F:209:LYS:NZ	2.16	0.79
1:F:197:LEU:HD22	1:F:376:LEU:HD12	1.65	0.79
1:J:308:HIS:HD2	1:J:313:MET:SD	2.06	0.78
1:J:299:LEU:HD12	1:J:305:LEU:CD2	2.10	0.78
1:I:292:LEU:C	1:I:295:ILE:CD1	2.48	0.78
1:J:155:LEU:HD23	1:J:205:LEU:HD21	1.64	0.78
1:E:333:ARG:HA	1:E:333:ARG:HH11	1.48	0.78
1:I:294:SER:O	1:I:296:GLU:N	2.17	0.78
1:B:135:ASP:HB3	1:B:150:ASN:HB2	1.66	0.78
1:D:70:VAL:HG12	1:D:71:PRO:HD3	1.65	0.78
1:E:298:ARG:O	1:E:301:ARG:HB2	1.84	0.78
1:H:78:GLU:O	1:H:81:LEU:N	2.17	0.78
1:J:155:LEU:HD21	1:J:205:LEU:CD2	1.86	0.77
1:I:326:ASP:OD1	1:I:327:ASP:N	2.17	0.77
1:H:237:LEU:HD22	1:H:327:ASP:HA	1.67	0.77
1:J:205:LEU:O	1:J:206:SER:C	2.21	0.77
1:C:227:ALA:HB1	1:C:230:GLU:HA	1.66	0.77
1:E:297:LYS:HE2	1:E:308:HIS:CE1	2.20	0.77
1:G:296:GLU:OE2	1:G:308:HIS:CE1	2.38	0.77
1:I:116:ARG:HB2	1:I:169:TYR:HE2	1.48	0.77
1:B:172:LYS:HD3	1:B:174:PHE:CZ	2.20	0.77
1:D:291:ARG:O	1:D:295:ILE:HG13	1.85	0.77
1:J:297:LYS:HG2	1:J:298:ARG:HA	1.66	0.76
1:E:70:VAL:HG12	1:E:71:PRO:HD3	1.67	0.76
1:G:78:GLU:HG3	1:G:298:ARG:NH2	2.01	0.76
1:J:204:GLU:O	1:J:207:ARG:HB2	1.85	0.76
1:E:175:PRO:O	1:E:178:SER:OG	2.04	0.76
1:B:300:HIS:CD2	1:B:311:GLU:HA	2.21	0.76
1:J:297:LYS:HD3	1:J:301:ARG:HG2	1.65	0.76
1:B:297:LYS:HE3	1:B:301:ARG:HA	1.66	0.76
1:B:297:LYS:HE3	1:B:301:ARG:CG	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LEU:O	1:F:203:LEU:N	2.18	0.76
1:J:187:SER:HB3	1:J:190:PRO:HG2	1.67	0.76
1:H:90:PRO:HB3	1:H:366:HIS:CD2	2.20	0.75
1:G:275:ASN:HD21	1:J:260:GLN:HE21	1.34	0.75
1:I:204:GLU:N	1:I:204:GLU:OE1	2.18	0.75
1:E:291:ARG:O	1:E:295:ILE:HG13	1.87	0.75
1:G:175:PRO:O	1:G:178:SER:OG	2.04	0.75
1:I:131:HIS:NE2	1:I:133:GLU:OE1	2.19	0.75
1:A:76:LEU:HG	1:A:378:GLU:HG3	1.67	0.75
1:J:79:ALA:O	1:J:81:LEU:N	2.20	0.75
1:J:297:LYS:CE	1:J:301:ARG:NH2	2.49	0.75
1:A:296:GLU:C	1:A:297:LYS:CG	2.50	0.75
1:J:83:ARG:NH2	1:J:204:GLU:OE2	2.19	0.75
1:X:140:SER:HB3	1:A:250:ILE:HD13	1.69	0.74
1:G:277:THR:OG1	1:G:344:THR:O	2.02	0.74
1:A:175:PRO:O	1:A:178:SER:OG	2.04	0.74
1:E:93:LEU:HD23	1:E:196:GLU:CB	2.16	0.74
1:H:70:VAL:CG1	1:H:298:ARG:HE	2.01	0.74
1:H:297:LYS:HZ3	1:H:301:ARG:NH2	1.66	0.74
1:H:300:HIS:CD2	1:H:311:GLU:HA	2.21	0.74
1:D:313:MET:O	1:D:316:GLN:NE2	2.21	0.74
1:G:297:LYS:HD2	1:G:311:GLU:CA	2.17	0.74
1:I:296:GLU:C	1:I:298:ARG:H	1.92	0.74
1:I:313:MET:O	1:I:316:GLN:NE2	2.20	0.74
1:B:297:LYS:CD	1:B:300:HIS:CD2	2.71	0.73
1:J:102:LEU:H	1:J:102:LEU:HD12	1.52	0.73
1:J:130:TRP:CZ2	1:J:205:LEU:HD11	2.24	0.73
1:B:297:LYS:CG	1:B:300:HIS:HD2	2.01	0.73
1:J:282:PHE:CE2	1:J:332:LEU:HD21	2.23	0.73
1:X:284:ARG:O	1:X:287:ARG:NH1	2.21	0.73
1:I:295:ILE:HD12	1:I:295:ILE:N	2.04	0.73
1:J:130:TRP:HZ2	1:J:205:LEU:HD11	1.52	0.73
1:J:116:ARG:NE	1:J:169:TYR:CE1	2.57	0.73
1:J:283:PRO:O	1:J:286:VAL:HG12	1.88	0.73
1:G:348:ALA:HA	1:J:284:ARG:HD3	1.70	0.73
1:H:70:VAL:HG13	1:H:298:ARG:CD	2.19	0.73
1:E:70:VAL:HG12	1:E:71:PRO:CD	2.17	0.73
1:H:297:LYS:HZ1	1:H:301:ARG:HH21	1.15	0.73
1:I:295:ILE:HG23	1:I:374:VAL:HG11	1.69	0.73
1:J:105:ARG:NH1	1:J:182:VAL:O	2.22	0.73
1:H:226:GLU:O	1:H:228:LEU:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:PRO:HB3	1:H:309:PRO:HG3	1.71	0.72
1:J:87:GLN:NE2	1:J:200:ALA:O	2.22	0.72
1:J:99:ARG:NE	1:J:357:GLU:OE1	2.23	0.72
1:J:76:LEU:HG	1:J:378:GLU:HG2	1.69	0.72
1:A:151:VAL:HB	1:A:221:PHE:HB2	1.71	0.72
1:G:275:ASN:ND2	1:J:260:GLN:HE21	1.87	0.72
1:B:107:PRO:O	1:B:109:SER:N	2.23	0.72
1:G:297:LYS:HA	1:G:298:ARG:C	2.06	0.71
1:B:297:LYS:CE	1:B:301:ARG:HG2	2.18	0.71
1:E:204:GLU:HB3	1:E:382:LEU:HB3	1.72	0.71
1:E:246:LEU:O	1:E:248:GLU:N	2.24	0.71
1:I:295:ILE:CG2	1:I:374:VAL:HG11	2.20	0.71
1:G:293:ARG:O	1:G:296:GLU:HB3	1.90	0.71
1:J:297:LYS:HE3	1:J:301:ARG:CD	2.20	0.71
1:F:126:LEU:HD11	1:F:198:ALA:HB1	1.73	0.71
1:G:87:GLN:OE1	1:G:87:GLN:N	2.22	0.71
1:A:297:LYS:HE2	1:A:312:VAL:HG23	1.71	0.71
1:B:70:VAL:HA	1:B:298:ARG:HG2	1.73	0.71
1:H:105:ARG:HG2	1:H:171:SER:HB3	1.73	0.71
1:G:297:LYS:CB	1:G:300:HIS:CB	2.68	0.71
1:H:158:ARG:HD2	1:H:159:ALA:N	2.06	0.71
1:J:297:LYS:HE3	1:J:301:ARG:NH2	2.01	0.71
1:E:296:GLU:O	1:E:297:LYS:C	2.28	0.70
1:F:135:ASP:HB3	1:F:150:ASN:HB2	1.73	0.70
1:I:357:GLU:O	1:I:359:ASN:N	2.25	0.70
1:I:141:THR:O	1:I:144:GLY:N	2.25	0.70
1:J:296:GLU:HA	1:J:297:LYS:C	2.11	0.70
1:A:275:ASN:OD1	1:F:260:GLN:NE2	2.18	0.70
1:B:210:LYS:HB3	1:C:211:GLN:OE1	1.90	0.70
1:F:361:HIS:CD2	1:F:363:PRO:HD2	2.26	0.70
1:E:97:TYR:O	1:E:101:LEU:HD12	1.92	0.70
1:J:295:ILE:O	1:J:298:ARG:HB3	1.91	0.70
1:B:160:ALA:HB1	1:B:254:PRO:HD2	1.73	0.70
1:G:80:ARG:HH12	1:G:84:VAL:HG21	1.57	0.70
1:H:252:HIS:CD2	1:H:261:ALA:HB2	2.27	0.70
1:J:299:LEU:CD1	1:J:305:LEU:HD21	2.13	0.70
1:A:87:GLN:NE2	1:A:204:GLU:OE2	2.20	0.70
1:A:300:HIS:HB2	1:A:305:LEU:HD12	1.74	0.70
1:G:233:PRO:HA	1:G:235:ASP:H	1.57	0.70
1:C:78:GLU:O	1:C:82:ARG:HG3	1.91	0.70
1:J:116:ARG:NE	1:J:169:TYR:HE1	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:O	1:B:295:ILE:HG13	1.91	0.69
1:C:142:PRO:O	1:C:144:GLY:N	2.25	0.69
1:G:296:GLU:O	1:G:299:LEU:HB2	1.92	0.69
1:B:93:LEU:HD23	1:B:196:GLU:HB2	1.74	0.69
1:E:210:LYS:O	1:E:212:ALA:N	2.25	0.69
1:I:300:HIS:CD2	1:I:311:GLU:HA	2.26	0.69
1:A:117:LYS:HE3	1:A:120:GLU:OE2	1.92	0.69
1:B:179:THR:HG22	1:B:180:PRO:HD2	1.75	0.69
1:D:300:HIS:ND1	1:D:311:GLU:HA	2.07	0.69
1:J:93:LEU:HD23	1:J:196:GLU:HB2	1.74	0.69
1:F:93:LEU:HD23	1:F:196:GLU:HB2	1.75	0.69
1:X:164:THR:OG1	1:X:218:GLN:OE1	2.09	0.69
1:B:175:PRO:O	1:B:178:SER:OG	2.10	0.69
1:B:252:HIS:N	1:B:256:PRO:O	2.25	0.69
1:G:82:ARG:HH21	1:G:302:LEU:HD13	1.57	0.69
1:I:273:ALA:HB2	1:I:347:PRO:HG3	1.74	0.69
1:J:187:SER:OG	1:J:269:ASP:OD1	2.09	0.69
1:B:77:PRO:HG3	1:C:71:PRO:HB2	1.74	0.69
1:C:135:ASP:HB3	1:C:150:ASN:HB2	1.75	0.69
1:C:99:ARG:HA	1:C:102:LEU:HD12	1.73	0.68
1:A:120:GLU:OE1	1:A:124:ARG:NH1	2.22	0.68
1:I:93:LEU:HD23	1:I:196:GLU:HB2	1.75	0.68
1:J:296:GLU:N	1:J:298:ARG:HB3	2.07	0.68
1:H:199:GLN:NE2	1:H:199:GLN:O	2.27	0.68
1:X:357:GLU:O	1:X:357:GLU:HG2	1.93	0.68
1:D:297:LYS:O	1:D:301:ARG:HG3	1.92	0.68
1:I:162:HIS:CD2	1:I:262:ILE:HA	2.29	0.68
1:G:297:LYS:HB2	1:G:300:HIS:HB3	1.76	0.68
1:G:313:MET:HE1	1:J:256:PRO:HD3	1.74	0.68
1:H:266:MET:HG3	1:H:339:LEU:HD12	1.74	0.68
1:B:297:LYS:HE2	1:B:301:ARG:HG2	1.72	0.68
1:E:298:ARG:HG3	1:E:302:LEU:HD13	1.75	0.68
1:H:134:LEU:HD23	1:H:135:ASP:N	2.09	0.68
1:J:155:LEU:HD22	1:J:205:LEU:HD22	1.33	0.68
1:J:299:LEU:O	1:J:300:HIS:C	2.32	0.68
1:F:298:ARG:O	1:F:301:ARG:N	2.27	0.68
1:G:248:GLU:HB2	1:G:259:ILE:HG13	1.75	0.67
1:J:298:ARG:O	1:J:301:ARG:N	2.25	0.67
1:E:184:ALA:O	1:E:189:VAL:HG23	1.94	0.67
1:H:70:VAL:HG13	1:H:298:ARG:HD2	1.77	0.67
1:C:326:ASP:OD1	1:C:327:ASP:N	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:NH2	1:B:311:GLU:OE1	2.27	0.67
1:G:78:GLU:HG3	1:G:298:ARG:HH21	1.60	0.67
1:G:205:LEU:O	1:G:208:ALA:N	2.28	0.67
1:H:300:HIS:HD2	1:H:311:GLU:HA	1.58	0.67
1:G:76:LEU:HD23	1:G:80:ARG:HH21	1.59	0.67
1:I:76:LEU:HD21	1:I:81:LEU:HD12	1.75	0.67
1:J:75:SER:HA	1:J:291:ARG:HH22	1.59	0.67
1:J:295:ILE:HA	1:J:298:ARG:HD2	1.77	0.67
1:J:339:LEU:HD23	1:J:340:HIS:N	2.09	0.67
1:A:281:HIS:HA	1:A:320:PRO:HG3	1.76	0.67
1:B:297:LYS:CE	1:B:301:ARG:N	2.51	0.67
1:E:93:LEU:HD23	1:E:196:GLU:HB3	1.75	0.67
1:B:210:LYS:NZ	1:C:211:GLN:HG2	2.10	0.67
1:E:120:GLU:OE1	1:E:124:ARG:NH1	2.26	0.67
1:G:294:SER:O	1:G:298:ARG:HB2	1.94	0.67
1:G:355:ASP:HA	1:G:359:ASN:HD22	1.60	0.66
1:B:70:VAL:CG1	1:B:71:PRO:HD3	2.23	0.66
1:H:101:LEU:HD12	1:H:101:LEU:N	2.10	0.66
1:J:297:LYS:CD	1:J:301:ARG:CG	2.51	0.66
1:G:293:ARG:HH12	1:G:317:PRO:CB	2.01	0.66
1:I:264:LEU:HA	1:I:337:PRO:HG2	1.76	0.66
1:G:211:GLN:O	1:G:213:ALA:N	2.28	0.66
1:G:296:GLU:OE2	1:G:308:HIS:HE1	1.76	0.66
1:J:99:ARG:NH2	1:J:357:GLU:OE2	2.29	0.66
1:J:297:LYS:CB	1:J:298:ARG:HA	2.25	0.66
1:G:142:PRO:C	1:G:144:GLY:H	1.99	0.66
1:I:360:LEU:O	1:I:362:PRO:HD3	1.96	0.66
1:J:280:SER:OG	1:J:282:PHE:O	2.14	0.66
1:E:291:ARG:NH1	1:E:378:GLU:OE1	2.29	0.65
1:F:70:VAL:HG13	1:F:298:ARG:NH1	2.09	0.65
1:E:283:PRO:O	1:E:286:VAL:HG12	1.95	0.65
1:H:235:ASP:O	1:H:236:SER:OG	2.13	0.65
1:H:240:SER:C	1:H:242:HIS:H	1.98	0.65
1:J:297:LYS:HB3	1:J:298:ARG:HB2	1.78	0.65
1:B:297:LYS:HA	1:B:298:ARG:C	2.17	0.65
1:I:116:ARG:HB2	1:I:169:TYR:CE2	2.31	0.65
1:E:298:ARG:O	1:E:301:ARG:N	2.29	0.65
1:X:120:GLU:HG2	1:X:124:ARG:NH1	2.11	0.65
1:E:71:PRO:HB3	1:E:298:ARG:HH21	1.62	0.65
1:D:70:VAL:HG21	1:D:301:ARG:HE	1.61	0.65
1:F:126:LEU:O	1:F:128:ALA:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:PRO:HG2	1:I:228:LEU:HD21	1.77	0.65
1:B:89:ASP:HB3	1:B:92:ARG:HB3	1.79	0.65
1:H:86:GLY:O	1:H:88:LEU:N	2.30	0.65
1:J:302:LEU:HG	1:J:304:LEU:HD13	1.78	0.65
1:B:294:SER:O	1:B:298:ARG:HB2	1.97	0.65
1:B:297:LYS:CG	1:B:300:HIS:CD2	2.80	0.65
1:D:116:ARG:HD3	1:D:134:LEU:HD11	1.79	0.65
1:E:105:ARG:HD2	1:E:169:TYR:O	1.97	0.65
1:E:172:LYS:H	1:E:181:PHE:HE2	1.45	0.65
1:J:337:PRO:O	1:J:338:VAL:HG23	1.97	0.65
1:J:116:ARG:NH2	1:J:223:ASP:CG	2.49	0.64
1:J:156:ASP:HB2	1:J:209:LYS:HG2	1.80	0.64
1:G:297:LYS:HB3	1:G:300:HIS:N	2.12	0.64
1:J:269:ASP:HB3	1:J:342:ILE:HD12	1.78	0.64
1:G:71:PRO:HB3	1:G:298:ARG:NE	2.12	0.64
1:H:297:LYS:HD3	1:H:311:GLU:CA	2.28	0.64
1:D:293:ARG:O	1:D:297:LYS:HG3	1.98	0.64
1:H:225:GLU:HG2	1:H:237:LEU:HD23	1.79	0.64
1:D:319:GLU:N	1:D:320:PRO:HD2	2.13	0.64
1:D:346:PHE:O	1:H:284:ARG:NH1	2.30	0.64
1:I:123:LEU:HD11	1:I:221:PHE:HE2	1.62	0.64
1:E:131:HIS:NE2	1:E:133:GLU:OE1	2.28	0.64
1:H:111:GLY:HA2	1:H:114:GLN:HB3	1.78	0.64
1:H:179:THR:HG22	1:H:180:PRO:HD2	1.80	0.64
1:J:130:TRP:O	1:J:132:VAL:N	2.30	0.64
1:E:123:LEU:HD13	1:E:153:ALA:HB2	1.79	0.64
1:E:246:LEU:O	1:E:249:SER:N	2.29	0.64
1:I:289:PHE:CE1	1:I:315:PHE:HD2	2.16	0.64
1:B:297:LYS:HD2	1:B:301:ARG:N	2.06	0.64
1:G:296:GLU:O	1:G:299:LEU:N	2.29	0.64
1:H:319:GLU:H	1:H:320:PRO:CD	2.10	0.64
1:G:297:LYS:NZ	1:G:311:GLU:CA	2.51	0.63
1:I:377:ALA:O	1:I:381:GLY:N	2.30	0.63
1:B:297:LYS:HE3	1:B:301:ARG:CB	2.28	0.63
1:G:112:ASN:O	1:G:114:GLN:N	2.32	0.63
1:H:297:LYS:CE	1:H:311:GLU:CG	2.70	0.63
1:H:97:TYR:O	1:H:101:LEU:HD11	1.99	0.63
1:H:279:TYR:CE1	1:H:316:GLN:HB2	2.33	0.63
1:J:297:LYS:HG2	1:J:298:ARG:CA	2.28	0.63
1:X:297:LYS:HB2	1:X:298:ARG:HB2	1.80	0.63
1:F:160:ALA:HB1	1:F:254:PRO:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:LEU:O	1:J:102:LEU:HD11	1.99	0.63
1:D:275:ASN:ND2	1:H:260:GLN:HG2	2.14	0.63
1:D:296:GLU:O	1:D:298:ARG:N	2.31	0.63
1:J:168:HIS:HD1	1:J:225:GLU:HB3	1.64	0.63
1:B:299:LEU:O	1:B:300:HIS:C	2.34	0.63
1:D:310:GLN:HB2	1:D:313:MET:HG3	1.80	0.63
1:G:141:THR:OG1	1:G:228:LEU:HD12	1.98	0.63
1:B:297:LYS:NZ	1:B:300:HIS:CD2	2.66	0.63
1:F:93:LEU:HD23	1:F:196:GLU:CB	2.29	0.63
1:F:230:GLU:HG3	3:F:402:A1D46:C15	2.29	0.63
1:F:291:ARG:N	1:F:291:ARG:HD2	2.12	0.63
1:H:220:LEU:HD13	1:H:243:LEU:HD21	1.79	0.63
1:F:70:VAL:CG1	1:F:298:ARG:NH1	2.61	0.63
1:X:105:ARG:HD2	1:X:115:VAL:HG21	1.80	0.62
1:G:76:LEU:HD23	1:G:80:ARG:NH2	2.14	0.62
1:H:166:ALA:HB1	1:H:222:LEU:HD11	1.81	0.62
1:J:308:HIS:CD2	1:J:313:MET:SD	2.90	0.62
1:B:166:ALA:O	1:B:267:LEU:HD12	1.99	0.62
1:G:352:THR:O	1:G:354:ALA:N	2.32	0.62
1:H:229:LYS:HG3	1:H:231:TRP:CZ3	2.34	0.62
1:X:318:GLY:O	1:X:319:GLU:HG2	1.99	0.62
1:E:296:GLU:O	1:E:297:LYS:O	2.17	0.62
1:F:134:LEU:O	1:F:136:PRO:HD3	1.98	0.62
1:E:79:ALA:HA	1:E:82:ARG:HB2	1.81	0.62
1:I:289:PHE:HE1	1:I:315:PHE:HD2	1.46	0.62
1:J:205:LEU:O	1:J:207:ARG:N	2.31	0.62
1:C:313:MET:O	1:C:316:GLN:NE2	2.33	0.62
1:D:156:ASP:OD1	1:D:158:ARG:NE	2.33	0.62
1:F:72:LEU:O	1:F:75:SER:HB2	2.00	0.62
1:X:120:GLU:HG2	1:X:124:ARG:HH12	1.65	0.62
1:C:120:GLU:OE1	1:C:124:ARG:NH1	2.27	0.62
1:F:360:LEU:O	1:F:362:PRO:HD3	1.99	0.62
1:J:267:LEU:HD23	1:J:340:HIS:CE1	2.35	0.62
1:A:134:LEU:O	1:A:136:PRO:HD3	2.00	0.62
1:B:92:ARG:HH22	1:B:200:ALA:HB2	1.65	0.62
1:E:326:ASP:H	1:E:329:ILE:HD13	1.64	0.62
1:G:268:LEU:HB3	1:G:271:LEU:HD11	1.82	0.61
1:G:297:LYS:HB3	1:G:300:HIS:H	1.63	0.61
1:X:291:ARG:O	1:X:295:ILE:HG13	2.00	0.61
1:C:297:LYS:O	1:C:301:ARG:HG3	1.99	0.61
1:I:296:GLU:O	1:I:299:LEU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:197:LEU:HD13	1:J:376:LEU:HD12	1.82	0.61
1:D:70:VAL:CG1	1:D:71:PRO:HD3	2.30	0.61
1:J:93:LEU:HD23	1:J:196:GLU:CB	2.29	0.61
1:D:270:LEU:HD12	1:D:346:PHE:CD1	2.36	0.61
1:H:240:SER:O	1:H:242:HIS:N	2.32	0.61
1:C:273:ALA:O	1:C:276:PRO:HD3	1.99	0.61
1:G:275:ASN:HD21	1:J:260:GLN:NE2	1.98	0.61
1:A:253:SER:HA	1:A:254:PRO:C	2.20	0.61
1:H:269:ASP:OD2	3:H:402:A1D46:N23	2.33	0.61
1:H:299:LEU:HD12	1:H:371:ILE:HG12	1.83	0.61
1:J:201:LEU:HD23	1:J:201:LEU:N	2.16	0.61
1:I:160:ALA:HB1	1:I:254:PRO:HD3	1.81	0.61
1:J:130:TRP:HZ2	1:J:205:LEU:CD1	2.14	0.61
1:X:141:THR:OG1	1:X:144:GLY:O	2.15	0.61
1:A:322:GLY:HA2	1:E:353:PRO:HG3	1.83	0.61
1:C:179:THR:HB	1:C:353:PRO:HB3	1.83	0.61
1:F:122:THR:O	1:F:125:SER:OG	2.17	0.61
1:G:219:LEU:O	1:G:220:LEU:HD23	2.01	0.61
1:I:227:ALA:CB	1:I:230:GLU:HA	2.30	0.61
1:I:349:VAL:O	1:I:355:ASP:HB2	2.01	0.61
1:A:225:GLU:HG3	1:A:327:ASP:OD2	2.00	0.61
1:H:296:GLU:OE2	1:H:308:HIS:NE2	2.26	0.61
1:G:77:PRO:HG2	1:G:80:ARG:HB2	1.83	0.60
1:H:298:ARG:O	1:H:301:ARG:N	2.33	0.60
1:C:142:PRO:C	1:C:144:GLY:H	2.05	0.60
1:E:156:ASP:O	1:E:216:THR:HG21	2.00	0.60
1:B:229:LYS:HB3	1:B:230:GLU:OE1	2.02	0.60
1:G:233:PRO:HA	1:G:235:ASP:N	2.17	0.60
1:I:97:TYR:CE2	1:I:196:GLU:HA	2.37	0.60
1:J:169:TYR:HD2	1:J:221:PHE:HB3	1.67	0.60
1:B:173:LEU:HD12	1:B:174:PHE:H	1.63	0.60
1:D:70:VAL:CG2	1:D:301:ARG:HE	2.13	0.60
1:I:174:PHE:CE2	1:I:353:PRO:HD3	2.36	0.60
1:I:267:LEU:HD22	1:I:328:HIS:HB3	1.84	0.60
1:E:270:LEU:HD13	1:E:347:PRO:HD2	1.83	0.60
1:J:98:LEU:O	1:J:102:LEU:CD1	2.50	0.60
1:J:153:ALA:HB3	1:J:219:LEU:HB2	1.83	0.60
1:J:299:LEU:C	1:J:301:ARG:N	2.52	0.60
1:F:134:LEU:HD11	1:F:151:VAL:HG22	1.83	0.60
1:J:374:VAL:O	1:J:378:GLU:HG3	2.02	0.60
1:X:119:LEU:O	1:X:123:LEU:HD12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:HIS:O	1:F:154:THR:N	2.35	0.60
1:G:227:ALA:HB2	1:G:231:TRP:HE3	1.66	0.60
1:H:92:ARG:HG2	1:H:97:TYR:CE2	2.37	0.60
1:H:229:LYS:O	1:H:231:TRP:HE3	1.85	0.60
1:H:274:PRO:HB3	1:H:361:HIS:HB2	1.84	0.60
1:J:204:GLU:OE1	1:J:204:GLU:N	2.34	0.60
1:H:93:LEU:O	1:H:98:LEU:N	2.35	0.59
1:I:155:LEU:O	1:I:209:LYS:NZ	2.24	0.59
1:B:70:VAL:HG21	1:B:301:ARG:HD2	1.83	0.59
1:C:227:ALA:CB	1:C:230:GLU:HA	2.32	0.59
1:F:156:ASP:OD1	1:F:158:ARG:NE	2.35	0.59
1:H:92:ARG:O	1:H:96:THR:OG1	2.19	0.59
1:I:309:PRO:HD2	1:I:313:MET:SD	2.42	0.59
1:J:99:ARG:HA	1:J:102:LEU:HD11	1.83	0.59
1:X:93:LEU:HD23	1:X:196:GLU:HB2	1.83	0.59
1:J:135:ASP:O	1:J:149:GLY:HA2	2.03	0.59
1:X:80:ARG:O	1:X:84:VAL:HG23	2.03	0.59
1:X:173:LEU:HD22	1:X:228:LEU:HD12	1.85	0.59
1:A:70:VAL:CG2	1:A:301:ARG:HD2	2.32	0.59
1:B:155:LEU:O	1:B:209:LYS:NZ	2.35	0.59
1:F:111:GLY:O	1:F:115:VAL:HG23	2.02	0.59
1:F:357:GLU:HA	1:F:360:LEU:HD12	1.83	0.59
1:A:127:THR:OG1	1:A:202:ASP:OD2	2.18	0.59
1:E:336:VAL:O	1:E:338:VAL:HG23	2.02	0.59
1:J:291:ARG:NH1	1:J:378:GLU:OE1	2.36	0.59
1:B:230:GLU:OE1	1:B:230:GLU:N	2.35	0.59
1:D:162:HIS:HB3	1:D:216:THR:HG22	1.85	0.59
1:G:291:ARG:CZ	1:G:295:ILE:HD11	2.32	0.59
1:H:196:GLU:O	1:H:200:ALA:N	2.35	0.59
1:J:101:LEU:O	1:J:103:VAL:N	2.28	0.59
1:G:112:ASN:O	1:G:115:VAL:N	2.35	0.59
1:G:308:HIS:HE2	1:G:313:MET:HB2	1.68	0.59
1:H:296:GLU:O	1:H:297:LYS:HB3	2.02	0.59
1:B:99:ARG:NH1	1:B:357:GLU:OE2	2.36	0.59
1:G:156:ASP:OD1	1:G:158:ARG:NE	2.35	0.59
1:H:361:HIS:ND1	1:H:363:PRO:HD2	2.18	0.59
1:X:313:MET:O	1:X:316:GLN:NE2	2.35	0.59
1:D:70:VAL:HG12	1:D:71:PRO:CD	2.31	0.59
1:D:275:ASN:HD21	1:H:260:GLN:HG2	1.66	0.59
1:F:298:ARG:O	1:F:299:LEU:C	2.41	0.59
1:G:113:LEU:O	1:G:117:LYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:LEU:CD2	1:H:378:GLU:HG3	2.30	0.59
1:E:78:GLU:O	1:E:81:LEU:N	2.36	0.59
1:H:103:VAL:C	1:H:182:VAL:HG12	2.23	0.59
1:H:161:ARG:O	1:H:215:VAL:HA	2.02	0.59
1:D:269:ASP:OD2	3:D:402:A1D46:N23	2.36	0.58
1:D:309:PRO:HD2	1:D:313:MET:SD	2.43	0.58
1:E:71:PRO:HB3	1:E:298:ARG:NH2	2.17	0.58
1:E:71:PRO:HB2	1:E:75:SER:CB	2.33	0.58
1:E:92:ARG:O	1:E:96:THR:HB	2.02	0.58
1:E:107:PRO:HA	1:E:112:ASN:ND2	2.17	0.58
1:H:297:LYS:HA	1:H:298:ARG:C	2.24	0.58
1:H:80:ARG:O	1:H:84:VAL:HG23	2.03	0.58
1:I:332:LEU:HG	1:I:332:LEU:O	2.02	0.58
1:J:92:ARG:NH2	1:J:196:GLU:OE2	2.35	0.58
1:A:70:VAL:HG21	1:A:301:ARG:HD2	1.84	0.58
1:D:85:VAL:HG13	1:D:370:ARG:NH1	2.18	0.58
1:H:97:TYR:OH	1:H:199:GLN:HG2	2.03	0.58
1:H:175:PRO:O	1:H:178:SER:OG	2.20	0.58
1:C:172:LYS:HD3	1:C:174:PHE:CZ	2.39	0.58
1:F:161:ARG:O	1:F:215:VAL:HA	2.02	0.58
1:I:295:ILE:CG2	1:I:374:VAL:CG1	2.81	0.58
1:I:301:ARG:NH2	1:I:311:GLU:OE1	2.36	0.58
1:B:279:TYR:CE1	1:B:316:GLN:HB2	2.37	0.58
1:D:150:ASN:ND2	1:D:239:GLY:O	2.32	0.58
1:E:381:GLY:O	1:E:382:LEU:HD23	2.04	0.58
1:H:298:ARG:O	1:H:299:LEU:C	2.41	0.58
1:C:296:GLU:O	1:C:297:LYS:CB	2.45	0.58
1:E:331:PHE:O	1:E:336:VAL:HG23	2.04	0.58
1:A:105:ARG:HB2	1:A:112:ASN:HA	1.85	0.58
1:A:105:ARG:HG2	1:A:171:SER:HB3	1.86	0.58
1:D:298:ARG:O	1:D:302:LEU:HG	2.03	0.58
1:E:306:GLN:O	1:E:367:ASN:ND2	2.34	0.58
1:J:130:TRP:CZ2	1:J:205:LEU:CD1	2.86	0.58
1:J:296:GLU:HA	1:J:298:ARG:CB	2.34	0.58
1:J:329:ILE:O	1:J:333:ARG:HG2	2.03	0.58
1:X:123:LEU:HA	1:X:126:LEU:HD12	1.86	0.58
1:G:80:ARG:NH1	1:G:84:VAL:HG21	2.18	0.58
1:G:291:ARG:C	1:G:295:ILE:HD13	2.24	0.58
1:H:111:GLY:O	1:H:115:VAL:HG23	2.03	0.58
1:J:305:LEU:HD12	1:J:308:HIS:CE1	2.39	0.58
1:J:83:ARG:HH22	1:J:204:GLU:CG	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ILE:HG22	1:C:299:LEU:HD12	1.83	0.58
1:I:164:THR:HG23	1:I:218:GLN:HB3	1.85	0.58
1:C:141:THR:HG22	1:C:238:TYR:HE2	1.69	0.57
1:C:295:ILE:HD12	1:C:295:ILE:H	1.69	0.57
1:E:223:ASP:OD1	1:E:224:GLY:N	2.37	0.57
1:J:82:ARG:HA	1:J:85:VAL:HB	1.85	0.57
1:A:155:LEU:HD21	1:A:205:LEU:HB3	1.84	0.57
1:F:150:ASN:OD1	1:F:222:LEU:HA	2.04	0.57
1:H:274:PRO:HB3	1:H:361:HIS:CB	2.34	0.57
1:J:282:PHE:HE2	1:J:332:LEU:HD21	1.66	0.57
1:G:89:ASP:HB3	1:G:92:ARG:HB2	1.86	0.57
1:I:222:LEU:HD13	1:I:240:SER:HB3	1.86	0.57
1:X:93:LEU:HD23	1:X:196:GLU:CB	2.34	0.57
1:A:162:HIS:HB3	1:A:216:THR:CG2	2.35	0.57
1:A:320:PRO:HA	1:A:321:PHE:HB2	1.85	0.57
1:G:309:PRO:HG2	1:J:256:PRO:HB2	1.85	0.57
1:G:350:TRP:CD2	1:G:351:HIS:HB2	2.39	0.57
1:A:155:LEU:O	1:A:209:LYS:HE3	2.04	0.57
1:A:322:GLY:CA	1:E:353:PRO:HG3	2.35	0.57
1:F:207:ARG:O	1:F:210:LYS:N	2.37	0.57
1:H:319:GLU:H	1:H:320:PRO:HD2	1.70	0.57
1:J:134:LEU:HA	1:J:150:ASN:O	2.04	0.57
1:J:200:ALA:C	1:J:201:LEU:CD2	2.72	0.57
1:G:70:VAL:CG1	1:G:71:PRO:HD2	2.34	0.57
1:G:105:ARG:HG2	1:G:171:SER:HB3	1.86	0.57
1:G:352:THR:C	1:G:354:ALA:H	2.08	0.57
1:F:126:LEU:C	1:F:128:ALA:H	2.08	0.57
1:H:168:HIS:ND1	1:H:170:ASP:OD1	2.38	0.57
1:J:101:LEU:HD21	1:J:118:PHE:CE2	2.39	0.57
1:J:112:ASN:O	1:J:116:ARG:HD3	2.04	0.57
1:X:106:THR:O	1:X:112:ASN:HB2	2.04	0.57
1:B:231:TRP:HZ2	1:B:325:GLU:HB3	1.69	0.57
1:C:70:VAL:N	1:C:71:PRO:HD3	2.19	0.57
1:J:370:ARG:O	1:J:374:VAL:HG23	2.04	0.57
1:D:142:PRO:O	1:D:144:GLY:N	2.36	0.57
1:E:76:LEU:HG	1:E:378:GLU:HG3	1.86	0.57
1:F:120:GLU:HB3	1:F:124:ARG:NH1	2.20	0.57
1:G:155:LEU:HD23	1:G:205:LEU:HD22	1.86	0.57
1:G:284:ARG:NH1	1:H:346:PHE:O	2.37	0.57
1:I:237:LEU:HD22	1:I:327:ASP:HA	1.85	0.57
1:J:203:LEU:O	1:J:206:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:HB3	1:A:92:ARG:HB3	1.87	0.56
1:D:160:ALA:HB1	1:D:254:PRO:HD2	1.87	0.56
1:E:172:LYS:HB2	1:E:226:GLU:HG3	1.87	0.56
1:F:199:GLN:O	1:F:201:LEU:N	2.38	0.56
1:H:375:PHE:HD1	1:H:376:LEU:HD23	1.69	0.56
1:X:94:TRP:CH2	1:X:362:PRO:HG3	2.40	0.56
1:X:298:ARG:O	1:X:302:LEU:HG	2.06	0.56
1:A:291:ARG:O	1:A:295:ILE:HG13	2.06	0.56
1:C:90:PRO:HB3	1:C:366:HIS:NE2	2.20	0.56
1:F:119:LEU:HD23	1:F:195:LEU:HD11	1.87	0.56
1:G:92:ARG:HH21	1:G:199:GLN:HB3	1.69	0.56
1:G:361:HIS:HE1	1:G:363:PRO:HB2	1.71	0.56
1:I:306:GLN:O	1:I:308:HIS:N	2.38	0.56
1:J:297:LYS:HB3	1:J:298:ARG:CB	2.35	0.56
1:J:305:LEU:HD12	1:J:308:HIS:ND1	2.20	0.56
1:E:78:GLU:O	1:E:80:ARG:N	2.38	0.56
1:G:78:GLU:CG	1:G:298:ARG:HH21	2.18	0.56
1:G:297:LYS:HB3	1:G:300:HIS:HB2	1.84	0.56
1:B:260:GLN:NE2	1:F:275:ASN:OD1	2.37	0.56
1:F:72:LEU:HG	1:F:291:ARG:HH22	1.69	0.56
1:G:184:ALA:O	1:G:189:VAL:HG23	2.05	0.56
1:G:302:LEU:O	1:G:304:LEU:N	2.39	0.56
1:H:162:HIS:HE1	1:H:262:ILE:HG12	1.68	0.56
1:J:184:ALA:N	1:J:355:ASP:OD2	2.25	0.56
1:D:105:ARG:NH1	1:D:182:VAL:O	2.39	0.56
1:I:295:ILE:O	1:I:299:LEU:HD12	2.06	0.56
1:A:207:ARG:HD2	1:A:207:ARG:N	2.21	0.56
1:C:291:ARG:NH2	1:C:378:GLU:OE1	2.39	0.56
1:E:269:ASP:OD2	3:E:402:A1D46:N23	2.39	0.56
1:G:300:HIS:HD2	1:G:311:GLU:CA	2.13	0.56
1:H:297:LYS:CE	1:H:311:GLU:HG2	2.21	0.56
1:J:237:LEU:HD22	1:J:327:ASP:HA	1.87	0.56
1:J:294:SER:C	1:J:296:GLU:H	2.09	0.56
1:A:252:HIS:O	1:A:255:GLY:HA3	2.05	0.56
1:B:92:ARG:NH2	1:B:200:ALA:HB2	2.20	0.56
1:H:107:PRO:HA	1:H:112:ASN:OD1	2.06	0.56
1:I:352:THR:C	1:I:354:ALA:H	2.08	0.56
1:A:320:PRO:HA	1:A:321:PHE:CB	2.35	0.56
1:A:358:VAL:HG13	1:A:359:ASN:OD1	2.06	0.56
1:H:113:LEU:O	1:H:116:ARG:HB3	2.06	0.56
1:J:142:PRO:HD2	1:J:228:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:TRP:CH2	1:D:362:PRO:HG3	2.42	0.55
1:G:291:ARG:O	1:G:295:ILE:HD13	2.05	0.55
1:H:94:TRP:HA	1:H:98:LEU:HB3	1.86	0.55
1:I:97:TYR:HE2	1:I:196:GLU:HA	1.70	0.55
1:J:112:ASN:C	1:J:116:ARG:HD3	2.25	0.55
1:A:162:HIS:HB3	1:A:216:THR:HG22	1.88	0.55
1:B:101:LEU:O	1:B:103:VAL:N	2.38	0.55
1:B:297:LYS:HD3	1:B:301:ARG:N	2.10	0.55
1:J:246:LEU:HG	1:J:250:ILE:HD11	1.89	0.55
1:F:234:LYS:HA	1:F:241:ARG:HH12	1.71	0.55
1:H:161:ARG:NH2	1:H:263:GLU:HG3	2.20	0.55
1:H:168:HIS:O	1:H:168:HIS:CD2	2.58	0.55
1:J:297:LYS:CB	1:J:298:ARG:CA	2.83	0.55
1:F:356:THR:OG1	1:F:358:VAL:HG12	2.06	0.55
1:G:93:LEU:HD23	1:G:196:GLU:HB2	1.86	0.55
1:G:355:ASP:HA	1:G:359:ASN:ND2	2.21	0.55
1:I:70:VAL:N	1:I:71:PRO:HD2	2.21	0.55
1:A:199:GLN:OE1	1:A:199:GLN:HA	2.07	0.55
1:D:190:PRO:O	1:D:193:LEU:HB2	2.06	0.55
1:F:298:ARG:O	1:F:300:HIS:N	2.39	0.55
1:G:299:LEU:O	1:G:300:HIS:C	2.42	0.55
1:H:299:LEU:CD1	1:H:371:ILE:HG12	2.37	0.55
1:X:283:PRO:O	1:X:286:VAL:HG12	2.07	0.55
1:D:283:PRO:O	1:D:286:VAL:HG12	2.06	0.55
1:G:293:ARG:NH1	1:G:317:PRO:HB3	2.01	0.55
1:A:297:LYS:HE2	1:A:312:VAL:CG2	2.37	0.55
1:E:194:LEU:HD23	1:E:194:LEU:N	2.22	0.55
1:H:304:LEU:C	1:H:370:ARG:HH12	2.07	0.55
1:B:298:ARG:O	1:B:301:ARG:HB2	2.07	0.55
1:E:71:PRO:O	1:E:72:LEU:HD23	2.07	0.55
1:H:189:VAL:HB	1:H:271:LEU:O	2.06	0.55
1:A:295:ILE:O	1:A:299:LEU:HD12	2.07	0.55
1:G:153:ALA:HB3	1:G:219:LEU:HB2	1.89	0.55
1:H:88:LEU:HD23	1:H:369:CYS:SG	2.46	0.55
1:H:184:ALA:O	1:H:189:VAL:HG23	2.07	0.55
1:I:166:ALA:O	1:I:267:LEU:HD12	2.05	0.55
1:X:110:PRO:O	1:X:114:GLN:NE2	2.40	0.54
1:B:141:THR:HB	1:B:228:LEU:HD12	1.87	0.54
1:E:141:THR:HG21	1:E:148:PHE:HZ	1.73	0.54
1:E:350:TRP:CD1	1:E:351:HIS:HB2	2.42	0.54
1:F:230:GLU:HG3	3:F:402:A1D46:C14	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:LYS:CE	1:G:311:GLU:CA	2.84	0.54
1:H:291:ARG:HH21	1:H:378:GLU:HB3	1.72	0.54
1:A:341:LEU:HD21	1:A:372:LEU:HD21	1.89	0.54
1:I:99:ARG:HB3	1:I:100:PRO:HD3	1.88	0.54
1:J:303:ASN:C	1:J:304:LEU:HD12	2.27	0.54
1:J:304:LEU:HB3	1:J:370:ARG:HH11	1.72	0.54
1:A:90:PRO:HB3	1:A:366:HIS:CD2	2.43	0.54
1:E:93:LEU:HD23	1:E:196:GLU:HB2	1.87	0.54
1:F:231:TRP:CZ3	3:F:402:A1D46:O01	2.61	0.54
1:G:356:THR:H	1:G:359:ASN:ND2	2.05	0.54
1:J:235:ASP:HA	1:J:238:TYR:OH	2.07	0.54
1:B:257:THR:OG1	1:B:260:GLN:OE1	2.13	0.54
1:E:309:PRO:HD2	1:E:313:MET:SD	2.48	0.54
1:F:206:SER:O	1:F:210:LYS:HG3	2.07	0.54
1:H:331:PHE:O	1:H:336:VAL:HG23	2.07	0.54
1:B:306:GLN:HB3	1:B:363:PRO:HB3	1.88	0.54
1:D:93:LEU:HD23	1:D:196:GLU:HB2	1.90	0.54
1:E:295:ILE:O	1:E:299:LEU:CD1	2.37	0.54
1:G:172:LYS:HG2	1:G:173:LEU:N	2.22	0.54
1:G:358:VAL:HG13	1:J:333:ARG:NH1	2.21	0.54
1:I:350:TRP:O	1:I:352:THR:HG23	2.07	0.54
1:J:169:TYR:HD2	1:J:221:PHE:CB	2.21	0.54
1:B:76:LEU:HG	1:B:378:GLU:HG2	1.90	0.54
1:B:324:VAL:HG11	1:B:346:PHE:CZ	2.43	0.54
1:F:153:ALA:O	1:F:218:GLN:HG3	2.08	0.54
1:H:150:ASN:ND2	1:H:239:GLY:O	2.41	0.54
1:H:174:PHE:CD2	1:H:181:PHE:CD2	2.95	0.54
1:B:296:GLU:HB2	1:B:371:ILE:HD13	1.90	0.54
1:C:334:ARG:HH11	1:C:334:ARG:HG3	1.73	0.54
1:H:203:LEU:O	1:H:206:SER:N	2.25	0.54
1:E:77:PRO:HG2	1:E:80:ARG:CZ	2.38	0.54
1:C:105:ARG:HD2	1:C:115:VAL:HG21	1.88	0.54
1:C:231:TRP:CD1	1:C:232:GLY:N	2.76	0.54
1:I:77:PRO:HB2	1:I:80:ARG:HB2	1.90	0.54
1:I:156:ASP:HA	1:I:209:LYS:NZ	2.23	0.54
1:I:269:ASP:O	1:I:342:ILE:HA	2.08	0.54
1:J:296:GLU:CA	1:J:298:ARG:CB	2.85	0.54
1:A:296:GLU:OE2	1:A:308:HIS:NE2	2.40	0.54
1:B:297:LYS:HG3	1:B:297:LYS:O	2.06	0.54
1:E:194:LEU:HD21	1:E:268:LEU:HD22	1.90	0.54
1:H:79:ALA:O	1:H:83:ARG:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:184:ALA:HB1	1:H:360:LEU:HD11	1.90	0.54
1:I:107:PRO:O	1:I:109:SER:N	2.41	0.54
1:I:357:GLU:O	1:I:360:LEU:N	2.33	0.54
1:A:310:GLN:HB2	1:A:313:MET:HG3	1.89	0.53
1:D:125:SER:OG	1:D:126:LEU:N	2.40	0.53
1:E:277:THR:OG1	1:E:344:THR:O	2.24	0.53
1:H:127:THR:O	1:H:129:GLY:N	2.41	0.53
1:J:94:TRP:CD1	1:J:98:LEU:HD23	2.43	0.53
1:J:316:GLN:OE1	1:J:317:PRO:HD2	2.08	0.53
1:G:90:PRO:HA	1:G:366:HIS:CD2	2.43	0.53
1:I:158:ARG:HH22	1:I:212:ALA:HA	1.74	0.53
1:B:87:GLN:NE2	1:B:204:GLU:OE2	2.39	0.53
1:H:112:ASN:HD22	1:H:112:ASN:C	2.11	0.53
1:I:101:LEU:O	1:I:105:ARG:NH1	2.41	0.53
1:J:283:PRO:HD2	1:J:284:ARG:H	1.73	0.53
1:J:349:VAL:HG11	1:J:359:ASN:HD22	1.73	0.53
1:C:88:LEU:HD23	1:C:200:ALA:CB	2.39	0.53
1:E:169:TYR:HE1	1:E:223:ASP:HB2	1.72	0.53
1:H:187:SER:HB3	1:H:190:PRO:HG3	1.88	0.53
1:I:352:THR:O	1:I:354:ALA:N	2.42	0.53
1:J:83:ARG:HH22	1:J:204:GLU:CD	2.11	0.53
1:J:278:PHE:O	1:J:316:GLN:HB2	2.07	0.53
1:X:225:GLU:HG2	1:X:225:GLU:O	2.07	0.53
1:B:80:ARG:HG3	1:C:73:ILE:HG23	1.89	0.53
1:F:70:VAL:CG1	1:F:298:ARG:HH11	2.14	0.53
1:G:315:PHE:HE1	1:G:371:ILE:HD13	1.74	0.53
1:H:229:LYS:HG3	1:H:231:TRP:CE3	2.43	0.53
1:J:295:ILE:HD13	1:J:374:VAL:HB	1.90	0.53
1:D:297:LYS:HG2	1:D:312:VAL:HG23	1.90	0.53
1:I:165:LEU:HD23	1:I:266:MET:HB3	1.89	0.53
1:I:190:PRO:HB3	1:I:268:LEU:O	2.09	0.53
1:B:123:LEU:HD11	1:B:221:PHE:CE1	2.44	0.53
1:B:217:LEU:HD12	1:B:218:GLN:H	1.74	0.53
1:B:297:LYS:HG2	1:B:311:GLU:HG2	1.89	0.53
1:H:70:VAL:CG1	1:H:298:ARG:NE	2.63	0.53
1:H:298:ARG:CG	1:H:302:LEU:HD11	2.39	0.53
1:I:207:ARG:O	1:I:210:LYS:N	2.42	0.53
1:A:76:LEU:O	1:A:298:ARG:NH1	2.41	0.53
1:A:379:TYR:HD1	1:A:380:LEU:HD23	1.74	0.53
1:B:160:ALA:HB1	1:B:254:PRO:CD	2.38	0.53
1:B:352:THR:HB	1:B:353:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:HD11	1:D:370:ARG:HA	1.91	0.53
1:F:269:ASP:OD2	1:F:326:ASP:OD2	2.26	0.53
1:J:116:ARG:N	1:J:116:ARG:HD2	2.24	0.53
1:X:246:LEU:O	1:X:250:ILE:HG13	2.09	0.53
1:B:297:LYS:HD3	1:B:300:HIS:HB3	1.88	0.53
1:E:161:ARG:O	1:E:215:VAL:HA	2.09	0.53
1:H:297:LYS:HZ3	1:H:301:ARG:CZ	2.11	0.53
1:J:185:THR:O	1:J:187:SER:HA	2.08	0.53
1:A:187:SER:HB3	1:A:190:PRO:HB2	1.90	0.53
1:B:251:PRO:HA	1:B:257:THR:HA	1.91	0.53
1:D:222:LEU:HD13	1:D:240:SER:HB3	1.91	0.53
1:G:297:LYS:CD	1:G:311:GLU:HB3	2.39	0.53
1:G:297:LYS:HD2	1:G:311:GLU:HB3	1.90	0.52
1:I:242:HIS:O	1:I:246:LEU:N	2.38	0.52
1:J:203:LEU:O	1:J:204:GLU:C	2.47	0.52
1:A:296:GLU:O	1:A:297:LYS:CB	2.52	0.52
1:G:203:LEU:CA	1:G:206:SER:HB3	2.36	0.52
1:I:281:HIS:CE1	1:I:340:HIS:CB	2.72	0.52
1:J:296:GLU:CA	1:J:298:ARG:HB3	2.39	0.52
1:D:80:ARG:HG2	1:D:83:ARG:HH11	1.74	0.52
1:G:299:LEU:O	1:G:301:ARG:N	2.41	0.52
1:H:281:HIS:HB3	1:H:323:SER:HB2	1.91	0.52
1:H:285:THR:HG21	1:H:338:VAL:O	2.09	0.52
1:J:201:LEU:N	1:J:201:LEU:CD2	2.73	0.52
1:J:297:LYS:HB3	1:J:298:ARG:HA	1.90	0.52
1:J:336:VAL:HG12	1:J:337:PRO:O	2.09	0.52
1:B:352:THR:C	1:B:354:ALA:H	2.13	0.52
1:E:362:PRO:HB2	1:E:363:PRO:HD3	1.91	0.52
1:G:309:PRO:HD2	1:G:313:MET:SD	2.49	0.52
1:B:99:ARG:HB3	1:B:100:PRO:CD	2.40	0.52
1:B:296:GLU:OE1	1:B:315:PHE:HD2	1.93	0.52
1:C:83:ARG:O	1:C:87:GLN:HG3	2.10	0.52
1:D:111:GLY:O	1:D:115:VAL:HG23	2.10	0.52
1:F:94:TRP:CH2	1:F:362:PRO:HG3	2.45	0.52
1:J:290:HIS:O	1:J:294:SER:N	2.39	0.52
1:E:129:GLY:O	1:E:209:LYS:NZ	2.41	0.52
1:E:137:PHE:CZ	1:E:148:PHE:HB2	2.45	0.52
1:H:86:GLY:C	1:H:88:LEU:H	2.12	0.52
1:I:295:ILE:H	1:I:295:ILE:CD1	2.03	0.52
1:X:250:ILE:HB	1:X:258:ARG:HD2	1.91	0.52
1:B:297:LYS:HE3	1:B:301:ARG:HG2	1.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:VAL:HB	1:D:221:PHE:HB2	1.92	0.52
1:E:168:HIS:O	1:E:187:SER:HB2	2.09	0.52
1:J:168:HIS:HD2	1:J:187:SER:HB2	1.74	0.52
1:D:134:LEU:O	1:D:136:PRO:HD3	2.10	0.52
1:E:259:ILE:HD11	1:E:334:ARG:HD3	1.92	0.52
1:H:269:ASP:O	1:H:342:ILE:HA	2.09	0.52
1:I:123:LEU:HD11	1:I:221:PHE:CE2	2.43	0.52
1:X:143:LEU:HD11	1:X:229:LYS:HG2	1.92	0.52
1:H:220:LEU:HD13	1:H:243:LEU:CD2	2.40	0.52
1:A:266:MET:CE	1:A:339:LEU:HD22	2.36	0.51
1:D:235:ASP:O	1:D:236:SER:HB3	2.10	0.51
1:D:352:THR:HG22	1:H:283:PRO:HD3	1.92	0.51
1:F:231:TRP:CD1	1:F:232:GLY:HA2	2.45	0.51
1:G:297:LYS:CD	1:G:311:GLU:CA	2.87	0.51
1:I:75:SER:HA	1:I:378:GLU:OE1	2.10	0.51
1:J:265:PHE:CE2	1:J:331:PHE:CD2	2.98	0.51
1:X:263:GLU:HG2	1:X:379:TYR:OH	2.09	0.51
1:C:229:LYS:O	1:C:230:GLU:HG2	2.09	0.51
1:E:333:ARG:C	1:E:335:GLY:H	2.13	0.51
1:G:90:PRO:O	1:G:366:HIS:NE2	2.41	0.51
1:G:304:LEU:O	1:G:305:LEU:HD23	2.09	0.51
1:G:361:HIS:CE1	1:G:363:PRO:HB2	2.45	0.51
1:H:243:LEU:O	1:H:247:MET:HG3	2.10	0.51
1:X:137:PHE:CE1	1:X:148:PHE:HB2	2.45	0.51
1:B:120:GLU:OE2	1:B:134:LEU:HD13	2.10	0.51
1:G:76:LEU:HD12	1:G:77:PRO:HD2	1.92	0.51
1:G:324:VAL:HG23	1:G:340:HIS:NE2	2.26	0.51
1:I:106:THR:O	1:I:107:PRO:O	2.29	0.51
1:I:268:LEU:HG	1:I:341:LEU:HD23	1.93	0.51
1:A:138:THR:OG1	1:A:147:ASP:OD1	2.20	0.51
1:B:293:ARG:HH12	1:B:317:PRO:HB3	1.74	0.51
1:D:92:ARG:HG3	1:D:96:THR:HG21	1.93	0.51
1:E:77:PRO:HG2	1:E:80:ARG:NH2	2.25	0.51
1:E:219:LEU:O	1:E:220:LEU:HD23	2.10	0.51
1:I:201:LEU:O	1:I:205:LEU:HG	2.09	0.51
1:C:142:PRO:HB2	1:C:229:LYS:HG3	1.92	0.51
1:D:90:PRO:HB3	1:D:366:HIS:CD2	2.46	0.51
1:I:257:THR:OG1	1:I:260:GLN:OE1	2.16	0.51
1:J:291:ARG:O	1:J:295:ILE:HG13	2.11	0.51
1:F:120:GLU:O	1:F:124:ARG:HG3	2.11	0.51
1:H:191:CYS:O	1:H:193:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:184:ALA:CB	1:X:360:LEU:HD21	2.41	0.51
1:A:90:PRO:HB3	1:A:366:HIS:NE2	2.26	0.51
1:C:122:THR:O	1:C:125:SER:OG	2.26	0.51
1:I:299:LEU:HB3	1:I:304:LEU:HB2	1.92	0.51
1:C:94:TRP:CH2	1:C:362:PRO:HG3	2.46	0.51
1:D:283:PRO:O	1:D:284:ARG:C	2.48	0.51
1:H:81:LEU:HD12	1:H:374:VAL:HG11	1.92	0.51
1:H:107:PRO:HB2	1:H:146:VAL:HG11	1.91	0.51
1:H:168:HIS:CD2	1:H:187:SER:OG	2.64	0.51
1:H:190:PRO:HB3	1:H:268:LEU:HB3	1.92	0.51
1:I:294:SER:C	1:I:296:GLU:H	2.12	0.51
1:I:228:LEU:H	1:I:235:ASP:CG	2.14	0.51
1:I:352:THR:OG1	1:I:354:ALA:HB3	2.11	0.51
1:J:224:GLY:O	1:J:238:TYR:N	2.25	0.51
1:X:80:ARG:NH1	1:X:382:LEU:OXT	2.43	0.51
1:E:332:LEU:HA	1:E:336:VAL:H	1.76	0.51
1:J:298:ARG:HD3	1:J:299:LEU:N	2.20	0.51
1:A:73:ILE:O	1:A:73:ILE:HG23	2.11	0.50
1:D:80:ARG:O	1:D:84:VAL:HG23	2.11	0.50
1:D:297:LYS:HG2	1:D:312:VAL:CG2	2.40	0.50
1:E:141:THR:O	1:E:144:GLY:N	2.43	0.50
1:B:297:LYS:HZ2	1:B:300:HIS:CD2	2.29	0.50
1:B:354:ALA:O	1:B:359:ASN:ND2	2.44	0.50
1:E:234:LYS:N	1:E:234:LYS:HD3	2.21	0.50
1:F:92:ARG:NH1	1:F:199:GLN:HG2	2.26	0.50
1:I:107:PRO:O	1:I:112:ASN:HB2	2.11	0.50
1:B:297:LYS:CG	1:B:311:GLU:CG	2.87	0.50
1:G:120:GLU:HB3	1:G:124:ARG:HH11	1.76	0.50
1:G:142:PRO:C	1:G:144:GLY:N	2.65	0.50
1:G:184:ALA:HB3	1:G:360:LEU:HD21	1.94	0.50
1:H:187:SER:O	1:H:190:PRO:HG2	2.12	0.50
1:X:113:LEU:O	1:X:117:LYS:HG2	2.12	0.50
1:D:103:VAL:HG23	1:D:104:VAL:O	2.11	0.50
1:H:174:PHE:HD1	1:H:175:PRO:HD2	1.77	0.50
1:A:223:ASP:OD1	1:A:224:GLY:N	2.44	0.50
1:B:324:VAL:HG11	1:B:346:PHE:HZ	1.76	0.50
1:E:324:VAL:HG21	1:E:342:ILE:HD13	1.93	0.50
1:G:297:LYS:HD2	1:G:311:GLU:CB	2.40	0.50
1:J:146:VAL:HB	1:J:148:PHE:CZ	2.47	0.50
1:J:252:HIS:CG	1:J:253:SER:N	2.79	0.50
1:C:115:VAL:HG12	1:C:169:TYR:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ALA:O	1:E:252:HIS:NE2	2.37	0.50
1:E:297:LYS:HE2	1:E:311:GLU:O	2.11	0.50
1:F:253:SER:HA	1:F:254:PRO:O	2.12	0.50
1:F:306:GLN:HB2	1:F:363:PRO:HB3	1.93	0.50
1:G:228:LEU:N	1:G:235:ASP:OD1	2.30	0.50
1:G:248:GLU:OE1	1:G:334:ARG:HG2	2.12	0.50
1:G:304:LEU:HD12	1:G:370:ARG:NH1	2.21	0.50
1:H:75:SER:HA	1:H:378:GLU:HG2	1.92	0.50
1:J:168:HIS:CD2	1:J:187:SER:HB2	2.47	0.50
1:J:246:LEU:O	1:J:250:ILE:HG13	2.12	0.50
1:J:361:HIS:CE1	1:J:363:PRO:HG2	2.46	0.50
1:B:80:ARG:O	1:B:84:VAL:HG23	2.11	0.50
1:B:93:LEU:HD23	1:B:196:GLU:CB	2.41	0.50
1:G:313:MET:HE1	1:J:256:PRO:CD	2.42	0.50
1:C:235:ASP:HA	1:C:238:TYR:OH	2.12	0.50
1:F:81:LEU:HD12	1:F:298:ARG:HH21	1.76	0.50
1:F:194:LEU:HD21	1:F:268:LEU:HD22	1.93	0.50
1:H:146:VAL:HB	1:H:148:PHE:CE1	2.47	0.50
1:H:248:GLU:O	1:H:257:THR:HB	2.11	0.50
1:H:269:ASP:C	1:H:271:LEU:HD23	2.32	0.50
1:J:120:GLU:HB3	1:J:124:ARG:HH12	1.76	0.50
1:J:265:PHE:HB3	1:J:338:VAL:HG22	1.94	0.50
1:B:210:LYS:HZ2	1:C:211:GLN:HG2	1.74	0.49
1:D:82:ARG:NH2	1:D:302:LEU:HB3	2.27	0.49
1:E:361:HIS:CE1	1:E:363:PRO:HB2	2.47	0.49
1:E:361:HIS:HB3	1:E:364:THR:HB	1.94	0.49
1:H:109:SER:OG	1:H:112:ASN:HB2	2.12	0.49
1:X:291:ARG:HG2	1:X:291:ARG:HH11	1.77	0.49
1:B:92:ARG:HH21	1:B:196:GLU:CD	2.14	0.49
1:B:320:PRO:HB2	1:B:321:PHE:CD1	2.47	0.49
1:C:295:ILE:O	1:C:296:GLU:HB3	2.12	0.49
1:D:367:ASN:O	1:D:370:ARG:N	2.45	0.49
1:F:234:LYS:HA	1:F:241:ARG:NH1	2.26	0.49
1:G:359:ASN:OD1	1:J:333:ARG:CZ	2.59	0.49
1:H:101:LEU:HD12	1:H:101:LEU:H	1.77	0.49
1:H:297:LYS:HZ3	1:H:301:ARG:NE	2.03	0.49
1:J:112:ASN:O	1:J:116:ARG:CD	2.59	0.49
1:C:295:ILE:HG22	1:C:299:LEU:CD1	2.42	0.49
1:G:329:ILE:HB	1:G:330:PRO:HD3	1.94	0.49
1:G:350:TRP:O	1:G:352:THR:HG23	2.12	0.49
1:H:141:THR:O	1:H:144:GLY:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:ARG:NH2	1:H:378:GLU:HB3	2.28	0.49
1:I:331:PHE:O	1:I:334:ARG:N	2.40	0.49
1:J:82:ARG:HH21	1:J:302:LEU:HB2	1.78	0.49
1:J:89:ASP:OD1	1:J:91:GLN:HB3	2.12	0.49
1:J:265:PHE:HE1	1:J:267:LEU:HD13	1.77	0.49
1:J:296:GLU:OE2	1:J:313:MET:N	2.26	0.49
1:H:350:TRP:HH2	3:H:402:A1D46:O06	1.94	0.49
1:I:229:LYS:N	1:I:235:ASP:OD2	2.44	0.49
1:I:296:GLU:HG3	1:I:371:ILE:CD1	2.43	0.49
1:J:106:THR:O	1:J:109:SER:HB3	2.13	0.49
1:A:89:ASP:HB3	1:A:92:ARG:CB	2.42	0.49
1:B:156:ASP:OD1	1:B:158:ARG:HG2	2.12	0.49
1:B:165:LEU:HD23	1:B:266:MET:HB3	1.94	0.49
1:G:155:LEU:HD21	1:G:205:LEU:HB3	1.94	0.49
1:I:134:LEU:HG	1:I:135:ASP:N	2.27	0.49
1:I:168:HIS:CD2	1:I:225:GLU:OE1	2.66	0.49
1:I:280:SER:HB2	1:I:289:PHE:CD2	2.48	0.49
1:J:75:SER:CA	1:J:291:ARG:HH22	2.25	0.49
1:X:270:LEU:HD12	1:X:346:PHE:CD1	2.46	0.49
1:D:119:LEU:CD2	1:D:195:LEU:HD11	2.43	0.49
1:G:267:LEU:HD23	1:G:340:HIS:CE1	2.47	0.49
1:I:295:ILE:O	1:I:295:ILE:HG22	2.12	0.49
1:J:297:LYS:CG	1:J:298:ARG:CA	2.85	0.49
1:H:297:LYS:HZ3	1:H:301:ARG:HE	1.51	0.49
1:I:156:ASP:HA	1:I:209:LYS:HZ2	1.77	0.49
1:J:84:VAL:HG12	1:J:373:ALA:HB1	1.93	0.49
1:J:113:LEU:HA	1:J:116:ARG:HB2	1.95	0.49
1:J:187:SER:HB3	1:J:190:PRO:CG	2.38	0.49
1:F:166:ALA:O	1:F:267:LEU:HD12	2.13	0.49
1:F:237:LEU:HD22	1:F:327:ASP:HA	1.95	0.49
1:H:76:LEU:HD23	1:H:76:LEU:H	1.77	0.49
1:H:162:HIS:HB3	1:H:216:THR:HG22	1.94	0.49
1:H:176:PRO:O	1:H:178:SER:N	2.45	0.49
1:J:160:ALA:HA	1:J:253:SER:O	2.13	0.49
1:X:90:PRO:HB3	1:X:366:HIS:CD2	2.48	0.49
1:X:142:PRO:O	1:A:251:PRO:HG2	2.11	0.49
1:C:106:THR:O	1:C:112:ASN:HB2	2.12	0.49
1:F:88:LEU:O	1:F:90:PRO:HD3	2.11	0.49
1:G:308:HIS:NE2	1:G:313:MET:HB2	2.28	0.49
1:I:284:ARG:O	1:I:284:ARG:HG2	2.13	0.49
1:J:104:VAL:HG21	1:J:180:PRO:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LYS:CE	1:B:301:ARG:CB	2.91	0.49
1:J:340:HIS:O	1:J:342:ILE:HG22	2.13	0.49
1:A:293:ARG:HG3	1:A:315:PHE:O	2.13	0.48
1:D:234:LYS:HA	1:D:234:LYS:HD2	1.52	0.48
1:D:296:GLU:O	1:D:297:LYS:C	2.51	0.48
1:E:70:VAL:HG12	1:E:71:PRO:HD2	1.94	0.48
1:F:85:VAL:HG11	1:F:304:LEU:HD22	1.94	0.48
1:G:266:MET:HE1	1:G:375:PHE:CE1	2.47	0.48
1:H:168:HIS:NE2	1:H:187:SER:OG	2.45	0.48
1:H:204:GLU:HB3	1:H:382:LEU:HD22	1.95	0.48
1:H:350:TRP:CH2	3:H:402:A1D46:O06	2.66	0.48
1:J:295:ILE:O	1:J:295:ILE:HG22	2.12	0.48
1:B:284:ARG:O	1:B:284:ARG:HG3	2.11	0.48
1:B:304:LEU:O	1:B:370:ARG:NH1	2.46	0.48
1:F:163:LEU:HD22	1:F:379:TYR:CD1	2.47	0.48
1:G:300:HIS:NE2	1:G:309:PRO:O	2.43	0.48
1:I:194:LEU:HB3	1:I:219:LEU:HD22	1.95	0.48
1:X:155:LEU:CD2	1:X:205:LEU:HB3	2.43	0.48
1:E:250:ILE:HG21	1:E:258:ARG:HH21	1.78	0.48
1:J:83:ARG:HH22	1:J:204:GLU:HG3	1.78	0.48
1:J:264:LEU:HG	1:J:265:PHE:N	2.29	0.48
1:J:291:ARG:O	1:J:294:SER:OG	2.17	0.48
1:J:299:LEU:C	1:J:301:ARG:H	2.14	0.48
1:A:360:LEU:O	1:A:362:PRO:HD3	2.14	0.48
1:B:259:ILE:O	1:B:262:ILE:HD12	2.13	0.48
1:I:283:PRO:O	1:I:285:THR:N	2.46	0.48
1:B:83:ARG:O	1:B:87:GLN:HG3	2.13	0.48
1:B:297:LYS:HG2	1:B:300:HIS:CD2	2.29	0.48
1:C:298:ARG:O	1:C:299:LEU:C	2.50	0.48
1:D:367:ASN:O	1:D:370:ARG:HB2	2.13	0.48
1:F:172:LYS:HE2	3:F:402:A1D46:C15	2.44	0.48
1:F:187:SER:CB	1:F:190:PRO:HG2	2.43	0.48
1:X:352:THR:HB	1:X:353:PRO:HD2	1.95	0.48
1:B:115:VAL:O	1:B:118:PHE:HB3	2.14	0.48
1:B:319:GLU:N	1:B:320:PRO:CD	2.77	0.48
1:D:300:HIS:CE1	1:D:311:GLU:HA	2.48	0.48
1:E:154:THR:HG21	1:E:157:PRO:HA	1.94	0.48
1:F:116:ARG:CZ	1:F:149:GLY:HA3	2.42	0.48
1:G:291:ARG:NE	1:G:295:ILE:HD11	2.29	0.48
1:H:218:GLN:OE1	1:H:220:LEU:HD21	2.14	0.48
1:J:297:LYS:HE2	1:J:301:ARG:NH2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:329:ILE:HB	1:J:330:PRO:HD3	1.94	0.48
1:B:99:ARG:HH11	1:B:357:GLU:CD	2.17	0.48
1:B:139:ALA:HB3	1:B:148:PHE:HE2	1.77	0.48
1:F:152:VAL:HG13	1:F:220:LEU:CD2	2.43	0.48
1:G:123:LEU:HD13	1:G:153:ALA:HB2	1.95	0.48
1:G:142:PRO:O	1:G:144:GLY:N	2.47	0.48
1:G:279:TYR:CE1	1:G:316:GLN:HB2	2.48	0.48
1:H:96:THR:O	1:H:100:PRO:HG2	2.14	0.48
1:H:187:SER:HB3	1:H:190:PRO:CG	2.44	0.48
1:H:269:ASP:O	1:H:271:LEU:HD23	2.14	0.48
1:A:298:ARG:O	1:A:301:ARG:N	2.47	0.48
1:C:284:ARG:NH1	1:C:337:PRO:HG3	2.29	0.48
1:D:149:GLY:O	1:D:223:ASP:HB2	2.14	0.48
1:G:189:VAL:HB	1:G:271:LEU:O	2.13	0.48
1:G:285:THR:HG21	1:G:338:VAL:O	2.14	0.48
1:H:103:VAL:O	1:H:105:ARG:HD3	2.13	0.48
1:J:151:VAL:HG13	1:J:221:PHE:HD1	1.76	0.48
1:J:189:VAL:HG21	1:J:360:LEU:HD13	1.95	0.48
1:X:225:GLU:HG2	1:X:237:LEU:HD23	1.95	0.48
1:A:380:LEU:HB3	1:A:382:LEU:HD21	1.96	0.48
1:E:199:GLN:O	1:E:202:ASP:HB2	2.13	0.48
1:E:297:LYS:CA	1:E:298:ARG:C	2.74	0.48
1:F:81:LEU:O	1:F:85:VAL:HG23	2.13	0.48
1:H:174:PHE:HD2	1:H:181:PHE:CD2	2.32	0.48
1:I:295:ILE:O	1:I:299:LEU:CD1	2.62	0.48
1:A:248:GLU:OE1	1:A:334:ARG:HG2	2.14	0.48
1:D:266:MET:HE3	1:D:339:LEU:HD13	1.96	0.48
1:H:236:SER:O	1:H:241:ARG:NH1	2.47	0.48
1:A:359:ASN:OD1	1:F:333:ARG:HD2	2.14	0.47
1:B:179:THR:HB	1:B:353:PRO:HB2	1.96	0.47
1:C:148:PHE:CD1	1:C:148:PHE:N	2.82	0.47
1:F:94:TRP:O	1:F:98:LEU:HB3	2.14	0.47
1:G:256:PRO:CB	1:H:309:PRO:HG3	2.42	0.47
1:H:168:HIS:ND1	1:H:225:GLU:HB3	2.29	0.47
1:H:299:LEU:HB3	1:H:305:LEU:HG	1.95	0.47
1:J:244:ALA:HB1	1:J:334:ARG:NH1	2.29	0.47
1:J:267:LEU:CD2	1:J:328:HIS:HD2	2.27	0.47
1:J:297:LYS:NZ	1:J:301:ARG:CZ	2.28	0.47
1:A:304:LEU:HB3	1:A:370:ARG:NH1	2.29	0.47
1:B:70:VAL:HG21	1:B:301:ARG:CD	2.43	0.47
1:B:179:THR:HG22	1:B:180:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:LYS:HD3	1:E:305:LEU:HD12	1.95	0.47
1:F:72:LEU:HG	1:F:291:ARG:NH2	2.29	0.47
1:F:296:GLU:O	1:F:297:LYS:C	2.52	0.47
1:G:250:ILE:HB	1:G:258:ARG:HG3	1.96	0.47
1:J:123:LEU:O	1:J:126:LEU:N	2.47	0.47
1:J:260:GLN:OE1	1:J:260:GLN:N	2.46	0.47
1:X:220:LEU:HD13	1:X:243:LEU:HD23	1.97	0.47
1:D:361:HIS:CD2	1:D:363:PRO:HD2	2.49	0.47
1:F:134:LEU:C	1:F:136:PRO:HD3	2.34	0.47
1:G:71:PRO:HB3	1:G:298:ARG:CD	2.44	0.47
1:G:103:VAL:C	1:G:182:VAL:HG12	2.35	0.47
1:H:105:ARG:HB2	1:H:112:ASN:HA	1.95	0.47
1:J:299:LEU:HD11	1:J:371:ILE:HG12	1.96	0.47
1:X:101:LEU:O	1:X:103:VAL:N	2.46	0.47
1:B:162:HIS:HB3	1:B:216:THR:HG22	1.97	0.47
1:E:80:ARG:O	1:E:83:ARG:HB3	2.14	0.47
1:G:172:LYS:HD2	1:G:351:HIS:CE1	2.48	0.47
1:H:227:ALA:HB1	1:H:230:GLU:HA	1.96	0.47
1:H:240:SER:C	1:H:242:HIS:N	2.67	0.47
1:H:298:ARG:HG3	1:H:302:LEU:HG	1.96	0.47
1:I:167:CYS:O	1:I:168:HIS:HB3	2.15	0.47
1:J:332:LEU:HD11	1:J:338:VAL:HB	1.95	0.47
1:X:184:ALA:HB1	1:X:360:LEU:HD21	1.95	0.47
1:A:291:ARG:HH21	1:A:378:GLU:HB3	1.78	0.47
1:F:273:ALA:HB1	1:F:274:PRO:HD2	1.97	0.47
1:G:314:TYR:OH	1:G:367:ASN:ND2	2.35	0.47
1:H:97:TYR:O	1:H:101:LEU:CD1	2.63	0.47
3:B:402:A1D46:O01	3:B:402:A1D46:C27	2.63	0.47
1:H:165:LEU:HB2	1:H:219:LEU:HD23	1.96	0.47
1:I:285:THR:O	1:I:287:ARG:N	2.48	0.47
1:I:292:LEU:HA	1:I:295:ILE:HD13	0.96	0.47
1:X:341:LEU:HD12	1:X:341:LEU:HA	1.79	0.47
1:B:300:HIS:HB2	1:B:305:LEU:HD12	1.96	0.47
1:C:269:ASP:OD2	1:C:326:ASP:OD2	2.33	0.47
1:E:71:PRO:HB2	1:E:75:SER:HB3	1.97	0.47
1:H:83:ARG:NH2	1:H:204:GLU:OE2	2.33	0.47
1:H:179:THR:O	1:H:180:PRO:O	2.31	0.47
1:H:245:GLN:O	1:H:248:GLU:HB3	2.14	0.47
1:H:298:ARG:HG3	1:H:302:LEU:CG	2.45	0.47
1:H:334:ARG:HH11	1:H:334:ARG:HG3	1.80	0.47
1:H:354:ALA:O	1:H:356:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:ASP:OD2	1:I:158:ARG:HG2	2.15	0.47
1:J:88:LEU:HD22	1:J:196:GLU:HG3	1.97	0.47
1:J:116:ARG:NH2	1:J:223:ASP:OD2	2.47	0.47
1:J:207:ARG:HB3	1:J:211:GLN:HE22	1.79	0.47
1:J:299:LEU:O	1:J:302:LEU:N	2.48	0.47
3:A:402:A1D46:C27	3:A:402:A1D46:C02	2.93	0.47
1:C:148:PHE:CZ	1:C:238:TYR:CD2	3.02	0.47
1:H:297:LYS:CA	1:H:298:ARG:C	2.82	0.47
1:J:297:LYS:CE	1:J:301:ARG:CD	2.87	0.47
1:J:297:LYS:CD	1:J:298:ARG:HA	2.45	0.47
1:X:235:ASP:O	1:X:236:SER:HB3	2.15	0.47
1:A:300:HIS:ND1	1:A:311:GLU:HA	2.29	0.47
1:B:99:ARG:HB3	1:B:100:PRO:HD3	1.96	0.47
1:C:156:ASP:HB2	1:C:209:LYS:HG3	1.97	0.47
1:D:123:LEU:HD13	1:D:153:ALA:HB2	1.97	0.47
1:D:352:THR:HB	1:D:353:PRO:HD2	1.96	0.47
1:F:101:LEU:O	1:F:105:ARG:NH1	2.48	0.47
1:F:141:THR:HG22	1:F:238:TYR:CE1	2.50	0.47
1:F:253:SER:HA	1:F:254:PRO:C	2.34	0.47
1:G:292:LEU:HA	1:G:295:ILE:HB	1.96	0.47
1:H:193:LEU:HD23	1:H:193:LEU:HA	1.71	0.47
1:H:309:PRO:HD2	1:H:313:MET:SD	2.55	0.47
1:I:163:LEU:CD1	1:I:264:LEU:HB3	2.44	0.47
1:I:204:GLU:HB3	1:I:382:LEU:HB3	1.95	0.47
1:X:187:SER:C	1:X:190:PRO:HD2	2.36	0.47
1:G:95:SER:O	1:G:100:PRO:HD3	2.15	0.47
1:G:83:ARG:O	1:G:87:GLN:OE1	2.33	0.46
1:G:156:ASP:CG	1:G:158:ARG:HE	2.16	0.46
1:G:293:ARG:O	1:G:296:GLU:N	2.44	0.46
1:I:139:ALA:O	1:I:145:PRO:HA	2.15	0.46
1:J:146:VAL:HB	1:J:148:PHE:CE1	2.49	0.46
1:J:297:LYS:HB3	1:J:298:ARG:CA	2.45	0.46
1:X:315:PHE:HE2	1:X:341:LEU:HD11	1.80	0.46
1:D:130:TRP:CE3	1:D:153:ALA:HB1	2.50	0.46
1:G:77:PRO:HG2	1:G:80:ARG:CB	2.44	0.46
1:H:172:LYS:HB3	1:H:181:PHE:CE2	2.49	0.46
1:J:298:ARG:N	1:J:300:HIS:HB3	2.29	0.46
1:X:193:LEU:O	1:X:197:LEU:HG	2.15	0.46
1:D:211:GLN:O	1:D:212:ALA:C	2.53	0.46
1:H:176:PRO:C	1:H:178:SER:H	2.17	0.46
1:J:248:GLU:HB2	1:J:259:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:O	1:B:206:SER:N	2.49	0.46
1:C:99:ARG:HB3	1:C:100:PRO:HD3	1.96	0.46
1:D:85:VAL:CG1	1:D:370:ARG:NH1	2.79	0.46
1:E:375:PHE:CD1	1:E:375:PHE:C	2.89	0.46
1:F:116:ARG:HD3	1:F:134:LEU:HD21	1.98	0.46
1:H:88:LEU:HA	1:H:196:GLU:OE2	2.15	0.46
1:I:185:THR:HG23	1:I:355:ASP:OD1	2.15	0.46
1:I:344:THR:O	1:I:344:THR:OG1	2.33	0.46
1:J:75:SER:O	1:J:76:LEU:HD23	2.16	0.46
1:A:297:LYS:O	1:A:297:LYS:HD2	2.15	0.46
1:C:137:PHE:CE1	1:C:148:PHE:HB2	2.50	0.46
1:I:76:LEU:HB2	1:I:77:PRO:HD2	1.98	0.46
1:I:255:GLY:HA3	1:I:256:PRO:C	2.35	0.46
1:J:297:LYS:HG2	1:J:298:ARG:N	2.29	0.46
1:B:376:LEU:HA	1:B:376:LEU:HD23	1.59	0.46
1:D:255:GLY:HA3	1:D:256:PRO:C	2.36	0.46
1:F:135:ASP:OD2	1:F:242:HIS:HD2	1.98	0.46
1:J:120:GLU:O	1:J:124:ARG:NH1	2.49	0.46
1:J:271:LEU:HD21	1:J:341:LEU:HG	1.97	0.46
1:B:224:GLY:HA3	1:B:238:TYR:HB2	1.98	0.46
1:D:80:ARG:NH1	1:D:382:LEU:OXT	2.49	0.46
1:E:333:ARG:HA	1:E:333:ARG:HD3	1.71	0.46
1:F:91:GLN:OE1	1:F:91:GLN:HA	2.16	0.46
1:F:357:GLU:HA	1:F:360:LEU:CD1	2.46	0.46
1:H:224:GLY:O	1:H:238:TYR:HD1	1.99	0.46
1:H:298:ARG:HG3	1:H:302:LEU:HD11	1.96	0.46
1:I:163:LEU:O	1:I:217:LEU:HD12	2.15	0.46
1:A:275:ASN:N	1:A:275:ASN:HD22	2.14	0.46
1:B:99:ARG:O	1:B:101:LEU:N	2.49	0.46
1:D:289:PHE:HA	1:D:292:LEU:HD12	1.98	0.46
1:J:88:LEU:HD21	1:J:197:LEU:HD23	1.97	0.46
1:B:253:SER:HA	1:B:254:PRO:C	2.35	0.46
1:E:172:LYS:HB3	1:E:181:PHE:CE2	2.51	0.46
3:E:402:A1D46:C27	3:E:402:A1D46:O01	2.64	0.46
1:F:119:LEU:CD2	1:F:195:LEU:HD11	2.45	0.46
1:G:205:LEU:O	1:G:207:ARG:N	2.49	0.46
1:H:372:LEU:O	1:H:376:LEU:HG	2.16	0.46
1:X:99:ARG:HA	1:X:102:LEU:HD12	1.97	0.46
1:X:269:ASP:HB3	1:X:342:ILE:HG13	1.97	0.46
1:B:107:PRO:HG2	1:B:228:LEU:HD21	1.98	0.46
1:F:139:ALA:O	1:F:145:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:TRP:HD1	1:J:98:LEU:HD23	1.81	0.46
1:C:123:LEU:HD13	1:C:153:ALA:HB2	1.98	0.45
1:C:166:ALA:O	1:C:267:LEU:HD12	2.16	0.45
1:D:165:LEU:HD23	1:D:266:MET:HB3	1.97	0.45
1:E:232:GLY:O	1:E:235:ASP:N	2.35	0.45
1:F:160:ALA:HB1	1:F:254:PRO:CD	2.46	0.45
1:G:207:ARG:O	1:G:210:LYS:N	2.41	0.45
1:H:106:THR:HG21	1:H:173:LEU:HA	1.97	0.45
1:J:126:LEU:HD23	1:J:126:LEU:HA	1.68	0.45
1:B:184:ALA:HB1	1:B:360:LEU:HD11	1.98	0.45
1:B:274:PRO:HD3	1:B:361:HIS:HB2	1.98	0.45
1:D:305:LEU:HB3	1:D:367:ASN:ND2	2.31	0.45
1:E:127:THR:O	1:E:129:GLY:N	2.48	0.45
1:E:297:LYS:HB2	1:E:297:LYS:HE3	1.68	0.45
1:F:92:ARG:HG2	1:F:97:TYR:CE2	2.51	0.45
1:H:354:ALA:O	1:H:359:ASN:ND2	2.49	0.45
1:J:99:ARG:HD3	1:J:102:LEU:HD13	1.97	0.45
1:J:101:LEU:HD22	1:J:115:VAL:CG1	2.47	0.45
1:X:243:LEU:HD12	1:X:243:LEU:HA	1.73	0.45
1:X:287:ARG:O	1:X:290:HIS:HB2	2.17	0.45
1:B:70:VAL:CA	1:B:298:ARG:HG2	2.45	0.45
1:B:374:VAL:O	1:B:377:ALA:N	2.48	0.45
1:C:292:LEU:HG	1:C:375:PHE:CD2	2.51	0.45
1:F:249:SER:O	1:F:251:PRO:HD3	2.16	0.45
1:G:291:ARG:CA	1:G:295:ILE:HD13	2.46	0.45
1:J:296:GLU:CA	1:J:297:LYS:C	2.81	0.45
1:G:294:SER:O	1:G:298:ARG:CB	2.62	0.45
1:G:328:HIS:ND1	1:G:329:ILE:N	2.64	0.45
1:H:298:ARG:HG3	1:H:302:LEU:CD1	2.47	0.45
1:I:81:LEU:O	1:I:84:VAL:HB	2.16	0.45
1:J:168:HIS:NE2	1:J:187:SER:N	2.65	0.45
1:J:263:GLU:O	1:J:337:PRO:HG2	2.17	0.45
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.62	0.45
1:C:222:LEU:HD13	1:C:240:SER:HB3	1.98	0.45
1:D:96:THR:O	1:D:100:PRO:HG3	2.16	0.45
1:D:283:PRO:O	1:D:286:VAL:N	2.22	0.45
1:D:304:LEU:O	1:D:305:LEU:HD23	2.16	0.45
1:E:298:ARG:HA	1:E:301:ARG:HB2	1.97	0.45
1:F:250:ILE:HG22	1:F:258:ARG:HG3	1.98	0.45
1:G:80:ARG:NH1	1:G:84:VAL:CG2	2.80	0.45
1:H:127:THR:C	1:H:129:GLY:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:269:ASP:HB3	1:H:342:ILE:HG13	1.98	0.45
1:A:270:LEU:HB2	1:A:342:ILE:HG13	1.98	0.45
1:D:93:LEU:CD2	1:D:196:GLU:HB2	2.46	0.45
1:F:76:LEU:HD22	1:F:80:ARG:HD2	1.98	0.45
1:F:80:ARG:O	1:F:84:VAL:HG23	2.16	0.45
1:G:359:ASN:OD1	1:J:333:ARG:NH2	2.49	0.45
1:H:179:THR:HG22	1:H:180:PRO:CD	2.44	0.45
1:I:116:ARG:NH2	1:I:148:PHE:O	2.49	0.45
1:X:274:PRO:HB3	1:X:361:HIS:HB2	1.98	0.45
1:A:350:TRP:O	1:A:352:THR:HG23	2.17	0.45
1:D:235:ASP:HA	1:D:238:TYR:OH	2.17	0.45
1:G:296:GLU:CG	1:G:297:LYS:N	2.78	0.45
1:I:89:ASP:HB3	1:I:92:ARG:HB3	1.98	0.45
1:J:270:LEU:HD13	1:J:347:PRO:HD2	1.97	0.45
1:X:207:ARG:NH2	1:I:145:PRO:O	2.49	0.45
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.17	0.45
1:B:240:SER:O	1:B:241:ARG:C	2.54	0.45
1:D:245:GLN:OE1	1:D:245:GLN:HA	2.17	0.45
1:E:235:ASP:HA	1:E:238:TYR:OH	2.17	0.45
1:E:264:LEU:HD12	1:E:264:LEU:HA	1.78	0.45
1:F:231:TRP:HD1	1:F:232:GLY:HA2	1.82	0.45
1:G:82:ARG:NH2	1:G:302:LEU:HB3	2.31	0.45
1:F:90:PRO:O	1:F:93:LEU:HB3	2.16	0.45
1:F:293:ARG:HH12	1:F:317:PRO:HB3	1.82	0.45
1:H:162:HIS:HB3	1:H:216:THR:CG2	2.47	0.45
1:I:184:ALA:HA	1:I:188:ALA:HB3	1.99	0.45
1:I:230:GLU:N	1:I:235:ASP:OD2	2.50	0.45
1:I:296:GLU:HB3	1:I:297:LYS:H	1.60	0.45
1:I:328:HIS:CE1	1:I:340:HIS:CD2	3.05	0.45
1:X:110:PRO:C	1:X:114:GLN:HE22	2.21	0.45
1:A:120:GLU:HG2	1:A:132:VAL:HG11	1.99	0.45
1:B:120:GLU:O	1:B:124:ARG:HG3	2.16	0.45
1:F:187:SER:HB3	1:F:190:PRO:HG2	1.98	0.45
1:G:204:GLU:HB3	1:G:382:LEU:HD13	1.98	0.45
1:G:352:THR:C	1:G:354:ALA:N	2.67	0.45
1:H:297:LYS:CD	1:H:311:GLU:CG	2.94	0.45
1:I:113:LEU:O	1:I:117:LYS:HG2	2.17	0.45
1:F:139:ALA:HB3	1:F:148:PHE:CE1	2.52	0.44
1:F:204:GLU:HG2	1:F:382:LEU:O	2.17	0.44
1:G:88:LEU:HD13	1:G:369:CYS:SG	2.57	0.44
1:H:134:LEU:HD23	1:H:135:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:ASP:O	1:H:158:ARG:N	2.44	0.44
1:I:138:THR:HA	1:I:146:VAL:O	2.18	0.44
1:J:294:SER:C	1:J:296:GLU:N	2.70	0.44
1:X:329:ILE:HB	1:X:330:PRO:HD3	1.98	0.44
1:A:80:ARG:O	1:A:84:VAL:HG23	2.17	0.44
1:D:374:VAL:O	1:D:377:ALA:N	2.50	0.44
1:E:168:HIS:CE1	1:E:187:SER:HG	2.33	0.44
1:H:264:LEU:HD12	1:H:265:PHE:N	2.32	0.44
1:I:352:THR:C	1:I:354:ALA:N	2.70	0.44
1:J:139:ALA:O	1:J:141:THR:HG23	2.17	0.44
1:J:205:LEU:O	1:J:208:ALA:N	2.49	0.44
1:A:232:GLY:O	1:A:234:LYS:N	2.50	0.44
1:C:223:ASP:O	1:C:239:GLY:HA3	2.17	0.44
1:D:81:LEU:O	1:D:84:VAL:N	2.49	0.44
1:E:83:ARG:NH2	1:E:204:GLU:OE2	2.47	0.44
1:G:233:PRO:HG3	1:G:236:SER:OG	2.18	0.44
1:X:331:PHE:O	1:X:336:VAL:HG23	2.17	0.44
1:B:156:ASP:O	1:B:216:THR:HG21	2.18	0.44
1:B:297:LYS:HD3	1:B:300:HIS:CA	2.47	0.44
1:C:329:ILE:HG23	1:C:333:ARG:HE	1.82	0.44
1:D:93:LEU:HD22	1:D:93:LEU:HA	1.79	0.44
1:J:96:THR:HG22	1:J:97:TYR:CE1	2.53	0.44
1:X:179:THR:O	1:X:180:PRO:C	2.53	0.44
1:A:207:ARG:O	1:A:210:LYS:N	2.51	0.44
1:B:325:GLU:HG2	1:B:329:ILE:HG13	1.98	0.44
1:C:142:PRO:C	1:C:144:GLY:N	2.70	0.44
1:C:321:PHE:O	1:C:322:GLY:O	2.36	0.44
1:D:292:LEU:HD22	1:D:315:PHE:CZ	2.53	0.44
1:E:164:THR:HB	1:E:262:ILE:HG23	1.99	0.44
1:G:84:VAL:HA	1:G:87:GLN:OE1	2.17	0.44
1:H:218:GLN:CD	1:H:220:LEU:HD21	2.37	0.44
1:I:161:ARG:HB2	1:I:215:VAL:HG12	1.99	0.44
1:I:276:PRO:HD3	1:I:364:THR:HG21	1.98	0.44
1:I:296:GLU:HG3	1:I:371:ILE:HD11	2.00	0.44
1:A:233:PRO:O	1:A:234:LYS:HD2	2.17	0.44
1:C:237:LEU:HD22	1:C:327:ASP:HA	1.99	0.44
1:D:252:HIS:HB2	1:D:258:ARG:HG2	2.00	0.44
1:D:293:ARG:HH12	1:D:317:PRO:HB3	1.83	0.44
1:D:301:ARG:O	1:D:303:ASN:N	2.51	0.44
1:E:117:LYS:HD2	1:E:117:LYS:HA	1.76	0.44
1:E:269:ASP:O	1:E:342:ILE:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:LEU:HD12	1:F:267:LEU:HA	1.75	0.44
1:F:354:ALA:O	1:F:356:THR:HG23	2.17	0.44
1:G:70:VAL:HG12	1:G:71:PRO:CD	2.38	0.44
1:G:349:VAL:O	1:G:355:ASP:HB2	2.18	0.44
1:H:93:LEU:HD23	1:H:196:GLU:HB2	1.98	0.44
1:I:220:LEU:O	1:I:221:PHE:CD1	2.70	0.44
1:J:163:LEU:O	1:J:218:GLN:N	2.50	0.44
1:X:193:LEU:HD23	1:X:193:LEU:HA	1.79	0.44
1:C:291:ARG:O	1:C:294:SER:HB3	2.17	0.44
1:E:70:VAL:HG21	1:E:301:ARG:HD2	1.98	0.44
1:E:105:ARG:HG3	1:E:171:SER:N	2.32	0.44
1:E:211:GLN:O	1:E:213:ALA:N	2.51	0.44
1:E:326:ASP:HB3	1:E:328:HIS:CE1	2.53	0.44
1:F:182:VAL:HG23	1:F:355:ASP:O	2.17	0.44
1:G:142:PRO:HD2	1:G:235:ASP:OD2	2.17	0.44
1:G:227:ALA:HB2	1:G:231:TRP:CE3	2.50	0.44
1:H:162:HIS:CE1	1:H:262:ILE:HG12	2.51	0.44
1:H:163:LEU:HD22	1:H:379:TYR:CD1	2.52	0.44
1:I:115:VAL:HG12	1:I:169:TYR:HD2	1.82	0.44
1:J:291:ARG:CZ	1:J:378:GLU:OE1	2.65	0.44
1:A:330:PRO:O	1:A:334:ARG:NH1	2.49	0.44
1:D:103:VAL:O	1:D:182:VAL:HG12	2.17	0.44
1:D:291:ARG:O	1:D:295:ILE:N	2.49	0.44
1:E:89:ASP:HB3	1:E:92:ARG:HB3	2.00	0.44
1:F:155:LEU:HD22	1:F:205:LEU:HD13	1.99	0.44
1:G:352:THR:CG2	1:J:283:PRO:HD3	2.48	0.44
1:I:107:PRO:HA	1:I:112:ASN:OD1	2.17	0.44
1:B:102:LEU:HD13	1:B:357:GLU:HB2	1.99	0.44
1:F:179:THR:HG22	1:F:180:PRO:HD2	1.99	0.44
1:F:199:GLN:O	1:F:202:ASP:HB2	2.17	0.44
1:G:120:GLU:OE2	1:G:134:LEU:HD21	2.18	0.44
1:H:279:TYR:HE1	1:H:316:GLN:HB2	1.81	0.44
1:I:292:LEU:C	1:I:295:ILE:HD13	1.78	0.44
1:J:99:ARG:C	1:J:101:LEU:H	2.21	0.44
1:J:306:GLN:O	1:J:367:ASN:ND2	2.41	0.44
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.89	0.43
1:B:185:THR:O	1:B:270:LEU:HA	2.17	0.43
1:D:301:ARG:C	1:D:303:ASN:H	2.21	0.43
1:E:161:ARG:HD2	1:E:260:GLN:O	2.18	0.43
1:G:267:LEU:CD2	1:G:328:HIS:HD2	2.31	0.43
1:I:370:ARG:O	1:I:373:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:151:VAL:CG1	1:J:221:PHE:HB2	2.48	0.43
1:J:237:LEU:O	1:J:241:ARG:HB2	2.19	0.43
1:J:272:GLY:O	1:J:360:LEU:HD22	2.19	0.43
1:X:156:ASP:HB2	1:X:209:LYS:HD2	2.00	0.43
1:A:155:LEU:CD2	1:A:205:LEU:HB3	2.47	0.43
1:A:280:SER:O	1:A:320:PRO:HD2	2.18	0.43
1:C:269:ASP:HB3	1:C:342:ILE:HG13	2.00	0.43
3:C:402:A1D46:C27	3:C:402:A1D46:O01	2.65	0.43
1:E:105:ARG:HG3	1:E:171:SER:H	1.83	0.43
1:F:156:ASP:HB2	1:F:216:THR:OG1	2.18	0.43
1:F:158:ARG:HD3	1:F:158:ARG:H	1.82	0.43
1:H:174:PHE:CD2	1:H:181:PHE:HD2	2.36	0.43
1:H:360:LEU:O	1:H:362:PRO:HD3	2.19	0.43
1:I:265:PHE:HB2	1:I:336:VAL:CG1	2.48	0.43
1:I:265:PHE:O	1:I:338:VAL:HA	2.18	0.43
1:X:231:TRP:CZ3	1:X:236:SER:HB2	2.52	0.43
1:A:352:THR:OG1	1:A:354:ALA:HB3	2.18	0.43
1:C:283:PRO:O	1:C:286:VAL:HG12	2.18	0.43
1:D:296:GLU:C	1:D:298:ARG:N	2.71	0.43
1:H:275:ASN:N	1:H:276:PRO:HD3	2.33	0.43
1:H:299:LEU:O	1:H:304:LEU:N	2.26	0.43
1:I:70:VAL:N	1:I:71:PRO:CD	2.81	0.43
1:I:82:ARG:NH2	1:I:302:LEU:HD23	2.24	0.43
1:I:227:ALA:HB1	1:I:230:GLU:CA	2.42	0.43
1:I:267:LEU:O	1:I:341:LEU:HB3	2.18	0.43
1:J:111:GLY:O	1:J:115:VAL:HG23	2.19	0.43
1:J:205:LEU:C	1:J:207:ARG:N	2.71	0.43
1:J:367:ASN:O	1:J:371:ILE:HG13	2.17	0.43
1:X:333:ARG:HA	1:C:359:ASN:OD1	2.18	0.43
1:B:300:HIS:O	1:B:303:ASN:N	2.51	0.43
1:G:220:LEU:HD13	1:G:243:LEU:CD2	2.47	0.43
1:H:80:ARG:CG	1:H:83:ARG:HH12	2.31	0.43
1:J:82:ARG:NH2	1:J:302:LEU:HB2	2.34	0.43
1:J:243:LEU:O	1:J:247:MET:HG3	2.18	0.43
1:J:252:HIS:CG	1:J:253:SER:H	2.36	0.43
1:A:156:ASP:HB2	1:A:209:LYS:HG3	1.99	0.43
1:B:94:TRP:CH2	1:B:362:PRO:HG3	2.53	0.43
1:B:174:PHE:O	1:B:175:PRO:C	2.56	0.43
1:C:295:ILE:O	1:C:296:GLU:CB	2.66	0.43
1:D:232:GLY:O	1:D:234:LYS:N	2.51	0.43
1:D:284:ARG:NH2	1:D:337:PRO:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:PRO:HB2	1:H:118:PHE:CE2	2.53	0.43
1:H:235:ASP:HA	1:H:238:TYR:OH	2.19	0.43
1:I:135:ASP:OD2	1:I:242:HIS:ND1	2.50	0.43
1:I:294:SER:C	1:I:296:GLU:N	2.69	0.43
1:J:235:ASP:HA	1:J:238:TYR:CZ	2.54	0.43
1:J:295:ILE:HG22	1:J:299:LEU:HG	1.99	0.43
1:B:187:SER:HB3	1:B:190:PRO:CG	2.41	0.43
1:D:111:GLY:O	1:D:114:GLN:HB2	2.18	0.43
1:E:127:THR:C	1:E:129:GLY:H	2.22	0.43
1:E:168:HIS:NE2	1:E:187:SER:OG	2.44	0.43
1:E:237:LEU:O	1:E:239:GLY:N	2.51	0.43
1:F:265:PHE:HB3	1:F:338:VAL:HG22	2.00	0.43
1:G:298:ARG:O	1:G:301:ARG:HB2	2.18	0.43
1:H:134:LEU:HD22	1:H:136:PRO:CG	2.42	0.43
1:H:224:GLY:HA3	1:H:238:TYR:HB2	1.99	0.43
1:H:288:TRP:CE3	1:H:288:TRP:HA	2.54	0.43
1:I:142:PRO:C	1:I:144:GLY:H	2.22	0.43
1:J:270:LEU:HD12	1:J:346:PHE:CD1	2.53	0.43
1:X:183:GLY:HA2	1:X:355:ASP:HB3	1.99	0.43
1:A:297:LYS:CE	1:A:312:VAL:CG2	2.97	0.43
1:C:152:VAL:HG13	1:C:220:LEU:CD2	2.48	0.43
1:C:168:HIS:HB3	1:C:225:GLU:HB2	2.01	0.43
1:D:223:ASP:O	1:D:239:GLY:HA3	2.19	0.43
1:E:268:LEU:HD21	1:E:372:LEU:CD1	2.49	0.43
1:E:341:LEU:HD21	1:E:372:LEU:HD21	1.99	0.43
1:F:174:PHE:HE2	1:F:353:PRO:HD3	1.83	0.43
1:G:106:THR:O	1:G:112:ASN:HB2	2.18	0.43
1:G:220:LEU:HD13	1:G:243:LEU:HD23	2.01	0.43
1:G:370:ARG:O	1:G:374:VAL:HG23	2.18	0.43
1:H:109:SER:HA	1:H:110:PRO:HD3	1.85	0.43
1:H:222:LEU:H	1:H:222:LEU:HG	1.61	0.43
1:H:251:PRO:HA	1:H:257:THR:HA	2.01	0.43
1:J:296:GLU:N	1:J:298:ARG:CB	2.81	0.43
1:X:226:GLU:O	1:X:227:ALA:HB2	2.19	0.43
1:A:231:TRP:CZ3	1:A:236:SER:HB2	2.53	0.43
1:B:93:LEU:O	1:B:97:TYR:HB2	2.19	0.43
1:C:243:LEU:HD12	1:C:243:LEU:HA	1.78	0.43
1:D:210:LYS:C	1:D:212:ALA:H	2.22	0.43
1:F:141:THR:HB	1:F:228:LEU:HD12	2.01	0.43
1:G:76:LEU:HD12	1:G:76:LEU:HA	1.76	0.43
1:I:305:LEU:HD12	1:I:308:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:LEU:HD22	1:J:205:LEU:CD1	2.48	0.43
1:X:143:LEU:CD1	1:X:229:LYS:HG2	2.47	0.43
1:B:297:LYS:CD	1:B:300:HIS:HB3	2.48	0.43
1:E:127:THR:C	1:E:129:GLY:N	2.72	0.43
1:E:298:ARG:O	1:E:301:ARG:CB	2.60	0.43
1:E:308:HIS:CE1	1:E:313:MET:HG3	2.54	0.43
1:F:234:LYS:HA	1:F:234:LYS:HZ2	1.84	0.43
1:F:235:ASP:O	1:F:236:SER:HB3	2.19	0.43
1:H:103:VAL:O	1:H:182:VAL:HG12	2.19	0.43
1:I:219:LEU:HA	1:I:219:LEU:HD23	1.77	0.43
1:J:296:GLU:HA	1:J:298:ARG:CA	2.49	0.43
1:X:318:GLY:C	1:X:319:GLU:HG2	2.40	0.43
1:A:300:HIS:CE1	1:A:311:GLU:HA	2.53	0.43
1:A:349:VAL:HG11	1:A:359:ASN:HD22	1.83	0.43
1:D:135:ASP:HB3	1:D:150:ASN:HB2	2.00	0.43
1:E:84:VAL:HG13	1:E:201:LEU:HD21	2.01	0.43
1:G:78:GLU:CG	1:G:298:ARG:NH2	2.77	0.43
1:H:82:ARG:NH1	1:H:304:LEU:HD21	2.34	0.43
1:H:115:VAL:O	1:H:118:PHE:HB3	2.19	0.43
1:H:168:HIS:HE1	1:H:226:GLU:OE2	2.02	0.43
1:H:280:SER:HB2	1:H:289:PHE:CG	2.54	0.43
1:I:258:ARG:O	1:I:261:ALA:HB3	2.19	0.43
1:I:295:ILE:HG21	1:I:374:VAL:CG1	2.48	0.43
1:X:282:PHE:CD1	1:C:352:THR:HG21	2.54	0.42
1:A:126:LEU:HA	1:A:126:LEU:HD23	1.71	0.42
1:B:319:GLU:H	1:B:320:PRO:CD	2.32	0.42
1:D:352:THR:HG21	1:H:282:PHE:HD1	1.84	0.42
1:G:135:ASP:OD1	1:G:242:HIS:HE1	2.02	0.42
1:I:190:PRO:HA	1:I:193:LEU:HD12	2.00	0.42
1:J:339:LEU:HD23	1:J:340:HIS:H	1.83	0.42
1:X:70:VAL:HG21	1:X:301:ARG:HD2	2.01	0.42
1:B:90:PRO:O	1:B:93:LEU:HB3	2.18	0.42
1:D:153:ALA:HB3	1:D:219:LEU:HB2	1.99	0.42
1:E:83:ARG:O	1:E:86:GLY:N	2.52	0.42
1:G:155:LEU:HD12	1:G:155:LEU:O	2.19	0.42
1:G:168:HIS:CD2	1:G:187:SER:HG	2.35	0.42
1:G:172:LYS:CD	1:G:351:HIS:CE1	3.02	0.42
1:G:252:HIS:O	1:G:254:PRO:O	2.37	0.42
1:H:361:HIS:CE1	1:H:363:PRO:HD2	2.54	0.42
1:J:118:PHE:CD2	1:J:119:LEU:HD23	2.54	0.42
1:J:203:LEU:HB3	1:J:207:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLY:HA2	1:E:353:PRO:CG	2.49	0.42
1:B:342:ILE:O	1:B:344:THR:HG23	2.19	0.42
1:B:381:GLY:O	1:C:80:ARG:NH2	2.52	0.42
1:E:105:ARG:HA	1:E:112:ASN:H	1.83	0.42
1:F:158:ARG:HG2	1:F:159:ALA:N	2.34	0.42
1:G:149:GLY:O	1:G:223:ASP:HB2	2.18	0.42
1:H:286:VAL:HG22	1:H:290:HIS:CD2	2.54	0.42
1:H:361:HIS:CE1	1:H:363:PRO:HG2	2.55	0.42
1:J:78:GLU:O	1:J:82:ARG:HG3	2.18	0.42
1:J:187:SER:HB3	1:J:190:PRO:HB2	2.00	0.42
1:J:293:ARG:NH1	1:J:317:PRO:HD3	2.34	0.42
1:J:297:LYS:HE2	1:J:297:LYS:HB2	1.85	0.42
1:J:361:HIS:O	1:J:361:HIS:ND1	2.49	0.42
1:X:216:THR:HG23	1:X:217:LEU:N	2.35	0.42
1:B:101:LEU:O	1:B:105:ARG:NH1	2.52	0.42
1:B:259:ILE:HD13	1:B:259:ILE:HA	1.78	0.42
1:D:334:ARG:HG3	1:D:334:ARG:HH11	1.84	0.42
1:E:248:GLU:HG3	1:E:259:ILE:HG13	2.01	0.42
1:E:326:ASP:HB3	1:E:328:HIS:ND1	2.35	0.42
1:F:172:LYS:HD3	1:F:174:PHE:HE1	1.84	0.42
1:G:243:LEU:HA	1:G:243:LEU:HD12	1.78	0.42
1:I:162:HIS:HA	1:I:216:THR:O	2.20	0.42
1:I:287:ARG:HH21	1:I:288:TRP:HE1	1.67	0.42
1:J:92:ARG:NH2	1:J:200:ALA:HB2	2.34	0.42
1:J:130:TRP:HE1	1:J:205:LEU:HD13	1.85	0.42
1:C:117:LYS:HE2	1:C:120:GLU:OE2	2.19	0.42
1:D:161:ARG:O	1:D:215:VAL:HA	2.19	0.42
1:D:300:HIS:HD2	1:D:308:HIS:HB3	1.83	0.42
1:E:122:THR:O	1:E:125:SER:OG	2.33	0.42
1:F:302:LEU:O	1:F:303:ASN:C	2.58	0.42
1:G:105:ARG:HD2	1:G:115:VAL:HG21	2.02	0.42
1:G:203:LEU:O	1:G:207:ARG:HD3	2.19	0.42
1:I:107:PRO:O	1:I:108:GLY:C	2.57	0.42
1:I:135:ASP:OD1	1:I:242:HIS:CE1	2.73	0.42
1:I:379:TYR:HD1	1:I:380:LEU:HD23	1.84	0.42
1:J:204:GLU:O	1:J:207:ARG:N	2.53	0.42
1:X:121:ALA:O	1:X:124:ARG:N	2.52	0.42
1:X:228:LEU:O	1:X:229:LYS:HB2	2.20	0.42
1:B:93:LEU:CD2	1:B:196:GLU:HB2	2.46	0.42
1:D:81:LEU:HD21	1:D:299:LEU:HD21	2.01	0.42
1:D:99:ARG:HA	1:D:102:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:PRO:O	1:F:80:ARG:N	2.51	0.42
1:H:180:PRO:O	1:H:181:PHE:HB2	2.19	0.42
1:I:357:GLU:C	1:I:359:ASN:H	2.21	0.42
1:J:207:ARG:HB3	1:J:211:GLN:NE2	2.35	0.42
1:X:203:LEU:HD23	1:X:203:LEU:HA	1.69	0.42
1:E:216:THR:HG23	1:E:217:LEU:N	2.35	0.42
1:E:370:ARG:O	1:E:373:ALA:HB3	2.19	0.42
1:G:150:ASN:OD1	1:G:222:LEU:HA	2.19	0.42
1:H:99:ARG:NE	1:H:357:GLU:OE2	2.52	0.42
1:I:156:ASP:H	1:I:216:THR:HG21	1.84	0.42
1:J:201:LEU:O	1:J:205:LEU:HB2	2.19	0.42
1:J:265:PHE:HB3	1:J:338:VAL:CG2	2.50	0.42
1:J:296:GLU:HA	1:J:298:ARG:HB3	2.01	0.42
1:X:184:ALA:HB1	1:X:360:LEU:HD11	2.02	0.42
1:X:196:GLU:OE1	1:X:196:GLU:HA	2.20	0.42
1:X:253:SER:HA	1:X:254:PRO:C	2.39	0.42
1:A:319:GLU:HA	1:A:320:PRO:HD2	1.80	0.42
1:B:141:THR:OG1	1:B:144:GLY:O	2.20	0.42
1:D:370:ARG:O	1:D:371:ILE:C	2.57	0.42
1:E:135:ASP:OD1	1:E:242:HIS:CE1	2.73	0.42
1:E:297:LYS:CE	1:E:311:GLU:O	2.68	0.42
1:G:184:ALA:CB	1:G:360:LEU:HD21	2.50	0.42
1:H:86:GLY:C	1:H:88:LEU:N	2.72	0.42
1:J:297:LYS:HD2	1:J:298:ARG:HA	2.02	0.42
1:X:352:THR:C	1:X:354:ALA:H	2.24	0.42
1:X:379:TYR:HD1	1:X:380:LEU:HD23	1.84	0.42
3:X:402:A1D46:C27	3:X:402:A1D46:O01	2.68	0.42
1:B:146:VAL:HG12	1:B:147:ASP:N	2.35	0.42
1:C:105:ARG:HB2	1:C:112:ASN:HA	2.01	0.42
1:D:85:VAL:HG13	1:D:370:ARG:HH11	1.85	0.42
1:D:142:PRO:HB2	1:D:229:LYS:HB2	2.01	0.42
1:F:123:LEU:HD13	1:F:153:ALA:HB2	2.02	0.42
1:F:326:ASP:HB3	1:F:328:HIS:ND1	2.35	0.42
1:G:158:ARG:HG2	1:G:159:ALA:N	2.35	0.42
1:G:172:LYS:HB3	1:G:181:PHE:HE2	1.84	0.42
1:H:82:ARG:HA	1:H:85:VAL:HB	2.02	0.42
1:H:136:PRO:O	1:H:137:PHE:HB3	2.20	0.42
1:H:252:HIS:HD2	1:H:261:ALA:HB2	1.80	0.42
1:H:291:ARG:O	1:H:295:ILE:HG13	2.19	0.42
1:I:115:VAL:O	1:I:117:LYS:N	2.53	0.42
1:J:339:LEU:HD22	1:J:341:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:HIS:ND1	1:B:170:ASP:OD1	2.35	0.42
1:D:81:LEU:HD21	1:D:299:LEU:CD2	2.50	0.42
1:F:161:ARG:NH1	1:F:260:GLN:O	2.53	0.42
1:H:186:ASP:N	1:H:187:SER:HA	2.33	0.42
1:X:204:GLU:OE1	1:X:204:GLU:N	2.49	0.41
1:C:300:HIS:CG	1:C:311:GLU:HA	2.55	0.41
1:D:359:ASN:OD1	1:H:333:ARG:HD2	2.20	0.41
1:E:270:LEU:HD12	1:E:346:PHE:CD1	2.55	0.41
1:F:381:GLY:O	1:F:382:LEU:HD23	2.20	0.41
1:I:76:LEU:HB2	1:I:77:PRO:CD	2.50	0.41
1:I:194:LEU:HD21	1:I:268:LEU:HD22	2.02	0.41
1:X:93:LEU:HD21	1:X:193:LEU:HD23	2.02	0.41
1:X:197:LEU:HA	1:X:197:LEU:HD23	1.67	0.41
1:C:194:LEU:N	1:C:194:LEU:HD23	2.35	0.41
1:D:80:ARG:HA	1:D:83:ARG:HB3	2.01	0.41
1:D:119:LEU:O	1:D:123:LEU:HG	2.21	0.41
1:D:189:VAL:HB	1:D:190:PRO:HD3	2.02	0.41
1:D:204:GLU:OE1	1:D:204:GLU:N	2.36	0.41
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.84	0.41
1:E:219:LEU:HA	1:E:219:LEU:HD23	1.82	0.41
1:E:279:TYR:CE1	1:E:320:PRO:HG2	2.55	0.41
1:E:377:ALA:HA	1:E:382:LEU:HG	2.01	0.41
1:G:275:ASN:ND2	1:J:260:GLN:NE2	2.60	0.41
1:I:76:LEU:H	1:I:298:ARG:HH22	1.67	0.41
1:I:297:LYS:O	1:I:301:ARG:HD2	2.19	0.41
1:J:155:LEU:HD23	1:J:205:LEU:CD2	2.23	0.41
1:D:193:LEU:HD23	1:D:193:LEU:HA	1.89	0.41
1:D:252:HIS:O	1:D:255:GLY:N	2.52	0.41
1:D:268:LEU:HD11	1:D:341:LEU:HD23	2.02	0.41
1:D:274:PRO:HB3	1:D:361:HIS:HB2	2.03	0.41
1:E:102:LEU:CD1	1:E:357:GLU:HB2	2.50	0.41
1:E:306:GLN:O	1:E:307:SER:C	2.58	0.41
1:F:99:ARG:HB3	1:F:100:PRO:HD3	2.02	0.41
1:F:283:PRO:HA	1:F:286:VAL:HB	2.02	0.41
1:G:185:THR:O	1:G:187:SER:HA	2.20	0.41
1:H:106:THR:CB	1:H:173:LEU:HD12	2.50	0.41
1:I:306:GLN:C	1:I:308:HIS:N	2.73	0.41
1:J:264:LEU:HD12	1:J:265:PHE:H	1.85	0.41
1:J:283:PRO:O	1:J:285:THR:N	2.53	0.41
1:X:135:ASP:O	1:X:149:GLY:HA2	2.19	0.41
1:X:162:HIS:HB3	1:X:216:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:HD3	1:A:134:LEU:HD11	2.02	0.41
1:E:263:GLU:HG2	1:E:379:TYR:OH	2.20	0.41
1:F:201:LEU:HA	1:F:201:LEU:HD23	1.77	0.41
1:G:112:ASN:O	1:G:113:LEU:C	2.59	0.41
1:G:137:PHE:CZ	1:G:148:PHE:HB2	2.56	0.41
1:G:141:THR:HG23	1:G:144:GLY:O	2.20	0.41
1:G:196:GLU:OE2	1:G:200:ALA:HB2	2.21	0.41
1:G:233:PRO:CA	1:G:235:ASP:H	2.30	0.41
1:H:107:PRO:HG2	1:H:148:PHE:CD2	2.55	0.41
1:H:204:GLU:HB3	1:H:382:LEU:CD2	2.51	0.41
1:J:123:LEU:O	1:J:126:LEU:HB2	2.19	0.41
1:X:151:VAL:HB	1:X:221:PHE:HB2	2.02	0.41
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.75	0.41
1:B:300:HIS:NE2	1:B:311:GLU:HA	2.34	0.41
1:D:185:THR:O	1:D:187:SER:HA	2.20	0.41
1:E:134:LEU:HB3	1:E:136:PRO:HD3	2.02	0.41
1:F:235:ASP:HA	1:F:238:TYR:OH	2.21	0.41
1:F:275:ASN:N	1:F:275:ASN:ND2	2.68	0.41
1:H:289:PHE:HE2	1:H:316:GLN:O	2.03	0.41
1:X:135:ASP:OD2	1:X:242:HIS:ND1	2.48	0.41
1:X:317:PRO:HA	1:X:318:GLY:HA2	1.74	0.41
1:A:116:ARG:O	1:A:116:ARG:HG2	2.19	0.41
1:A:235:ASP:HA	1:A:238:TYR:OH	2.19	0.41
1:B:184:ALA:O	1:B:189:VAL:HG23	2.20	0.41
1:F:92:ARG:HA	1:F:96:THR:OG1	2.19	0.41
1:F:118:PHE:O	1:F:122:THR:OG1	2.25	0.41
1:F:237:LEU:O	1:F:241:ARG:HB2	2.19	0.41
1:G:324:VAL:HG23	1:G:340:HIS:CD2	2.55	0.41
1:H:293:ARG:HG2	1:H:293:ARG:O	2.20	0.41
1:I:158:ARG:HH12	1:I:212:ALA:CB	2.34	0.41
1:I:162:HIS:CE1	1:I:261:ALA:HB1	2.55	0.41
1:I:346:PHE:N	1:I:346:PHE:CD1	2.87	0.41
1:J:101:LEU:HD22	1:J:115:VAL:HG13	2.01	0.41
1:B:163:LEU:HB2	1:B:379:TYR:CE1	2.55	0.41
1:B:297:LYS:HZ3	1:B:300:HIS:CD2	2.39	0.41
1:C:263:GLU:HG2	1:C:379:TYR:OH	2.21	0.41
1:C:297:LYS:O	1:C:301:ARG:N	2.36	0.41
1:F:184:ALA:O	1:F:188:ALA:HB3	2.21	0.41
1:G:101:LEU:HD23	1:G:115:VAL:HG13	2.03	0.41
1:H:318:GLY:O	1:H:319:GLU:HB2	2.21	0.41
1:H:375:PHE:CD1	1:H:376:LEU:HD23	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:GLU:OE1	1:I:334:ARG:NE	2.50	0.41
1:A:199:GLN:O	1:A:202:ASP:N	2.53	0.41
1:G:117:LYS:HA	1:G:117:LYS:HD2	1.66	0.41
1:G:367:ASN:O	1:G:370:ARG:N	2.54	0.41
1:H:174:PHE:CE2	1:H:181:PHE:CE2	3.09	0.41
1:H:186:ASP:HB2	1:H:270:LEU:CD2	2.50	0.41
1:H:196:GLU:HG2	1:H:369:CYS:SG	2.61	0.41
1:H:243:LEU:O	1:H:243:LEU:HG	2.20	0.41
1:H:303:ASN:O	1:H:304:LEU:HD23	2.20	0.41
1:I:76:LEU:H	1:I:298:ARG:NH1	2.18	0.41
1:J:76:LEU:HD22	1:J:80:ARG:HD2	2.02	0.41
1:J:79:ALA:C	1:J:81:LEU:N	2.74	0.41
1:J:330:PRO:HA	1:J:333:ARG:HG2	2.03	0.41
1:X:140:SER:OG	1:A:133:GLU:OE2	2.38	0.41
1:B:230:GLU:O	1:B:235:ASP:HB3	2.21	0.41
1:C:196:GLU:OE1	1:C:196:GLU:HA	2.21	0.41
1:D:299:LEU:HD23	1:D:299:LEU:HA	1.86	0.41
1:D:302:LEU:HB2	1:D:304:LEU:HD12	2.03	0.41
1:E:76:LEU:HA	1:E:77:PRO:HD2	1.90	0.41
1:E:101:LEU:O	1:E:103:VAL:N	2.51	0.41
1:E:168:HIS:ND1	1:E:170:ASP:OD1	2.52	0.41
1:E:250:ILE:CG2	1:E:258:ARG:HD2	2.51	0.41
1:E:310:GLN:O	1:E:311:GLU:O	2.39	0.41
1:G:154:THR:HA	1:G:218:GLN:HG3	2.02	0.41
1:G:292:LEU:HA	1:G:292:LEU:HD23	1.90	0.41
1:G:368:LEU:H	1:G:368:LEU:HG	1.73	0.41
1:H:141:THR:OG1	1:H:144:GLY:O	2.20	0.41
1:H:183:GLY:HA2	1:H:355:ASP:HB3	2.02	0.41
1:H:361:HIS:O	1:H:362:PRO:C	2.59	0.41
1:I:76:LEU:HD22	1:I:378:GLU:OE2	2.20	0.41
1:I:122:THR:O	1:I:124:ARG:N	2.54	0.41
1:I:152:VAL:HG13	1:I:220:LEU:CD2	2.51	0.41
1:I:155:LEU:O	1:I:155:LEU:HD12	2.21	0.41
1:I:160:ALA:HB1	1:I:254:PRO:CD	2.48	0.41
1:I:246:LEU:O	1:I:250:ILE:HG13	2.21	0.41
1:I:266:MET:HE2	1:I:339:LEU:HD13	2.02	0.41
1:I:288:TRP:CZ3	1:I:379:TYR:CD2	3.09	0.41
1:J:79:ALA:C	1:J:81:LEU:H	2.23	0.41
1:J:168:HIS:CD2	1:J:168:HIS:O	2.74	0.41
1:J:353:PRO:C	1:J:355:ASP:H	2.24	0.41
1:X:103:VAL:O	1:X:105:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:CG	1:A:297:LYS:O	2.69	0.41
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.59	0.41
1:D:315:PHE:HE1	1:D:341:LEU:HD11	1.85	0.41
1:D:319:GLU:N	1:D:320:PRO:CD	2.82	0.41
1:F:354:ALA:C	1:F:356:THR:HG23	2.41	0.41
1:G:172:LYS:HB3	1:G:181:PHE:CE2	2.56	0.41
1:G:203:LEU:HB3	1:G:207:ARG:NH1	2.36	0.41
1:I:217:LEU:HD22	1:I:380:LEU:HD11	2.02	0.41
1:J:187:SER:HB3	1:J:190:PRO:CB	2.51	0.41
1:J:344:THR:O	1:J:344:THR:OG1	2.35	0.41
1:C:207:ARG:O	1:C:210:LYS:HB2	2.22	0.40
3:C:402:A1D46:C27	3:C:402:A1D46:C02	2.99	0.40
1:E:156:ASP:OD1	1:E:158:ARG:HG3	2.21	0.40
1:E:266:MET:HE1	1:E:375:PHE:CZ	2.56	0.40
1:F:375:PHE:CD1	1:F:375:PHE:C	2.94	0.40
1:G:195:LEU:HD23	1:G:195:LEU:HA	1.56	0.40
1:G:275:ASN:N	1:G:276:PRO:HD3	2.36	0.40
1:G:356:THR:HG22	1:G:357:GLU:H	1.87	0.40
1:G:368:LEU:O	1:G:372:LEU:HG	2.21	0.40
1:J:184:ALA:HB3	1:J:355:ASP:OD1	2.21	0.40
1:X:298:ARG:HA	1:X:298:ARG:HD2	1.65	0.40
1:B:163:LEU:N	1:B:216:THR:O	2.49	0.40
1:E:126:LEU:O	1:E:129:GLY:N	2.50	0.40
1:E:137:PHE:CE1	1:E:148:PHE:HB2	2.56	0.40
1:E:249:SER:O	1:E:251:PRO:HD3	2.22	0.40
1:F:95:SER:O	1:F:100:PRO:HD3	2.20	0.40
1:G:286:VAL:HG22	1:G:290:HIS:CD2	2.55	0.40
1:G:313:MET:HE2	1:G:313:MET:HB3	1.94	0.40
1:I:324:VAL:O	1:I:326:ASP:N	2.53	0.40
1:J:270:LEU:HD12	1:J:346:PHE:CE1	2.56	0.40
1:J:364:THR:O	1:J:367:ASN:HB2	2.20	0.40
1:X:136:PRO:HA	1:X:148:PHE:O	2.20	0.40
1:B:70:VAL:HG21	1:B:301:ARG:NE	2.35	0.40
1:B:217:LEU:HD12	1:B:218:GLN:N	2.36	0.40
1:D:243:LEU:HD12	1:D:246:LEU:HD23	2.02	0.40
1:D:280:SER:HB2	1:D:289:PHE:CD2	2.57	0.40
1:E:99:ARG:HH11	1:E:99:ARG:HD2	1.61	0.40
1:E:207:ARG:HH22	1:E:210:LYS:HZ3	1.68	0.40
1:I:146:VAL:HG12	1:I:147:ASP:N	2.36	0.40
1:I:336:VAL:HG13	1:I:337:PRO:HD2	2.03	0.40
1:J:99:ARG:O	1:J:101:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:81:LEU:HD23	1:X:81:LEU:C	2.42	0.40
1:A:199:GLN:O	1:A:202:ASP:HB2	2.21	0.40
1:C:152:VAL:HG13	1:C:220:LEU:HD21	2.04	0.40
1:C:284:ARG:HH12	1:C:337:PRO:HG3	1.84	0.40
1:D:170:ASP:HB3	1:D:223:ASP:OD1	2.21	0.40
1:E:265:PHE:CE2	1:E:331:PHE:CD2	3.09	0.40
1:E:329:ILE:O	1:E:333:ARG:HG2	2.21	0.40
1:G:149:GLY:O	1:G:169:TYR:OH	2.17	0.40
1:G:231:TRP:CD1	1:G:232:GLY:N	2.90	0.40
1:G:270:LEU:HD23	1:G:270:LEU:N	2.37	0.40
1:H:155:LEU:O	1:H:156:ASP:HB2	2.22	0.40
1:I:186:ASP:OD1	3:I:402:A1D46:C24	2.69	0.40
1:I:259:ILE:HD13	1:I:259:ILE:HA	1.88	0.40
1:I:292:LEU:HG	1:I:375:PHE:CD2	2.56	0.40
1:J:134:LEU:HD12	1:J:150:ASN:O	2.21	0.40
1:J:259:ILE:HD13	1:J:259:ILE:HA	1.92	0.40
1:X:136:PRO:HA	1:X:149:GLY:HA2	2.04	0.40
1:X:237:LEU:O	1:X:241:ARG:HG3	2.21	0.40
1:A:275:ASN:N	1:A:276:PRO:CD	2.85	0.40
1:A:292:LEU:HG	1:A:375:PHE:CD2	2.57	0.40
1:B:121:ALA:O	1:B:125:SER:N	2.54	0.40
1:B:295:ILE:HD13	1:B:374:VAL:HG12	2.04	0.40
1:C:109:SER:OG	1:C:112:ASN:HB2	2.22	0.40
1:D:217:LEU:HA	1:D:217:LEU:HD12	1.80	0.40
1:D:361:HIS:NE2	1:D:363:PRO:HG2	2.36	0.40
1:E:229:LYS:O	1:E:230:GLU:O	2.39	0.40
1:H:298:ARG:HB3	1:H:299:LEU:H	1.48	0.40
1:J:287:ARG:HG2	1:J:288:TRP:H	1.86	0.40
1:J:354:ALA:O	1:J:359:ASN:ND2	2.55	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)
1:C:158:ARG:NH1	1:G:114:GLN:OE1[2_455]	1.91	0.29
1:X:359:ASN:OD1	1:D:333:ARG:NH2[2_454]	2.09	0.11

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	311/313 (99%)	256 (82%)	38 (12%)	17 (6%)	2 10
1	B	311/313 (99%)	243 (78%)	47 (15%)	21 (7%)	1 6
1	C	311/313 (99%)	260 (84%)	36 (12%)	15 (5%)	2 13
1	D	311/313 (99%)	228 (73%)	56 (18%)	27 (9%)	1 4
1	E	311/313 (99%)	228 (73%)	51 (16%)	32 (10%)	0 2
1	F	311/313 (99%)	251 (81%)	36 (12%)	24 (8%)	1 5
1	G	311/313 (99%)	217 (70%)	58 (19%)	36 (12%)	0 1
1	H	311/313 (99%)	220 (71%)	60 (19%)	31 (10%)	0 3
1	I	311/313 (99%)	210 (68%)	69 (22%)	32 (10%)	0 2
1	J	311/313 (99%)	218 (70%)	68 (22%)	25 (8%)	1 4
1	X	311/313 (99%)	254 (82%)	42 (14%)	15 (5%)	2 13
All	All	3421/3443 (99%)	2585 (76%)	561 (16%)	275 (8%)	1 4

All (275) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	72	LEU
1	X	227	ALA
1	X	236	SER
1	X	254	PRO
1	X	298	ARG
1	X	321	PHE
1	X	324	VAL
1	A	231	TRP
1	A	298	ARG
1	B	108	GLY
1	B	204	GLU
1	C	75	SER
1	C	230	GLU

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Mol	Chain	Res	Type
1	C	254	PRO
1	C	297	LYS
1	D	95	SER
1	D	96	THR
1	D	178	SER
1	D	255	GLY
1	D	314	TYR
1	D	319	GLU
1	D	321	PHE
1	E	78	GLU
1	E	127	THR
1	E	211	GLN
1	E	212	ALA
1	E	230	GLU
1	E	231	TRP
1	E	233	PRO
1	E	238	TYR
1	E	246	LEU
1	E	247	MET
1	E	298	ARG
1	E	320	PRO
1	F	127	THR
1	F	178	SER
1	F	202	ASP
1	F	231	TRP
1	F	233	PRO
1	F	234	LYS
1	F	254	PRO
1	F	303	ASN
1	G	112	ASN
1	G	113	LEU
1	G	145	PRO
1	G	206	SER
1	G	212	ALA
1	G	254	PRO
1	G	303	ASN
1	G	319	GLU
1	G	320	PRO
1	G	322	GLY
1	G	353	PRO
1	H	78	GLU
1	H	180	PRO

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Mol	Chain	Res	Type
1	H	181	PHE
1	H	183	GLY
1	H	191	CYS
1	H	192	ALA
1	H	227	ALA
1	H	228	LEU
1	H	241	ARG
1	H	254	PRO
1	H	298	ARG
1	H	299	LEU
1	H	319	GLU
1	I	73	ILE
1	I	107	PRO
1	I	295	ILE
1	I	297	LYS
1	I	349	VAL
1	I	358	VAL
1	J	79	ALA
1	J	80	ARG
1	J	130	TRP
1	J	131	HIS
1	J	297	LYS
1	J	299	LEU
1	J	300	HIS
1	J	320	PRO
1	X	130	TRP
1	A	207	ARG
1	A	230	GLU
1	A	297	LYS
1	A	299	LEU
1	A	351	HIS
1	B	86	GLY
1	B	112	ASN
1	B	183	GLY
1	B	203	LEU
1	C	321	PHE
1	C	322	GLY
1	D	236	SER
1	D	297	LYS
1	D	320	PRO
1	D	367	ASN
1	D	368	LEU

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Mol	Chain	Res	Type
1	D	370	ARG
1	D	371	ILE
1	D	375	PHE
1	E	79	ALA
1	E	84	VAL
1	E	128	ALA
1	E	297	LYS
1	E	311	GLU
1	E	334	ARG
1	E	355	ASP
1	F	73	ILE
1	F	125	SER
1	F	200	ALA
1	F	207	ARG
1	F	232	GLY
1	F	236	SER
1	F	355	ASP
1	F	381	GLY
1	G	72	LEU
1	G	75	SER
1	G	183	GLY
1	G	205	LEU
1	G	230	GLU
1	G	298	ARG
1	G	367	ASN
1	G	368	LEU
1	H	87	GLN
1	H	128	ALA
1	H	175	PRO
1	H	236	SER
1	H	259	ILE
1	H	349	VAL
1	I	108	GLY
1	I	129	GLY
1	I	183	GLY
1	I	255	GLY
1	I	307	SER
1	I	314	TYR
1	I	325	GLU
1	I	377	ALA
1	J	204	GLU
1	J	298	ARG

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Mol	Chain	Res	Type
1	J	319	GLU
1	J	349	VAL
1	J	354	ALA
1	J	357	GLU
1	J	358	VAL
1	J	360	LEU
1	X	79	ALA
1	X	102	LEU
1	X	136	PRO
1	X	303	ASN
1	A	236	SER
1	B	297	LYS
1	B	375	PHE
1	C	143	LEU
1	C	178	SER
1	C	234	LYS
1	D	71	PRO
1	D	126	LEU
1	D	302	LEU
1	D	317	PRO
1	D	357	GLU
1	E	71	PRO
1	E	77	PRO
1	E	178	SER
1	E	183	GLY
1	E	307	SER
1	F	78	GLU
1	F	208	ALA
1	F	230	GLU
1	G	143	LEU
1	G	178	SER
1	G	300	HIS
1	G	325	GLU
1	G	374	VAL
1	H	120	GLU
1	H	137	PHE
1	H	212	ALA
1	H	377	ALA
1	I	227	ALA
1	I	300	HIS
1	I	302	LEU
1	I	320	PRO

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Mol	Chain	Res	Type
1	I	353	PRO
1	I	367	ASN
1	I	375	PHE
1	J	177	GLY
1	J	272	GLY
1	A	199	GLN
1	B	113	LEU
1	B	176	PRO
1	B	275	ASN
1	B	301	ARG
1	B	319	GLU
1	C	204	GLU
1	D	292	LEU
1	E	210	LYS
1	E	259	ILE
1	E	347	PRO
1	E	381	GLY
1	F	199	GLN
1	G	106	THR
1	G	140	SER
1	G	296	GLU
1	G	375	PHE
1	H	112	ASN
1	H	233	PRO
1	I	149	GLY
1	I	168	HIS
1	I	178	SER
1	I	198	ALA
1	I	231	TRP
1	I	327	ASP
1	J	196	GLU
1	J	275	ASN
1	X	318	GLY
1	X	381	GLY
1	A	71	PRO
1	A	93	LEU
1	A	178	SER
1	B	102	LEU
1	B	115	VAL
1	C	142	PRO
1	D	273	ALA
1	F	71	PRO

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Mol	Chain	Res	Type
1	G	196	GLU
1	G	211	GLN
1	H	156	ASP
1	H	167	CYS
1	I	236	SER
1	J	102	LEU
1	J	203	LEU
1	J	307	SER
1	X	107	PRO
1	A	84	VAL
1	B	374	VAL
1	D	143	LEU
1	E	333	ARG
1	F	76	LEU
1	G	93	LEU
1	G	207	ARG
1	H	160	ALA
1	H	309	PRO
1	I	175	PRO
1	I	233	PRO
1	A	85	VAL
1	A	107	PRO
1	A	233	PRO
1	B	107	PRO
1	D	374	VAL
1	D	381	GLY
1	G	233	PRO
1	G	349	VAL
1	J	100	PRO
1	B	322	GLY
1	C	232	GLY
1	C	233	PRO
1	C	381	GLY
1	F	190	PRO
1	H	142	PRO
1	H	273	ALA
1	I	84	VAL
1	J	183	GLY
1	D	275	ASN
1	E	90	PRO
1	G	317	PRO
1	E	319	GLU

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Mol	Chain	Res	Type
1	F	353	PRO
1	G	347	PRO
1	B	100	PRO
1	B	349	VAL
1	I	256	PRO
1	B	254	PRO
1	D	256	PRO
1	A	254	PRO
1	E	254	PRO
1	C	256	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/271 (100%)	260 (96%)	11 (4%)	30	61
1	B	271/271 (100%)	268 (99%)	3 (1%)	73	88
1	C	271/271 (100%)	265 (98%)	6 (2%)	52	77
1	D	271/271 (100%)	261 (96%)	10 (4%)	34	65
1	E	271/271 (100%)	260 (96%)	11 (4%)	30	61
1	F	271/271 (100%)	263 (97%)	8 (3%)	41	70
1	G	271/271 (100%)	259 (96%)	12 (4%)	28	59
1	H	271/271 (100%)	255 (94%)	16 (6%)	19	48
1	I	271/271 (100%)	259 (96%)	12 (4%)	28	59
1	J	271/271 (100%)	250 (92%)	21 (8%)	13	39
1	X	271/271 (100%)	263 (97%)	8 (3%)	41	70
All	All	2981/2981 (100%)	2863 (96%)	118 (4%)	31	62

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	179	THR

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Mol	Chain	Res	Type
1	X	269	ASP
1	X	287	ARG
1	X	291	ARG
1	X	298	ARG
1	X	319	GLU
1	X	321	PHE
1	X	340	HIS
1	A	93	LEU
1	A	99	ARG
1	A	114	GLN
1	A	117	LYS
1	A	158	ARG
1	A	207	ARG
1	A	234	LYS
1	A	297	LYS
1	A	320	PRO
1	A	321	PHE
1	A	339	LEU
1	B	210	LYS
1	B	298	ARG
1	B	370	ARG
1	C	99	ARG
1	C	114	GLN
1	C	211	GLN
1	C	297	LYS
1	C	321	PHE
1	C	370	ARG
1	D	75	SER
1	D	76	LEU
1	D	158	ARG
1	D	207	ARG
1	D	241	ARG
1	D	291	ARG
1	D	293	ARG
1	D	308	HIS
1	D	321	PHE
1	D	340	HIS
1	E	99	ARG
1	E	169	TYR
1	E	207	ARG
1	E	225	GLU
1	E	230	GLU

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Mol	Chain	Res	Type
1	E	234	LYS
1	E	287	ARG
1	E	294	SER
1	E	297	LYS
1	E	298	ARG
1	E	333	ARG
1	F	83	ARG
1	F	137	PHE
1	F	158	ARG
1	F	161	ARG
1	F	180	PRO
1	F	231	TRP
1	F	291	ARG
1	F	298	ARG
1	G	80	ARG
1	G	117	LYS
1	G	147	ASP
1	G	158	ARG
1	G	229	LYS
1	G	258	ARG
1	G	280	SER
1	G	297	LYS
1	G	298	ARG
1	G	300	HIS
1	G	333	ARG
1	G	340	HIS
1	H	76	LEU
1	H	112	ASN
1	H	148	PHE
1	H	158	ARG
1	H	168	HIS
1	H	181	PHE
1	H	193	LEU
1	H	223	ASP
1	H	231	TRP
1	H	275	ASN
1	H	287	ARG
1	H	291	ARG
1	H	298	ARG
1	H	300	HIS
1	H	326	ASP
1	H	366	HIS

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Mol	Chain	Res	Type
1	I	82	ARG
1	I	112	ASN
1	I	158	ARG
1	I	162	HIS
1	I	199	GLN
1	I	207	ARG
1	I	281	HIS
1	I	282	PHE
1	I	289	PHE
1	I	290	HIS
1	I	294	SER
1	I	295	ILE
1	J	83	ARG
1	J	114	GLN
1	J	116	ARG
1	J	148	PHE
1	J	158	ARG
1	J	168	HIS
1	J	201	LEU
1	J	205	LEU
1	J	209	LYS
1	J	210	LYS
1	J	231	TRP
1	J	258	ARG
1	J	287	ARG
1	J	298	ARG
1	J	302	LEU
1	J	319	GLU
1	J	327	ASP
1	J	351	HIS
1	J	369	CYS
1	J	370	ARG
1	J	376	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	114	GLN
1	X	361	HIS
1	B	300	HIS
1	C	112	ASN
1	D	275	ASN

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Mol	Chain	Res	Type
1	D	300	HIS
1	E	162	HIS
1	E	340	HIS
1	G	275	ASN
1	G	308	HIS
1	G	351	HIS
1	H	275	ASN
1	I	281	HIS
1	I	328	HIS
1	J	162	HIS
1	J	211	GLN
1	J	308	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 for Mogul analysis.

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	$\#\|Z\| > 2$
3	A1D46	H	402	-	29,31,31	2.98	9 (31%)	34,44,44	2.40	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A1D46	B	402	2	29,31,31	3.28	13 (44%)	34,44,44	2.94	14 (41%)
3	A1D46	E	402	-	29,31,31	2.80	8 (27%)	34,44,44	2.16	11 (32%)
3	A1D46	A	402	-	29,31,31	3.03	10 (34%)	34,44,44	2.79	11 (32%)
3	A1D46	J	402	2	29,31,31	3.10	9 (31%)	34,44,44	1.98	11 (32%)
3	A1D46	D	402	-	29,31,31	3.05	11 (37%)	34,44,44	2.15	7 (20%)
3	A1D46	X	402	2	29,31,31	2.97	7 (24%)	34,44,44	2.62	14 (41%)
3	A1D46	G	402	-	29,31,31	3.17	10 (34%)	34,44,44	1.89	7 (20%)
3	A1D46	F	402	2	29,31,31	3.22	13 (44%)	34,44,44	3.29	11 (32%)
3	A1D46	C	402	-	29,31,31	3.37	14 (48%)	34,44,44	3.07	11 (32%)
3	A1D46	I	402	2	29,31,31	2.80	8 (27%)	34,44,44	2.21	6 (17%)

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
3	A1D46	H	402	-	-	3/8/28/28	1/5/5/5
3	A1D46	B	402	2	-	2/8/28/28	0/5/5/5
3	A1D46	E	402	-	-	0/8/28/28	0/5/5/5
3	A1D46	A	402	-	-	4/8/28/28	0/5/5/5
3	A1D46	J	402	2	-	5/8/28/28	0/5/5/5
3	A1D46	D	402	-	-	6/8/28/28	0/5/5/5
3	A1D46	X	402	2	-	2/8/28/28	0/5/5/5
3	A1D46	G	402	-	-	5/8/28/28	0/5/5/5
3	A1D46	F	402	2	-	2/8/28/28	0/5/5/5
3	A1D46	C	402	-	-	3/8/28/28	0/5/5/5
3	A1D46	I	402	2	-	4/8/28/28	0/5/5/5

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	402	A1D46	C02-N17	9.72	1.46	1.36
3	G	402	A1D46	C02-N17	9.64	1.46	1.36
3	A	402	A1D46	C02-N17	9.53	1.46	1.36
3	B	402	A1D46	C02-N17	8.84	1.45	1.36
3	F	402	A1D46	C19-C18	8.50	1.63	1.46
3	J	402	A1D46	C02-N17	8.50	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	A1D46	C02-N17	8.40	1.45	1.36
3	D	402	A1D46	C02-N17	8.31	1.45	1.36
3	I	402	A1D46	C02-N17	8.23	1.45	1.36
3	E	402	A1D46	C02-N17	8.20	1.45	1.36
3	J	402	A1D46	C16-N17	8.10	1.53	1.38
3	I	402	A1D46	C16-N17	7.78	1.53	1.38
3	B	402	A1D46	C16-N17	7.68	1.52	1.38
3	H	402	A1D46	C02-N17	7.64	1.44	1.36
3	A	402	A1D46	C16-N17	7.58	1.52	1.38
3	C	402	A1D46	C19-C18	7.54	1.61	1.46
3	X	402	A1D46	C16-N17	7.53	1.52	1.38
3	F	402	A1D46	C02-N17	7.41	1.44	1.36
3	B	402	A1D46	C19-C18	7.37	1.61	1.46
3	E	402	A1D46	C16-N17	7.30	1.52	1.38
3	C	402	A1D46	C16-N17	7.29	1.52	1.38
3	G	402	A1D46	C16-N17	7.25	1.52	1.38
3	D	402	A1D46	C19-C18	7.19	1.60	1.46
3	H	402	A1D46	C16-N17	7.19	1.51	1.38
3	F	402	A1D46	C16-N17	7.01	1.51	1.38
3	G	402	A1D46	C19-C18	6.95	1.60	1.46
3	D	402	A1D46	C16-N17	6.74	1.51	1.38
3	H	402	A1D46	C19-C18	6.62	1.59	1.46
3	C	402	A1D46	O06-C05	6.01	1.47	1.37
3	J	402	A1D46	C19-C18	5.72	1.57	1.46
3	J	402	A1D46	O06-C05	5.52	1.47	1.37
3	A	402	A1D46	C19-C18	5.45	1.57	1.46
3	H	402	A1D46	O06-C05	5.35	1.46	1.37
3	E	402	A1D46	C19-C18	5.21	1.56	1.46
3	I	402	A1D46	C19-C18	5.11	1.56	1.46
3	X	402	A1D46	C19-C18	5.02	1.56	1.46
3	I	402	A1D46	O06-C05	4.93	1.46	1.37
3	F	402	A1D46	C04-C03	4.82	1.55	1.45
3	H	402	A1D46	C04-C05	4.73	1.49	1.40
3	D	402	A1D46	C04-C03	4.69	1.54	1.45
3	C	402	A1D46	C04-C03	4.69	1.54	1.45
3	F	402	A1D46	O06-C05	4.58	1.45	1.37
3	B	402	A1D46	C04-C03	4.45	1.54	1.45
3	G	402	A1D46	O06-C05	4.43	1.45	1.37
3	X	402	A1D46	O06-C05	4.37	1.45	1.37
3	D	402	A1D46	O06-C05	4.30	1.44	1.37
3	J	402	A1D46	C04-C05	4.28	1.48	1.40
3	E	402	A1D46	O06-C05	4.20	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	A1D46	O06-C05	4.08	1.44	1.37
3	H	402	A1D46	C04-C03	4.04	1.53	1.45
3	B	402	A1D46	O06-C05	4.02	1.44	1.37
3	G	402	A1D46	C04-C03	3.96	1.53	1.45
3	C	402	A1D46	C14-C13	3.83	1.47	1.38
3	F	402	A1D46	O01-C02	-3.76	1.16	1.23
3	G	402	A1D46	C14-C13	3.69	1.46	1.38
3	D	402	A1D46	C04-C05	3.63	1.47	1.40
3	C	402	A1D46	C04-C05	3.54	1.47	1.40
3	J	402	A1D46	C14-C13	3.51	1.46	1.38
3	X	402	A1D46	C14-C13	3.48	1.46	1.38
3	B	402	A1D46	C14-C13	3.47	1.46	1.38
3	E	402	A1D46	C14-C13	3.43	1.46	1.38
3	J	402	A1D46	C04-C03	3.40	1.52	1.45
3	A	402	A1D46	C04-C03	3.38	1.52	1.45
3	F	402	A1D46	C04-C05	3.35	1.46	1.40
3	B	402	A1D46	C18-C03	3.21	1.39	1.34
3	I	402	A1D46	C14-C13	3.12	1.45	1.38
3	C	402	A1D46	O01-C02	-3.06	1.17	1.23
3	D	402	A1D46	O01-C02	-3.05	1.17	1.23
3	F	402	A1D46	C14-C13	3.04	1.45	1.38
3	E	402	A1D46	C04-C03	3.04	1.51	1.45
3	D	402	A1D46	C14-C13	3.01	1.45	1.38
3	E	402	A1D46	O01-C02	-3.01	1.17	1.23
3	J	402	A1D46	O01-C02	-2.98	1.17	1.23
3	A	402	A1D46	C14-C13	2.93	1.45	1.38
3	F	402	A1D46	C04-C16	2.89	1.46	1.41
3	C	402	A1D46	C04-C16	2.87	1.46	1.41
3	I	402	A1D46	C04-C05	2.82	1.45	1.40
3	X	402	A1D46	C04-C03	2.81	1.51	1.45
3	B	402	A1D46	C04-C05	2.76	1.45	1.40
3	C	402	A1D46	C18-C03	2.73	1.38	1.34
3	G	402	A1D46	C18-C03	2.71	1.38	1.34
3	B	402	A1D46	C04-C16	2.69	1.46	1.41
3	H	402	A1D46	C14-C13	2.69	1.44	1.38
3	A	402	A1D46	C03-C02	2.64	1.54	1.50
3	G	402	A1D46	O01-C02	-2.58	1.18	1.23
3	A	402	A1D46	C04-C05	2.58	1.45	1.40
3	B	402	A1D46	O01-C02	-2.53	1.18	1.23
3	I	402	A1D46	C04-C03	2.51	1.50	1.45
3	G	402	A1D46	C04-C05	2.51	1.45	1.40
3	J	402	A1D46	C04-C16	2.47	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	A1D46	C21-C20	2.47	1.41	1.36
3	B	402	A1D46	C15-C16	2.46	1.43	1.39
3	E	402	A1D46	C04-C05	2.42	1.45	1.40
3	A	402	A1D46	C27-C26	-2.42	1.38	1.41
3	I	402	A1D46	O01-C02	-2.41	1.19	1.23
3	C	402	A1D46	C26-C22	-2.38	1.34	1.42
3	F	402	A1D46	C18-C03	2.30	1.38	1.34
3	D	402	A1D46	C21-C20	2.29	1.41	1.36
3	G	402	A1D46	C04-C16	2.25	1.45	1.41
3	B	402	A1D46	C21-C20	2.24	1.41	1.36
3	H	402	A1D46	O01-C02	-2.21	1.19	1.23
3	D	402	A1D46	C27-C19	2.21	1.43	1.38
3	C	402	A1D46	C21-C20	2.21	1.41	1.36
3	D	402	A1D46	C04-C16	2.19	1.45	1.41
3	X	402	A1D46	C03-C02	2.18	1.54	1.50
3	H	402	A1D46	C27-C19	2.17	1.43	1.38
3	F	402	A1D46	C26-C22	-2.14	1.35	1.42
3	F	402	A1D46	C27-C19	2.12	1.43	1.38
3	A	402	A1D46	C04-C16	2.04	1.45	1.41
3	B	402	A1D46	C03-C02	2.04	1.53	1.50
3	C	402	A1D46	C27-C26	-2.03	1.38	1.41
3	C	402	A1D46	C11-N10	2.02	1.54	1.47

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	402	A1D46	C03-C02-N17	11.60	113.38	106.88
3	C	402	A1D46	C03-C02-N17	9.86	112.41	106.88
3	A	402	A1D46	C16-N17-C02	-9.29	105.54	111.38
3	F	402	A1D46	C16-N17-C02	-9.23	105.58	111.38
3	B	402	A1D46	C03-C02-N17	9.12	111.99	106.88
3	X	402	A1D46	C16-N17-C02	-8.60	105.98	111.38
3	C	402	A1D46	C16-N17-C02	-8.15	106.26	111.38
3	A	402	A1D46	C19-C18-C03	-7.85	113.88	129.63
3	B	402	A1D46	C16-N17-C02	-7.83	106.46	111.38
3	H	402	A1D46	C19-C18-C03	-7.58	114.42	129.63
3	I	402	A1D46	C19-C18-C03	-7.20	115.19	129.63
3	D	402	A1D46	C03-C02-N17	6.96	110.78	106.88
3	H	402	A1D46	C16-N17-C02	-6.70	107.17	111.38
3	E	402	A1D46	C19-C18-C03	-6.65	116.30	129.63
3	D	402	A1D46	C16-N17-C02	-6.58	107.24	111.38
3	X	402	A1D46	C03-C02-N17	6.31	110.42	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	402	A1D46	C03-C02-N17	6.22	110.37	106.88
3	A	402	A1D46	C03-C02-N17	6.01	110.25	106.88
3	G	402	A1D46	C16-N17-C02	-5.71	107.79	111.38
3	J	402	A1D46	C16-N17-C02	-5.65	107.83	111.38
3	H	402	A1D46	C04-C03-C02	5.57	108.47	105.31
3	I	402	A1D46	C04-C03-C02	5.45	108.40	105.31
3	E	402	A1D46	C16-N17-C02	-5.36	108.01	111.38
3	J	402	A1D46	C04-C03-C02	5.36	108.35	105.31
3	I	402	A1D46	C16-N17-C02	-5.33	108.03	111.38
3	B	402	A1D46	C19-C18-C03	-5.16	119.28	129.63
3	F	402	A1D46	C19-C18-C03	-5.15	119.30	129.63
3	F	402	A1D46	O01-C02-N17	-4.61	119.04	126.36
3	F	402	A1D46	C04-C03-C02	-4.59	102.70	105.31
3	B	402	A1D46	C04-C03-C02	-4.52	102.73	105.31
3	X	402	A1D46	C19-C18-C03	-4.50	120.61	129.63
3	B	402	A1D46	O01-C02-N17	-4.42	119.35	126.36
3	C	402	A1D46	C19-C18-C03	-4.41	120.78	129.63
3	A	402	A1D46	C12-C11-N10	4.41	119.56	110.64
3	C	402	A1D46	C19-C27-C26	4.24	128.25	120.57
3	C	402	A1D46	O06-C07-C12	4.23	117.67	108.31
3	C	402	A1D46	C04-C03-C02	-4.22	102.90	105.31
3	E	402	A1D46	C03-C02-N17	4.14	109.20	106.88
3	B	402	A1D46	C08-C09-N10	3.90	118.53	110.64
3	D	402	A1D46	C19-C18-C03	-3.85	121.91	129.63
3	F	402	A1D46	C20-C19-C27	-3.77	113.57	118.58
3	C	402	A1D46	O01-C02-N17	-3.72	120.46	126.36
3	F	402	A1D46	C19-C27-C26	3.58	127.05	120.57
3	C	402	A1D46	C12-C11-N10	3.54	117.80	110.64
3	X	402	A1D46	C08-C09-N10	3.51	117.75	110.64
3	E	402	A1D46	O06-C07-C12	-3.43	100.73	108.31
3	I	402	A1D46	C16-C04-C05	3.36	120.98	117.79
3	X	402	A1D46	C16-C04-C05	3.30	120.93	117.79
3	C	402	A1D46	C20-C19-C27	-3.28	114.22	118.58
3	H	402	A1D46	O06-C07-C12	3.25	115.48	108.31
3	H	402	A1D46	O06-C05-C13	-3.18	116.40	123.87
3	H	402	A1D46	O06-C05-C04	3.14	124.40	117.70
3	B	402	A1D46	C15-C14-C13	-3.09	115.86	120.25
3	X	402	A1D46	O01-C02-N17	-3.05	121.52	126.36
3	X	402	A1D46	C05-C04-C03	-3.03	129.18	136.13
3	G	402	A1D46	C04-C03-C02	-3.02	103.59	105.31
3	F	402	A1D46	C16-C04-C05	-2.97	114.98	117.79
3	I	402	A1D46	C05-O06-C07	-2.93	110.29	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	402	A1D46	C18-C03-C02	2.86	131.46	119.96
3	X	402	A1D46	O06-C05-C04	-2.77	111.81	117.70
3	E	402	A1D46	C08-C09-N10	2.76	116.23	110.64
3	E	402	A1D46	C12-C11-N10	2.74	116.20	110.64
3	B	402	A1D46	C19-C27-C26	2.72	125.48	120.57
3	J	402	A1D46	C08-C09-N10	2.66	116.02	110.64
3	G	402	A1D46	C18-C03-C02	2.63	130.54	119.96
3	G	402	A1D46	C16-C04-C03	2.61	110.78	106.61
3	J	402	A1D46	O06-C05-C04	2.57	123.19	117.70
3	G	402	A1D46	O01-C02-N17	-2.56	122.30	126.36
3	I	402	A1D46	C08-C09-N10	2.55	115.80	110.64
3	J	402	A1D46	C12-C07-C08	-2.52	106.89	111.74
3	A	402	A1D46	O01-C02-N17	-2.50	122.40	126.36
3	J	402	A1D46	C16-C04-C05	2.49	120.16	117.79
3	C	402	A1D46	C21-C22-N23	2.49	137.69	130.80
3	E	402	A1D46	C05-C04-C03	-2.48	130.46	136.13
3	X	402	A1D46	O06-C07-C12	2.45	113.73	108.31
3	X	402	A1D46	O06-C05-C13	2.43	129.58	123.87
3	A	402	A1D46	O06-C07-C12	2.40	113.60	108.31
3	D	402	A1D46	O06-C05-C13	-2.39	118.25	123.87
3	J	402	A1D46	C27-C19-C18	2.39	125.47	118.94
3	A	402	A1D46	O06-C05-C13	-2.39	118.26	123.87
3	F	402	A1D46	C15-C16-N17	-2.39	126.01	130.87
3	D	402	A1D46	C05-O06-C07	-2.36	112.23	120.21
3	A	402	A1D46	O06-C05-C04	2.35	122.70	117.70
3	X	402	A1D46	C19-C27-C26	2.33	124.79	120.57
3	E	402	A1D46	C16-C04-C05	2.33	120.01	117.79
3	B	402	A1D46	O06-C07-C08	2.32	113.43	108.31
3	H	402	A1D46	C12-C11-N10	2.30	115.30	110.64
3	G	402	A1D46	C05-C04-C03	-2.29	130.89	136.13
3	H	402	A1D46	C04-C16-N17	2.28	111.44	108.04
3	A	402	A1D46	C21-C20-C19	-2.27	117.73	120.90
3	X	402	A1D46	O06-C07-C08	-2.26	103.31	108.31
3	B	402	A1D46	C16-C04-C03	2.22	110.17	106.61
3	F	402	A1D46	C21-C22-N23	2.20	136.89	130.80
3	E	402	A1D46	C18-C03-C02	2.20	128.79	119.96
3	H	402	A1D46	C03-C02-N17	2.19	108.11	106.88
3	J	402	A1D46	O06-C07-C08	2.18	113.12	108.31
3	E	402	A1D46	C12-C07-C08	2.16	115.92	111.74
3	J	402	A1D46	C03-C02-N17	2.16	108.09	106.88
3	J	402	A1D46	C12-C11-N10	2.16	115.02	110.64
3	B	402	A1D46	C11-N10-C09	2.15	116.53	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	402	A1D46	O01-C02-N17	-2.14	122.97	126.36
3	C	402	A1D46	C20-C19-C18	2.09	128.34	121.22
3	B	402	A1D46	C21-C22-N23	2.09	136.58	130.80
3	A	402	A1D46	C05-O06-C07	-2.08	113.18	120.21
3	A	402	A1D46	C18-C03-C02	2.05	128.21	119.96
3	X	402	A1D46	C16-C04-C03	2.04	109.88	106.61
3	B	402	A1D46	C14-C13-C05	2.04	123.47	119.71
3	D	402	A1D46	C19-C27-C26	2.01	124.21	120.57
3	B	402	A1D46	C16-C04-C05	-2.01	115.89	117.79
3	F	402	A1D46	C15-C14-C13	-2.01	117.39	120.25
3	J	402	A1D46	C18-C03-C02	2.01	128.03	119.96
3	D	402	A1D46	O01-C02-N17	-2.00	123.19	126.36

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	402	A1D46	C02-C03-C18-C19
3	A	402	A1D46	C02-C03-C18-C19
3	A	402	A1D46	C04-C03-C18-C19
3	C	402	A1D46	C02-C03-C18-C19
3	C	402	A1D46	C04-C03-C18-C19
3	D	402	A1D46	C02-C03-C18-C19
3	F	402	A1D46	C02-C03-C18-C19
3	F	402	A1D46	C04-C03-C18-C19
3	G	402	A1D46	C02-C03-C18-C19
3	H	402	A1D46	C02-C03-C18-C19
3	H	402	A1D46	C04-C03-C18-C19
3	I	402	A1D46	C02-C03-C18-C19
3	I	402	A1D46	C04-C03-C18-C19
3	J	402	A1D46	C02-C03-C18-C19
3	J	402	A1D46	C04-C03-C18-C19
3	I	402	A1D46	C13-C05-O06-C07
3	D	402	A1D46	C08-C07-O06-C05
3	X	402	A1D46	C04-C03-C18-C19
3	D	402	A1D46	C04-C03-C18-C19
3	G	402	A1D46	C04-C03-C18-C19
3	I	402	A1D46	C04-C05-O06-C07
3	B	402	A1D46	C04-C05-O06-C07
3	G	402	A1D46	C04-C05-O06-C07
3	B	402	A1D46	C13-C05-O06-C07
3	A	402	A1D46	C04-C05-O06-C07

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Mol	Chain	Res	Type	Atoms
3	D	402	A1D46	C04-C05-O06-C07
3	C	402	A1D46	C12-C07-O06-C05
3	D	402	A1D46	C12-C07-O06-C05
3	G	402	A1D46	C12-C07-O06-C05
3	G	402	A1D46	C13-C05-O06-C07
3	A	402	A1D46	C13-C05-O06-C07
3	D	402	A1D46	C13-C05-O06-C07
3	J	402	A1D46	C13-C05-O06-C07
3	J	402	A1D46	C12-C07-O06-C05
3	J	402	A1D46	C04-C05-O06-C07
3	H	402	A1D46	C13-C05-O06-C07

All (1) ring outliers are listed below:

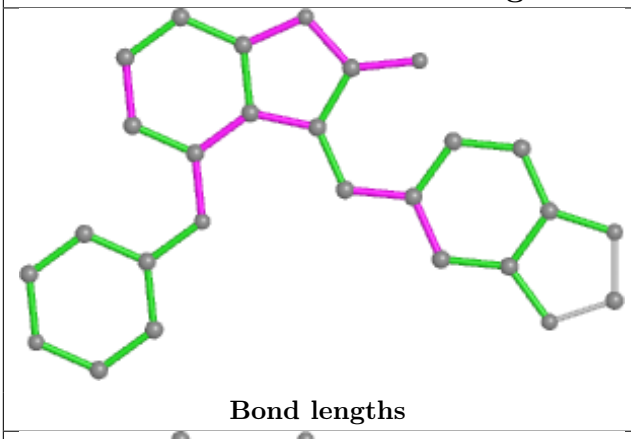
Mol	Chain	Res	Type	Atoms
3	H	402	A1D46	C07-C08-C09-C11-C12-N10

9 monomers are involved in 16 short contacts:

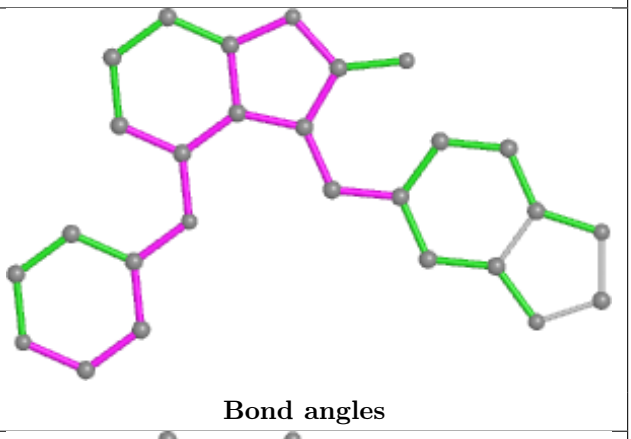
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	402	A1D46	3	0
3	B	402	A1D46	1	0
3	E	402	A1D46	2	0
3	A	402	A1D46	1	0
3	D	402	A1D46	1	0
3	X	402	A1D46	1	0
3	F	402	A1D46	4	0
3	C	402	A1D46	2	0
3	I	402	A1D46	1	0

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

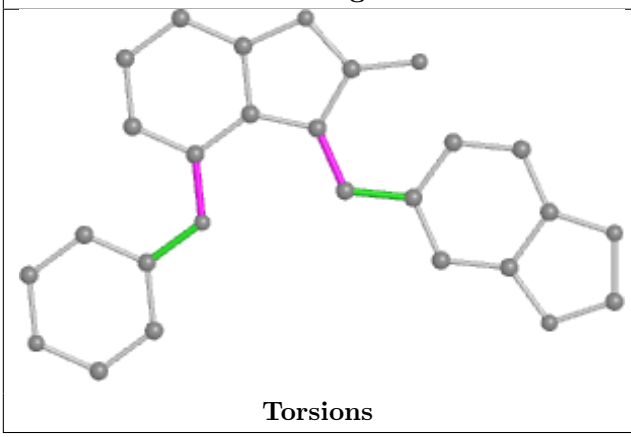
Ligand A1D46 H 402



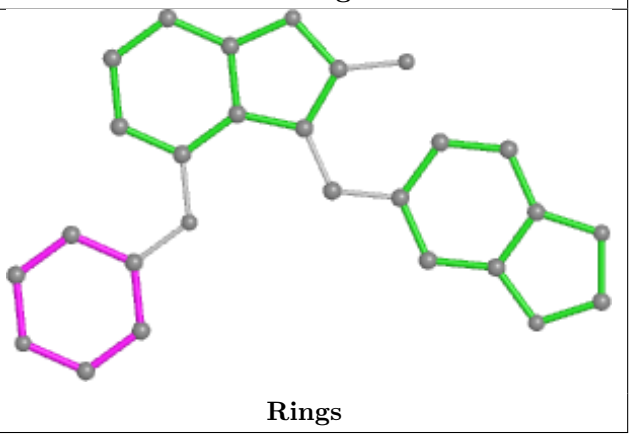
Bond lengths



Bond angles

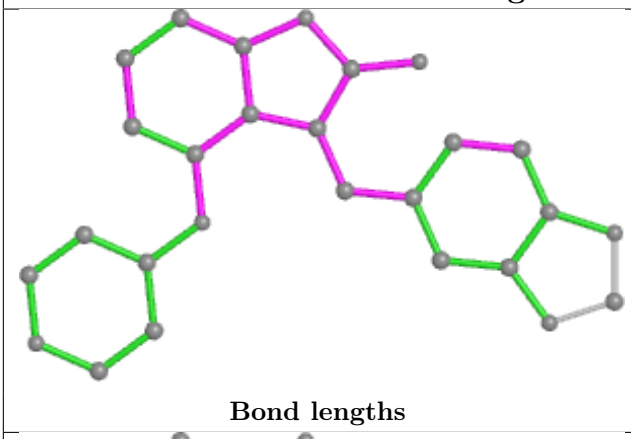


Torsions

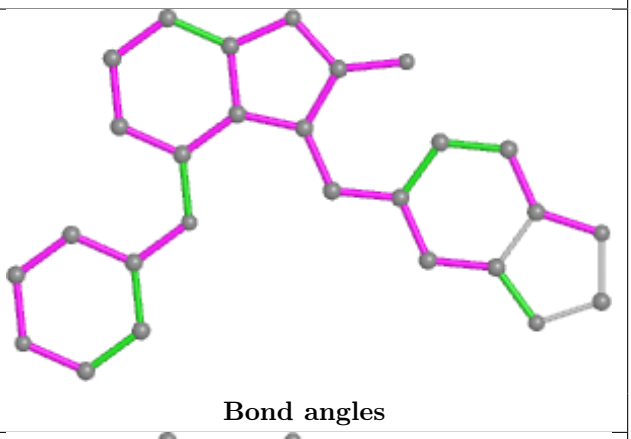


Rings

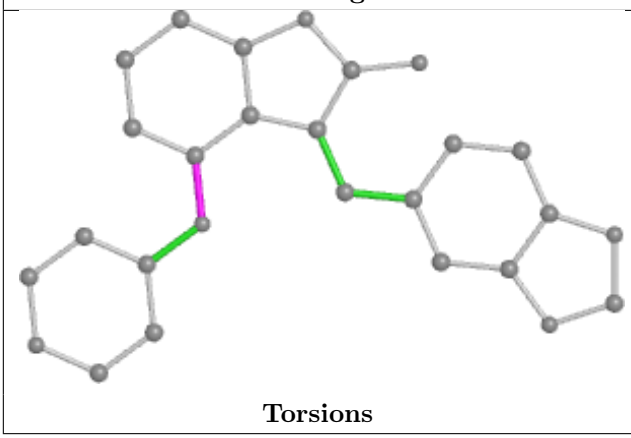
Ligand A1D46 B 402



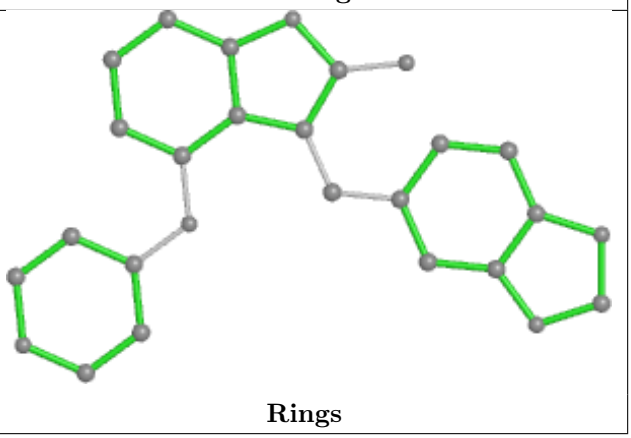
Bond lengths



Bond angles

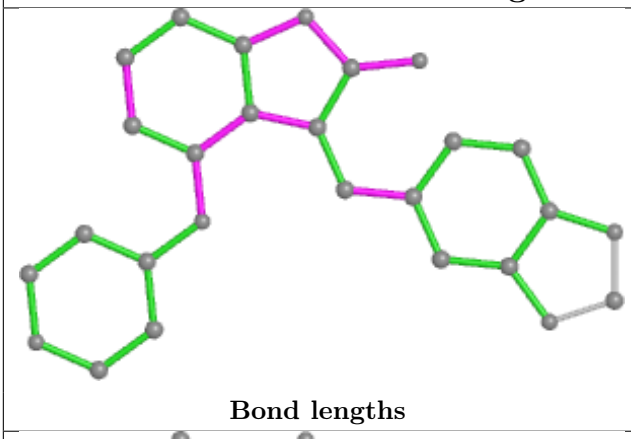


Torsions

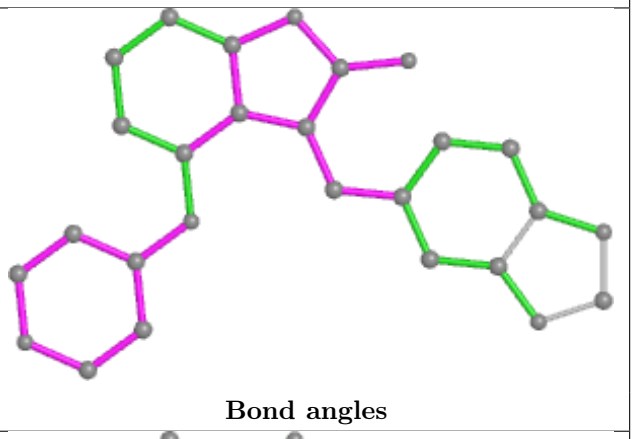


Rings

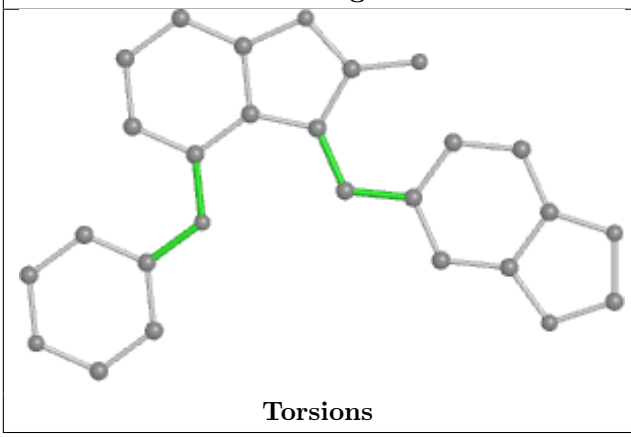
Ligand A1D46 E 402



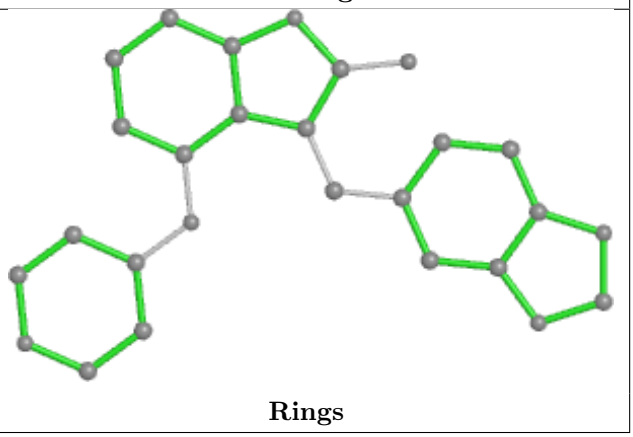
Bond lengths



Bond angles

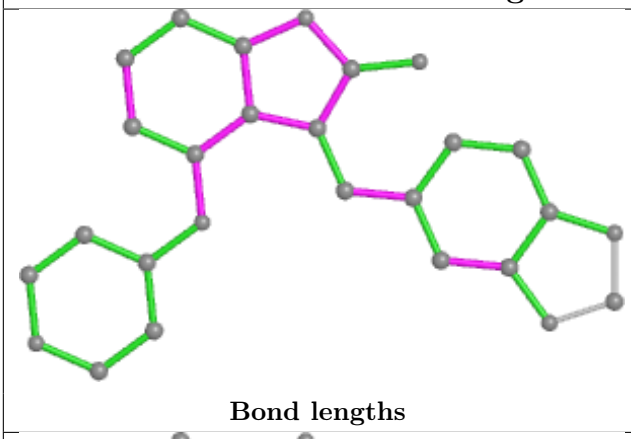


Torsions

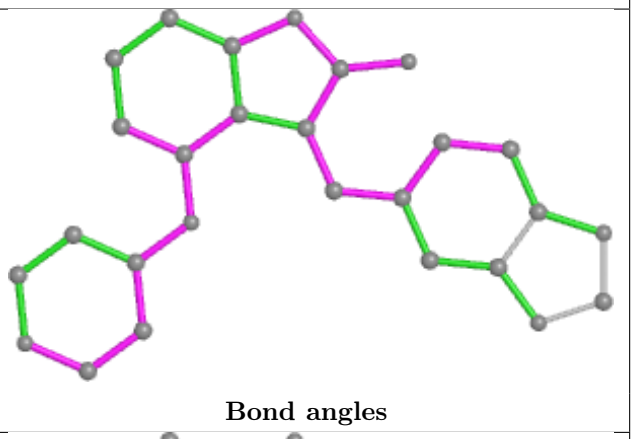


Rings

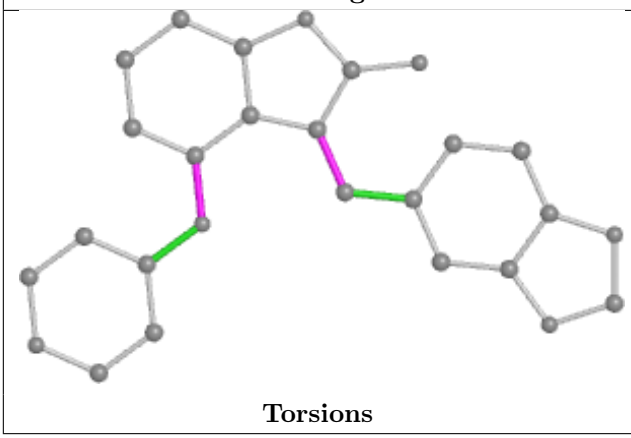
Ligand A1D46 A 402



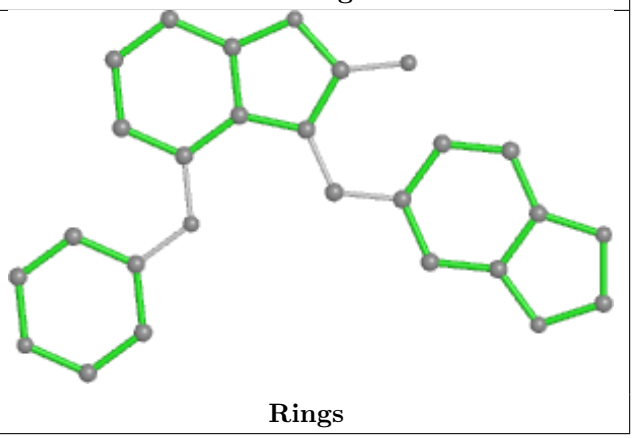
Bond lengths



Bond angles

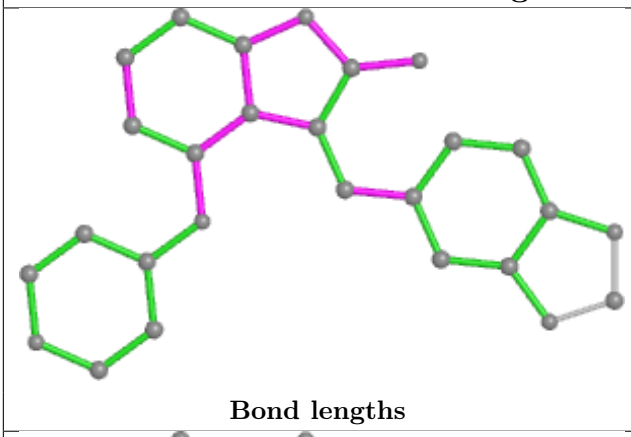


Torsions

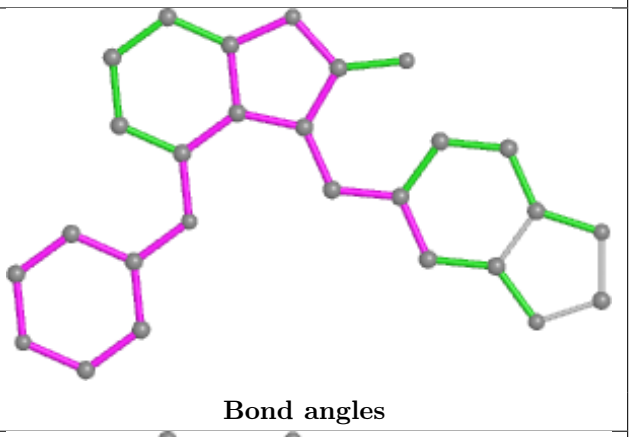


Rings

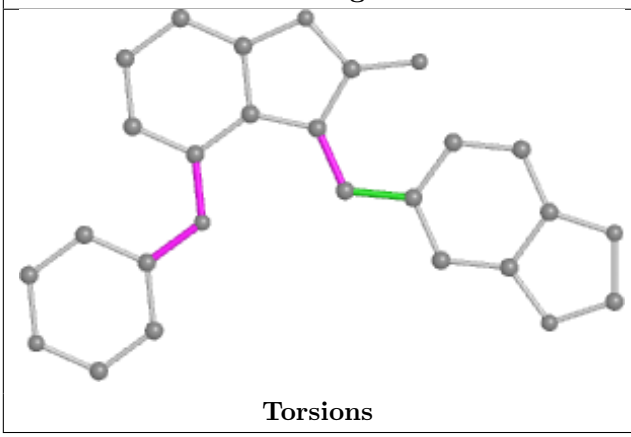
Ligand A1D46 J 402



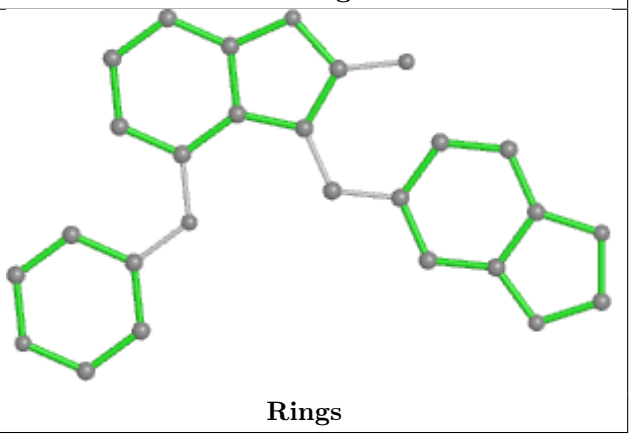
Bond lengths



Bond angles

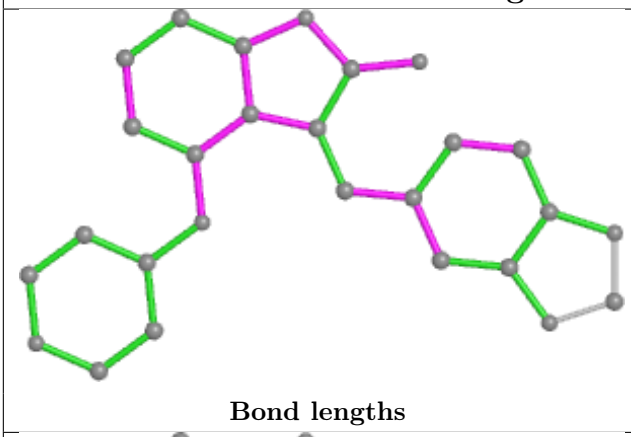


Torsions

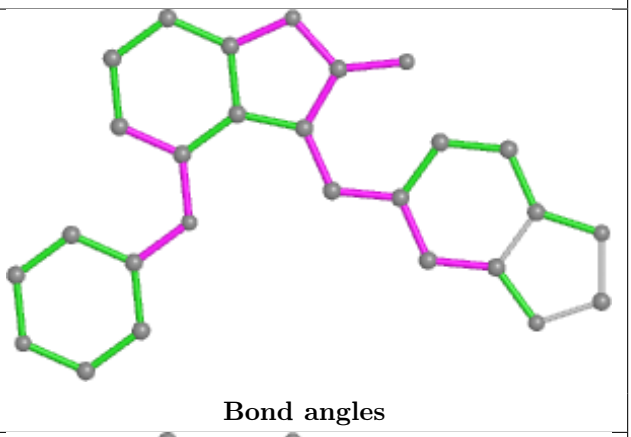


Rings

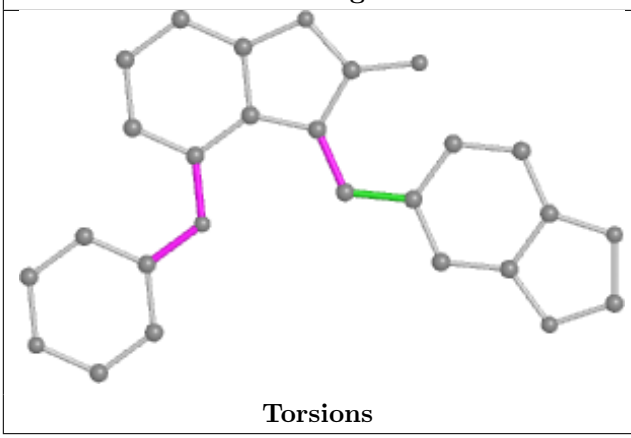
Ligand A1D46 D 402



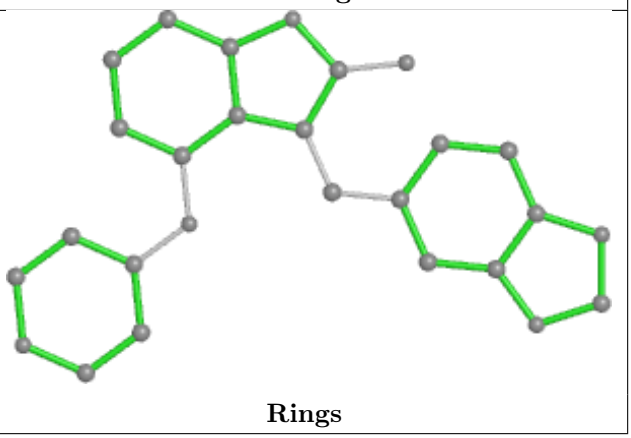
Bond lengths



Bond angles

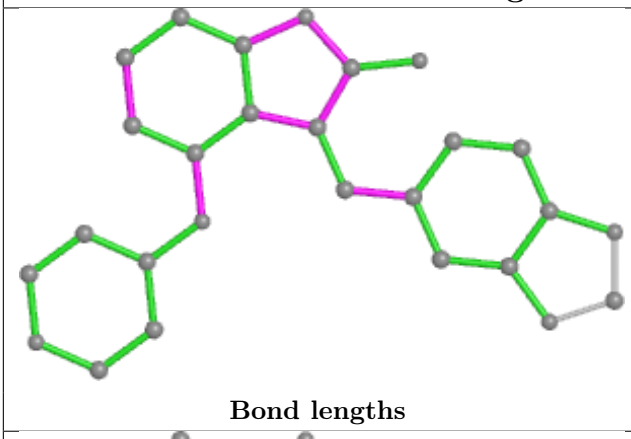


Torsions

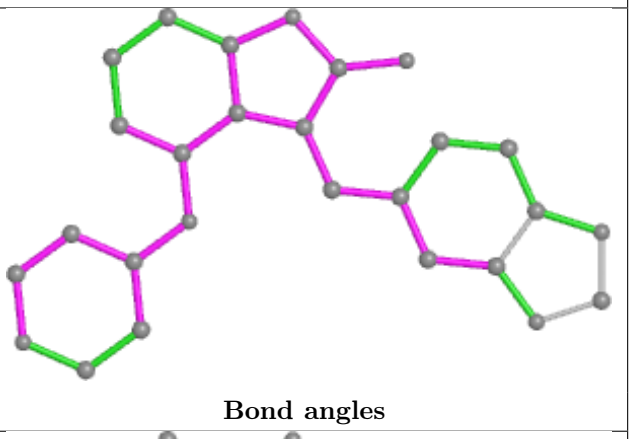


Rings

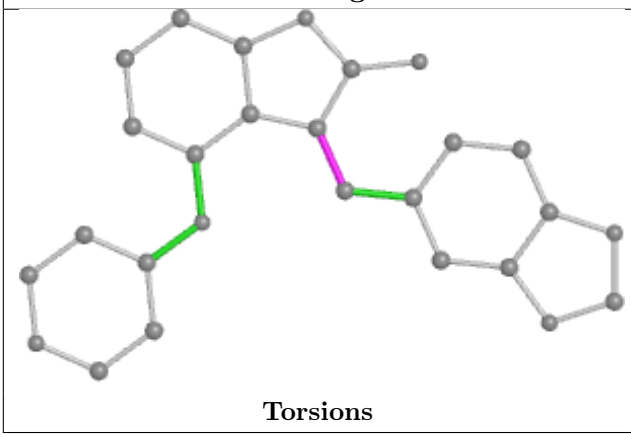
Ligand A1D46 X 402



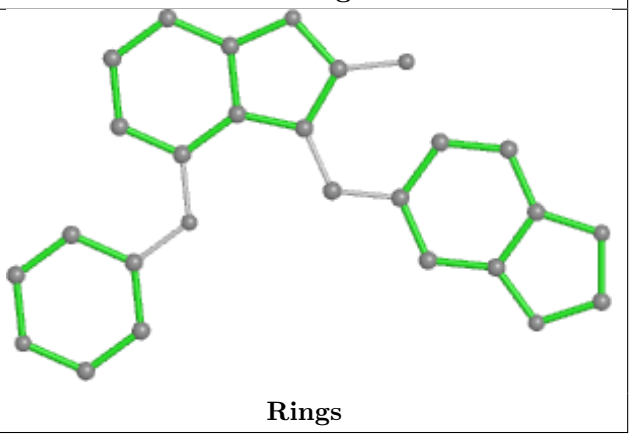
Bond lengths



Bond angles

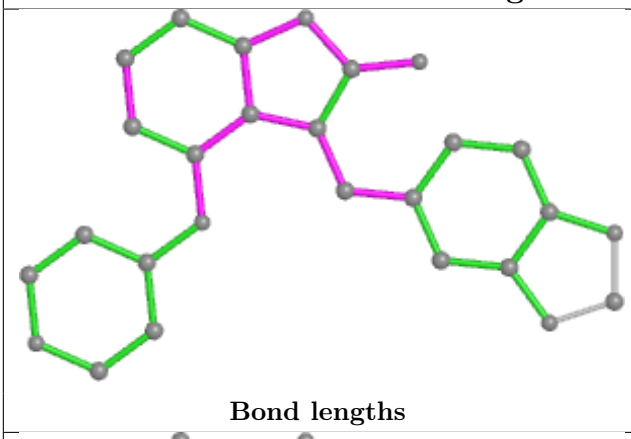


Torsions

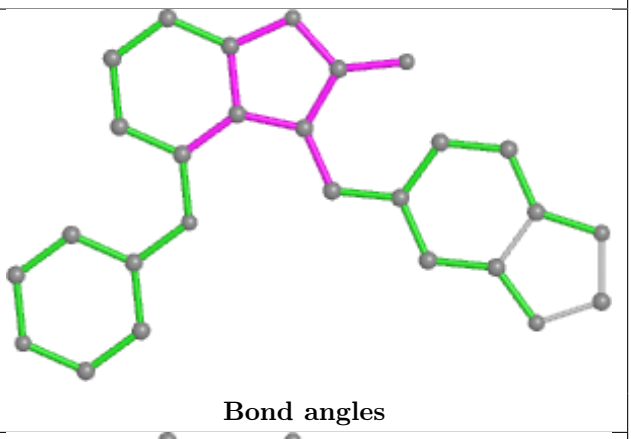


Rings

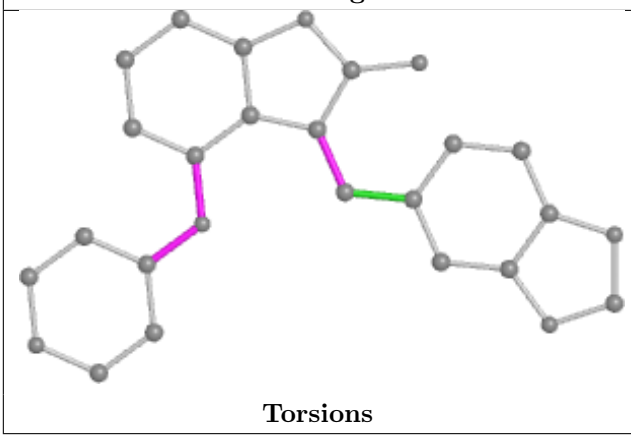
Ligand A1D46 G 402



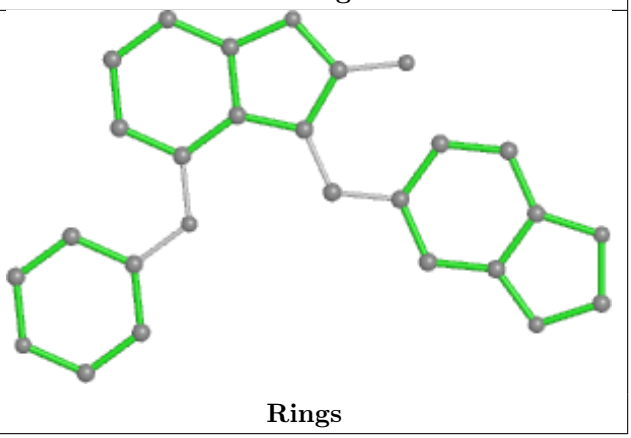
Bond lengths



Bond angles

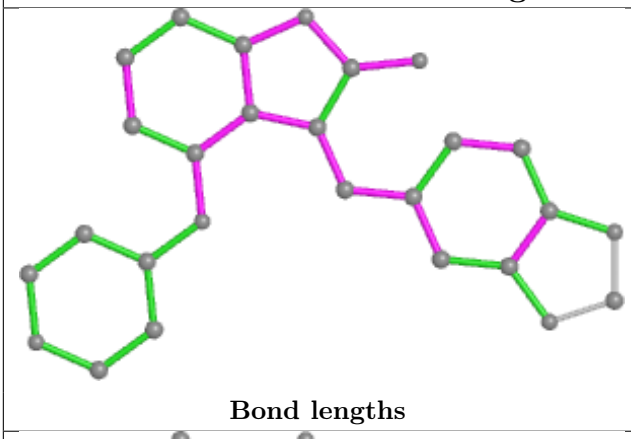


Torsions

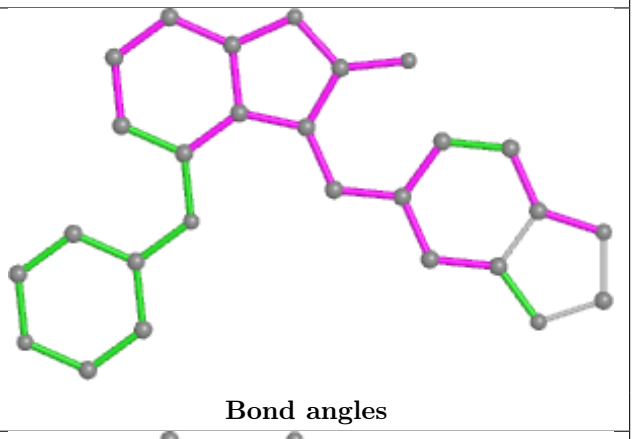


Rings

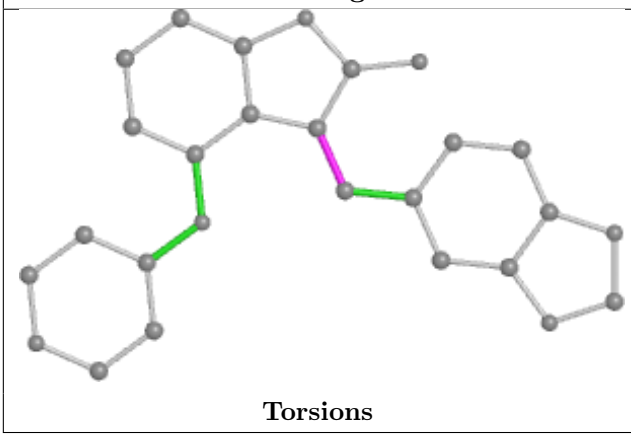
Ligand A1D46 F 402



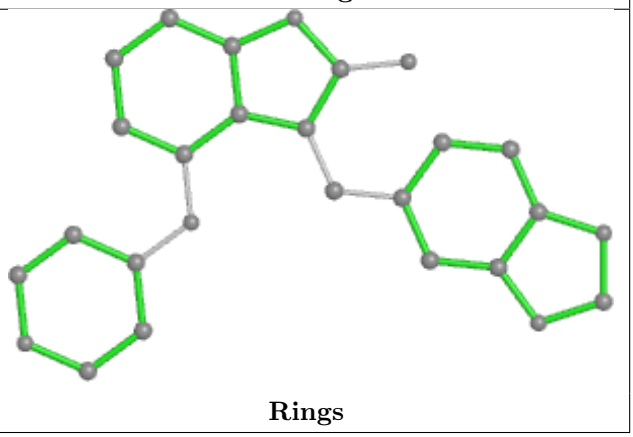
Bond lengths



Bond angles

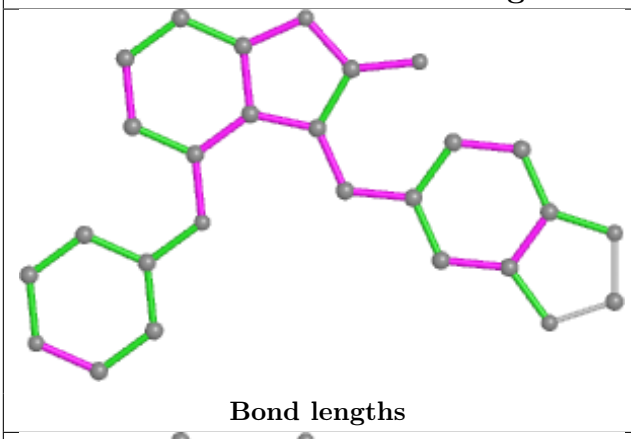


Torsions

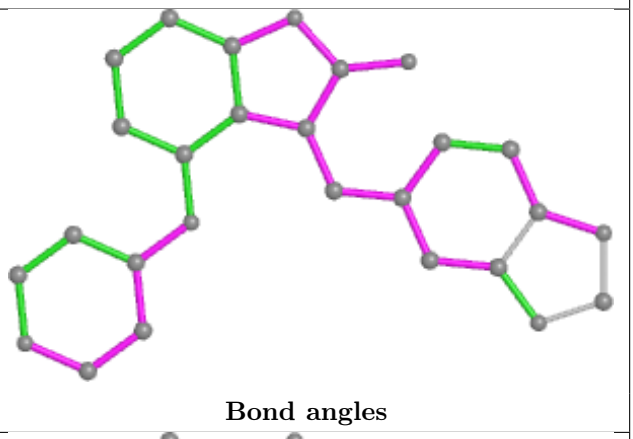


Rings

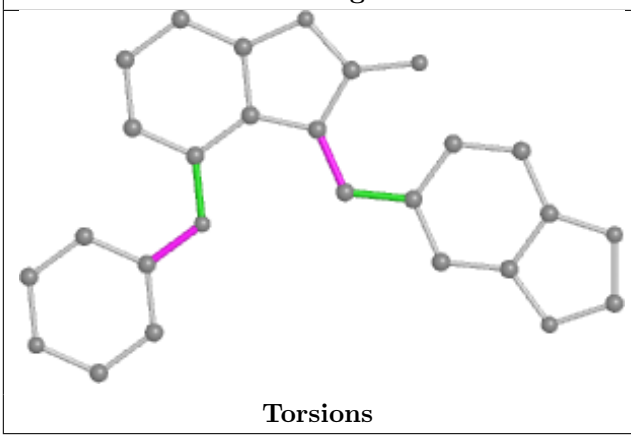
Ligand A1D46 C 402



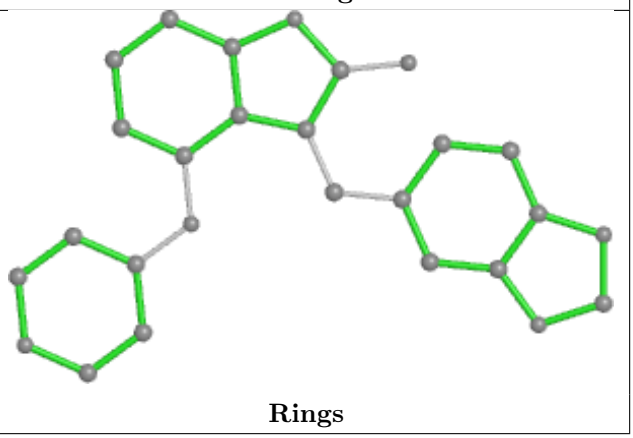
Bond lengths



Bond angles

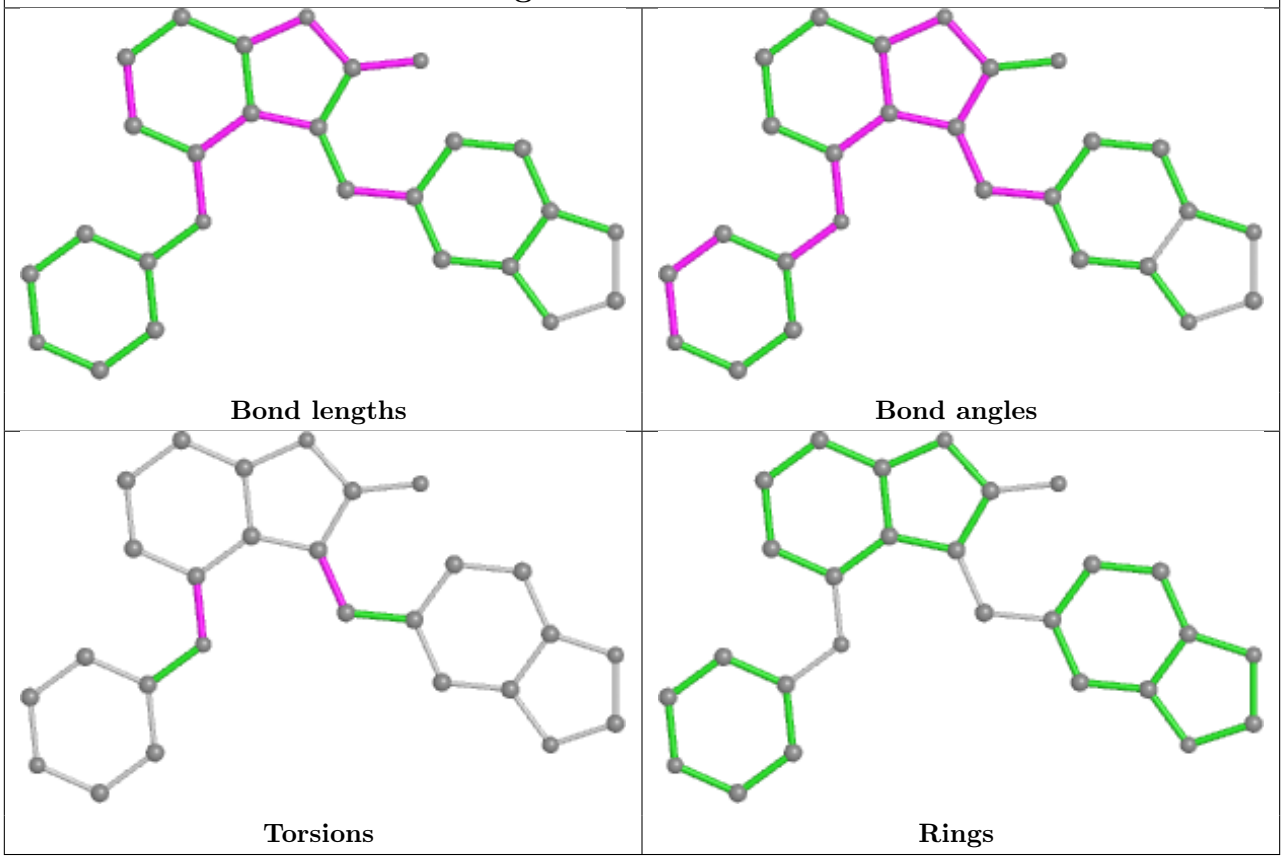


Torsions



Rings

Ligand A1D46 I 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	312/313 (99%)	-0.43	4 (1%)	77	61	30, 44, 67, 115	0
1	B	312/313 (99%)	-0.53	2 (0%)	89	80	33, 45, 68, 108	0
1	C	312/313 (99%)	-0.44	3 (0%)	82	70	26, 37, 58, 95	0
1	D	312/313 (99%)	-0.42	4 (1%)	77	61	31, 51, 76, 121	0
1	E	312/313 (99%)	-0.23	5 (1%)	72	53	34, 59, 84, 120	0
1	F	312/313 (99%)	-0.30	3 (0%)	82	70	36, 58, 84, 126	0
1	G	312/313 (99%)	-0.02	12 (3%)	40	21	42, 68, 111, 140	0
1	H	312/313 (99%)	-0.01	10 (3%)	47	26	44, 72, 100, 136	0
1	I	312/313 (99%)	0.25	11 (3%)	44	23	57, 96, 118, 131	0
1	J	312/313 (99%)	0.57	35 (11%)	5	2	65, 109, 132, 148	0
1	X	313/313 (100%)	-0.38	4 (1%)	77	61	25, 44, 63, 122	0
All	All	3433/3443 (99%)	-0.18	93 (2%)	54	32	25, 58, 114, 148	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	322	GLY	7.2
1	H	72	LEU	7.1
1	E	70	VAL	7.0
1	J	231	TRP	6.8
1	E	72	LEU	6.3
1	A	71	PRO	6.2
1	D	71	PRO	6.2
1	F	71	PRO	6.0
1	F	70	VAL	5.9
1	X	71	PRO	5.9
1	E	71	PRO	5.9
1	A	72	LEU	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	231	TRP	5.6
1	G	71	PRO	5.4
1	D	73	ILE	5.3
1	H	231	TRP	5.3
1	C	70	VAL	5.1
1	G	73	ILE	5.0
1	X	70	VAL	4.9
1	G	72	LEU	4.6
1	G	382	LEU	4.4
1	B	71	PRO	4.4
1	H	73	ILE	4.3
1	I	320	PRO	4.2
1	J	382	LEU	4.2
1	D	70	VAL	4.2
1	I	232	GLY	4.2
1	C	71	PRO	3.9
1	I	322	GLY	3.8
1	D	72	LEU	3.8
1	J	72	LEU	3.8
1	G	70	VAL	3.7
1	G	80	ARG	3.7
1	G	320	PRO	3.5
1	G	322	GLY	3.5
1	X	72	LEU	3.4
1	I	176	PRO	3.4
1	J	211	GLN	3.3
1	A	73	ILE	3.3
1	J	198	ALA	3.3
1	J	81	LEU	3.3
1	I	70	VAL	3.3
1	J	157	PRO	3.2
1	J	135	ASP	3.2
1	X	73	ILE	3.2
1	J	70	VAL	3.0
1	J	380	LEU	2.9
1	J	251	PRO	2.9
1	J	228	LEU	2.9
1	I	234	LYS	2.9
1	E	320	PRO	2.9
1	J	312	VAL	2.8
1	J	212	ALA	2.8
1	J	305	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	323	SER	2.7
1	J	253	SER	2.7
1	J	210	LYS	2.7
1	J	71	PRO	2.7
1	J	84	VAL	2.7
1	J	73	ILE	2.7
1	H	71	PRO	2.7
1	J	322	GLY	2.7
1	A	70	VAL	2.6
1	H	78	GLU	2.6
1	J	194	LEU	2.5
1	J	154	THR	2.5
1	I	149	GLY	2.5
1	G	321	PHE	2.5
1	B	72	LEU	2.5
1	I	73	ILE	2.5
1	H	70	VAL	2.4
1	C	72	LEU	2.4
1	J	129	GLY	2.4
1	G	76	LEU	2.4
1	J	107	PRO	2.3
1	J	252	HIS	2.3
1	F	73	ILE	2.3
1	J	140	SER	2.3
1	J	357	GLU	2.3
1	H	228	LEU	2.2
1	G	294	SER	2.2
1	J	220	LEU	2.2
1	I	236	SER	2.2
1	J	176	PRO	2.1
1	G	301	ARG	2.1
1	J	206	SER	2.1
1	E	382	LEU	2.1
1	J	173	LEU	2.1
1	H	234	LYS	2.0
1	J	250	ILE	2.0
1	J	301	ARG	2.0
1	J	195	LEU	2.0
1	I	129	GLY	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)

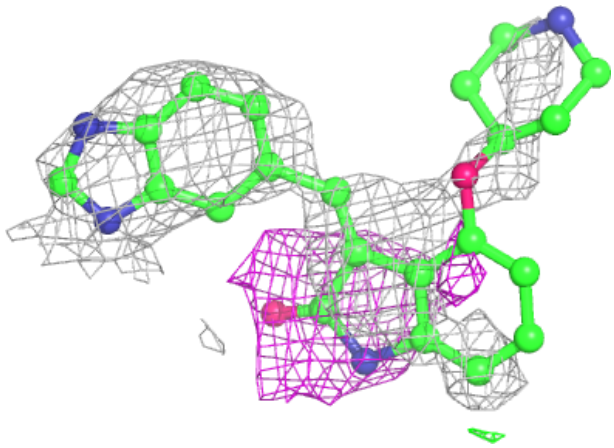
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

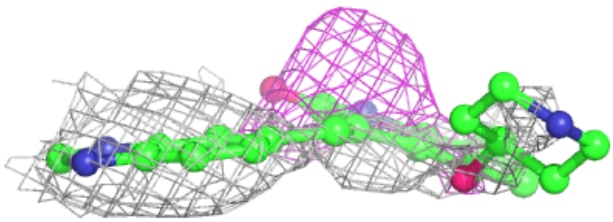
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1D46	G	402	27/27	0.66	0.58	70,90,100,105	0
3	A1D46	B	402	27/27	0.67	0.44	55,79,105,116	0
3	A1D46	H	402	27/27	0.67	0.58	77,106,118,122	0
2	ZN	H	401	1/1	0.69	0.38	142,142,142,142	0
3	A1D46	J	402	27/27	0.70	0.53	100,112,120,122	0
3	A1D46	F	402	27/27	0.72	0.49	61,81,93,94	0
3	A1D46	I	402	27/27	0.74	0.39	95,101,112,115	0
3	A1D46	A	402	27/27	0.79	0.41	59,76,94,102	0
3	A1D46	C	402	27/27	0.81	0.34	47,74,87,89	0
2	ZN	I	401	1/1	0.82	0.17	138,138,138,138	0
3	A1D46	X	402	27/27	0.86	0.31	49,62,70,72	0
2	ZN	X	401	1/1	0.87	0.08	86,86,86,86	0
3	A1D46	D	402	27/27	0.88	0.35	53,78,101,106	0
3	A1D46	E	402	27/27	0.89	0.28	66,75,83,86	0
2	ZN	F	401	1/1	0.92	0.14	105,105,105,105	0
2	ZN	E	401	1/1	0.92	0.09	107,107,107,107	0
2	ZN	G	401	1/1	0.93	0.19	121,121,121,121	0
2	ZN	J	401	1/1	0.95	0.06	130,130,130,130	0
2	ZN	A	401	1/1	0.96	0.06	100,100,100,100	0
2	ZN	C	401	1/1	0.97	0.09	102,102,102,102	0
2	ZN	B	401	1/1	0.97	0.17	93,93,93,93	0
2	ZN	D	401	1/1	0.98	0.07	98,98,98,98	0

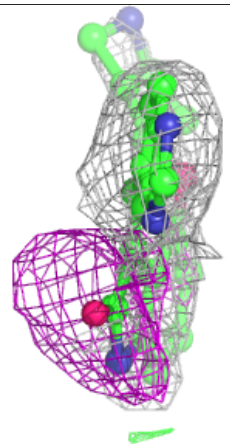
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1D46 G 402:

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

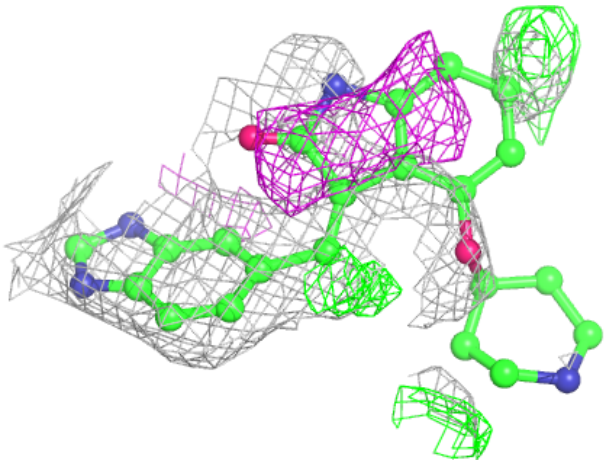


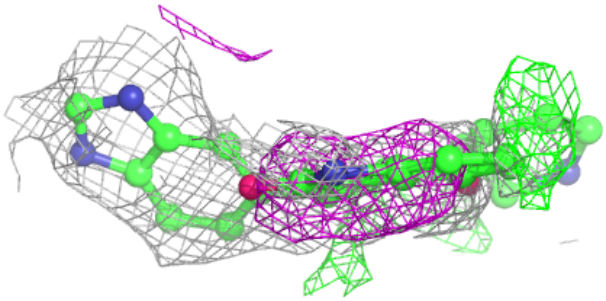


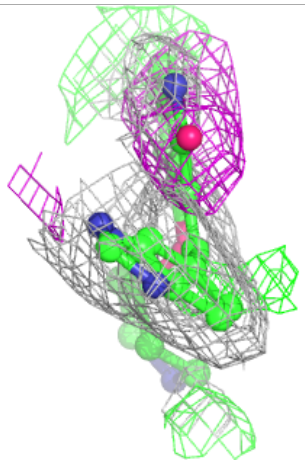


Electron density around A1D46 B 402:

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

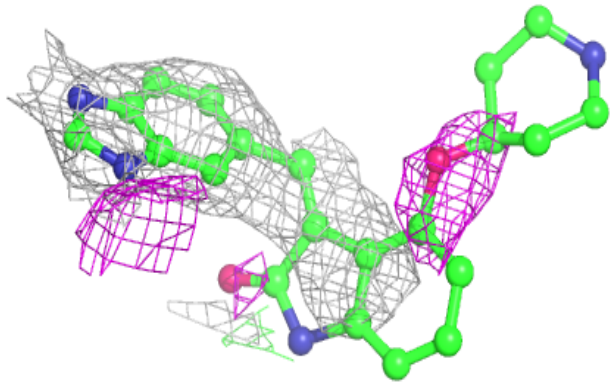


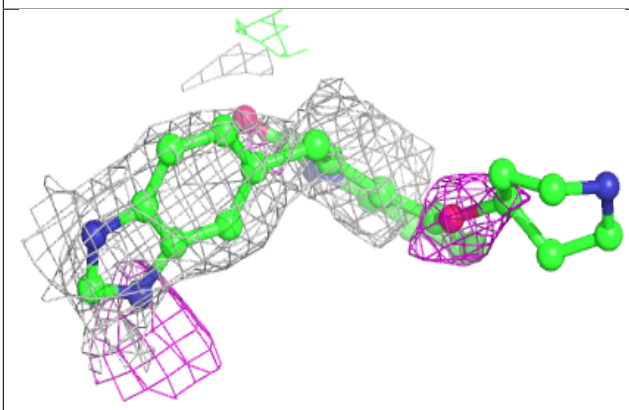


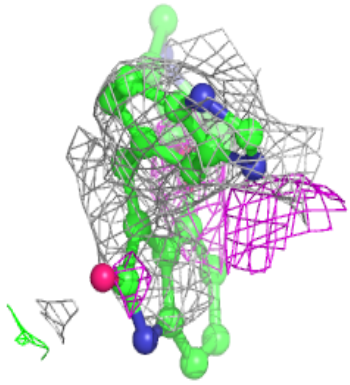


Electron density around A1D46 H 402:

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

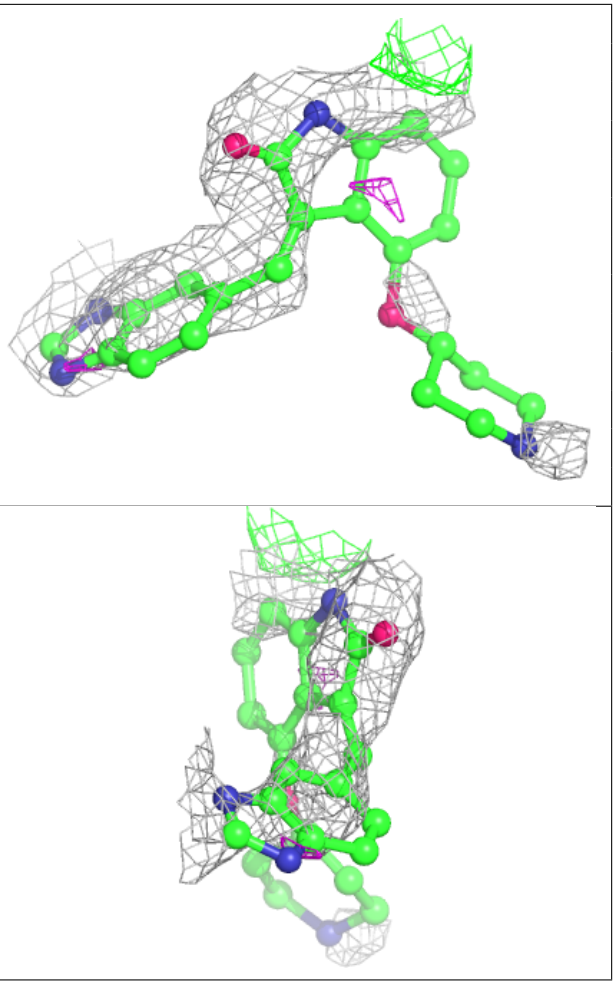


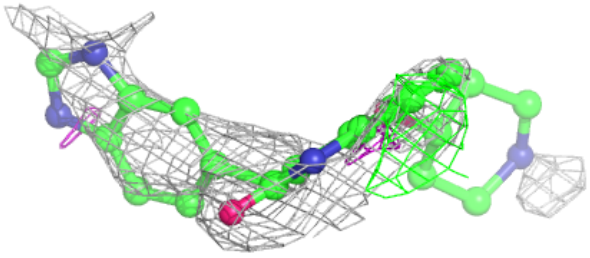




Electron density around A1D46 J 402:

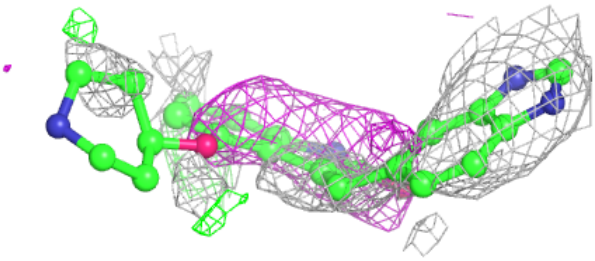
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

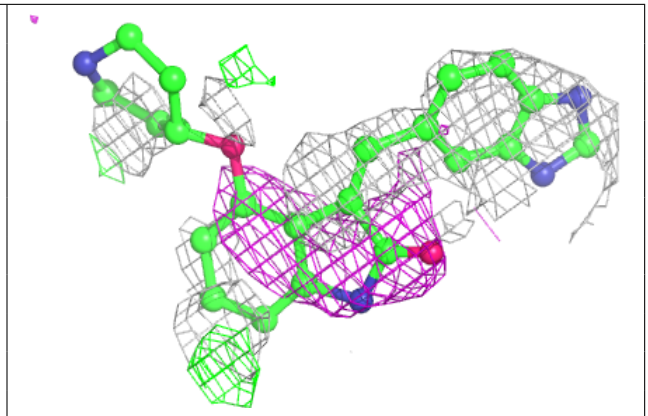


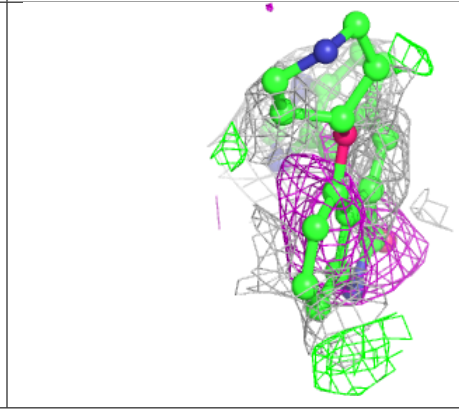


Electron density around A1D46 F 402:

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

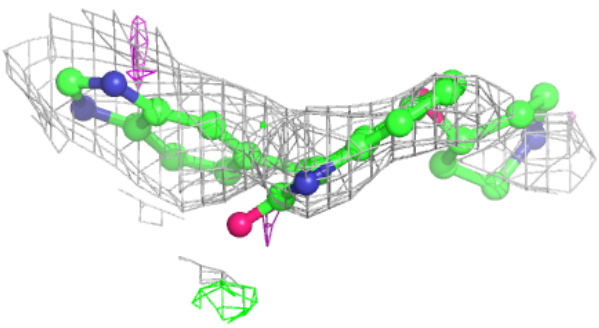


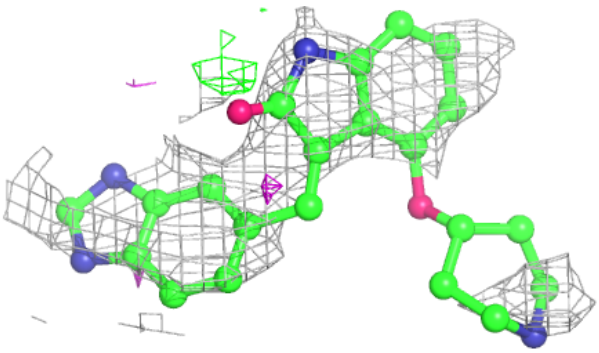


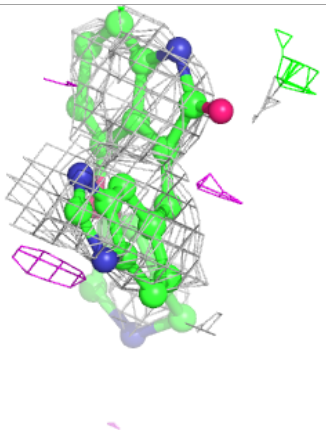


Electron density around A1D46 I 402:

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

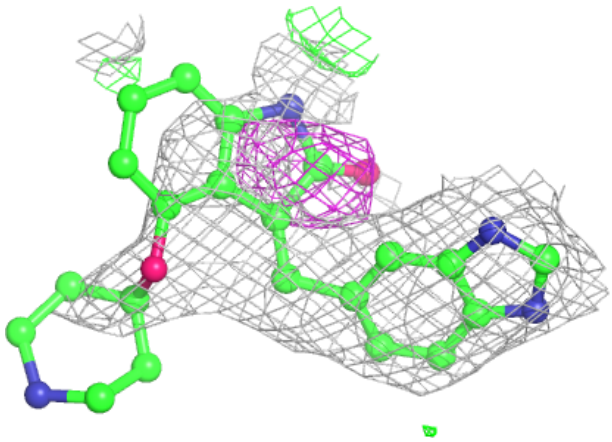


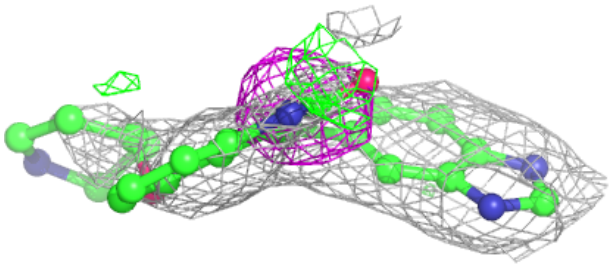


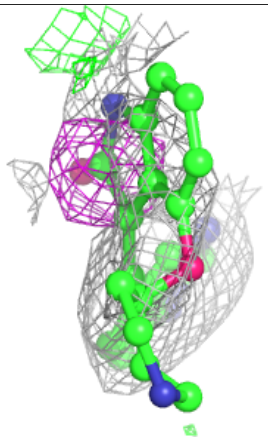


Electron density around A1D46 A 402:

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

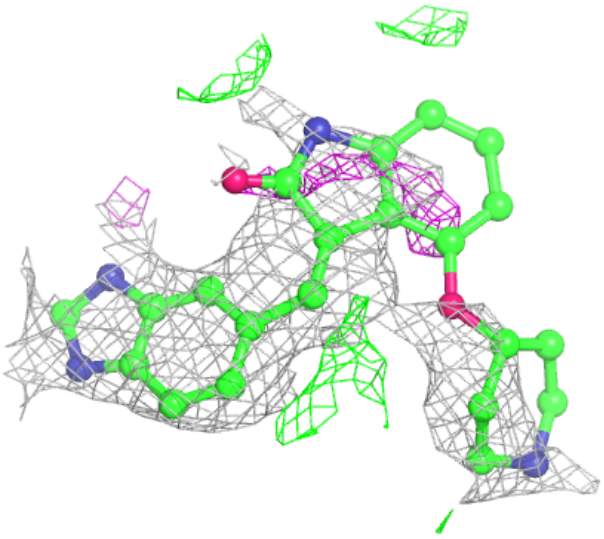


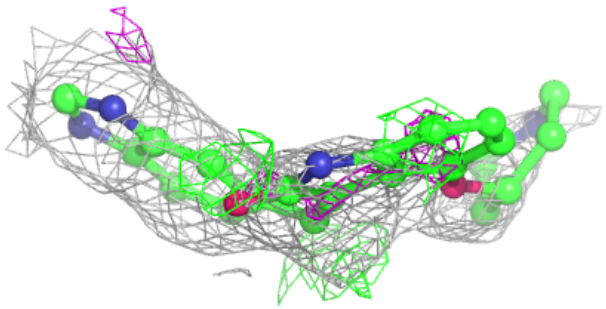


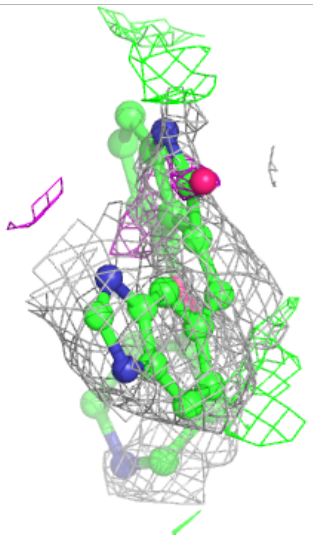


Electron density around A1D46 C 402:

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

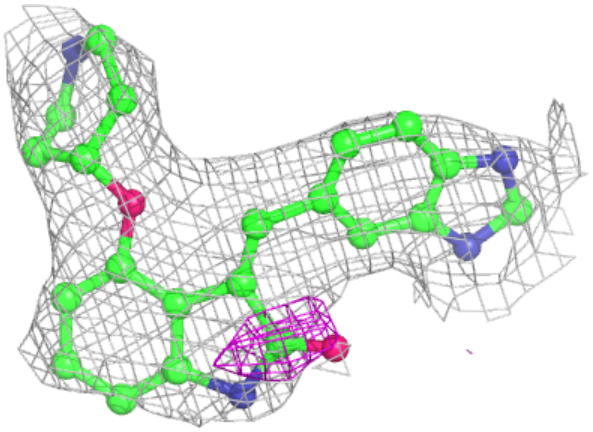


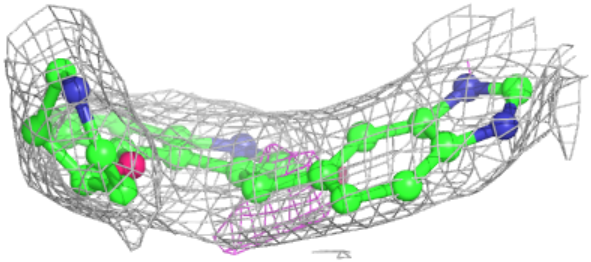


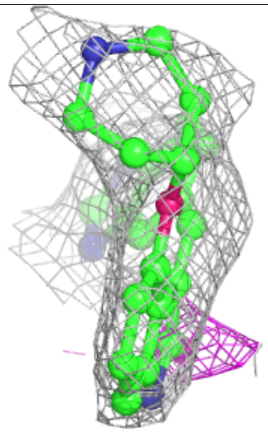


Electron density around A1D46 X 402:

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

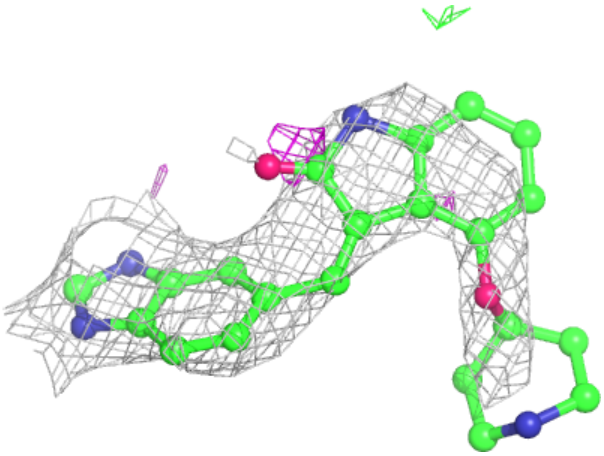


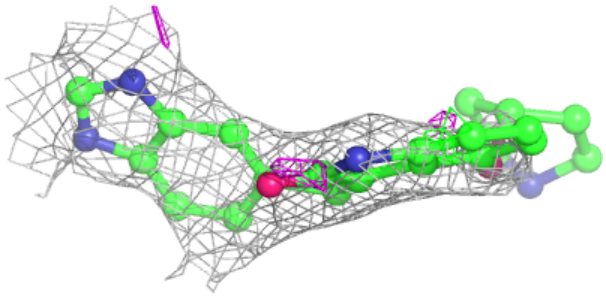


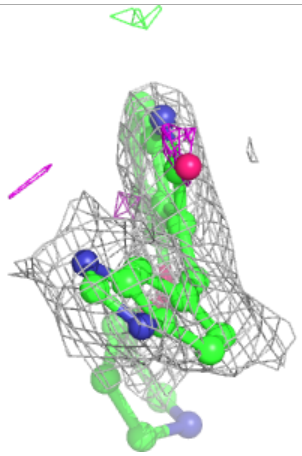


Electron density around A1D46 D 402:

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

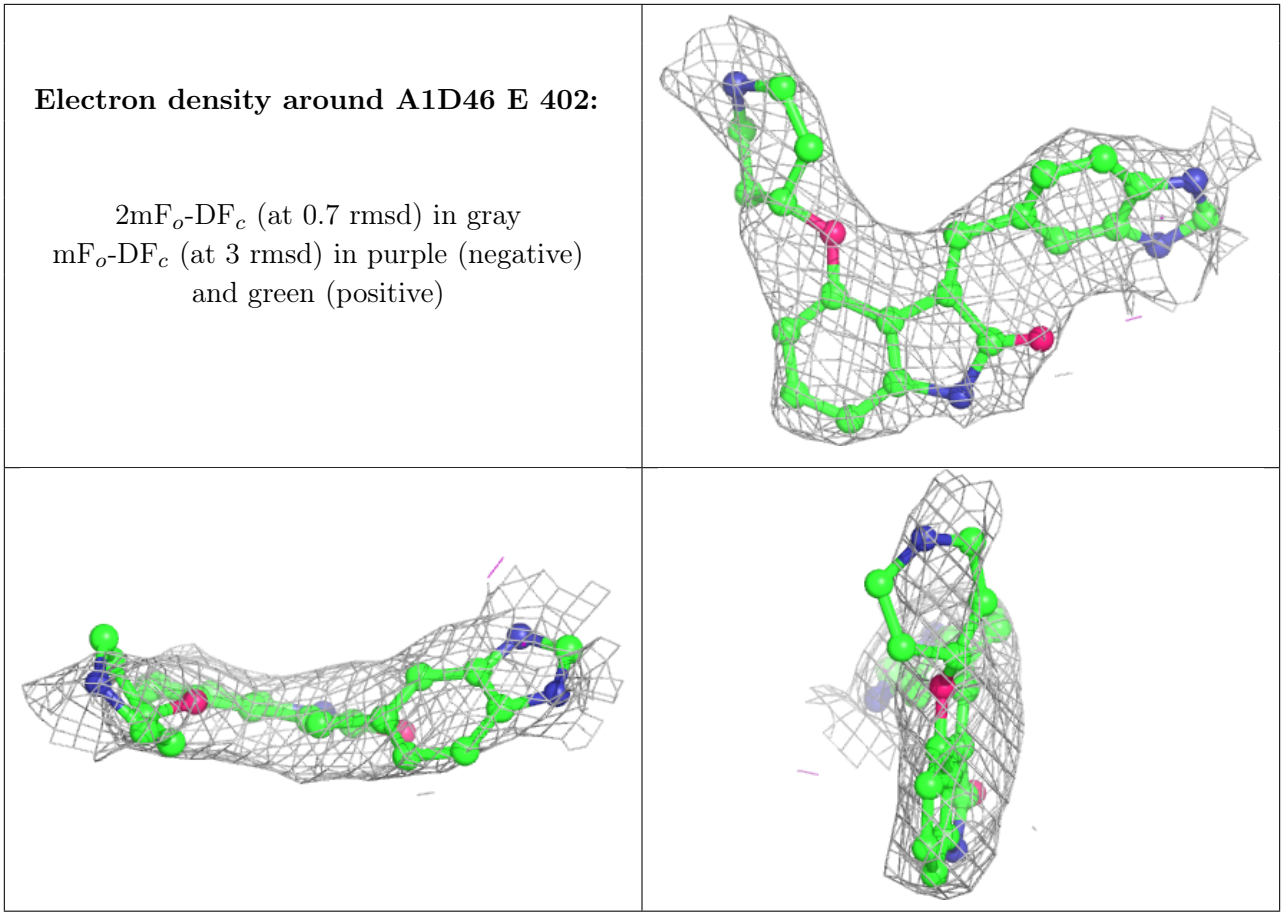






Electron density around A1D46 E 402:

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



6.5 Other polymers

There are no such residues in this entry.