



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:06 AM UTC

PDB ID : 2ZBK / pdb_00002zbk
Title : Crystal structure of an intact type II DNA topoisomerase: insights into DNA transfer mechanisms
Authors : Graille, M.; Cladiere, L.; Durand, D.; Lecointe, F.; Forterre, P.; van Tilbeurgh, H.; Paris-Sud Yeast Structural Genomics (YSG)
Deposited on : 2007-10-22
Resolution : 3.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

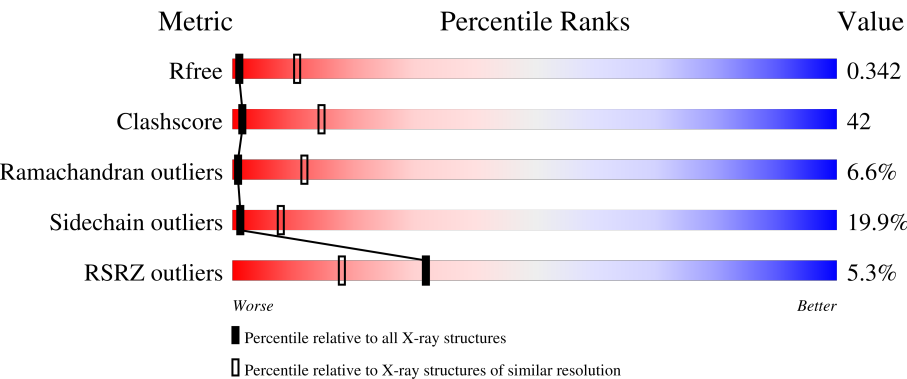
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.56 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	389	7% 21%43%23%•11%
1	C	389	7% 21%43%21%•11%
1	E	389	6% 22%43%21%•11%
1	G	389	5% 23%42%20%•11%

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Mol	Chain	Length	Quality of chain
2	B	530	4% 48% 38% 8% 5%
2	D	530	4% 49% 39% 7% 5%
2	F	530	3% 49% 38% 8% 5%
2	H	530	6% 48% 39% 8% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27776 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.

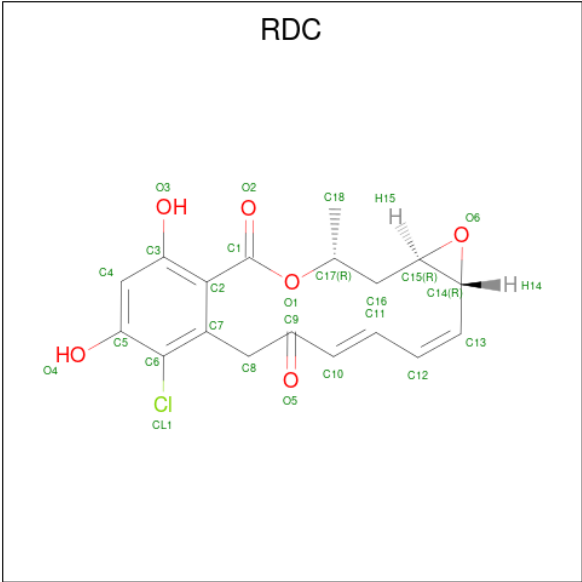
- Molecule 1 is a protein called Type II DNA topoisomerase VI subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			
1	C	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			
1	E	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			
1	G	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			

- Molecule 2 is a protein called Type 2 DNA topoisomerase 6 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			
2	D	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			
2	F	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			
2	H	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			

- Molecule 3 is RADICICOL (CCD ID: RDC) (formula: C₁₈H₁₇ClO₆).

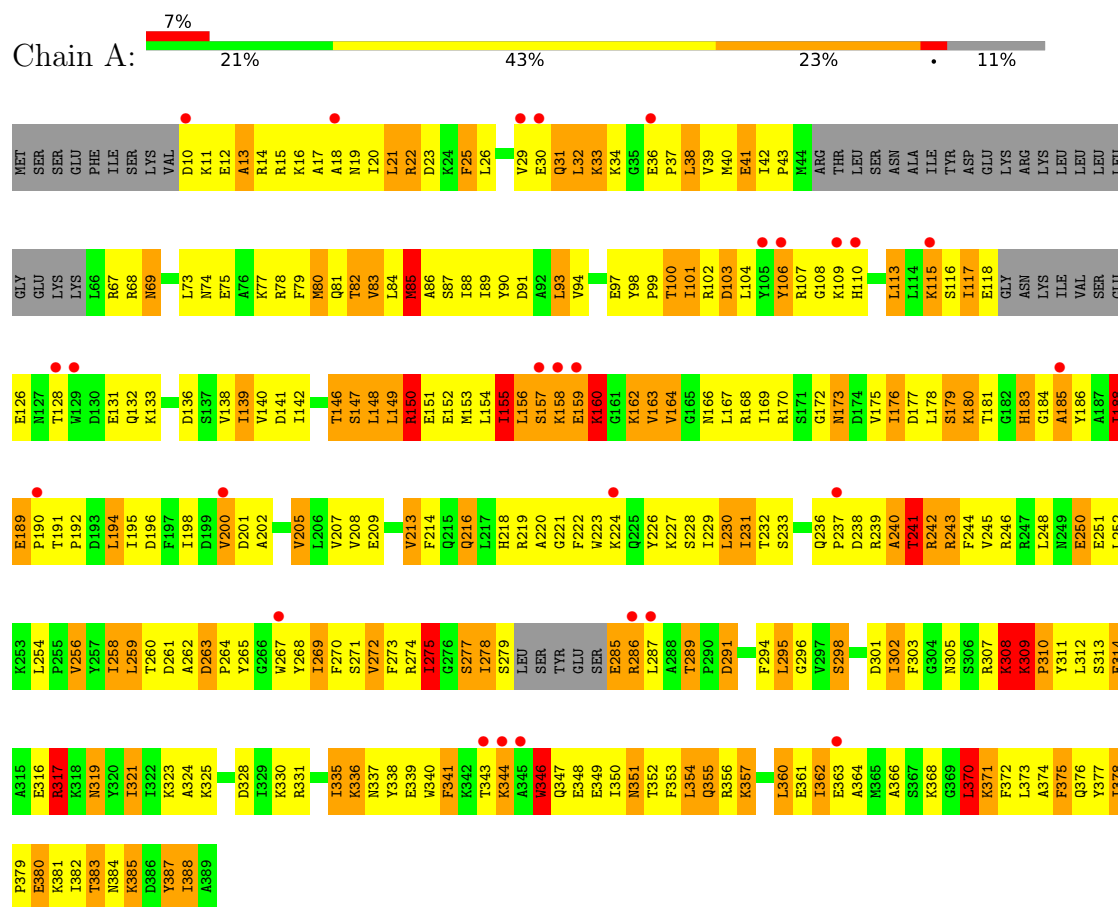


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	Cl	O	0	0
			25	18	1	6		
3	D	1	Total	C	Cl	O	0	0
			25	18	1	6		
3	F	1	Total	C	Cl	O	0	0
			25	18	1	6		
3	H	1	Total	C	Cl	O	0	0
			25	18	1	6		

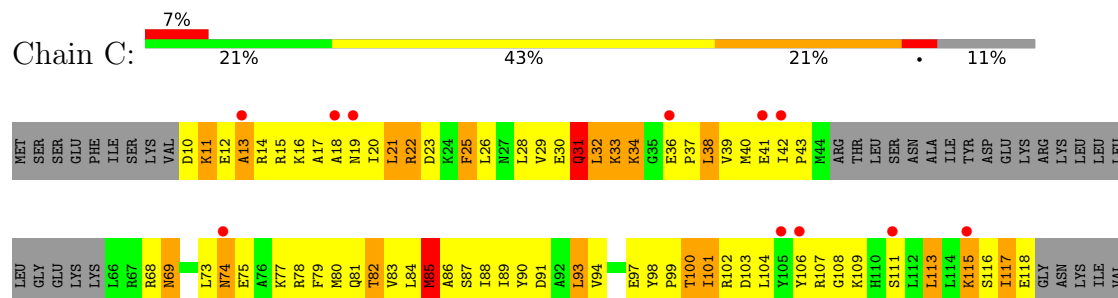
3 Residue-property plots

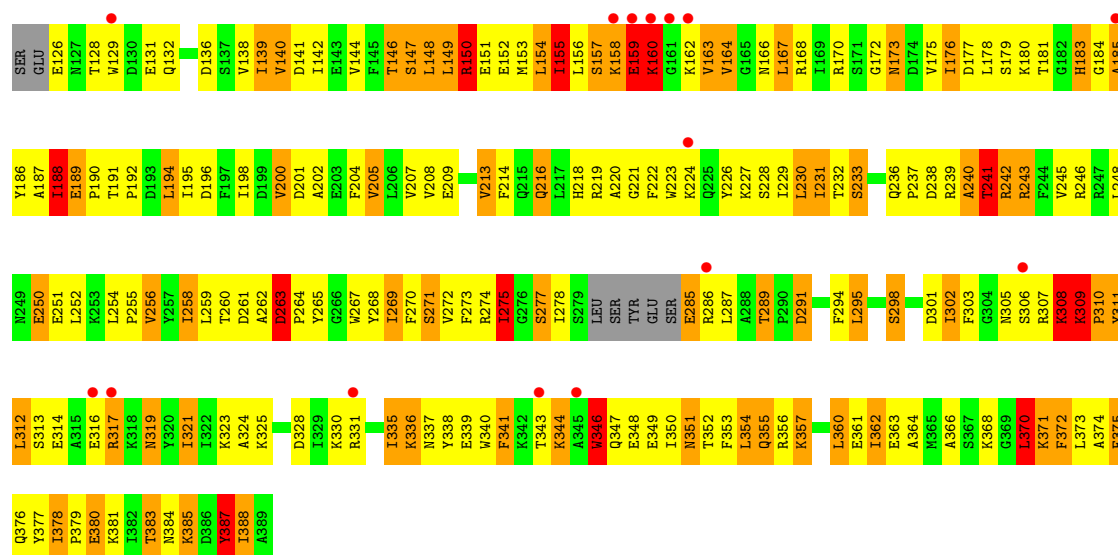
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Type II DNA topoisomerase VI subunit A

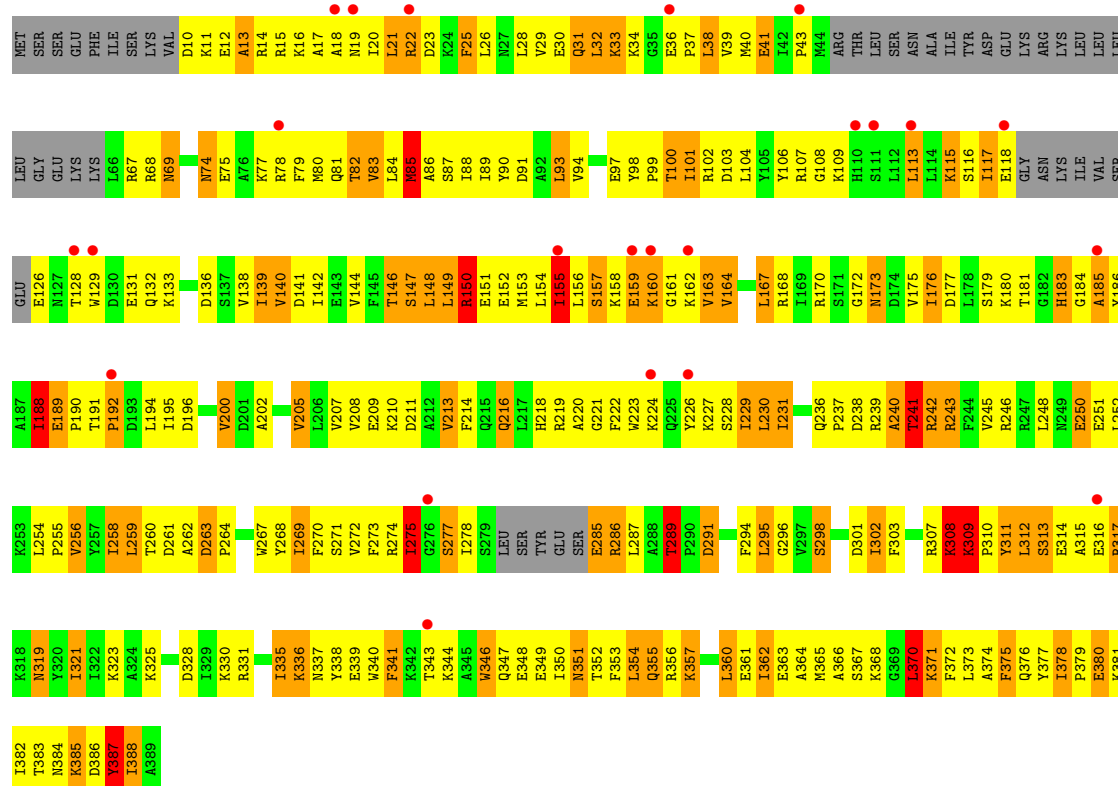
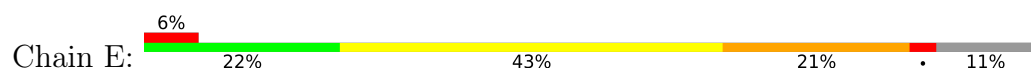


• Molecule 1: Type II DNA topoisomerase VI subunit A

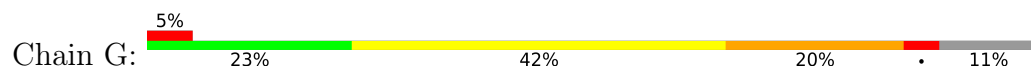


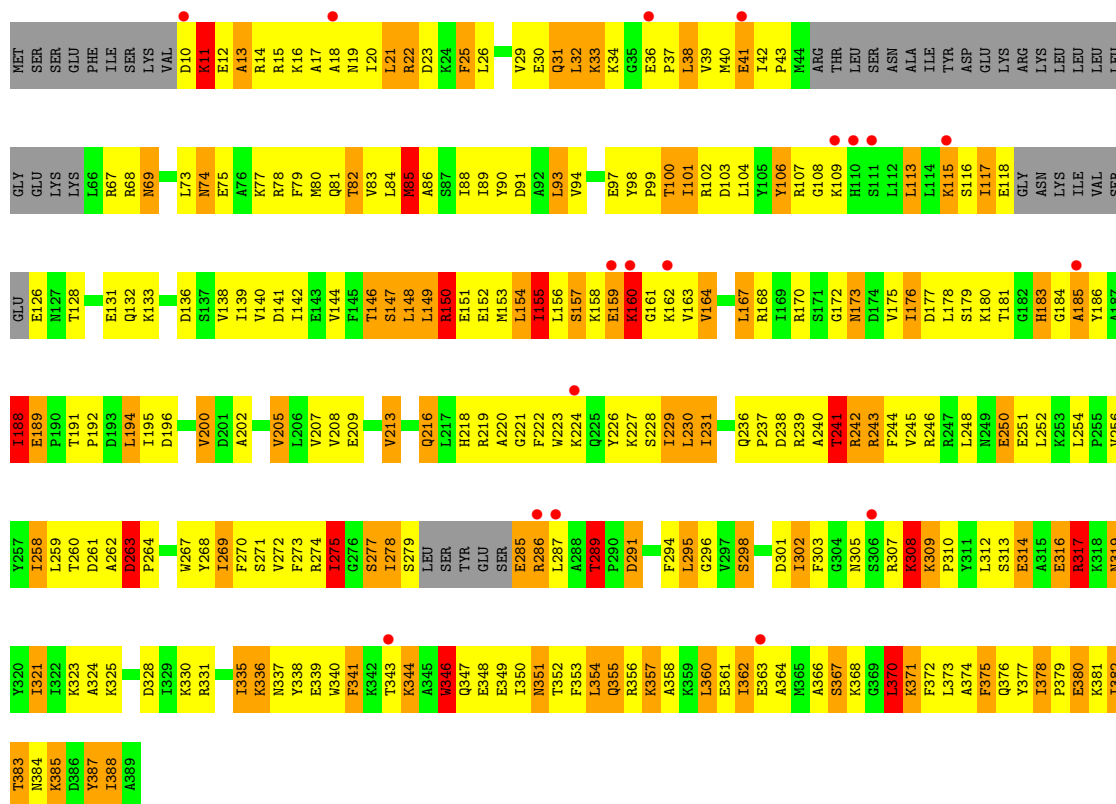


• Molecule 1: Type II DNA topoisomerase VI subunit A

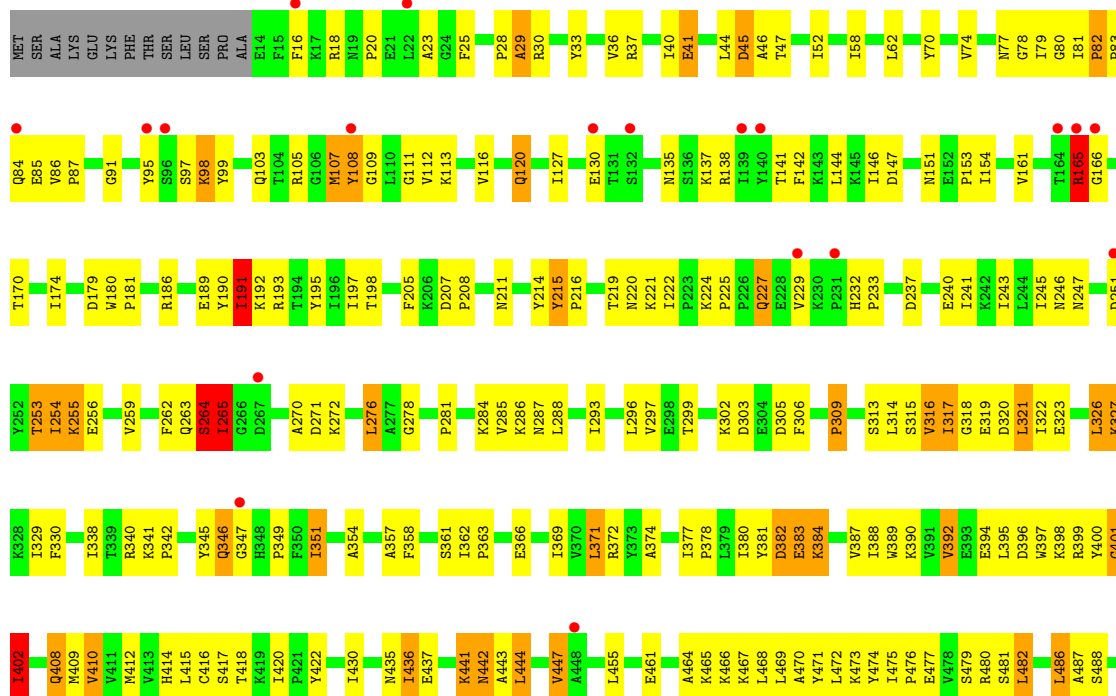


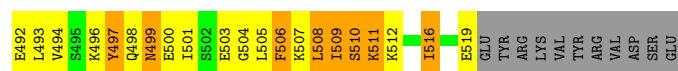
• Molecule 1: Type II DNA topoisomerase VI subunit A



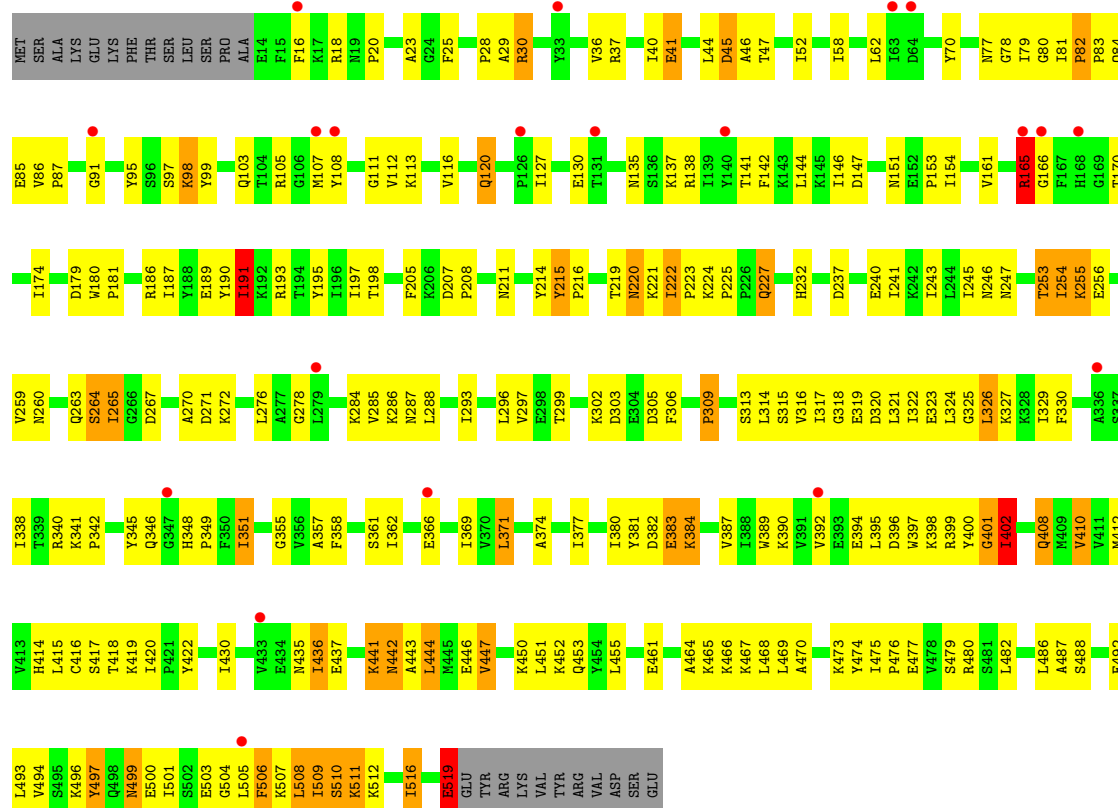


• Molecule 2: Type 2 DNA topoisomerase 6 subunit B

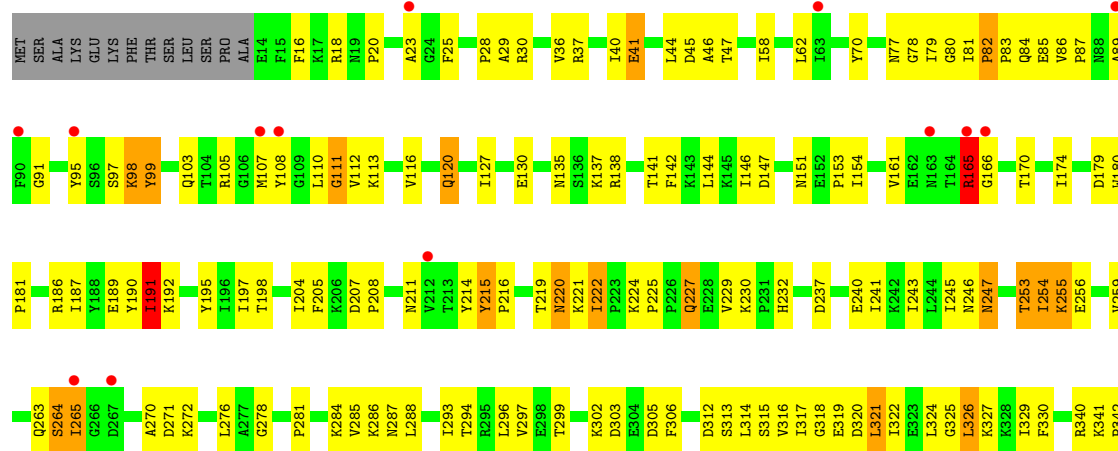




• Molecule 2: Type 2 DNA topoisomerase 6 subunit B



• Molecule 2: Type 2 DNA topoisomerase 6 subunit B





• Molecule 2: Type 2 DNA topoisomerase 6 subunit B

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.96Å 200.53Å 329.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.56 19.99 – 3.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-3.56) 97.1 (19.99-3.56)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.312 , 0.333 0.339 , 0.342	Depositor DCC
R_{free} test set	4435 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	27776	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.95	5/2893 (0.2%)	1.17	22/3890 (0.6%)
1	C	0.94	3/2893 (0.1%)	1.29	20/3890 (0.5%)
1	E	0.88	2/2893 (0.1%)	1.15	15/3890 (0.4%)
1	G	0.82	0/2893	1.13	15/3890 (0.4%)
2	B	0.62	0/4161	0.93	10/5623 (0.2%)
2	D	0.68	2/4161 (0.0%)	0.89	6/5623 (0.1%)
2	F	0.54	0/4161	0.90	9/5623 (0.2%)
2	H	0.50	1/4161 (0.0%)	0.88	7/5623 (0.1%)
All	All	0.73	13/28216 (0.0%)	1.03	104/38052 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	2
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	519	GLU	C-O	28.01	1.79	1.23
1	A	317	ARG	C-N	14.55	1.53	1.34
1	C	158	LYS	C-N	12.59	1.54	1.33
1	C	310	PRO	C-N	9.67	1.48	1.33
1	E	317	ARG	C-N	9.07	1.46	1.34
1	E	311	TYR	C-N	-8.09	1.21	1.33
1	A	162	LYS	C-N	6.67	1.37	1.33
1	A	310	PRO	C-N	-6.58	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	519	GLU	CA-CB	6.35	1.66	1.53
2	H	458	LYS	N-CA	6.34	1.54	1.46
1	A	159	GLU	N-CA	5.77	1.52	1.45
1	C	160	LYS	N-CA	5.35	1.52	1.45
1	A	160	LYS	CA-CB	-5.29	1.46	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	LYS	O-C-N	-32.41	81.30	123.10
1	E	311	TYR	O-C-N	-17.18	98.93	122.46
1	C	160	LYS	CA-C-N	14.50	149.82	121.41
1	C	160	LYS	C-N-CA	14.50	149.82	121.41
1	A	241	THR	N-CA-C	-10.62	99.72	112.89
1	C	241	THR	N-CA-C	-10.58	100.32	113.01
2	D	519	GLU	CA-C-O	-10.00	103.80	120.80
1	G	241	THR	N-CA-C	-8.99	101.74	112.89
2	B	232	HIS	CA-C-N	8.98	131.06	119.84
2	B	232	HIS	C-N-CA	8.98	131.06	119.84
2	D	232	HIS	CA-C-N	8.92	130.99	119.84
2	D	232	HIS	C-N-CA	8.92	130.99	119.84
2	F	232	HIS	CA-C-N	8.91	130.97	119.84
2	F	232	HIS	C-N-CA	8.91	130.97	119.84
2	H	232	HIS	CA-C-N	8.83	130.88	119.84
2	H	232	HIS	C-N-CA	8.83	130.88	119.84
1	A	296	GLY	N-CA-C	-8.76	103.63	111.95
1	A	346	TRP	N-CA-C	-8.75	101.67	111.82
1	E	159	GLU	N-CA-C	8.54	123.33	109.59
1	A	341	PHE	N-CA-C	-8.07	103.26	113.43
1	E	241	THR	N-CA-C	-7.72	103.32	112.89
1	E	346	TRP	N-CA-C	-7.47	103.15	111.82
2	F	450	LYS	N-CA-C	-7.47	104.16	113.28
1	G	346	TRP	N-CA-C	-7.46	103.17	111.82
1	E	308	LYS	N-CA-C	7.38	120.45	108.34
1	E	341	PHE	N-CA-C	-7.34	104.18	113.43
1	C	341	PHE	N-CA-C	-7.21	104.35	113.43
1	C	346	TRP	N-CA-C	-7.20	103.47	111.82
1	G	296	GLY	N-CA-C	-7.16	104.27	112.29
1	G	159	GLU	N-CA-C	7.13	121.46	109.76
1	G	341	PHE	N-CA-C	-7.05	104.54	113.43
1	C	31	GLN	N-CA-C	-6.67	107.02	114.62
1	A	159	GLU	N-CA-C	6.55	120.72	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	LYS	N-CA-C	6.55	119.14	108.26
2	H	82	PRO	CA-C-N	6.51	127.97	119.84
2	H	82	PRO	C-N-CA	6.51	127.97	119.84
1	A	286	ARG	N-CA-C	-6.49	103.43	112.25
1	A	308	LYS	N-CA-C	6.49	118.98	108.34
1	E	286	ARG	N-CA-C	-6.39	103.56	112.25
1	C	309	LYS	CA-C-N	6.36	126.54	120.31
1	C	309	LYS	C-N-CA	6.36	126.54	120.31
1	G	263	ASP	CA-C-N	6.34	125.97	119.56
1	G	263	ASP	C-N-CA	6.34	125.97	119.56
1	G	308	LYS	N-CA-C	6.34	118.73	108.34
2	B	327	LYS	N-CA-C	-6.25	105.31	113.12
2	F	82	PRO	CA-C-N	6.17	127.55	119.84
2	F	82	PRO	C-N-CA	6.17	127.55	119.84
2	D	82	PRO	CA-C-N	6.16	127.55	119.84
2	D	82	PRO	C-N-CA	6.16	127.55	119.84
2	H	456	SER	N-CA-C	-6.09	106.18	113.97
1	E	296	GLY	N-CA-C	-6.05	105.51	112.29
1	C	159	GLU	N-CA-C	6.04	118.99	107.75
1	G	160	LYS	CB-CA-C	-6.02	108.40	117.07
1	A	220	ALA	N-CA-C	-5.94	105.03	112.93
1	A	310	PRO	O-C-N	-5.93	115.66	123.13
2	D	165	ARG	N-CA-C	5.85	123.27	110.80
2	B	82	PRO	CA-C-N	5.85	127.16	119.84
2	B	82	PRO	C-N-CA	5.85	127.16	119.84
1	E	313	SER	N-CA-C	-5.83	102.83	110.53
1	A	310	PRO	CA-C-N	5.79	132.27	122.26
1	A	310	PRO	C-N-CA	5.79	132.27	122.26
1	C	220	ALA	N-CA-C	-5.77	105.25	112.93
1	G	157	SER	CA-C-O	5.74	121.27	117.94
1	A	157	SER	CB-CA-C	-5.74	108.81	117.07
2	B	321	LEU	N-CA-C	-5.73	105.12	111.71
1	C	163	VAL	CB-CA-C	-5.73	106.36	111.74
1	C	157	SER	CB-CA-C	-5.72	108.84	117.07
1	A	309	LYS	CA-C-N	5.69	126.17	120.14
1	A	309	LYS	C-N-CA	5.69	126.17	120.14
1	G	157	SER	CB-CA-C	-5.68	108.89	117.07
1	G	220	ALA	N-CA-C	-5.65	105.41	112.93
1	E	289	THR	N-CA-C	5.60	117.02	109.24
2	B	229	VAL	N-CA-C	5.55	115.53	107.88
1	A	157	SER	CA-C-O	5.47	121.11	117.94
2	B	165	ARG	N-CA-C	5.41	122.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	PRO	CA-C-N	-5.40	112.92	122.26
1	C	310	PRO	C-N-CA	-5.40	112.92	122.26
1	E	309	LYS	N-CA-C	5.40	115.81	109.60
1	E	163	VAL	CB-CA-C	-5.39	106.67	111.74
2	F	165	ARG	N-CA-C	5.39	122.28	110.80
2	H	165	ARG	N-CA-C	5.38	122.27	110.80
1	G	289	THR	N-CA-C	5.36	116.69	109.24
1	A	272	VAL	CB-CA-C	-5.34	105.05	112.04
2	F	321	LEU	N-CA-C	-5.33	105.58	111.71
1	E	157	SER	CB-CA-C	-5.32	109.41	117.07
2	F	230	LYS	N-CA-C	5.28	115.67	109.60
1	A	163	VAL	CB-CA-C	-5.26	106.79	111.74
1	G	317	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	C	256	VAL	N-CA-C	5.22	115.10	107.37
1	A	256	VAL	N-CA-C	5.22	115.10	107.37
1	A	158	LYS	N-CA-CB	-5.21	103.25	111.23
1	A	317	ARG	O-C-N	-5.21	115.90	122.20
1	A	156	LEU	CA-C-N	-5.20	117.42	123.04
1	A	156	LEU	C-N-CA	-5.20	117.42	123.04
2	H	459	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	C	263	ASP	CA-C-N	5.11	124.77	119.56
1	C	263	ASP	C-N-CA	5.11	124.77	119.56
2	F	393	GLU	N-CA-C	-5.10	107.18	113.41
1	E	256	VAL	N-CA-C	5.10	114.91	107.37
1	C	306	SER	N-CA-C	-5.07	106.36	112.54
1	G	286	ARG	N-CA-C	-5.07	105.36	112.25
2	B	29	ALA	N-CA-C	5.04	116.47	110.97
2	B	265	ILE	N-CA-C	5.02	119.78	109.34
1	E	220	ALA	N-CA-C	-5.02	106.25	112.93

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	160	LYS	Peptide,Mainchain
1	E	311	TYR	Mainchain
1	E	315	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2842	0	2895	409	0
1	C	2842	0	2894	421	0
1	E	2842	0	2895	389	0
1	G	2842	0	2895	388	0
2	B	4077	0	4181	212	0
2	D	4077	0	4181	204	0
2	F	4077	0	4181	208	0
2	H	4077	0	4181	222	0
3	B	25	0	15	5	0
3	D	25	0	15	7	0
3	F	25	0	15	5	0
3	H	25	0	17	4	0
All	All	27776	0	28365	2354	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (2354) 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:E:302:ILE:CG2	1:E:312:LEU:HD11	1.58	1.32
1:C:312:LEU:CD2	1:C:317:ARG:HD3	1.63	1.28
2:D:519:GLU:C	2:D:519:GLU:O	1.79	1.23
1:C:106:TYR:O	1:C:107:ARG:HD3	1.41	1.20
2:H:455:LEU:CD1	2:H:459:ARG:HH12	1.54	1.20
1:G:106:TYR:O	1:G:107:ARG:HD3	1.44	1.16
1:A:106:TYR:O	1:A:107:ARG:HD3	1.45	1.16
1:C:160:LYS:O	1:C:160:LYS:HG2	1.33	1.15
1:C:22:ARG:HG3	1:C:23:ASP:H	1.11	1.15
1:E:22:ARG:HG3	1:E:23:ASP:H	1.12	1.13
1:C:155:ILE:H	1:C:155:ILE:HD12	1.13	1.13
1:C:312:LEU:CD1	1:C:312:LEU:H	1.61	1.13
1:A:22:ARG:HG3	1:A:23:ASP:H	1.10	1.11
1:E:106:TYR:O	1:E:107:ARG:HD3	1.47	1.11
1:G:22:ARG:HG3	1:G:23:ASP:H	1.10	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ILE:HG22	1:C:312:LEU:HD21	1.27	1.10
2:F:401:GLY:HA3	2:F:455:LEU:HD21	1.16	1.10
2:D:400:TYR:HA	2:D:452:LYS:HE2	1.34	1.09
1:E:155:ILE:HD12	1:E:155:ILE:H	1.15	1.09
1:E:302:ILE:HG22	1:E:312:LEU:HD11	1.30	1.09
1:A:155:ILE:H	1:A:155:ILE:HD12	1.14	1.09
1:A:307:ARG:HD2	1:A:308:LYS:HZ3	0.99	1.09
1:E:176:ILE:HD11	1:G:176:ILE:HD11	1.11	1.09
1:A:176:ILE:HD11	1:C:176:ILE:HD11	1.11	1.08
1:E:238:ASP:OD1	1:E:241:THR:HB	1.54	1.08
1:E:307:ARG:HD2	1:E:308:LYS:NZ	1.69	1.07
1:E:302:ILE:HG23	1:E:312:LEU:HD11	1.35	1.07
1:A:238:ASP:OD1	1:A:241:THR:HB	1.54	1.07
1:A:298:SER:O	1:A:301:ASP:HB2	1.53	1.07
1:C:307:ARG:HD2	1:C:308:LYS:NZ	1.70	1.06
1:G:307:ARG:HD2	1:G:308:LYS:NZ	1.70	1.06
1:C:312:LEU:HD22	1:C:317:ARG:HD3	1.30	1.05
1:E:307:ARG:HD2	1:E:308:LYS:HZ3	0.93	1.05
1:G:298:SER:O	1:G:301:ASP:HB2	1.55	1.05
1:C:307:ARG:HD2	1:C:308:LYS:HZ3	0.93	1.05
1:E:176:ILE:HD11	1:G:176:ILE:CD1	1.87	1.05
1:A:176:ILE:HD11	1:C:176:ILE:CD1	1.87	1.03
1:A:176:ILE:CD1	1:C:176:ILE:HD11	1.89	1.03
1:C:238:ASP:OD1	1:C:241:THR:HB	1.56	1.03
1:E:298:SER:O	1:E:301:ASP:HB2	1.55	1.03
1:C:312:LEU:H	1:C:312:LEU:HD12	1.17	1.03
1:G:238:ASP:OD1	1:G:241:THR:HB	1.58	1.03
2:H:455:LEU:HD13	2:H:459:ARG:HH12	1.22	1.03
1:C:312:LEU:CD2	1:C:317:ARG:CD	2.36	1.02
1:A:14:ARG:NH2	1:C:183:HIS:CG	2.25	1.02
1:E:176:ILE:CD1	1:G:176:ILE:HD11	1.89	1.01
1:C:312:LEU:HD12	1:C:312:LEU:N	1.72	1.01
1:G:155:ILE:H	1:G:155:ILE:HD12	1.22	1.00
1:G:160:LYS:CB	1:G:160:LYS:HZ3	1.74	0.99
1:A:14:ARG:NH2	1:C:183:HIS:CD2	2.30	0.98
1:C:302:ILE:HA	1:C:312:LEU:HD11	1.43	0.98
1:C:298:SER:O	1:C:301:ASP:HB2	1.62	0.98
1:A:316:GLU:O	1:A:319:ASN:ND2	1.95	0.98
1:C:335:ILE:HG22	1:C:338:TYR:CE1	1.98	0.98
2:D:480:ARG:HB2	2:D:497:TYR:HE1	1.28	0.98
1:G:307:ARG:HD2	1:G:308:LYS:HZ3	0.83	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:314:GLU:HG3	1:G:317:ARG:HH12	1.29	0.97
1:G:160:LYS:O	1:G:188:ILE:HD11	1.62	0.97
1:E:14:ARG:NH2	1:G:183:HIS:CG	2.32	0.97
1:A:31:GLN:HG3	1:A:38:LEU:HD13	1.46	0.96
2:F:401:GLY:HA3	2:F:455:LEU:CD2	1.94	0.96
2:H:79:ILE:HG13	2:H:80:GLY:H	1.31	0.96
1:A:31:GLN:O	1:A:33:LYS:N	1.99	0.95
1:G:307:ARG:CD	1:G:308:LYS:HZ3	1.79	0.95
1:G:314:GLU:HG3	1:G:317:ARG:NH1	1.81	0.95
1:C:312:LEU:HD21	1:C:317:ARG:CD	1.96	0.95
1:E:31:GLN:O	1:E:33:LYS:N	1.99	0.95
1:E:224:LYS:O	1:E:224:LYS:HD2	1.64	0.94
1:A:218:HIS:HD2	1:A:223:TRP:HE1	1.13	0.94
1:E:335:ILE:HG22	1:E:338:TYR:CE1	2.02	0.94
1:A:307:ARG:HD2	1:A:308:LYS:NZ	1.83	0.94
1:E:183:HIS:CG	1:G:14:ARG:NH2	2.36	0.93
1:E:160:LYS:CB	1:E:160:LYS:NZ	2.31	0.93
1:A:155:ILE:H	1:A:155:ILE:CD1	1.82	0.93
2:B:480:ARG:HB2	2:B:497:TYR:HE1	1.31	0.93
1:G:31:GLN:O	1:G:33:LYS:N	2.01	0.93
1:A:224:LYS:HD2	1:A:224:LYS:O	1.68	0.93
1:E:150:ARG:HB2	1:E:150:ARG:HH21	1.34	0.92
1:C:31:GLN:O	1:C:33:LYS:N	2.01	0.92
1:E:218:HIS:HD2	1:E:223:TRP:HE1	1.09	0.92
1:G:218:HIS:HD2	1:G:223:TRP:HE1	1.12	0.92
1:E:370:LEU:HD23	1:E:370:LEU:H	1.33	0.92
2:F:480:ARG:HB2	2:F:497:TYR:HE1	1.34	0.92
1:G:224:LYS:HD2	1:G:224:LYS:O	1.69	0.92
2:H:455:LEU:CD1	2:H:459:ARG:NH1	2.32	0.92
1:A:335:ILE:HG22	1:A:338:TYR:CE1	2.04	0.92
1:C:150:ARG:HH21	1:C:150:ARG:HB2	1.35	0.91
2:B:383:GLU:HG3	2:B:384:LYS:HD3	1.50	0.91
1:E:160:LYS:CB	1:E:160:LYS:HZ3	1.82	0.91
2:H:480:ARG:HB2	2:H:497:TYR:HE1	1.34	0.91
1:A:160:LYS:HB2	1:A:160:LYS:NZ	1.86	0.91
1:A:183:HIS:CG	1:C:14:ARG:NH2	2.37	0.91
1:A:22:ARG:HG3	1:A:23:ASP:N	1.81	0.91
1:E:155:ILE:H	1:E:155:ILE:CD1	1.81	0.91
1:A:32:LEU:HD11	2:B:486:LEU:HD11	1.50	0.91
1:C:316:GLU:O	1:C:319:ASN:ND2	2.04	0.91
1:C:218:HIS:HD2	1:C:223:TRP:HE1	1.13	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:455:LEU:HD12	2:H:459:ARG:HH12	1.33	0.91
1:C:31:GLN:HG3	1:C:38:LEU:HD13	1.52	0.90
1:C:155:ILE:H	1:C:155:ILE:CD1	1.82	0.90
1:G:335:ILE:HG22	1:G:338:TYR:CE1	2.05	0.90
1:C:155:ILE:HD12	1:C:155:ILE:N	1.87	0.90
1:G:22:ARG:HG3	1:G:23:ASP:N	1.84	0.90
1:C:22:ARG:HG3	1:C:23:ASP:N	1.84	0.90
1:E:22:ARG:HG3	1:E:23:ASP:N	1.83	0.90
2:D:500:GLU:HA	2:D:503:GLU:HB3	1.54	0.90
2:F:79:ILE:HG13	2:F:80:GLY:H	1.34	0.90
2:B:500:GLU:HA	2:B:503:GLU:HB3	1.54	0.90
2:H:198:THR:O	2:H:198:THR:HG22	1.71	0.90
1:A:150:ARG:HH21	1:A:150:ARG:HB2	1.36	0.89
2:F:198:THR:O	2:F:198:THR:HG22	1.71	0.89
1:E:155:ILE:HD12	1:E:155:ILE:N	1.88	0.89
1:G:160:LYS:CB	1:G:160:LYS:NZ	2.28	0.89
1:C:307:ARG:CD	1:C:308:LYS:HZ3	1.84	0.89
2:H:500:GLU:HA	2:H:503:GLU:HB3	1.53	0.89
1:E:319:ASN:H	1:E:319:ASN:HD22	1.18	0.88
2:B:198:THR:HG22	2:B:198:THR:O	1.73	0.88
1:E:85:MET:HE1	1:E:104:LEU:HD23	1.54	0.88
1:G:150:ARG:HH21	1:G:150:ARG:HB2	1.37	0.88
1:C:181:THR:HG22	1:C:181:THR:O	1.72	0.88
2:D:79:ILE:HG13	2:D:80:GLY:H	1.38	0.88
2:F:516:ILE:HD13	2:F:516:ILE:H	1.38	0.88
1:A:368:LYS:HD3	1:A:372:PHE:HE2	1.37	0.88
1:C:224:LYS:O	1:C:224:LYS:HD2	1.74	0.88
1:C:335:ILE:HG22	1:C:338:TYR:CD1	2.09	0.88
2:D:383:GLU:HG3	2:D:384:LYS:HD3	1.56	0.88
1:E:307:ARG:CD	1:E:308:LYS:HZ3	1.85	0.88
1:E:261:ASP:OD1	1:E:361:GLU:HA	1.72	0.88
2:B:138:ARG:HB3	2:B:161:VAL:O	1.74	0.88
1:G:31:GLN:HG3	1:G:38:LEU:HD13	1.54	0.87
2:H:383:GLU:HG3	2:H:384:LYS:HD3	1.57	0.87
1:C:302:ILE:HG22	1:C:317:ARG:HD2	1.57	0.87
1:C:312:LEU:CD1	1:C:312:LEU:N	2.26	0.87
1:A:160:LYS:HB2	1:A:160:LYS:HZ3	1.37	0.87
1:C:319:ASN:HD22	1:C:319:ASN:H	1.19	0.87
1:E:368:LYS:HD3	1:E:372:PHE:HE2	1.38	0.87
2:F:500:GLU:HA	2:F:503:GLU:HB3	1.55	0.87
1:A:370:LEU:HD23	1:A:370:LEU:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ARG:HH21	1:E:150:ARG:CB	1.88	0.87
1:G:155:ILE:H	1:G:155:ILE:CD1	1.88	0.87
2:D:414:HIS:HD2	2:D:415:LEU:N	1.72	0.86
1:C:101:ILE:HD12	1:C:101:ILE:N	1.91	0.86
2:B:41:GLU:OE1	2:B:105:ARG:HB3	1.75	0.86
1:E:31:GLN:HG3	1:E:38:LEU:HD13	1.56	0.86
1:A:150:ARG:HH21	1:A:150:ARG:CB	1.87	0.86
1:G:160:LYS:HZ3	1:G:160:LYS:HB3	1.38	0.86
1:E:368:LYS:HD3	1:E:372:PHE:CE2	2.10	0.86
1:G:261:ASP:OD1	1:G:361:GLU:HA	1.75	0.86
1:A:160:LYS:O	1:A:238:ASP:OD2	1.94	0.86
1:G:153:MET:O	1:G:154:LEU:HB2	1.76	0.86
2:B:414:HIS:HD2	2:B:415:LEU:N	1.72	0.86
2:D:219:THR:HG23	2:D:220:ASN:N	1.90	0.85
1:A:155:ILE:HD12	1:A:155:ILE:N	1.89	0.85
1:A:261:ASP:OD1	1:A:361:GLU:HA	1.77	0.85
1:E:101:ILE:HD12	1:E:101:ILE:N	1.92	0.85
1:A:319:ASN:HD22	1:A:319:ASN:H	1.20	0.85
1:A:374:ALA:C	1:A:375:PHE:HD1	1.82	0.85
1:A:368:LYS:HD3	1:A:372:PHE:CE2	2.11	0.85
1:E:181:THR:O	1:E:181:THR:HG22	1.76	0.84
2:H:219:THR:HG23	2:H:220:ASN:N	1.90	0.84
2:H:138:ARG:HB3	2:H:161:VAL:O	1.77	0.84
2:B:79:ILE:HG13	2:B:80:GLY:H	1.40	0.84
1:C:368:LYS:HD3	1:C:372:PHE:HE2	1.42	0.84
2:B:506:PHE:O	2:B:509:ILE:HG13	1.77	0.84
2:F:41:GLU:OE1	2:F:105:ARG:HB3	1.77	0.84
1:A:31:GLN:HB2	1:A:38:LEU:HD22	1.59	0.84
2:F:138:ARG:HB3	2:F:161:VAL:O	1.76	0.84
2:F:221:LYS:HD2	2:F:321:LEU:HD21	1.59	0.84
2:D:198:THR:HG22	2:D:198:THR:O	1.75	0.84
1:E:218:HIS:CD2	1:E:223:TRP:HE1	1.96	0.84
2:F:383:GLU:HG3	2:F:384:LYS:HD3	1.59	0.84
1:G:146:THR:O	1:G:147:SER:HB2	1.78	0.84
2:D:516:ILE:HD13	2:D:516:ILE:H	1.42	0.83
2:B:516:ILE:HD13	2:B:516:ILE:H	1.41	0.83
1:E:316:GLU:O	1:E:319:ASN:ND2	2.11	0.83
2:F:219:THR:HG23	2:F:220:ASN:N	1.92	0.83
1:C:22:ARG:CG	1:C:23:ASP:H	1.91	0.83
1:A:376:GLN:O	1:A:380:GLU:HB2	1.78	0.83
1:E:159:GLU:OE1	1:E:240:ALA:HB3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:MET:O	1:E:154:LEU:HB2	1.78	0.83
1:C:377:TYR:CE2	1:C:381:LYS:HD2	2.14	0.83
1:G:150:ARG:HH21	1:G:150:ARG:CB	1.91	0.83
1:G:181:THR:O	1:G:181:THR:HG22	1.76	0.83
2:D:506:PHE:O	2:D:509:ILE:HG13	1.79	0.83
2:H:516:ILE:H	2:H:516:ILE:HD13	1.41	0.83
1:A:219:ARG:CZ	1:C:14:ARG:HH21	1.92	0.83
1:C:312:LEU:HD21	1:C:317:ARG:HD2	1.61	0.83
1:C:370:LEU:HD23	1:C:370:LEU:H	1.44	0.83
1:C:153:MET:O	1:C:154:LEU:HB2	1.76	0.82
1:C:376:GLN:O	1:C:380:GLU:HB2	1.77	0.82
1:G:218:HIS:CD2	1:G:223:TRP:HE1	1.96	0.82
1:C:99:PRO:HB2	1:C:104:LEU:HD11	1.62	0.82
1:C:150:ARG:HH21	1:C:150:ARG:CB	1.92	0.82
1:E:374:ALA:HB1	1:E:375:PHE:CE1	2.14	0.82
2:H:455:LEU:HD13	2:H:459:ARG:NH1	1.92	0.82
2:B:340:ARG:NH2	2:B:442:ASN:HB2	1.92	0.82
1:G:335:ILE:HG22	1:G:338:TYR:CD1	2.13	0.82
1:C:302:ILE:O	1:C:317:ARG:CZ	2.28	0.82
1:A:377:TYR:CE2	1:A:381:LYS:HD2	2.14	0.82
2:F:475:ILE:O	2:F:479:SER:OG	1.97	0.82
1:G:155:ILE:HD12	1:G:155:ILE:N	1.92	0.82
1:G:319:ASN:H	1:G:319:ASN:HD22	1.24	0.82
1:A:84:LEU:O	1:A:86:ALA:N	2.13	0.82
1:A:181:THR:HG22	1:A:181:THR:O	1.79	0.82
1:E:374:ALA:C	1:E:375:PHE:HD1	1.88	0.82
2:F:516:ILE:HD13	2:F:516:ILE:N	1.95	0.82
2:D:41:GLU:OE1	2:D:105:ARG:HB3	1.80	0.82
1:E:84:LEU:O	1:E:86:ALA:N	2.13	0.82
2:D:138:ARG:HB3	2:D:161:VAL:O	1.79	0.81
1:E:22:ARG:CG	1:E:23:ASP:H	1.93	0.81
1:G:160:LYS:NZ	1:G:160:LYS:HB2	1.94	0.81
2:D:224:LYS:HG3	2:D:225:PRO:HD2	1.63	0.81
2:F:224:LYS:HG3	2:F:225:PRO:HD2	1.62	0.81
1:G:22:ARG:CG	1:G:23:ASP:H	1.92	0.81
1:G:149:LEU:HD12	1:G:149:LEU:H	1.43	0.81
1:C:160:LYS:O	1:C:160:LYS:CG	2.20	0.81
1:E:160:LYS:O	1:E:188:ILE:HD11	1.79	0.81
2:B:475:ILE:O	2:B:479:SER:OG	1.95	0.81
1:C:218:HIS:CD2	1:C:223:TRP:HE1	1.98	0.81
1:E:335:ILE:C	1:E:337:ASN:H	1.86	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:VAL:HG13	1:C:68:ARG:O	1.81	0.81
1:G:376:GLN:O	1:G:380:GLU:HB2	1.80	0.81
2:H:414:HIS:HD2	2:H:415:LEU:N	1.78	0.81
1:C:374:ALA:HB1	1:C:375:PHE:CE1	2.16	0.81
1:C:146:THR:O	1:C:147:SER:HB2	1.78	0.81
1:A:22:ARG:CG	1:A:23:ASP:H	1.92	0.80
1:E:377:TYR:CE2	1:E:381:LYS:HD2	2.15	0.80
1:G:377:TYR:CE2	1:G:381:LYS:HD2	2.15	0.80
1:A:374:ALA:HB1	1:A:375:PHE:CE1	2.16	0.80
1:E:335:ILE:HG22	1:E:338:TYR:CD1	2.15	0.80
2:B:265:ILE:HG22	2:B:270:ALA:HB2	1.64	0.80
2:H:455:LEU:HD12	2:H:459:ARG:NH1	1.95	0.80
1:A:14:ARG:HH21	1:C:219:ARG:CZ	1.95	0.80
2:H:475:ILE:O	2:H:479:SER:OG	1.99	0.80
2:H:506:PHE:O	2:H:509:ILE:HG13	1.81	0.80
1:A:153:MET:O	1:A:154:LEU:HB2	1.81	0.80
2:B:219:THR:HG23	2:B:220:ASN:N	1.97	0.80
1:C:335:ILE:C	1:C:337:ASN:H	1.89	0.80
2:D:475:ILE:O	2:D:479:SER:OG	1.98	0.80
2:D:516:ILE:HD13	2:D:516:ILE:N	1.97	0.80
1:A:218:HIS:CD2	1:A:223:TRP:HE1	2.00	0.80
1:G:368:LYS:HD3	1:G:372:PHE:CE2	2.17	0.80
1:G:243:ARG:NH2	1:G:287:LEU:HD22	1.97	0.80
2:H:79:ILE:HG13	2:H:80:GLY:N	1.97	0.80
1:A:101:ILE:N	1:A:101:ILE:HD12	1.96	0.80
1:A:314:GLU:HA	1:A:317:ARG:HH11	1.47	0.80
1:C:31:GLN:HB2	1:C:38:LEU:HD22	1.62	0.80
1:G:368:LYS:HD3	1:G:372:PHE:HE2	1.47	0.80
2:H:41:GLU:OE1	2:H:105:ARG:HB3	1.82	0.80
1:E:17:ALA:HA	1:E:20:ILE:HG22	1.64	0.79
1:G:374:ALA:C	1:G:375:PHE:HD1	1.91	0.79
1:A:335:ILE:HG22	1:A:338:TYR:CD1	2.16	0.79
1:C:368:LYS:HD3	1:C:372:PHE:CE2	2.18	0.79
1:E:370:LEU:HD23	1:E:370:LEU:N	1.97	0.79
2:H:516:ILE:HD13	2:H:516:ILE:N	1.97	0.79
2:F:506:PHE:O	2:F:509:ILE:HG13	1.81	0.79
1:E:14:ARG:NH2	1:G:183:HIS:CD2	2.51	0.79
2:D:480:ARG:HB2	2:D:497:TYR:CE1	2.16	0.79
1:A:99:PRO:HB2	1:A:104:LEU:HD11	1.63	0.79
2:H:197:ILE:HB	2:H:317:ILE:HD12	1.63	0.79
2:B:516:ILE:HD13	2:B:516:ILE:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ASP:OD1	1:C:361:GLU:HA	1.83	0.79
1:A:160:LYS:HZ3	1:A:160:LYS:CB	1.94	0.78
1:C:302:ILE:CG2	1:C:312:LEU:HD21	2.12	0.78
1:E:160:LYS:NZ	1:E:160:LYS:HB2	1.97	0.78
1:E:160:LYS:HZ3	1:E:160:LYS:HB3	1.48	0.78
1:G:73:LEU:HD21	2:H:467:LYS:HE3	1.63	0.78
1:C:378:ILE:HD13	1:C:378:ILE:H	1.48	0.78
1:E:335:ILE:O	1:E:337:ASN:N	2.16	0.78
1:A:85:MET:HE1	1:A:104:LEU:HD23	1.65	0.78
2:F:480:ARG:HB2	2:F:497:TYR:CE1	2.19	0.78
1:A:335:ILE:C	1:A:337:ASN:H	1.88	0.78
2:F:414:HIS:HD2	2:F:415:LEU:N	1.81	0.78
2:B:116:VAL:O	2:B:120:GLN:NE2	2.16	0.78
1:G:101:ILE:HD12	1:G:101:ILE:N	1.98	0.78
1:A:335:ILE:O	1:A:337:ASN:N	2.16	0.78
2:B:480:ARG:HB2	2:B:497:TYR:CE1	2.18	0.78
1:C:84:LEU:O	1:C:86:ALA:N	2.17	0.78
1:C:243:ARG:NH2	1:C:287:LEU:HD22	1.97	0.78
1:C:374:ALA:C	1:C:375:PHE:HD1	1.92	0.78
1:A:160:LYS:NZ	1:A:160:LYS:CB	2.37	0.78
1:A:353:PHE:C	1:A:355:GLN:H	1.90	0.78
1:A:372:PHE:CD1	1:A:372:PHE:C	2.60	0.78
1:E:146:THR:O	1:E:147:SER:HB2	1.83	0.78
1:A:102:ARG:HD2	1:C:363:GLU:HG3	1.66	0.77
2:F:340:ARG:NH2	2:F:442:ASN:HB2	1.98	0.77
1:E:375:PHE:HD1	1:E:375:PHE:N	1.82	0.77
1:C:85:MET:HE1	1:C:104:LEU:HD23	1.65	0.77
1:E:97:GLU:OE1	1:G:370:LEU:HG	1.85	0.77
1:C:378:ILE:HD13	1:C:378:ILE:N	1.98	0.77
1:C:39:VAL:HG22	1:C:69:ASN:HA	1.66	0.77
1:E:302:ILE:HG22	1:E:312:LEU:CD1	2.14	0.77
2:H:265:ILE:HG22	2:H:270:ALA:HB2	1.67	0.77
1:A:149:LEU:H	1:A:149:LEU:HD12	1.46	0.77
1:A:13:ALA:HA	1:A:16:LYS:HG3	1.67	0.77
1:C:335:ILE:O	1:C:337:ASN:N	2.17	0.77
1:A:146:THR:O	1:A:147:SER:HB2	1.85	0.76
1:E:183:HIS:CD2	1:G:14:ARG:NH2	2.53	0.76
2:H:455:LEU:O	2:H:459:ARG:NH1	2.18	0.76
2:H:103:GLN:NE2	2:H:315:SER:H	1.84	0.76
2:F:79:ILE:HG13	2:F:80:GLY:N	2.01	0.76
1:G:335:ILE:O	1:G:337:ASN:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:PHE:HD1	1:A:375:PHE:N	1.84	0.76
1:C:372:PHE:CD1	1:C:372:PHE:C	2.60	0.76
1:E:31:GLN:HB2	1:E:38:LEU:HD22	1.65	0.76
1:G:353:PHE:C	1:G:355:GLN:H	1.93	0.76
2:H:493:LEU:HG	2:H:494:VAL:HG13	1.67	0.76
1:A:14:ARG:CZ	1:C:183:HIS:CE1	2.69	0.76
2:B:91:GLY:HA3	2:B:153:PRO:HB3	1.68	0.76
1:G:370:LEU:HD23	1:G:370:LEU:H	1.51	0.76
1:C:312:LEU:H	1:C:312:LEU:HD13	1.49	0.76
2:B:340:ARG:HH22	2:B:442:ASN:CB	1.99	0.76
1:C:149:LEU:H	1:C:149:LEU:HD12	1.49	0.76
1:A:68:ARG:NH2	1:A:141:ASP:OD1	2.19	0.75
1:A:243:ARG:NH2	1:A:287:LEU:HD22	2.01	0.75
1:E:99:PRO:HB2	1:E:104:LEU:HD11	1.66	0.75
1:A:14:ARG:HH22	1:C:183:HIS:CG	2.04	0.75
2:F:37:ARG:O	2:F:41:GLU:HG3	1.86	0.75
1:G:17:ALA:HA	1:G:20:ILE:HG22	1.68	0.75
1:G:335:ILE:C	1:G:337:ASN:H	1.91	0.75
2:D:36:VAL:O	2:D:40:ILE:HD12	1.86	0.75
2:D:265:ILE:HG22	2:D:270:ALA:HB2	1.68	0.75
2:H:37:ARG:O	2:H:41:GLU:HG3	1.87	0.75
2:H:480:ARG:HB2	2:H:497:TYR:CE1	2.20	0.75
1:C:307:ARG:C	1:C:308:LYS:HD3	2.10	0.75
1:C:353:PHE:C	1:C:355:GLN:H	1.91	0.75
1:E:149:LEU:H	1:E:149:LEU:HD12	1.49	0.75
2:B:116:VAL:HG13	2:B:127:ILE:HG13	1.69	0.75
2:H:193:ARG:HD3	2:H:371:LEU:HD23	1.69	0.75
1:E:32:LEU:HD11	2:F:486:LEU:HD11	1.69	0.75
1:G:374:ALA:HB1	1:G:375:PHE:CE1	2.21	0.75
2:H:116:VAL:O	2:H:120:GLN:NE2	2.19	0.75
1:A:183:HIS:CD2	1:C:14:ARG:NH2	2.55	0.74
2:B:493:LEU:HG	2:B:494:VAL:HG13	1.68	0.74
1:C:101:ILE:HD12	1:C:101:ILE:H	1.52	0.74
1:C:374:ALA:HB1	1:C:375:PHE:CD1	2.22	0.74
1:G:319:ASN:H	1:G:319:ASN:ND2	1.86	0.74
1:E:68:ARG:NH2	1:E:141:ASP:OD1	2.21	0.74
1:G:378:ILE:HD13	1:G:378:ILE:N	2.03	0.74
2:B:414:HIS:CD2	2:B:415:LEU:N	2.56	0.74
1:G:31:GLN:HB2	1:G:38:LEU:HD22	1.67	0.74
1:E:77:LYS:NZ	1:E:126:GLU:OE1	2.20	0.74
1:E:353:PHE:C	1:E:355:GLN:H	1.92	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:MET:HE1	1:G:104:LEU:HD23	1.69	0.74
1:A:295:LEU:O	1:A:295:LEU:HD22	1.88	0.73
2:D:414:HIS:CD2	2:D:415:LEU:N	2.55	0.73
1:A:319:ASN:ND2	1:A:319:ASN:H	1.87	0.73
2:D:79:ILE:HG13	2:D:80:GLY:N	2.01	0.73
1:E:13:ALA:HA	1:E:16:LYS:HG3	1.70	0.73
2:F:340:ARG:HH22	2:F:442:ASN:CB	2.01	0.73
1:G:202:ALA:HB1	1:G:228:SER:HA	1.69	0.73
2:H:103:GLN:NE2	2:H:315:SER:N	2.36	0.73
1:A:17:ALA:HA	1:A:20:ILE:HG22	1.68	0.73
1:A:25:PHE:HD1	1:A:25:PHE:C	1.96	0.73
1:C:378:ILE:N	1:C:378:ILE:CD1	2.49	0.73
1:C:319:ASN:ND2	1:C:319:ASN:H	1.85	0.73
2:D:37:ARG:O	2:D:41:GLU:HG3	1.87	0.73
1:G:99:PRO:HB2	1:G:104:LEU:HD11	1.69	0.73
1:G:378:ILE:HD13	1:G:378:ILE:H	1.54	0.73
1:E:319:ASN:H	1:E:319:ASN:ND2	1.85	0.73
2:F:36:VAL:O	2:F:40:ILE:HD12	1.89	0.73
2:F:499:ASN:C	2:F:499:ASN:HD22	1.97	0.73
1:C:374:ALA:CB	1:C:375:PHE:CD1	2.72	0.73
2:H:340:ARG:NH2	2:H:442:ASN:HB2	2.03	0.72
2:B:37:ARG:O	2:B:41:GLU:HG3	1.89	0.72
1:C:202:ALA:HB1	1:C:228:SER:HA	1.71	0.72
1:E:374:ALA:HB1	1:E:375:PHE:CD1	2.24	0.72
1:C:335:ILE:CG2	1:C:338:TYR:CE1	2.71	0.72
2:H:116:VAL:HG13	2:H:127:ILE:HG13	1.72	0.72
2:D:91:GLY:HA3	2:D:153:PRO:HB3	1.71	0.72
2:F:91:GLY:HA3	2:F:153:PRO:HB3	1.70	0.72
1:G:200:VAL:HG11	1:G:252:LEU:HD23	1.71	0.72
1:A:84:LEU:C	1:A:86:ALA:H	1.98	0.72
1:C:380:GLU:O	1:C:384:ASN:HB2	1.89	0.72
1:E:375:PHE:N	1:E:375:PHE:CD1	2.55	0.72
1:G:84:LEU:O	1:G:86:ALA:N	2.23	0.72
2:H:91:GLY:HA3	2:H:153:PRO:HB3	1.70	0.72
2:B:499:ASN:C	2:B:499:ASN:HD22	1.98	0.72
1:C:84:LEU:C	1:C:86:ALA:H	1.95	0.72
1:C:17:ALA:HA	1:C:20:ILE:HG22	1.71	0.72
2:D:116:VAL:O	2:D:120:GLN:NE2	2.22	0.72
1:A:12:GLU:C	1:A:14:ARG:H	1.98	0.71
1:A:370:LEU:HD23	1:A:370:LEU:N	2.05	0.71
1:A:374:ALA:HB1	1:A:375:PHE:CD1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ALA:HB1	1:E:228:SER:HA	1.72	0.71
1:G:68:ARG:NH2	1:G:141:ASP:OD1	2.23	0.71
1:C:302:ILE:CA	1:C:312:LEU:HD11	2.20	0.71
2:F:116:VAL:O	2:F:120:GLN:NE2	2.23	0.71
1:A:375:PHE:N	1:A:375:PHE:CD1	2.55	0.71
2:B:193:ARG:HD3	2:B:371:LEU:HD23	1.72	0.71
2:B:224:LYS:HG3	2:B:225:PRO:HD2	1.72	0.71
1:G:271:SER:HB3	1:G:340:TRP:CH2	2.25	0.71
1:E:219:ARG:CZ	1:G:14:ARG:HH21	2.04	0.71
1:E:376:GLN:O	1:E:380:GLU:HB2	1.90	0.71
1:G:25:PHE:HD1	1:G:25:PHE:C	1.97	0.71
2:B:79:ILE:HG13	2:B:80:GLY:N	2.06	0.71
1:C:25:PHE:C	1:C:25:PHE:HD1	1.97	0.71
1:E:101:ILE:HD12	1:E:101:ILE:H	1.55	0.71
1:E:84:LEU:C	1:E:86:ALA:H	1.97	0.71
2:F:116:VAL:HG13	2:F:127:ILE:HG13	1.72	0.71
2:F:265:ILE:HG22	2:F:270:ALA:HB2	1.71	0.71
1:C:13:ALA:HA	1:C:16:LYS:HG3	1.73	0.71
1:C:271:SER:HB3	1:C:340:TRP:CH2	2.26	0.71
2:F:86:VAL:HB	2:F:87:PRO:HD3	1.72	0.71
1:G:246:ARG:HG2	1:G:246:ARG:O	1.89	0.71
1:E:243:ARG:NH2	1:E:287:LEU:HD22	2.05	0.71
1:E:200:VAL:HG11	1:E:252:LEU:HD23	1.73	0.71
1:E:264:PRO:HA	1:E:267:TRP:CE3	2.26	0.71
2:D:400:TYR:HA	2:D:452:LYS:CE	2.16	0.71
1:E:370:LEU:HG	1:G:97:GLU:OE1	1.91	0.71
1:E:319:ASN:HD22	1:E:319:ASN:N	1.86	0.70
1:G:335:ILE:C	1:G:337:ASN:N	2.47	0.70
1:C:264:PRO:HA	1:C:267:TRP:CE3	2.26	0.70
1:E:378:ILE:HD13	1:E:378:ILE:N	2.06	0.70
1:C:77:LYS:NZ	1:C:126:GLU:OE1	2.24	0.70
1:C:335:ILE:C	1:C:337:ASN:N	2.46	0.70
1:E:351:ASN:HA	1:E:354:LEU:HB2	1.73	0.70
2:D:116:VAL:HG13	2:D:127:ILE:HG13	1.73	0.70
1:G:73:LEU:CD2	2:H:467:LYS:HG2	2.22	0.70
1:A:291:ASP:OD1	1:A:291:ASP:O	2.10	0.70
1:E:271:SER:HB3	1:E:340:TRP:CH2	2.27	0.70
1:E:335:ILE:C	1:E:337:ASN:N	2.44	0.70
2:H:86:VAL:HB	2:H:87:PRO:HD3	1.72	0.70
2:H:499:ASN:C	2:H:499:ASN:HD22	1.99	0.70
1:A:77:LYS:NZ	1:A:126:GLU:OE1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:O	1:A:246:ARG:HG2	1.91	0.70
1:C:68:ARG:NH2	1:C:141:ASP:OD1	2.25	0.70
2:D:499:ASN:HD22	2:D:499:ASN:C	1.99	0.70
2:H:224:LYS:HG3	2:H:225:PRO:HD2	1.74	0.70
1:C:181:THR:HG21	1:C:185:ALA:HA	1.73	0.70
2:D:493:LEU:HG	2:D:494:VAL:HG13	1.71	0.70
1:E:25:PHE:C	1:E:25:PHE:HD1	2.00	0.70
1:G:378:ILE:N	1:G:378:ILE:CD1	2.55	0.70
1:C:181:THR:O	1:C:181:THR:CG2	2.38	0.70
1:E:372:PHE:C	1:E:372:PHE:CD1	2.67	0.70
1:A:238:ASP:OD1	1:A:241:THR:CB	2.38	0.69
2:B:36:VAL:O	2:B:40:ILE:HD12	1.92	0.69
1:E:291:ASP:O	1:E:291:ASP:OD1	2.09	0.69
2:F:493:LEU:HG	2:F:494:VAL:HG13	1.73	0.69
1:G:149:LEU:O	1:G:150:ARG:C	2.32	0.69
1:C:375:PHE:HD1	1:C:375:PHE:N	1.90	0.69
1:E:21:LEU:HD21	1:E:153:MET:HA	1.74	0.69
1:A:31:GLN:HG3	1:A:38:LEU:CD1	2.22	0.69
1:A:380:GLU:O	1:A:384:ASN:HB2	1.92	0.69
1:C:39:VAL:HG13	1:C:68:ARG:C	2.17	0.69
1:G:25:PHE:C	1:G:25:PHE:CD1	2.70	0.69
1:A:246:ARG:O	1:A:250:GLU:HB2	1.92	0.69
1:C:302:ILE:HB	1:C:303:PHE:CD2	2.27	0.69
1:A:115:LYS:NZ	1:A:115:LYS:HB3	2.07	0.69
1:E:372:PHE:HA	1:E:376:GLN:OE1	1.92	0.69
2:H:103:GLN:HE22	2:H:315:SER:H	1.38	0.69
1:C:25:PHE:C	1:C:25:PHE:CD1	2.70	0.69
1:E:363:GLU:HG3	1:G:102:ARG:HD2	1.73	0.69
2:F:264:SER:C	2:F:265:ILE:HG12	2.17	0.69
1:G:209:GLU:HB3	1:G:260:THR:HG22	1.75	0.69
1:E:335:ILE:CG2	1:E:338:TYR:CE1	2.76	0.69
2:F:475:ILE:N	2:F:476:PRO:HD2	2.06	0.69
1:A:370:LEU:HG	1:C:97:GLU:OE1	1.92	0.69
2:B:197:ILE:HB	2:B:317:ILE:HD12	1.74	0.69
1:C:374:ALA:CB	1:C:375:PHE:HD1	2.06	0.69
2:B:500:GLU:HA	2:B:503:GLU:CB	2.23	0.69
1:C:21:LEU:HD21	1:C:153:MET:HA	1.75	0.69
1:A:172:GLY:CA	1:C:183:HIS:HE1	2.06	0.68
1:E:238:ASP:OD1	1:E:241:THR:CB	2.37	0.68
1:A:202:ALA:HB1	1:A:228:SER:HA	1.75	0.68
2:D:340:ARG:NH2	2:D:442:ASN:HB2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ALA:CB	1:A:375:PHE:CD1	2.76	0.68
1:E:246:ARG:O	1:E:250:GLU:HB2	1.93	0.68
1:E:374:ALA:CB	1:E:375:PHE:CD1	2.75	0.68
1:G:181:THR:O	1:G:181:THR:CG2	2.42	0.68
1:A:351:ASN:O	1:A:355:GLN:HB2	1.93	0.68
1:C:370:LEU:HD23	1:C:370:LEU:N	2.08	0.68
1:A:307:ARG:C	1:A:308:LYS:HD3	2.18	0.68
1:G:335:ILE:CG2	1:G:338:TYR:CE1	2.77	0.68
1:A:363:GLU:HG3	1:C:102:ARG:HD2	1.76	0.68
2:B:475:ILE:N	2:B:476:PRO:HD2	2.09	0.68
2:F:508:LEU:C	2:F:510:SER:H	2.02	0.68
1:A:302:ILE:HB	1:A:303:PHE:CD2	2.29	0.68
1:E:307:ARG:C	1:E:308:LYS:HD3	2.18	0.68
1:A:385:LYS:HG3	1:A:387:TYR:HE2	1.58	0.68
1:E:208:VAL:HG21	1:E:213:VAL:CG1	2.24	0.68
1:E:303:PHE:CE1	1:E:356:ARG:HD2	2.28	0.68
1:G:115:LYS:HB3	1:G:115:LYS:NZ	2.09	0.68
1:G:264:PRO:HA	1:G:267:TRP:CE3	2.29	0.68
2:H:36:VAL:O	2:H:40:ILE:HD12	1.94	0.68
1:A:351:ASN:HA	1:A:354:LEU:HB2	1.76	0.68
1:C:246:ARG:O	1:C:246:ARG:HG2	1.93	0.68
2:B:340:ARG:NH2	2:B:442:ASN:CB	2.56	0.68
1:C:200:VAL:HG11	1:C:252:LEU:HD23	1.75	0.68
2:D:86:VAL:HB	2:D:87:PRO:HD3	1.75	0.68
2:D:500:GLU:HA	2:D:503:GLU:CB	2.24	0.68
2:H:414:HIS:CD2	2:H:415:LEU:N	2.61	0.68
1:A:335:ILE:CG2	1:A:338:TYR:CE1	2.77	0.67
2:B:86:VAL:HB	2:B:87:PRO:HD3	1.75	0.67
1:G:146:THR:O	1:G:147:SER:CB	2.43	0.67
1:G:317:ARG:O	1:G:321:ILE:HG13	1.94	0.67
1:A:271:SER:HB3	1:A:340:TRP:CH2	2.28	0.67
1:A:340:TRP:HZ3	1:A:341:PHE:CZ	2.13	0.67
1:C:146:THR:O	1:C:147:SER:CB	2.43	0.67
1:E:351:ASN:O	1:E:355:GLN:HB2	1.93	0.67
1:G:291:ASP:OD1	1:G:291:ASP:O	2.12	0.67
1:G:375:PHE:HD1	1:G:375:PHE:N	1.91	0.67
1:E:84:LEU:C	1:E:86:ALA:N	2.50	0.67
1:C:149:LEU:O	1:C:150:ARG:C	2.37	0.67
1:C:291:ASP:OD1	1:C:291:ASP:O	2.12	0.67
1:G:12:GLU:C	1:G:14:ARG:H	2.03	0.67
1:G:77:LYS:NZ	1:G:126:GLU:OE1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:O	1:A:374:ALA:N	2.25	0.67
2:F:500:GLU:HA	2:F:503:GLU:CB	2.24	0.67
1:G:351:ASN:O	1:G:355:GLN:HB2	1.95	0.67
2:D:475:ILE:N	2:D:476:PRO:HD2	2.10	0.67
1:G:73:LEU:HD21	2:H:467:LYS:HG2	1.75	0.67
1:A:377:TYR:HE2	1:A:381:LYS:HD2	1.57	0.67
2:F:390:LYS:HG2	2:F:394:GLU:HG3	1.77	0.67
1:C:85:MET:CE	1:C:104:LEU:HB3	2.25	0.67
2:D:197:ILE:HB	2:D:317:ILE:HD12	1.75	0.67
1:G:84:LEU:C	1:G:86:ALA:H	2.02	0.67
2:H:455:LEU:HD12	2:H:455:LEU:O	1.94	0.67
2:H:475:ILE:N	2:H:476:PRO:HD2	2.09	0.67
1:A:84:LEU:C	1:A:86:ALA:N	2.51	0.66
1:G:372:PHE:CD1	1:G:372:PHE:C	2.69	0.66
1:E:160:LYS:HZ3	1:E:160:LYS:HB2	1.53	0.66
1:G:13:ALA:HA	1:G:16:LYS:HG3	1.76	0.66
1:A:175:VAL:HG23	1:A:175:VAL:O	1.96	0.66
1:E:183:HIS:HB2	1:G:189:GLU:HB3	1.77	0.66
1:G:246:ARG:O	1:G:246:ARG:CG	2.43	0.66
1:A:264:PRO:HA	1:A:267:TRP:CE3	2.29	0.66
1:A:374:ALA:C	1:A:375:PHE:CD1	2.70	0.66
2:B:221:LYS:HD2	2:B:321:LEU:HD21	1.76	0.66
1:E:21:LEU:HD12	1:E:93:LEU:CD1	2.24	0.66
1:C:351:ASN:HA	1:C:354:LEU:HB2	1.78	0.66
2:D:496:LYS:O	2:D:499:ASN:ND2	2.28	0.66
1:G:181:THR:HG21	1:G:185:ALA:HA	1.77	0.66
2:H:390:LYS:HG2	2:H:394:GLU:HG3	1.78	0.66
3:H:531:RDC:O1	3:H:531:RDC:H81	1.95	0.66
1:C:101:ILE:H	1:C:101:ILE:CD1	2.07	0.66
1:E:181:THR:O	1:E:181:THR:CG2	2.42	0.66
1:E:370:LEU:O	1:E:374:ALA:N	2.21	0.66
2:B:508:LEU:C	2:B:510:SER:H	2.02	0.66
1:C:375:PHE:CD1	1:C:375:PHE:N	2.62	0.66
1:E:353:PHE:C	1:E:355:GLN:N	2.52	0.66
1:G:237:PRO:O	1:G:242:ARG:NH2	2.27	0.66
1:E:302:ILE:HG23	1:E:312:LEU:CD1	2.21	0.66
1:G:230:LEU:CD2	1:G:230:LEU:C	2.69	0.66
1:C:115:LYS:NZ	1:C:115:LYS:HB3	2.10	0.66
1:C:208:VAL:HG21	1:C:213:VAL:CG1	2.26	0.66
2:D:390:LYS:HG2	2:D:394:GLU:HG3	1.78	0.66
1:E:12:GLU:C	1:E:14:ARG:H	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:ARG:O	1:E:246:ARG:HG2	1.95	0.66
1:A:303:PHE:CE1	1:A:356:ARG:HD2	2.31	0.66
1:C:85:MET:HE1	1:C:104:LEU:HB3	1.77	0.66
1:E:13:ALA:HB1	1:E:16:LYS:HE2	1.78	0.66
2:F:165:ARG:HG2	2:F:166:GLY:H	1.61	0.66
2:H:500:GLU:HA	2:H:503:GLU:CB	2.22	0.66
1:E:149:LEU:O	1:E:150:ARG:C	2.40	0.65
1:E:149:LEU:HD13	1:E:152:GLU:HG3	1.77	0.65
1:E:181:THR:HG21	1:E:185:ALA:HA	1.77	0.65
1:G:374:ALA:HB1	1:G:375:PHE:CD1	2.31	0.65
2:H:259:VAL:HG13	2:H:265:ILE:O	1.96	0.65
2:B:444:LEU:O	2:B:447:VAL:HG23	1.96	0.65
1:C:351:ASN:O	1:C:355:GLN:HB2	1.95	0.65
1:G:340:TRP:HZ3	1:G:341:PHE:CZ	2.13	0.65
1:G:377:TYR:HE2	1:G:381:LYS:HD2	1.60	0.65
1:A:181:THR:O	1:A:181:THR:CG2	2.45	0.65
1:E:85:MET:CE	1:E:104:LEU:HB3	2.26	0.65
2:H:340:ARG:HH22	2:H:442:ASN:CB	2.09	0.65
1:A:85:MET:HE1	1:A:104:LEU:HB3	1.79	0.65
1:A:172:GLY:N	1:C:183:HIS:HE1	1.93	0.65
1:A:183:HIS:CE1	1:C:14:ARG:CZ	2.79	0.65
1:E:25:PHE:C	1:E:25:PHE:CD1	2.72	0.65
1:G:160:LYS:HZ3	1:G:160:LYS:HB2	1.49	0.65
1:A:85:MET:CE	1:A:104:LEU:HB3	2.27	0.65
1:A:319:ASN:HD22	1:A:319:ASN:N	1.87	0.65
1:A:372:PHE:HA	1:A:376:GLN:OE1	1.96	0.65
1:G:101:ILE:HD12	1:G:101:ILE:H	1.60	0.65
1:A:270:PHE:CE2	1:A:294:PHE:HB2	2.31	0.65
2:D:508:LEU:C	2:D:510:SER:H	2.04	0.65
2:F:496:LYS:O	2:F:499:ASN:ND2	2.30	0.65
1:G:230:LEU:C	1:G:230:LEU:HD23	2.21	0.65
1:G:270:PHE:CE2	1:G:294:PHE:HB2	2.31	0.65
1:A:14:ARG:NH2	1:C:219:ARG:CZ	2.59	0.65
1:C:246:ARG:O	1:C:250:GLU:HB2	1.97	0.65
1:G:351:ASN:HA	1:G:354:LEU:HB2	1.77	0.65
1:A:68:ARG:NH1	1:A:78:ARG:HB3	2.11	0.65
1:A:101:ILE:HD12	1:A:101:ILE:H	1.59	0.65
2:D:415:LEU:HD23	2:D:430:ILE:HD13	1.78	0.65
1:E:209:GLU:HB3	1:E:260:THR:HG22	1.78	0.65
1:E:224:LYS:HD2	1:E:224:LYS:C	2.22	0.65
2:D:165:ARG:HG2	2:D:166:GLY:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:THR:O	1:E:147:SER:CB	2.46	0.65
1:E:188:ILE:HD12	1:E:188:ILE:O	1.97	0.65
1:E:237:PRO:O	1:E:242:ARG:NH2	2.29	0.65
1:E:374:ALA:C	1:E:375:PHE:CD1	2.75	0.65
1:E:380:GLU:O	1:E:384:ASN:HB2	1.96	0.65
1:G:149:LEU:HD13	1:G:152:GLU:HG3	1.78	0.64
1:C:246:ARG:O	1:C:246:ARG:CG	2.45	0.64
1:C:372:PHE:HA	1:C:376:GLN:OE1	1.97	0.64
2:D:165:ARG:HG2	2:D:166:GLY:H	1.63	0.64
1:G:85:MET:HE1	1:G:104:LEU:HB3	1.79	0.64
1:E:268:TYR:O	1:E:269:ILE:C	2.39	0.64
2:F:455:LEU:HD12	2:F:455:LEU:O	1.97	0.64
1:A:25:PHE:C	1:A:25:PHE:CD1	2.69	0.64
1:A:97:GLU:OE1	1:C:370:LEU:HG	1.96	0.64
1:A:150:ARG:CB	1:A:150:ARG:NH2	2.60	0.64
1:A:200:VAL:HG11	1:A:252:LEU:HD23	1.79	0.64
1:C:175:VAL:O	1:C:175:VAL:HG23	1.97	0.64
1:G:13:ALA:O	1:G:16:LYS:HB2	1.96	0.64
1:C:21:LEU:CD2	1:C:153:MET:HA	2.28	0.64
1:A:149:LEU:O	1:A:150:ARG:C	2.40	0.64
1:C:353:PHE:C	1:C:355:GLN:N	2.52	0.64
2:F:475:ILE:N	2:F:476:PRO:CD	2.61	0.64
1:G:85:MET:CE	1:G:104:LEU:HB3	2.28	0.64
1:G:302:ILE:HB	1:G:303:PHE:CD2	2.33	0.64
1:G:208:VAL:HG21	1:G:213:VAL:CG1	2.27	0.64
2:B:455:LEU:HD12	2:B:455:LEU:O	1.98	0.63
1:C:31:GLN:HG3	1:C:38:LEU:CD1	2.28	0.63
1:C:356:ARG:O	1:C:357:LYS:C	2.40	0.63
2:D:444:LEU:O	2:D:447:VAL:HG23	1.98	0.63
1:E:150:ARG:CB	1:E:150:ARG:NH2	2.60	0.63
2:H:508:LEU:C	2:H:510:SER:H	2.05	0.63
1:C:209:GLU:HB3	1:C:260:THR:HG22	1.78	0.63
1:C:370:LEU:O	1:C:374:ALA:N	2.29	0.63
2:F:165:ARG:HG2	2:F:166:GLY:N	2.12	0.63
1:A:73:LEU:HD21	2:B:467:LYS:HE3	1.78	0.63
1:E:39:VAL:HG13	1:E:68:ARG:O	1.98	0.63
2:F:340:ARG:NH2	2:F:442:ASN:CB	2.60	0.63
1:G:150:ARG:O	1:G:152:GLU:N	2.31	0.63
1:A:189:GLU:HB3	1:C:183:HIS:HB2	1.81	0.63
2:F:414:HIS:CD2	2:F:415:LEU:N	2.63	0.63
3:F:531:RDC:H81	3:F:531:RDC:O1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD12	1:A:188:ILE:O	1.98	0.63
2:B:496:LYS:O	2:B:499:ASN:ND2	2.31	0.63
1:E:189:GLU:HB3	1:G:183:HIS:HB2	1.81	0.63
1:G:246:ARG:O	1:G:250:GLU:HB2	1.98	0.63
1:A:335:ILE:C	1:A:337:ASN:N	2.46	0.63
1:C:100:THR:OG1	1:C:101:ILE:HD12	1.98	0.63
2:F:414:HIS:HE2	2:F:416:CYS:HB3	1.62	0.63
1:A:181:THR:HG21	1:A:185:ALA:HA	1.80	0.63
2:B:259:VAL:HG13	2:B:265:ILE:O	1.99	0.63
1:E:302:ILE:HB	1:E:303:PHE:CD2	2.34	0.63
1:G:39:VAL:HG13	1:G:68:ARG:O	1.99	0.63
1:G:268:TYR:O	1:G:269:ILE:C	2.40	0.63
2:H:444:LEU:O	2:H:447:VAL:HG23	1.98	0.63
1:A:12:GLU:C	1:A:14:ARG:N	2.57	0.63
1:A:314:GLU:HA	1:A:317:ARG:NH1	2.13	0.63
1:E:31:GLN:O	1:E:32:LEU:C	2.42	0.63
1:E:270:PHE:CE2	1:E:294:PHE:HB2	2.34	0.63
1:E:374:ALA:CB	1:E:375:PHE:HD1	2.11	0.63
1:G:31:GLN:HG3	1:G:38:LEU:CD1	2.27	0.63
1:G:370:LEU:HD23	1:G:370:LEU:N	2.14	0.63
1:G:374:ALA:CB	1:G:375:PHE:CD1	2.82	0.63
1:A:268:TYR:O	1:A:269:ILE:C	2.41	0.62
2:B:264:SER:C	2:B:265:ILE:HG12	2.22	0.62
2:B:381:TYR:O	2:B:382:ASP:HB2	1.97	0.62
2:B:390:LYS:HG2	2:B:394:GLU:HG3	1.80	0.62
1:E:230:LEU:HD23	1:E:230:LEU:C	2.24	0.62
1:A:21:LEU:HD21	1:A:153:MET:HA	1.80	0.62
1:A:183:HIS:HB2	1:C:189:GLU:HB3	1.79	0.62
2:F:198:THR:O	2:F:198:THR:CG2	2.45	0.62
1:A:230:LEU:HD23	1:A:230:LEU:C	2.24	0.62
1:C:21:LEU:HD21	1:C:153:MET:HG2	1.81	0.62
2:H:191:ILE:H	2:H:191:ILE:HD13	1.64	0.62
2:H:414:HIS:HE2	2:H:416:CYS:HB3	1.64	0.62
1:A:14:ARG:HH21	1:C:183:HIS:CD2	2.15	0.62
2:B:480:ARG:CB	2:B:497:TYR:HE1	2.10	0.62
1:E:14:ARG:CZ	1:G:183:HIS:CE1	2.82	0.62
1:E:14:ARG:HH21	1:G:219:ARG:CZ	2.11	0.62
1:E:101:ILE:H	1:E:101:ILE:CD1	2.10	0.62
1:E:183:HIS:CE1	1:G:14:ARG:CZ	2.81	0.62
2:F:381:TYR:O	2:F:382:ASP:HB2	2.00	0.62
1:G:84:LEU:C	1:G:86:ALA:N	2.56	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:ARG:C	1:G:308:LYS:HD3	2.24	0.62
1:A:230:LEU:C	1:A:230:LEU:CD2	2.72	0.62
1:C:84:LEU:C	1:C:86:ALA:N	2.51	0.62
1:E:102:ARG:HD2	1:G:363:GLU:HG3	1.80	0.62
1:E:150:ARG:HH12	1:E:157:SER:HB3	1.64	0.62
1:G:149:LEU:H	1:G:149:LEU:CD1	2.12	0.62
2:H:496:LYS:O	2:H:499:ASN:ND2	2.32	0.62
1:C:22:ARG:O	1:C:25:PHE:HB3	2.00	0.62
2:D:264:SER:C	2:D:265:ILE:HG12	2.24	0.62
1:E:12:GLU:C	1:E:14:ARG:N	2.56	0.62
1:E:378:ILE:N	1:E:378:ILE:CD1	2.62	0.62
2:H:493:LEU:HG	2:H:494:VAL:N	2.14	0.62
1:A:146:THR:O	1:A:147:SER:CB	2.48	0.62
3:F:531:RDC:CL1	3:F:531:RDC:O5	2.55	0.62
2:H:401:GLY:HA3	2:H:455:LEU:HD21	1.80	0.62
2:B:318:GLY:O	2:B:320:ASP:N	2.33	0.62
1:C:149:LEU:HD12	1:C:149:LEU:N	2.15	0.62
2:D:480:ARG:CB	2:D:497:TYR:HE1	2.09	0.62
3:D:531:RDC:H81	3:D:531:RDC:O1	1.99	0.62
1:G:375:PHE:N	1:G:375:PHE:CD1	2.64	0.62
2:H:511:LYS:HB2	2:H:512:LYS:HD2	1.82	0.62
1:A:31:GLN:O	1:A:32:LEU:C	2.43	0.62
2:B:441:LYS:O	2:B:442:ASN:C	2.43	0.62
1:E:183:HIS:ND1	1:E:183:HIS:N	2.48	0.62
1:A:149:LEU:HD12	1:A:149:LEU:N	2.15	0.61
2:D:191:ILE:HD13	2:D:191:ILE:H	1.64	0.61
1:E:378:ILE:HD13	1:E:378:ILE:H	1.63	0.61
3:B:531:RDC:O1	3:B:531:RDC:H81	1.99	0.61
2:D:259:VAL:HG13	2:D:265:ILE:O	2.00	0.61
1:G:13:ALA:HB1	1:G:16:LYS:HE2	1.82	0.61
1:A:229:ILE:HD11	1:A:248:LEU:HD13	1.83	0.61
1:A:237:PRO:O	1:A:242:ARG:NH2	2.33	0.61
2:D:112:VAL:HG11	3:D:531:RDC:CL1	2.37	0.61
1:G:22:ARG:O	1:G:25:PHE:HB3	1.99	0.61
2:B:475:ILE:N	2:B:476:PRO:CD	2.64	0.61
1:C:42:ILE:HD11	1:C:68:ARG:HG3	1.83	0.61
1:A:136:ASP:O	1:A:139:ILE:HB	2.00	0.61
1:A:353:PHE:C	1:A:355:GLN:N	2.51	0.61
2:D:511:LYS:HB2	2:D:512:LYS:HD2	1.82	0.61
1:E:13:ALA:O	1:E:16:LYS:HB2	2.01	0.61
1:E:377:TYR:HE2	1:E:381:LYS:HD2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PRO:CB	1:A:104:LEU:HD11	2.31	0.61
1:A:246:ARG:O	1:A:246:ARG:CG	2.49	0.61
2:B:241:ILE:O	2:B:245:ILE:HG13	2.00	0.61
1:E:115:LYS:NZ	1:E:115:LYS:HB3	2.14	0.61
2:H:480:ARG:CB	2:H:497:TYR:HE1	2.12	0.61
2:D:340:ARG:HH22	2:D:442:ASN:CB	2.14	0.61
1:G:163:VAL:HG23	1:G:231:ILE:HB	1.82	0.61
2:H:264:SER:C	2:H:265:ILE:HG12	2.24	0.61
1:A:101:ILE:H	1:A:101:ILE:CD1	2.12	0.61
2:B:493:LEU:HG	2:B:494:VAL:N	2.15	0.61
2:B:511:LYS:HB2	2:B:512:LYS:HD2	1.83	0.61
1:C:268:TYR:O	1:C:269:ILE:C	2.43	0.61
2:D:381:TYR:O	2:D:382:ASP:HB2	2.01	0.61
2:F:318:GLY:C	2:F:320:ASP:H	2.09	0.61
1:E:172:GLY:CA	1:G:183:HIS:HE1	2.13	0.61
1:G:21:LEU:HD21	1:G:153:MET:HA	1.83	0.61
2:H:475:ILE:N	2:H:476:PRO:CD	2.63	0.61
1:A:21:LEU:HD12	1:A:93:LEU:HG	1.83	0.61
1:E:85:MET:CE	1:E:104:LEU:HD23	2.28	0.61
1:E:208:VAL:HG21	1:E:213:VAL:HG11	1.83	0.61
2:F:493:LEU:HG	2:F:494:VAL:N	2.15	0.61
1:A:298:SER:O	1:A:301:ASP:CB	2.40	0.60
1:E:230:LEU:C	1:E:230:LEU:CD2	2.74	0.60
1:A:303:PHE:HA	1:A:317:ARG:HH21	1.65	0.60
1:E:21:LEU:CD2	1:E:153:MET:HA	2.31	0.60
2:F:243:ILE:O	2:F:247:ASN:HB2	2.00	0.60
2:F:511:LYS:HB2	2:F:512:LYS:HD2	1.84	0.60
1:G:12:GLU:C	1:G:14:ARG:N	2.58	0.60
3:H:531:RDC:CL1	3:H:531:RDC:O5	2.55	0.60
1:A:149:LEU:HD13	1:A:152:GLU:HG3	1.82	0.60
1:A:209:GLU:HB3	1:A:260:THR:HG22	1.84	0.60
1:A:274:ARG:C	1:A:275:ILE:HG12	2.26	0.60
2:B:255:LYS:O	2:B:256:GLU:C	2.44	0.60
2:B:263:GLN:O	2:B:264:SER:CB	2.49	0.60
2:B:345:TYR:O	2:B:346:GLN:C	2.44	0.60
1:C:31:GLN:O	1:C:32:LEU:C	2.44	0.60
1:E:14:ARG:HH21	1:G:183:HIS:CD2	2.19	0.60
1:C:150:ARG:O	1:C:152:GLU:N	2.35	0.60
1:C:319:ASN:HD22	1:C:319:ASN:N	1.86	0.60
1:G:31:GLN:O	1:G:32:LEU:C	2.43	0.60
1:A:353:PHE:O	1:A:355:GLN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ALA:CB	1:A:375:PHE:HD1	2.13	0.60
1:C:12:GLU:C	1:C:14:ARG:H	2.09	0.60
1:C:238:ASP:OD1	1:C:241:THR:CB	2.41	0.60
1:C:303:PHE:CE1	1:C:356:ARG:HD2	2.35	0.60
2:D:493:LEU:HG	2:D:494:VAL:N	2.17	0.60
1:E:22:ARG:O	1:E:25:PHE:HB3	2.01	0.60
2:F:318:GLY:O	2:F:320:ASP:N	2.34	0.60
2:B:191:ILE:H	2:B:191:ILE:HD13	1.66	0.60
2:B:318:GLY:C	2:B:320:ASP:H	2.09	0.60
2:D:243:ILE:O	2:D:247:ASN:HB2	2.01	0.60
1:E:17:ALA:C	1:E:19:ASN:H	2.10	0.60
2:F:516:ILE:N	2:F:516:ILE:CD1	2.63	0.60
1:G:353:PHE:C	1:G:355:GLN:N	2.53	0.60
1:A:208:VAL:HG21	1:A:213:VAL:CG1	2.31	0.60
1:A:13:ALA:O	1:A:16:LYS:HB2	2.02	0.60
1:A:356:ARG:O	1:A:357:LYS:C	2.43	0.60
1:C:17:ALA:C	1:C:19:ASN:H	2.10	0.60
1:C:353:PHE:O	1:C:355:GLN:N	2.34	0.60
2:D:475:ILE:N	2:D:476:PRO:CD	2.65	0.60
1:G:21:LEU:HD12	1:G:93:LEU:HG	1.84	0.60
2:B:243:ILE:O	2:B:247:ASN:HB2	2.02	0.60
1:C:385:LYS:HG3	1:C:387:TYR:HE2	1.66	0.60
2:F:444:LEU:O	2:F:447:VAL:HG23	2.01	0.60
1:G:238:ASP:OD1	1:G:238:ASP:N	2.35	0.60
1:C:245:VAL:HG12	1:C:246:ARG:N	2.17	0.60
1:A:13:ALA:HB1	1:A:16:LYS:HE2	1.83	0.59
1:A:219:ARG:CZ	1:C:14:ARG:NH2	2.65	0.59
1:C:39:VAL:HG12	1:C:40:MET:N	2.17	0.59
2:D:18:ARG:O	2:D:20:PRO:HD3	2.02	0.59
1:E:85:MET:HE1	1:E:104:LEU:HB3	1.82	0.59
1:E:374:ALA:HB1	1:E:375:PHE:HE1	1.64	0.59
2:F:18:ARG:O	2:F:20:PRO:HD3	2.03	0.59
1:G:150:ARG:CB	1:G:150:ARG:NH2	2.64	0.59
1:A:31:GLN:HE21	2:B:482:LEU:HD21	1.67	0.59
1:C:99:PRO:CB	1:C:104:LEU:HD11	2.32	0.59
2:D:267:ASP:HB2	2:H:204:ILE:HD13	1.84	0.59
1:E:175:VAL:HG23	1:E:175:VAL:O	2.01	0.59
1:A:224:LYS:HD2	1:A:224:LYS:C	2.27	0.59
1:E:172:GLY:N	1:G:183:HIS:HE1	2.01	0.59
1:G:242:ARG:O	1:G:243:ARG:C	2.43	0.59
1:G:372:PHE:HA	1:G:376:GLN:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:ILE:HG22	2:B:326:LEU:HD21	1.84	0.59
2:B:492:GLU:HB3	2:B:496:LYS:HG2	1.85	0.59
1:E:239:ARG:HH22	1:E:277:SER:HB3	1.67	0.59
1:E:246:ARG:O	1:E:246:ARG:CG	2.50	0.59
1:A:149:LEU:H	1:A:149:LEU:CD1	2.15	0.59
2:B:18:ARG:O	2:B:20:PRO:HD3	2.02	0.59
1:C:150:ARG:CB	1:C:150:ARG:NH2	2.64	0.59
2:F:180:TRP:HB3	2:F:181:PRO:HD3	1.85	0.59
1:C:163:VAL:HG22	1:C:164:VAL:H	1.66	0.59
2:H:415:LEU:HD23	2:H:430:ILE:HD13	1.84	0.59
1:C:237:PRO:HG2	1:C:272:VAL:HG11	1.83	0.59
1:C:274:ARG:C	1:C:275:ILE:HG12	2.27	0.59
1:C:374:ALA:C	1:C:375:PHE:CD1	2.78	0.59
2:D:46:ALA:HB2	3:D:531:RDC:H162	1.84	0.59
2:F:293:ILE:O	2:F:296:LEU:HB3	2.03	0.59
2:F:303:ASP:HB3	2:F:306:PHE:HE2	1.67	0.59
2:H:243:ILE:O	2:H:247:ASN:HB2	2.02	0.59
2:H:342:PRO:HA	2:H:351:ILE:HG23	1.85	0.59
2:H:381:TYR:O	2:H:382:ASP:HB2	2.01	0.59
2:H:516:ILE:N	2:H:516:ILE:CD1	2.65	0.59
1:C:230:LEU:C	1:C:230:LEU:CD2	2.76	0.59
1:E:113:LEU:HD22	1:E:115:LYS:O	2.03	0.59
1:E:356:ARG:O	1:E:357:LYS:C	2.45	0.59
2:D:455:LEU:HD12	2:D:455:LEU:O	2.03	0.59
2:H:303:ASP:HB3	2:H:306:PHE:HE2	1.68	0.59
1:A:17:ALA:C	1:A:19:ASN:H	2.10	0.58
1:A:150:ARG:HH12	1:A:157:SER:HB3	1.67	0.58
1:A:309:LYS:HB2	1:A:309:LYS:NZ	2.17	0.58
1:C:150:ARG:HH12	1:C:157:SER:HB3	1.68	0.58
2:F:259:VAL:HG13	2:F:265:ILE:O	2.02	0.58
2:F:263:GLN:O	2:F:264:SER:CB	2.50	0.58
2:B:516:ILE:N	2:B:516:ILE:CD1	2.66	0.58
1:E:31:GLN:HG3	1:E:38:LEU:CD1	2.32	0.58
2:F:255:LYS:O	2:F:256:GLU:C	2.45	0.58
2:F:448:ALA:O	2:F:451:LEU:HB3	2.03	0.58
1:G:274:ARG:C	1:G:275:ILE:HG12	2.26	0.58
1:C:115:LYS:HB3	1:C:115:LYS:HZ3	1.68	0.58
2:D:303:ASP:HB3	2:D:306:PHE:HE2	1.69	0.58
1:C:312:LEU:HD22	1:C:317:ARG:HH11	1.67	0.58
1:C:340:TRP:HZ3	1:C:341:PHE:CZ	2.21	0.58
1:A:21:LEU:HD12	1:A:93:LEU:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:LEU:HD12	1:G:149:LEU:N	2.15	0.58
1:G:163:VAL:HG22	1:G:164:VAL:H	1.69	0.58
1:G:270:PHE:CD1	1:G:270:PHE:C	2.81	0.58
1:G:374:ALA:C	1:G:375:PHE:CD1	2.77	0.58
1:A:183:HIS:ND1	1:A:183:HIS:N	2.52	0.58
2:B:441:LYS:O	2:B:443:ALA:N	2.35	0.58
1:C:12:GLU:C	1:C:14:ARG:N	2.60	0.58
1:C:351:ASN:OD1	1:C:351:ASN:N	2.29	0.58
1:E:21:LEU:HD12	1:E:93:LEU:HG	1.84	0.58
1:G:183:HIS:ND1	1:G:183:HIS:N	2.51	0.58
1:G:353:PHE:O	1:G:355:GLN:N	2.37	0.58
1:C:230:LEU:C	1:C:230:LEU:HD23	2.28	0.58
2:D:241:ILE:O	2:D:245:ILE:HG13	2.04	0.58
1:E:31:GLN:HE21	2:F:482:LEU:HD21	1.69	0.58
2:F:18:ARG:C	2:F:20:PRO:HD3	2.29	0.58
1:G:73:LEU:HD21	2:H:467:LYS:CE	2.34	0.58
1:G:356:ARG:O	1:G:357:LYS:C	2.45	0.58
2:H:103:GLN:HE22	2:H:315:SER:N	2.01	0.58
3:B:531:RDC:O5	3:B:531:RDC:CL1	2.58	0.58
1:C:224:LYS:HD2	1:C:224:LYS:C	2.29	0.58
3:D:531:RDC:CL1	3:D:531:RDC:O5	2.59	0.58
1:E:39:VAL:HG12	1:E:40:MET:N	2.18	0.58
1:G:189:GLU:O	1:G:191:THR:N	2.36	0.58
1:A:32:LEU:O	1:A:33:LYS:C	2.46	0.57
1:A:239:ARG:HH22	1:A:277:SER:HB3	1.69	0.57
2:F:197:ILE:HB	2:F:317:ILE:HD12	1.85	0.57
1:G:224:LYS:HD2	1:G:224:LYS:C	2.28	0.57
1:A:106:TYR:C	1:A:107:ARG:HD3	2.24	0.57
1:A:374:ALA:HB1	1:A:375:PHE:HE1	1.69	0.57
2:D:400:TYR:CA	2:D:452:LYS:HE2	2.23	0.57
2:D:516:ILE:N	2:D:516:ILE:CD1	2.65	0.57
2:F:480:ARG:CB	2:F:497:TYR:HE1	2.12	0.57
2:H:263:GLN:O	2:H:264:SER:CB	2.51	0.57
1:A:21:LEU:CD2	1:A:153:MET:HA	2.35	0.57
1:A:183:HIS:HE1	1:C:172:GLY:CA	2.16	0.57
1:C:32:LEU:O	1:C:33:LYS:C	2.46	0.57
1:C:303:PHE:HA	1:C:317:ARG:NH2	2.19	0.57
2:D:263:GLN:O	2:D:264:SER:CB	2.51	0.57
1:E:170:ARG:HG3	1:E:196:ASP:HB2	1.86	0.57
1:A:39:VAL:HG13	1:A:68:ARG:O	2.05	0.57
1:A:163:VAL:HG22	1:A:164:VAL:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:LEU:H	1:E:149:LEU:CD1	2.17	0.57
1:E:325:LYS:O	1:E:328:ASP:HB2	2.04	0.57
2:H:322:ILE:HD13	2:H:412:MET:HE1	1.86	0.57
1:C:80:MET:CE	2:D:477:GLU:HB3	2.34	0.57
2:D:46:ALA:CB	3:D:531:RDC:H162	2.35	0.57
1:E:138:VAL:O	1:E:142:ILE:HG13	2.04	0.57
1:E:385:LYS:HG3	1:E:387:TYR:HE2	1.70	0.57
2:F:415:LEU:HD23	2:F:430:ILE:HD13	1.85	0.57
1:G:17:ALA:C	1:G:19:ASN:H	2.12	0.57
1:G:150:ARG:HH12	1:G:157:SER:HB3	1.68	0.57
2:D:18:ARG:C	2:D:20:PRO:HD3	2.29	0.57
1:E:340:TRP:HZ3	1:E:341:PHE:CZ	2.22	0.57
2:H:487:ALA:HB3	2:H:492:GLU:HB2	1.85	0.57
1:C:295:LEU:O	1:C:295:LEU:HD22	2.05	0.57
1:E:183:HIS:N	1:E:183:HIS:HD1	2.02	0.57
1:E:353:PHE:O	1:E:355:GLN:N	2.37	0.57
2:F:492:GLU:HB3	2:F:496:LYS:HG2	1.85	0.57
1:G:13:ALA:CB	1:G:16:LYS:HE2	2.35	0.57
2:H:180:TRP:HB3	2:H:181:PRO:HD3	1.85	0.57
2:H:340:ARG:HH22	2:H:442:ASN:HB2	1.69	0.57
2:B:401:GLY:HA3	2:B:455:LEU:HD21	1.87	0.57
1:C:69:ASN:N	1:C:69:ASN:OD1	2.38	0.57
1:C:149:LEU:HD13	1:C:152:GLU:HG3	1.86	0.57
1:E:13:ALA:CB	1:E:16:LYS:HE2	2.34	0.57
1:G:303:PHE:CE1	1:G:356:ARG:HD2	2.40	0.57
1:A:22:ARG:O	1:A:25:PHE:HB3	2.04	0.57
1:A:36:GLU:HB3	1:A:37:PRO:HD2	1.87	0.57
1:A:85:MET:CE	1:A:104:LEU:HD23	2.35	0.57
2:B:18:ARG:C	2:B:20:PRO:HD3	2.30	0.57
2:B:112:VAL:HG21	3:B:531:RDC:CL1	2.42	0.57
2:B:322:ILE:HD13	2:B:412:MET:HE1	1.87	0.57
2:B:340:ARG:HH22	2:B:442:ASN:HB3	1.70	0.57
2:B:420:ILE:HB	2:B:422:TYR:HE2	1.70	0.57
1:C:13:ALA:O	1:C:16:LYS:HB2	2.05	0.57
1:E:99:PRO:CB	1:E:104:LEU:HD11	2.33	0.57
1:E:238:ASP:O	1:E:242:ARG:NH2	2.38	0.57
1:E:270:PHE:C	1:E:270:PHE:CD1	2.82	0.57
1:G:21:LEU:HD12	1:G:93:LEU:CD1	2.34	0.57
1:E:262:ALA:HB2	1:E:360:LEU:HD12	1.86	0.57
1:A:307:ARG:CD	1:A:308:LYS:HZ3	1.94	0.56
1:C:17:ALA:O	1:C:19:ASN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:THR:OG1	1:E:101:ILE:HD12	2.05	0.56
2:F:401:GLY:CA	2:F:455:LEU:HD21	2.11	0.56
1:G:177:ASP:C	1:G:177:ASP:OD1	2.47	0.56
1:G:239:ARG:HH22	1:G:277:SER:HB3	1.70	0.56
1:G:374:ALA:CB	1:G:375:PHE:HD1	2.18	0.56
2:H:318:GLY:C	2:H:320:ASP:H	2.12	0.56
2:H:455:LEU:HD13	2:H:459:ARG:HH22	1.70	0.56
1:C:39:VAL:CG2	1:C:69:ASN:HA	2.35	0.56
1:C:246:ARG:HB2	1:C:289:THR:HG22	1.87	0.56
1:E:298:SER:O	1:E:301:ASP:CB	2.44	0.56
1:A:13:ALA:CB	1:A:16:LYS:HE2	2.36	0.56
1:C:183:HIS:N	1:C:183:HIS:ND1	2.53	0.56
1:E:69:ASN:N	1:E:69:ASN:OD1	2.38	0.56
1:E:98:TYR:HB3	1:E:156:LEU:CD2	2.35	0.56
1:E:183:HIS:HE1	1:G:172:GLY:CA	2.18	0.56
1:E:319:ASN:ND2	1:E:319:ASN:N	2.47	0.56
2:F:142:PHE:HB3	2:F:144:LEU:CD1	2.36	0.56
2:F:322:ILE:HD13	2:F:412:MET:HE1	1.86	0.56
1:G:12:GLU:C	1:G:12:GLU:CD	2.74	0.56
1:G:99:PRO:CB	1:G:104:LEU:HD11	2.35	0.56
1:G:106:TYR:C	1:G:107:ARG:HD3	2.27	0.56
1:G:270:PHE:HE2	1:G:294:PHE:HB2	1.71	0.56
1:A:274:ARG:O	1:A:275:ILE:HG23	2.05	0.56
1:C:262:ALA:HB2	1:C:360:LEU:HD12	1.88	0.56
2:D:255:LYS:O	2:D:256:GLU:C	2.47	0.56
1:E:246:ARG:HB2	1:E:289:THR:HG22	1.86	0.56
1:E:274:ARG:C	1:E:275:ILE:HG12	2.29	0.56
1:G:272:VAL:HG13	1:G:277:SER:H	1.69	0.56
1:G:309:LYS:HG3	1:G:310:PRO:HD2	1.87	0.56
1:A:221:GLY:O	1:A:222:PHE:C	2.47	0.56
1:A:331:ARG:O	1:A:335:ILE:HG12	2.05	0.56
1:C:237:PRO:O	1:C:242:ARG:NH2	2.39	0.56
1:C:270:PHE:CE2	1:C:294:PHE:HB2	2.41	0.56
2:D:112:VAL:HG21	3:D:531:RDC:CL1	2.43	0.56
2:D:318:GLY:C	2:D:320:ASP:H	2.13	0.56
2:D:342:PRO:HA	2:D:351:ILE:HG23	1.88	0.56
1:E:183:HIS:HE1	1:G:172:GLY:N	2.03	0.56
2:F:467:LYS:O	2:F:469:LEU:N	2.39	0.56
1:A:113:LEU:HD22	1:A:115:LYS:O	2.05	0.56
1:C:113:LEU:HD22	1:C:115:LYS:O	2.06	0.56
1:E:21:LEU:HB3	1:E:93:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:LEU:C	2:F:46:ALA:H	2.14	0.56
2:F:441:LYS:O	2:F:442:ASN:C	2.49	0.56
1:G:32:LEU:O	1:G:33:LYS:C	2.48	0.56
1:G:36:GLU:HB3	1:G:37:PRO:HD2	1.88	0.56
1:G:68:ARG:NH1	1:G:78:ARG:HB3	2.20	0.56
1:A:262:ALA:HB2	1:A:360:LEU:HD12	1.88	0.56
2:D:180:TRP:HB3	2:D:181:PRO:HD3	1.87	0.56
2:D:221:LYS:HD2	2:D:321:LEU:HD21	1.87	0.56
1:G:100:THR:OG1	1:G:101:ILE:HD12	2.05	0.56
1:A:14:ARG:CZ	1:C:183:HIS:CD2	2.89	0.56
1:C:142:ILE:O	1:C:146:THR:HG23	2.05	0.56
1:G:208:VAL:HG21	1:G:213:VAL:HG11	1.88	0.56
2:H:322:ILE:CG2	2:H:412:MET:HE2	2.36	0.56
2:B:414:HIS:CD2	2:B:414:HIS:C	2.84	0.56
1:C:319:ASN:ND2	1:C:319:ASN:N	2.46	0.56
1:C:377:TYR:HE2	1:C:381:LYS:HD2	1.69	0.56
1:E:351:ASN:OD1	1:E:351:ASN:N	2.34	0.56
1:G:192:PRO:HG3	1:G:240:ALA:HB1	1.87	0.56
2:H:420:ILE:HB	2:H:422:TYR:HE2	1.71	0.56
1:C:17:ALA:C	1:C:19:ASN:N	2.63	0.55
1:C:106:TYR:C	1:C:107:ARG:HD3	2.26	0.55
1:C:374:ALA:HB1	1:C:375:PHE:HE1	1.68	0.55
1:C:378:ILE:O	1:C:379:PRO:C	2.49	0.55
2:F:285:VAL:HG13	2:F:286:LYS:N	2.21	0.55
1:C:208:VAL:HG21	1:C:213:VAL:HG11	1.88	0.55
2:D:492:GLU:HB3	2:D:496:LYS:HG2	1.88	0.55
1:E:136:ASP:O	1:E:139:ILE:HB	2.06	0.55
1:E:150:ARG:O	1:E:152:GLU:N	2.39	0.55
1:A:101:ILE:N	1:A:101:ILE:CD1	2.63	0.55
1:C:149:LEU:H	1:C:149:LEU:CD1	2.18	0.55
1:C:163:VAL:HG23	1:C:231:ILE:HB	1.88	0.55
1:C:191:THR:OG1	1:C:194:LEU:HD21	2.06	0.55
2:D:322:ILE:CG2	2:D:412:MET:HE2	2.36	0.55
2:D:441:LYS:O	2:D:442:ASN:C	2.49	0.55
2:H:112:VAL:HG21	3:H:531:RDC:CL1	2.43	0.55
1:A:21:LEU:HD21	1:A:153:MET:HG2	1.88	0.55
2:D:142:PHE:HB3	2:D:144:LEU:CD1	2.36	0.55
2:D:191:ILE:H	2:D:191:ILE:CD1	2.16	0.55
1:E:163:VAL:HG23	1:E:231:ILE:HB	1.88	0.55
2:F:342:PRO:HA	2:F:351:ILE:HG23	1.88	0.55
1:G:295:LEU:O	1:G:295:LEU:HD22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:293:ILE:O	2:H:296:LEU:HB3	2.06	0.55
1:A:82:THR:HA	1:A:138:VAL:CG1	2.37	0.55
1:A:142:ILE:O	1:A:146:THR:HG23	2.07	0.55
1:C:136:ASP:O	1:C:139:ILE:HB	2.06	0.55
2:D:227:GLN:O	2:D:313:SER:HA	2.06	0.55
1:G:113:LEU:HD22	1:G:115:LYS:O	2.06	0.55
1:G:238:ASP:OD1	1:G:241:THR:CB	2.45	0.55
2:B:44:LEU:C	2:B:46:ALA:H	2.15	0.55
1:C:13:ALA:HB1	1:C:16:LYS:HE2	1.89	0.55
1:C:21:LEU:HB3	1:C:93:LEU:HD11	1.88	0.55
1:C:36:GLU:HB3	1:C:37:PRO:HD2	1.88	0.55
1:C:170:ARG:CG	1:C:196:ASP:HB2	2.36	0.55
1:C:261:ASP:OD1	1:C:362:ILE:N	2.39	0.55
1:E:142:ILE:O	1:E:146:THR:HG23	2.07	0.55
1:E:149:LEU:HD12	1:E:149:LEU:N	2.18	0.55
1:E:163:VAL:HG22	1:E:164:VAL:H	1.71	0.55
1:A:42:ILE:HD11	1:A:68:ARG:HG3	1.88	0.55
1:C:73:LEU:HD21	2:D:467:LYS:HG2	1.88	0.55
1:C:101:ILE:N	1:C:101:ILE:CD1	2.59	0.55
1:A:339:GLU:HG3	1:A:339:GLU:O	2.07	0.55
2:B:342:PRO:HA	2:B:351:ILE:HG23	1.89	0.55
2:D:420:ILE:HB	2:D:422:TYR:HE2	1.71	0.55
2:D:487:ALA:HB3	2:D:492:GLU:HB2	1.88	0.55
2:H:441:LYS:O	2:H:442:ASN:C	2.50	0.55
2:H:492:GLU:O	2:H:493:LEU:C	2.50	0.55
1:C:85:MET:CE	1:C:104:LEU:HD23	2.36	0.55
2:B:227:GLN:O	2:B:313:SER:HA	2.07	0.55
1:C:366:ALA:C	1:C:368:LYS:N	2.63	0.55
1:G:183:HIS:N	1:G:183:HIS:HD1	2.04	0.55
2:H:255:LYS:O	2:H:256:GLU:C	2.50	0.55
1:A:39:VAL:HG22	1:A:69:ASN:HA	1.88	0.54
1:C:138:VAL:O	1:C:142:ILE:HG13	2.07	0.54
2:D:293:ILE:O	2:D:296:LEU:HB3	2.07	0.54
2:D:318:GLY:O	2:D:320:ASP:N	2.40	0.54
2:D:401:GLY:HA3	2:D:455:LEU:HD11	1.88	0.54
1:G:32:LEU:HD11	2:H:486:LEU:HD11	1.88	0.54
1:A:21:LEU:HB3	1:A:93:LEU:HD11	1.88	0.54
1:A:69:ASN:OD1	1:A:69:ASN:N	2.39	0.54
2:B:180:TRP:HB3	2:B:181:PRO:HD3	1.88	0.54
2:B:198:THR:O	2:B:198:THR:CG2	2.47	0.54
2:B:293:ILE:O	2:B:296:LEU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLY:O	1:C:222:PHE:C	2.51	0.54
2:B:285:VAL:O	2:B:288:LEU:HG	2.07	0.54
1:C:148:LEU:HD12	1:C:148:LEU:N	2.22	0.54
1:C:307:ARG:C	1:C:308:LYS:CD	2.80	0.54
2:D:215:TYR:CD2	2:D:215:TYR:N	2.74	0.54
1:E:221:GLY:O	1:E:222:PHE:C	2.50	0.54
1:E:366:ALA:C	1:E:368:LYS:N	2.65	0.54
1:G:85:MET:CE	1:G:104:LEU:HD23	2.37	0.54
1:G:229:ILE:HD11	1:G:248:LEU:HD13	1.90	0.54
1:A:270:PHE:HE2	1:A:294:PHE:HB2	1.73	0.54
2:B:330:PHE:O	2:B:361:SER:HB2	2.08	0.54
2:D:414:HIS:CD2	2:D:414:HIS:C	2.85	0.54
1:E:176:ILE:CD1	1:G:176:ILE:CD1	2.67	0.54
2:F:215:TYR:N	2:F:215:TYR:CD2	2.75	0.54
1:G:69:ASN:OD1	1:G:69:ASN:N	2.39	0.54
1:G:175:VAL:HG23	1:G:175:VAL:O	2.06	0.54
1:A:86:ALA:O	1:A:89:ILE:HB	2.08	0.54
1:A:270:PHE:CD1	1:A:270:PHE:C	2.85	0.54
1:C:229:ILE:HD11	1:C:248:LEU:HD13	1.88	0.54
1:E:36:GLU:HB3	1:E:37:PRO:HD2	1.89	0.54
2:F:326:LEU:HD12	2:F:357:ALA:HB2	1.89	0.54
2:F:508:LEU:C	2:F:510:SER:N	2.65	0.54
2:H:492:GLU:HB3	2:H:496:LYS:HG2	1.90	0.54
1:A:100:THR:OG1	1:A:101:ILE:HD12	2.08	0.54
1:C:242:ARG:O	1:C:243:ARG:C	2.49	0.54
1:E:17:ALA:C	1:E:19:ASN:N	2.63	0.54
2:B:396:ASP:HB3	2:B:399:ARG:HH11	1.73	0.54
1:C:21:LEU:HD12	1:C:93:LEU:HG	1.90	0.54
1:E:309:LYS:HG3	1:E:310:PRO:HD2	1.89	0.54
2:F:240:GLU:O	2:F:241:ILE:C	2.51	0.54
1:G:43:PRO:O	1:G:144:VAL:HG11	2.08	0.54
1:G:245:VAL:HG12	1:G:246:ARG:N	2.22	0.54
1:G:261:ASP:OD1	1:G:362:ILE:N	2.40	0.54
1:A:189:GLU:O	1:A:191:THR:N	2.40	0.54
2:B:303:ASP:HB3	2:B:306:PHE:HE2	1.72	0.54
1:C:309:LYS:HG3	1:C:310:PRO:HD2	1.90	0.54
1:E:32:LEU:O	1:E:33:LYS:C	2.50	0.54
1:G:339:GLU:O	1:G:339:GLU:HG3	2.07	0.54
2:H:44:LEU:C	2:H:46:ALA:H	2.16	0.54
2:H:191:ILE:H	2:H:191:ILE:CD1	2.21	0.54
1:A:309:LYS:HG3	1:A:310:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:ILE:HG22	2:B:408:GLN:HB3	1.90	0.54
1:G:366:ALA:C	1:G:368:LYS:N	2.65	0.54
2:H:18:ARG:O	2:H:20:PRO:HD3	2.08	0.54
1:A:176:ILE:CD1	1:C:176:ILE:CD1	2.67	0.53
2:B:415:LEU:HD23	2:B:430:ILE:HD13	1.90	0.53
2:F:330:PHE:O	2:F:361:SER:HB2	2.07	0.53
2:H:285:VAL:O	2:H:288:LEU:HG	2.08	0.53
2:B:467:LYS:O	2:B:470:ALA:N	2.41	0.53
1:C:12:GLU:CG	1:C:13:ALA:N	2.70	0.53
2:D:44:LEU:C	2:D:46:ALA:H	2.16	0.53
2:F:369:ILE:HB	2:F:410:VAL:HG13	1.90	0.53
2:H:322:ILE:HG22	2:H:326:LEU:HD21	1.90	0.53
1:A:188:ILE:O	1:A:188:ILE:CD1	2.56	0.53
1:A:291:ASP:OD1	1:A:291:ASP:C	2.52	0.53
2:B:142:PHE:HB3	2:B:144:LEU:CD1	2.37	0.53
1:C:148:LEU:N	1:C:148:LEU:CD1	2.71	0.53
1:E:68:ARG:NH1	1:E:78:ARG:HB3	2.24	0.53
2:F:395:LEU:HD12	2:F:396:ASP:H	1.72	0.53
1:G:86:ALA:O	1:G:89:ILE:HB	2.08	0.53
1:G:262:ALA:HB2	1:G:360:LEU:HD12	1.89	0.53
2:H:18:ARG:C	2:H:20:PRO:HD3	2.33	0.53
2:B:508:LEU:C	2:B:510:SER:N	2.65	0.53
1:E:170:ARG:CG	1:E:196:ASP:HB2	2.38	0.53
2:F:492:GLU:O	2:F:493:LEU:C	2.51	0.53
1:A:183:HIS:HE1	1:C:172:GLY:N	2.06	0.53
1:A:184:GLY:O	1:A:185:ALA:HB2	2.09	0.53
1:A:237:PRO:HG2	1:A:272:VAL:HG11	1.89	0.53
3:B:531:RDC:CL1	3:B:531:RDC:C9	2.94	0.53
1:C:80:MET:CE	2:D:477:GLU:CB	2.86	0.53
1:C:268:TYR:O	1:C:271:SER:N	2.41	0.53
2:D:285:VAL:O	2:D:288:LEU:HG	2.08	0.53
1:E:188:ILE:O	1:E:188:ILE:CD1	2.56	0.53
1:G:101:ILE:H	1:G:101:ILE:CD1	2.14	0.53
2:H:318:GLY:O	2:H:320:ASP:N	2.39	0.53
1:A:17:ALA:C	1:A:19:ASN:N	2.63	0.53
1:A:138:VAL:O	1:A:142:ILE:HG13	2.09	0.53
1:E:39:VAL:HG22	1:E:69:ASN:HA	1.90	0.53
1:E:295:LEU:O	1:E:295:LEU:HD22	2.09	0.53
1:E:347:GLN:O	1:E:348:GLU:C	2.52	0.53
2:F:302:LYS:O	2:F:303:ASP:C	2.51	0.53
1:G:21:LEU:CD2	1:G:153:MET:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:ASP:OD1	2:H:105:ARG:HD2	2.09	0.53
2:B:322:ILE:CG2	2:B:412:MET:HE2	2.38	0.53
1:C:42:ILE:CD1	1:C:68:ARG:HG3	2.38	0.53
1:E:339:GLU:HG3	1:E:339:GLU:O	2.08	0.53
1:G:243:ARG:HH22	1:G:287:LEU:HD22	1.73	0.53
1:E:242:ARG:O	1:E:243:ARG:C	2.50	0.53
1:E:245:VAL:HG12	1:E:246:ARG:N	2.24	0.53
1:E:291:ASP:OD1	1:E:291:ASP:C	2.51	0.53
2:F:47:THR:HG22	2:F:78:GLY:HA2	1.91	0.53
2:H:142:PHE:HB3	2:H:144:LEU:CD1	2.39	0.53
1:A:172:GLY:N	1:C:183:HIS:CE1	2.76	0.53
2:B:467:LYS:O	2:B:469:LEU:N	2.42	0.53
1:C:163:VAL:HG22	1:C:164:VAL:N	2.23	0.53
2:D:492:GLU:O	2:D:493:LEU:C	2.50	0.53
1:E:17:ALA:O	1:E:19:ASN:N	2.42	0.53
2:F:414:HIS:CD2	2:F:414:HIS:C	2.87	0.53
1:G:39:VAL:HG12	1:G:40:MET:N	2.23	0.53
2:B:47:THR:HG22	2:B:78:GLY:HA2	1.91	0.53
2:D:322:ILE:HG22	2:D:326:LEU:HD21	1.91	0.53
1:E:160:LYS:HB2	1:E:160:LYS:HZ2	1.73	0.53
2:H:165:ARG:HG2	2:H:166:GLY:H	1.73	0.53
1:A:246:ARG:HB2	1:A:289:THR:HG22	1.91	0.52
1:A:259:LEU:CD1	1:A:259:LEU:O	2.57	0.52
1:C:89:ILE:HD13	1:C:104:LEU:HD21	1.92	0.52
1:C:98:TYR:HB3	1:C:156:LEU:CD2	2.39	0.52
1:C:302:ILE:HG22	1:C:312:LEU:CD2	2.19	0.52
1:E:366:ALA:C	1:E:368:LYS:H	2.17	0.52
1:G:270:PHE:CD2	1:G:294:PHE:HD1	2.27	0.52
1:G:370:LEU:O	1:G:374:ALA:N	2.33	0.52
1:A:12:GLU:O	1:A:14:ARG:N	2.41	0.52
1:A:170:ARG:CG	1:A:196:ASP:HB2	2.39	0.52
1:A:177:ASP:C	1:A:177:ASP:OD1	2.52	0.52
1:A:385:LYS:HG3	1:A:387:TYR:CE2	2.42	0.52
2:D:326:LEU:HD12	2:D:357:ALA:HB2	1.90	0.52
2:D:402:ILE:O	2:D:402:ILE:HG22	2.10	0.52
2:D:467:LYS:O	2:D:469:LEU:N	2.43	0.52
2:F:191:ILE:HD13	2:F:191:ILE:H	1.73	0.52
1:G:37:PRO:HD3	2:H:507:LYS:NZ	2.23	0.52
1:G:221:GLY:O	1:G:222:PHE:C	2.51	0.52
2:H:165:ARG:HG2	2:H:166:GLY:N	2.24	0.52
2:H:340:ARG:NH2	2:H:442:ASN:CB	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG23	1:A:231:ILE:HB	1.91	0.52
1:A:379:PRO:O	1:A:383:THR:HG22	2.09	0.52
2:B:165:ARG:HG2	2:B:166:GLY:N	2.23	0.52
1:E:85:MET:HE1	1:E:104:LEU:CD2	2.33	0.52
1:E:378:ILE:HB	1:E:379:PRO:CD	2.40	0.52
2:F:322:ILE:HG22	2:F:326:LEU:HD21	1.91	0.52
1:A:39:VAL:HG12	1:A:40:MET:N	2.23	0.52
1:A:325:LYS:O	1:A:328:ASP:HB2	2.09	0.52
2:B:40:ILE:O	2:B:41:GLU:C	2.52	0.52
2:B:487:ALA:HB3	2:B:492:GLU:HB2	1.90	0.52
2:F:286:LYS:HG3	2:F:287:ASN:HD22	1.74	0.52
1:G:142:ILE:O	1:G:146:THR:HG23	2.10	0.52
1:G:374:ALA:HB1	1:G:375:PHE:HE1	1.70	0.52
2:H:215:TYR:N	2:H:215:TYR:CD2	2.77	0.52
2:H:241:ILE:O	2:H:245:ILE:HG13	2.09	0.52
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.09	0.52
1:C:12:GLU:HG3	1:C:13:ALA:N	2.25	0.52
1:C:68:ARG:NH1	1:C:78:ARG:HB3	2.25	0.52
2:D:193:ARG:HD3	2:D:371:LEU:HD23	1.91	0.52
2:D:340:ARG:NH2	2:D:442:ASN:CB	2.71	0.52
2:D:340:ARG:HH22	2:D:442:ASN:HB2	1.75	0.52
1:E:184:GLY:O	1:E:185:ALA:HB2	2.09	0.52
1:G:136:ASP:O	1:G:139:ILE:HB	2.10	0.52
2:H:402:ILE:O	2:H:402:ILE:HG22	2.09	0.52
2:B:326:LEU:HD12	2:B:357:ALA:HB2	1.90	0.52
2:B:437:GLU:O	2:B:437:GLU:HG3	2.10	0.52
2:D:302:LYS:O	2:D:303:ASP:C	2.53	0.52
2:D:322:ILE:HD13	2:D:412:MET:HE1	1.90	0.52
1:E:159:GLU:HG2	1:E:238:ASP:HB2	1.90	0.52
2:F:382:ASP:C	2:F:384:LYS:H	2.16	0.52
1:A:191:THR:OG1	1:A:194:LEU:HD21	2.10	0.52
1:C:80:MET:HE3	2:D:477:GLU:CB	2.40	0.52
1:A:14:ARG:CZ	1:C:183:HIS:NE2	2.73	0.52
2:B:253:THR:OG1	2:B:254:ILE:N	2.42	0.52
1:C:98:TYR:HB3	1:C:156:LEU:HD21	1.91	0.52
1:C:216:GLN:HG2	1:C:370:LEU:HD11	1.92	0.52
1:E:312:LEU:N	1:E:312:LEU:HD23	2.24	0.52
2:F:340:ARG:HH22	2:F:442:ASN:HB3	1.72	0.52
1:G:331:ARG:O	1:G:335:ILE:HG12	2.10	0.52
1:G:385:LYS:HG3	1:G:387:TYR:HE2	1.75	0.52
1:A:270:PHE:CD2	1:A:294:PHE:HD1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LYS:O	2:B:303:ASP:C	2.52	0.52
2:B:492:GLU:O	2:B:493:LEU:C	2.52	0.52
3:D:531:RDC:CL1	3:D:531:RDC:C9	2.95	0.52
2:F:322:ILE:CG2	2:F:412:MET:HE2	2.40	0.52
2:F:362:ILE:HG22	2:F:408:GLN:HB3	1.92	0.52
2:H:396:ASP:HB3	2:H:399:ARG:HH11	1.75	0.52
1:C:307:ARG:O	1:C:308:LYS:HD2	2.10	0.52
2:D:224:LYS:CG	2:D:225:PRO:HD2	2.38	0.52
2:D:286:LYS:HG3	2:D:287:ASN:HD22	1.75	0.52
1:E:115:LYS:HB3	1:E:115:LYS:HZ3	1.75	0.52
2:F:467:LYS:O	2:F:470:ALA:N	2.43	0.52
1:C:302:ILE:HB	1:C:303:PHE:HD2	1.72	0.51
1:C:325:LYS:O	1:C:328:ASP:HB2	2.10	0.51
2:D:505:LEU:O	2:D:508:LEU:HB2	2.10	0.51
1:E:219:ARG:CZ	1:G:14:ARG:NH2	2.72	0.51
1:G:307:ARG:HG3	1:G:308:LYS:N	2.24	0.51
1:G:378:ILE:O	1:G:379:PRO:C	2.52	0.51
3:H:531:RDC:CL1	3:H:531:RDC:C9	2.95	0.51
1:C:238:ASP:OD1	1:C:238:ASP:N	2.42	0.51
2:D:508:LEU:C	2:D:510:SER:N	2.67	0.51
1:E:101:ILE:N	1:E:101:ILE:CD1	2.60	0.51
1:E:331:ARG:O	1:E:335:ILE:HG12	2.09	0.51
2:H:286:LYS:HG3	2:H:287:ASN:HD22	1.74	0.51
1:A:89:ILE:O	1:A:93:LEU:HB2	2.10	0.51
1:C:270:PHE:CD2	1:C:294:PHE:HD1	2.29	0.51
2:D:207:ASP:HB2	2:D:208:PRO:CD	2.40	0.51
2:F:219:THR:CG2	2:F:220:ASN:N	2.62	0.51
1:C:291:ASP:OD1	1:C:291:ASP:C	2.53	0.51
1:E:118:GLU:OE1	1:E:118:GLU:HA	2.10	0.51
1:G:17:ALA:C	1:G:19:ASN:N	2.65	0.51
1:G:351:ASN:N	1:G:351:ASN:OD1	2.38	0.51
2:H:240:GLU:O	2:H:241:ILE:C	2.54	0.51
2:H:395:LEU:HD12	2:H:396:ASP:H	1.75	0.51
1:A:183:HIS:N	1:A:183:HIS:HD1	2.08	0.51
1:C:239:ARG:HH22	1:C:277:SER:HB3	1.76	0.51
1:C:261:ASP:OD1	1:C:362:ILE:HG13	2.10	0.51
2:D:362:ILE:HG22	2:D:408:GLN:HB3	1.92	0.51
1:G:263:ASP:HB2	1:G:264:PRO:HD2	1.92	0.51
2:H:508:LEU:C	2:H:510:SER:N	2.68	0.51
1:A:268:TYR:O	1:A:271:SER:N	2.44	0.51
2:B:395:LEU:HD12	2:B:396:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:PHE:CD2	1:E:294:PHE:HD1	2.29	0.51
2:F:103:GLN:NE2	2:F:315:SER:H	2.08	0.51
3:F:531:RDC:CL1	3:F:531:RDC:C9	2.95	0.51
1:A:12:GLU:C	1:A:12:GLU:CD	2.79	0.51
1:A:80:MET:CE	2:B:477:GLU:HB3	2.41	0.51
2:B:240:GLU:O	2:B:243:ILE:HG12	2.11	0.51
2:D:219:THR:HG23	2:D:220:ASN:H	1.73	0.51
2:D:382:ASP:C	2:D:384:LYS:H	2.19	0.51
2:D:441:LYS:O	2:D:443:ALA:N	2.43	0.51
1:E:89:ILE:O	1:E:93:LEU:HB2	2.11	0.51
1:E:229:ILE:HD11	1:E:248:LEU:HD13	1.93	0.51
1:E:378:ILE:O	1:E:379:PRO:C	2.49	0.51
1:G:31:GLN:HE21	2:H:482:LEU:HD21	1.76	0.51
1:G:37:PRO:CD	2:H:507:LYS:HZ1	2.24	0.51
1:G:319:ASN:ND2	1:G:319:ASN:N	2.52	0.51
1:A:160:LYS:HB2	1:A:160:LYS:HZ2	1.72	0.51
1:E:192:PRO:HG3	1:E:240:ALA:HB1	1.92	0.51
1:G:118:GLU:OE1	1:G:118:GLU:HA	2.10	0.51
2:H:362:ILE:HG22	2:H:408:GLN:HB3	1.93	0.51
1:A:347:GLN:O	1:A:348:GLU:C	2.52	0.51
1:C:170:ARG:HG3	1:C:196:ASP:HB2	1.92	0.51
2:D:467:LYS:O	2:D:470:ALA:N	2.44	0.51
1:E:309:LYS:NZ	1:E:309:LYS:HB2	2.26	0.51
2:F:99:TYR:HH	2:F:348:HIS:HE2	1.57	0.51
1:G:159:GLU:CG	1:G:238:ASP:HB2	2.40	0.51
1:G:271:SER:HB3	1:G:340:TRP:HH2	1.75	0.51
2:H:414:HIS:CD2	2:H:414:HIS:C	2.88	0.51
2:H:505:LEU:O	2:H:508:LEU:HB2	2.11	0.51
1:A:295:LEU:HD23	1:A:387:TYR:HB3	1.92	0.51
1:C:12:GLU:C	1:C:12:GLU:CD	2.78	0.51
1:C:294:PHE:HB3	1:C:388:ILE:HG13	1.92	0.51
1:E:89:ILE:HD13	1:E:104:LEU:HD21	1.93	0.51
1:G:98:TYR:HB3	1:G:156:LEU:HD21	1.93	0.51
1:A:208:VAL:HG22	1:A:209:GLU:N	2.26	0.50
1:A:238:ASP:O	1:A:242:ARG:NH2	2.44	0.50
1:A:243:ARG:HH22	1:A:287:LEU:HD22	1.75	0.50
1:E:21:LEU:HD21	1:E:153:MET:HG2	1.93	0.50
2:F:401:GLY:O	2:F:402:ILE:C	2.54	0.50
1:A:89:ILE:HD13	1:A:104:LEU:HD21	1.93	0.50
1:A:205:VAL:CG1	1:A:256:VAL:HG22	2.41	0.50
1:A:317:ARG:O	1:A:321:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ILE:O	2:B:205:PHE:HA	2.10	0.50
1:C:274:ARG:O	1:C:275:ILE:HG23	2.11	0.50
2:D:84:GLN:HE21	2:D:85:GLU:HG3	1.76	0.50
1:E:154:LEU:O	1:E:156:LEU:N	2.44	0.50
1:E:294:PHE:HB3	1:E:388:ILE:HG13	1.92	0.50
2:F:99:TYR:HE2	2:F:348:HIS:CE1	2.29	0.50
2:B:286:LYS:HG3	2:B:287:ASN:HD22	1.76	0.50
1:C:13:ALA:CB	1:C:16:LYS:HE2	2.40	0.50
1:C:118:GLU:OE1	1:C:118:GLU:HA	2.11	0.50
1:C:154:LEU:O	1:C:156:LEU:N	2.44	0.50
2:D:348:HIS:ND1	2:D:419:LYS:HB2	2.27	0.50
1:E:183:HIS:CD2	1:G:14:ARG:HH21	2.28	0.50
1:E:336:LYS:O	1:E:336:LYS:HG2	2.12	0.50
1:G:316:GLU:O	1:G:319:ASN:ND2	2.44	0.50
1:G:368:LYS:CB	1:G:372:PHE:HD2	2.24	0.50
2:H:302:LYS:O	2:H:303:ASP:C	2.54	0.50
1:A:17:ALA:O	1:A:19:ASN:N	2.45	0.50
2:B:192:LYS:O	2:B:195:TYR:HB3	2.11	0.50
2:B:369:ILE:HB	2:B:410:VAL:HG13	1.93	0.50
2:D:240:GLU:O	2:D:241:ILE:C	2.53	0.50
1:E:363:GLU:O	1:E:364:ALA:C	2.53	0.50
2:F:395:LEU:HD12	2:F:396:ASP:N	2.26	0.50
1:G:363:GLU:O	1:G:364:ALA:C	2.52	0.50
1:A:150:ARG:O	1:A:152:GLU:N	2.44	0.50
1:A:238:ASP:OD1	1:A:238:ASP:N	2.45	0.50
2:B:84:GLN:HE21	2:B:85:GLU:HG3	1.77	0.50
2:D:255:LYS:HG2	2:H:214:TYR:CE2	2.46	0.50
2:F:103:GLN:NE2	2:F:315:SER:N	2.60	0.50
1:G:21:LEU:HD21	1:G:153:MET:HG2	1.94	0.50
1:G:366:ALA:C	1:G:368:LYS:H	2.19	0.50
1:C:347:GLN:O	1:C:348:GLU:C	2.53	0.50
1:G:17:ALA:O	1:G:19:ASN:N	2.45	0.50
1:G:160:LYS:HB2	1:G:160:LYS:HZ2	1.73	0.50
2:H:467:LYS:O	2:H:469:LEU:N	2.45	0.50
1:C:205:VAL:CG1	1:C:256:VAL:HG22	2.42	0.50
1:C:366:ALA:C	1:C:368:LYS:H	2.20	0.50
1:E:98:TYR:HB3	1:E:156:LEU:HD21	1.92	0.50
1:E:381:LYS:HE2	1:E:386:ASP:CG	2.37	0.50
1:G:80:MET:CE	2:H:477:GLU:HB3	2.41	0.50
1:G:80:MET:CE	2:H:477:GLU:CB	2.89	0.50
1:G:163:VAL:HG22	1:G:164:VAL:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:ILE:HG22	2:B:402:ILE:O	2.10	0.50
1:C:177:ASP:C	1:C:177:ASP:OD1	2.54	0.50
2:D:44:LEU:O	2:D:46:ALA:N	2.45	0.50
1:G:148:LEU:N	1:G:148:LEU:HD12	2.26	0.50
1:G:294:PHE:HB3	1:G:388:ILE:HG13	1.93	0.50
1:C:90:TYR:CD2	1:C:90:TYR:C	2.90	0.50
1:C:243:ARG:HH21	1:C:287:LEU:HD22	1.74	0.50
2:D:40:ILE:O	2:D:41:GLU:C	2.54	0.50
2:D:198:THR:O	2:D:198:THR:CG2	2.48	0.50
2:D:345:TYR:O	2:D:346:GLN:C	2.55	0.50
1:G:323:LYS:H	1:G:323:LYS:HD3	1.77	0.50
2:H:309:PRO:O	2:H:349:PRO:HB3	2.12	0.50
1:A:200:VAL:HG11	1:A:252:LEU:CD2	2.42	0.49
1:A:222:PHE:CZ	1:A:378:ILE:HG21	2.47	0.49
1:A:261:ASP:OD1	1:A:362:ILE:N	2.44	0.49
2:B:130:GLU:HG2	2:B:141:THR:HG22	1.94	0.49
2:B:215:TYR:CD2	2:B:215:TYR:N	2.79	0.49
1:C:39:VAL:CG1	1:C:40:MET:N	2.75	0.49
1:C:102:ARG:O	1:C:103:ASP:C	2.54	0.49
1:C:183:HIS:N	1:C:183:HIS:HD1	2.09	0.49
1:C:272:VAL:HG13	1:C:277:SER:H	1.77	0.49
1:E:82:THR:HA	1:E:138:VAL:CG1	2.41	0.49
1:E:183:HIS:CG	1:G:14:ARG:HH22	2.24	0.49
1:E:237:PRO:HG2	1:E:272:VAL:HG11	1.93	0.49
1:G:148:LEU:N	1:G:148:LEU:CD1	2.74	0.49
2:H:326:LEU:HD12	2:H:357:ALA:HB2	1.93	0.49
2:H:500:GLU:CA	2:H:503:GLU:HB3	2.36	0.49
1:A:183:HIS:CG	1:C:14:ARG:HH22	2.22	0.49
1:C:26:LEU:HD23	1:C:26:LEU:C	2.38	0.49
1:C:189:GLU:O	1:C:191:THR:N	2.45	0.49
2:D:285:VAL:HG13	2:D:286:LYS:N	2.27	0.49
1:E:238:ASP:OD1	1:E:238:ASP:N	2.44	0.49
1:E:251:GLU:C	1:E:252:LEU:HD12	2.36	0.49
2:F:44:LEU:O	2:F:46:ALA:N	2.45	0.49
2:F:285:VAL:O	2:F:288:LEU:HG	2.11	0.49
1:G:98:TYR:HB3	1:G:156:LEU:CD2	2.41	0.49
1:G:177:ASP:OD1	1:G:178:LEU:N	2.46	0.49
1:G:347:GLN:O	1:G:348:GLU:C	2.54	0.49
1:A:175:VAL:O	1:A:175:VAL:CG2	2.59	0.49
2:B:191:ILE:H	2:B:191:ILE:CD1	2.22	0.49
2:B:240:GLU:O	2:B:241:ILE:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:GLY:O	2:B:402:ILE:C	2.55	0.49
1:G:154:LEU:O	1:G:156:LEU:N	2.45	0.49
1:G:246:ARG:HB2	1:G:289:THR:HG22	1.94	0.49
1:A:242:ARG:O	1:A:243:ARG:C	2.53	0.49
1:A:263:ASP:HB2	1:A:264:PRO:HD2	1.95	0.49
1:C:271:SER:HB3	1:C:340:TRP:HH2	1.75	0.49
1:C:370:LEU:H	1:C:370:LEU:CD2	2.19	0.49
2:D:58:ILE:O	2:D:205:PHE:HA	2.12	0.49
1:E:14:ARG:HH22	1:G:183:HIS:CG	2.27	0.49
1:E:148:LEU:N	1:E:148:LEU:CD1	2.75	0.49
2:F:240:GLU:O	2:F:243:ILE:N	2.46	0.49
2:F:240:GLU:O	2:F:243:ILE:HG12	2.12	0.49
2:F:253:THR:OG1	2:F:254:ILE:N	2.45	0.49
2:F:372:ARG:HH21	2:F:383:GLU:HB3	1.78	0.49
1:G:238:ASP:O	1:G:242:ARG:NH2	2.45	0.49
1:A:42:ILE:CD1	1:A:68:ARG:HG3	2.43	0.49
2:B:436:ILE:HG22	2:B:437:GLU:N	2.28	0.49
1:C:209:GLU:CB	1:C:260:THR:HG22	2.42	0.49
2:F:44:LEU:C	2:F:46:ALA:N	2.71	0.49
2:F:314:LEU:HD21	2:F:417:SER:HA	1.94	0.49
1:G:31:GLN:HG2	1:G:32:LEU:N	2.27	0.49
1:A:230:LEU:HD23	1:A:231:ILE:N	2.26	0.49
1:C:323:LYS:H	1:C:323:LYS:HD3	1.77	0.49
2:D:506:PHE:C	2:D:508:LEU:H	2.21	0.49
1:G:295:LEU:HD23	1:G:387:TYR:HB3	1.93	0.49
2:H:47:THR:HG22	2:H:78:GLY:HA2	1.95	0.49
2:H:382:ASP:C	2:H:384:LYS:H	2.21	0.49
1:A:83:VAL:O	2:B:481:SER:HB3	2.13	0.49
1:A:163:VAL:HG22	1:A:164:VAL:N	2.27	0.49
1:A:272:VAL:HG13	1:A:277:SER:H	1.77	0.49
2:B:382:ASP:C	2:B:384:LYS:H	2.21	0.49
1:C:86:ALA:O	1:C:89:ILE:HB	2.12	0.49
1:C:108:GLY:O	1:C:109:LYS:HB2	2.13	0.49
1:C:270:PHE:CD1	1:C:270:PHE:C	2.90	0.49
2:D:47:THR:HG22	2:D:78:GLY:HA2	1.94	0.49
2:D:103:GLN:NE2	2:D:315:SER:H	2.10	0.49
2:D:127:ILE:HG23	2:D:174:ILE:HG12	1.93	0.49
1:E:106:TYR:C	1:E:107:ARG:HD3	2.31	0.49
2:F:190:TYR:O	2:F:191:ILE:C	2.56	0.49
1:G:189:GLU:C	1:G:191:THR:N	2.71	0.49
2:H:369:ILE:HB	2:H:410:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:O	1:A:85:MET:C	2.56	0.49
1:G:325:LYS:O	1:G:328:ASP:HB2	2.12	0.49
1:G:371:LYS:H	1:G:371:LYS:CD	2.25	0.49
2:B:165:ARG:HG2	2:B:166:GLY:H	1.76	0.49
1:C:175:VAL:O	1:C:175:VAL:CG2	2.61	0.49
1:C:214:PHE:CE1	1:C:230:LEU:HD22	2.48	0.49
1:E:148:LEU:N	1:E:148:LEU:HD12	2.27	0.49
1:A:154:LEU:O	1:A:156:LEU:N	2.46	0.49
1:A:208:VAL:HG21	1:A:213:VAL:HG11	1.93	0.49
1:A:378:ILE:HD13	1:A:378:ILE:N	2.27	0.49
1:E:216:GLN:HG2	1:E:370:LEU:HD11	1.94	0.49
2:F:40:ILE:O	2:F:41:GLU:C	2.56	0.49
1:G:82:THR:HA	1:G:138:VAL:CG1	2.43	0.49
1:G:85:MET:SD	1:G:104:LEU:HD23	2.53	0.49
1:G:188:ILE:HD12	1:G:188:ILE:O	2.13	0.49
1:G:379:PRO:O	1:G:383:THR:HG22	2.13	0.49
2:H:311:ALA:O	2:H:314:LEU:HB2	2.11	0.49
1:A:363:GLU:O	1:A:364:ALA:C	2.54	0.48
2:B:127:ILE:HG23	2:B:174:ILE:HG12	1.95	0.48
1:C:89:ILE:O	1:C:93:LEU:HB2	2.12	0.48
1:E:21:LEU:HD12	1:E:93:LEU:CG	2.42	0.48
1:E:68:ARG:NH1	1:E:78:ARG:O	2.46	0.48
2:F:222:ILE:H	2:F:222:ILE:HG13	1.46	0.48
2:F:487:ALA:HB3	2:F:492:GLU:HB2	1.93	0.48
1:G:380:GLU:O	1:G:384:ASN:HB2	2.13	0.48
2:H:441:LYS:O	2:H:444:LEU:N	2.45	0.48
2:H:467:LYS:O	2:H:470:ALA:N	2.45	0.48
1:C:243:ARG:HH22	1:C:287:LEU:HD22	1.76	0.48
2:D:97:SER:O	2:D:98:LYS:C	2.56	0.48
2:D:401:GLY:O	2:D:402:ILE:C	2.55	0.48
1:E:295:LEU:HD23	1:E:387:TYR:HB3	1.95	0.48
2:F:506:PHE:C	2:F:508:LEU:H	2.21	0.48
1:A:12:GLU:CG	1:A:13:ALA:N	2.76	0.48
1:C:285:GLU:HB3	1:C:286:ARG:H	1.47	0.48
1:C:295:LEU:HD23	1:C:387:TYR:HB3	1.96	0.48
2:D:253:THR:OG1	2:D:254:ILE:N	2.46	0.48
2:D:474:TYR:N	2:D:474:TYR:HD1	2.12	0.48
1:E:39:VAL:CG1	1:E:40:MET:N	2.76	0.48
1:E:262:ALA:CB	1:E:360:LEU:H	2.26	0.48
1:E:268:TYR:O	1:E:271:SER:N	2.47	0.48
1:G:89:ILE:O	1:G:93:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:ASP:OD1	1:G:291:ASP:C	2.56	0.48
2:H:127:ILE:HG23	2:H:174:ILE:HG12	1.95	0.48
2:H:285:VAL:HG13	2:H:286:LYS:N	2.29	0.48
1:A:14:ARG:NH1	1:C:183:HIS:CE1	2.81	0.48
1:C:91:ASP:C	1:C:93:LEU:N	2.70	0.48
1:E:25:PHE:O	1:E:26:LEU:C	2.55	0.48
1:E:200:VAL:HG11	1:E:252:LEU:CD2	2.41	0.48
1:E:286:ARG:C	1:E:287:LEU:HG	2.39	0.48
2:F:441:LYS:O	2:F:443:ALA:N	2.45	0.48
1:G:115:LYS:HB3	1:G:115:LYS:HZ3	1.76	0.48
1:G:274:ARG:O	1:G:275:ILE:HG23	2.14	0.48
2:H:237:ASP:HA	2:H:297:VAL:HG21	1.95	0.48
2:H:348:HIS:ND1	2:H:419:LYS:HB2	2.29	0.48
1:A:98:TYR:HB3	1:A:156:LEU:HD21	1.96	0.48
1:A:294:PHE:HB3	1:A:388:ILE:HG13	1.95	0.48
2:B:398:LYS:C	2:B:400:TYR:N	2.70	0.48
1:C:21:LEU:HD12	1:C:93:LEU:CD1	2.42	0.48
1:C:214:PHE:CD1	1:C:230:LEU:HD21	2.48	0.48
1:C:336:LYS:HG2	1:C:336:LYS:O	2.14	0.48
2:D:240:GLU:O	2:D:243:ILE:HG12	2.14	0.48
2:F:237:ASP:HA	2:F:297:VAL:HG21	1.95	0.48
2:F:505:LEU:O	2:F:508:LEU:HB2	2.14	0.48
2:H:455:LEU:HD13	2:H:459:ARG:NH2	2.27	0.48
2:H:506:PHE:C	2:H:508:LEU:H	2.20	0.48
2:B:44:LEU:C	2:B:46:ALA:N	2.72	0.48
2:B:467:LYS:C	2:B:469:LEU:N	2.72	0.48
1:C:302:ILE:HA	1:C:312:LEU:CD1	2.31	0.48
1:C:307:ARG:O	1:C:308:LYS:CD	2.61	0.48
1:E:159:GLU:CD	1:E:240:ALA:HB3	2.38	0.48
1:E:307:ARG:HG3	1:E:308:LYS:N	2.27	0.48
2:F:276:LEU:HB3	2:F:299:THR:HG21	1.96	0.48
2:F:382:ASP:C	2:F:384:LYS:N	2.71	0.48
2:F:402:ILE:O	2:F:402:ILE:HG22	2.12	0.48
1:G:21:LEU:HB3	1:G:93:LEU:HD11	1.95	0.48
1:G:68:ARG:NH1	1:G:78:ARG:O	2.46	0.48
2:H:240:GLU:O	2:H:243:ILE:HG12	2.13	0.48
2:H:496:LYS:O	2:H:500:GLU:HG3	2.14	0.48
2:B:237:ASP:HA	2:B:297:VAL:HG21	1.96	0.48
2:B:285:VAL:HG13	2:B:286:LYS:N	2.29	0.48
2:D:474:TYR:N	2:D:474:TYR:CD1	2.81	0.48
1:E:108:GLY:O	1:E:109:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:GLU:O	1:E:132:GLN:C	2.55	0.48
1:E:163:VAL:HG22	1:E:164:VAL:N	2.29	0.48
1:E:271:SER:HB3	1:E:340:TRP:HH2	1.78	0.48
2:F:324:LEU:O	2:F:325:GLY:C	2.56	0.48
2:F:467:LYS:C	2:F:469:LEU:N	2.71	0.48
2:H:474:TYR:N	2:H:474:TYR:CD1	2.80	0.48
1:A:91:ASP:C	1:A:93:LEU:N	2.71	0.48
1:E:103:ASP:O	1:G:367:SER:HB2	2.13	0.48
2:F:146:ILE:HG12	2:F:147:ASP:N	2.29	0.48
2:F:241:ILE:O	2:F:245:ILE:HG13	2.13	0.48
2:H:97:SER:O	2:H:98:LYS:C	2.57	0.48
2:H:253:THR:OG1	2:H:254:ILE:N	2.47	0.48
2:H:506:PHE:C	2:H:508:LEU:N	2.71	0.48
1:A:189:GLU:C	1:A:191:THR:N	2.71	0.48
1:A:378:ILE:N	1:A:379:PRO:HD2	2.29	0.48
2:D:130:GLU:HG2	2:D:141:THR:HG22	1.96	0.48
1:E:188:ILE:CD1	1:E:188:ILE:C	2.87	0.48
1:E:214:PHE:CE1	1:E:230:LEU:HD22	2.49	0.48
2:F:127:ILE:HG23	2:F:174:ILE:HG12	1.95	0.48
2:F:504:GLY:O	2:F:505:LEU:C	2.57	0.48
1:G:191:THR:OG1	1:G:194:LEU:HD21	2.14	0.48
2:H:374:ALA:O	2:H:377:ILE:HG13	2.14	0.48
2:B:318:GLY:C	2:B:320:ASP:N	2.72	0.48
2:B:496:LYS:O	2:B:500:GLU:HG3	2.13	0.48
1:E:43:PRO:O	1:E:144:VAL:HG11	2.14	0.48
2:F:396:ASP:HB3	2:F:399:ARG:HH11	1.78	0.48
2:H:77:ASN:OD1	2:H:77:ASN:N	2.46	0.48
1:C:200:VAL:HG11	1:C:252:LEU:CD2	2.43	0.47
2:D:77:ASN:OD1	2:D:77:ASN:N	2.47	0.47
2:F:16:PHE:CE1	2:F:23:ALA:HB3	2.49	0.47
1:G:39:VAL:HG22	1:G:69:ASN:HA	1.97	0.47
1:G:286:ARG:C	1:G:287:LEU:HG	2.39	0.47
2:H:58:ILE:O	2:H:205:PHE:HA	2.13	0.47
2:H:82:PRO:HA	2:H:83:PRO:HD2	1.73	0.47
1:A:98:TYR:HB3	1:A:156:LEU:CD2	2.43	0.47
2:D:44:LEU:C	2:D:46:ALA:N	2.72	0.47
1:E:153:MET:HB2	1:E:155:ILE:HD13	1.96	0.47
1:E:323:LYS:HD3	1:E:323:LYS:H	1.78	0.47
2:F:412:MET:HE3	2:F:412:MET:HB3	1.80	0.47
2:F:474:TYR:N	2:F:474:TYR:HD1	2.13	0.47
1:G:89:ILE:HD13	1:G:104:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:ILE:O	2:H:41:GLU:C	2.57	0.47
1:A:188:ILE:CD1	1:A:188:ILE:C	2.87	0.47
1:A:261:ASP:OD1	1:A:361:GLU:CA	2.58	0.47
1:A:372:PHE:C	1:A:372:PHE:HD1	2.18	0.47
1:C:207:VAL:HB	1:C:258:ILE:HB	1.97	0.47
1:C:302:ILE:O	1:C:317:ARG:NE	2.47	0.47
1:C:339:GLU:HG3	1:C:339:GLU:O	2.14	0.47
1:G:170:ARG:CG	1:G:196:ASP:HB2	2.44	0.47
2:H:190:TYR:O	2:H:191:ILE:C	2.57	0.47
2:H:474:TYR:N	2:H:474:TYR:HD1	2.11	0.47
1:A:179:SER:OG	1:A:180:LYS:N	2.46	0.47
2:B:414:HIS:NE2	2:B:416:CYS:HB3	2.29	0.47
1:C:331:ARG:O	1:C:335:ILE:HG12	2.15	0.47
1:C:370:LEU:N	1:C:370:LEU:CD2	2.77	0.47
2:D:436:ILE:HG22	2:D:437:GLU:N	2.29	0.47
1:E:91:ASP:C	1:E:93:LEU:N	2.71	0.47
1:E:350:ILE:O	1:E:353:PHE:HB3	2.15	0.47
1:G:263:ASP:HB2	1:G:264:PRO:CD	2.45	0.47
2:H:401:GLY:O	2:H:402:ILE:C	2.56	0.47
1:A:37:PRO:HD3	2:B:507:LYS:NZ	2.30	0.47
1:A:85:MET:SD	1:A:104:LEU:HD23	2.55	0.47
1:A:148:LEU:CD1	1:A:148:LEU:N	2.78	0.47
1:A:177:ASP:OD1	1:A:178:LEU:N	2.48	0.47
2:B:397:TRP:O	2:B:402:ILE:HB	2.14	0.47
2:D:499:ASN:C	2:D:499:ASN:ND2	2.70	0.47
1:G:37:PRO:HD3	2:H:507:LYS:HZ1	1.79	0.47
1:G:226:TYR:O	1:G:227:LYS:C	2.58	0.47
1:G:268:TYR:O	1:G:271:SER:N	2.48	0.47
1:A:148:LEU:N	1:A:148:LEU:HD12	2.29	0.47
1:A:176:ILE:HG21	1:A:186:TYR:CE1	2.50	0.47
1:A:336:LYS:HG2	1:A:336:LYS:O	2.14	0.47
2:B:372:ARG:HH21	2:B:383:GLU:HB3	1.78	0.47
1:C:263:ASP:HB2	1:C:264:PRO:HD2	1.96	0.47
1:C:294:PHE:O	1:C:387:TYR:HB2	2.14	0.47
1:C:372:PHE:CD1	1:C:372:PHE:O	2.67	0.47
2:D:322:ILE:HG21	2:D:412:MET:HE2	1.96	0.47
1:E:14:ARG:NH2	1:G:219:ARG:CZ	2.77	0.47
1:E:183:HIS:CD2	1:G:189:GLU:OE2	2.67	0.47
1:E:370:LEU:N	1:E:370:LEU:CD2	2.70	0.47
1:E:378:ILE:HB	1:E:379:PRO:HD3	1.96	0.47
1:G:387:TYR:N	1:G:387:TYR:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:CD2	1:A:90:TYR:C	2.93	0.47
1:A:319:ASN:ND2	1:A:319:ASN:N	2.48	0.47
1:A:340:TRP:HZ3	1:A:341:PHE:CE1	2.33	0.47
2:B:383:GLU:CG	2:B:384:LYS:HD3	2.32	0.47
2:B:505:LEU:O	2:B:508:LEU:HB2	2.14	0.47
1:C:226:TYR:O	1:C:227:LYS:C	2.55	0.47
2:D:237:ASP:HA	2:D:297:VAL:HG21	1.97	0.47
1:E:26:LEU:C	1:E:26:LEU:HD23	2.40	0.47
1:E:102:ARG:C	1:E:104:LEU:N	2.72	0.47
1:E:175:VAL:O	1:E:175:VAL:CG2	2.63	0.47
1:E:261:ASP:OD1	1:E:362:ILE:N	2.47	0.47
1:E:272:VAL:HG13	1:E:277:SER:H	1.79	0.47
1:E:302:ILE:HB	1:E:303:PHE:HD2	1.77	0.47
2:F:112:VAL:HG11	3:F:531:RDC:O5	2.13	0.47
2:F:348:HIS:ND1	2:F:419:LYS:HB2	2.30	0.47
2:F:441:LYS:O	2:F:444:LEU:N	2.45	0.47
1:A:166:ASN:HB3	1:A:201:ASP:HB3	1.96	0.47
1:A:323:LYS:H	1:A:323:LYS:HD3	1.80	0.47
2:B:362:ILE:O	2:B:408:GLN:HG2	2.15	0.47
1:C:73:LEU:CD2	2:D:467:LYS:HG2	2.44	0.47
1:C:363:GLU:O	1:C:364:ALA:C	2.57	0.47
1:G:26:LEU:HD23	1:G:26:LEU:C	2.40	0.47
1:G:274:ARG:HE	1:G:274:ARG:HB2	1.55	0.47
2:H:207:ASP:HB2	2:H:208:PRO:CD	2.44	0.47
1:A:25:PHE:O	1:A:26:LEU:C	2.57	0.47
1:A:80:MET:HE3	2:B:477:GLU:CB	2.45	0.47
1:A:366:ALA:C	1:A:368:LYS:N	2.72	0.47
1:A:378:ILE:O	1:A:379:PRO:C	2.57	0.47
2:B:33:TYR:CZ	2:B:37:ARG:HD3	2.49	0.47
2:B:387:VAL:HG12	2:B:430:ILE:HB	1.97	0.47
1:C:102:ARG:C	1:C:104:LEU:N	2.68	0.47
2:D:441:LYS:O	2:D:444:LEU:N	2.45	0.47
2:D:467:LYS:C	2:D:469:LEU:N	2.72	0.47
1:E:100:THR:O	1:E:103:ASP:HB2	2.15	0.47
1:E:230:LEU:HD23	1:E:231:ILE:N	2.29	0.47
1:G:42:ILE:CD1	1:G:68:ARG:HG3	2.45	0.47
1:G:209:GLU:CB	1:G:260:THR:HG22	2.44	0.47
1:G:237:PRO:HG2	1:G:272:VAL:HG11	1.95	0.47
1:G:372:PHE:HD1	1:G:376:GLN:HB2	1.80	0.47
1:A:251:GLU:C	1:A:252:LEU:HD12	2.40	0.47
1:A:309:LYS:HB2	1:A:309:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ASN:C	1:C:21:LEU:N	2.73	0.47
1:C:173:ASN:HD22	1:C:173:ASN:HA	1.57	0.47
1:E:160:LYS:NZ	1:E:160:LYS:HB3	2.14	0.47
1:A:85:MET:HE1	1:A:104:LEU:CD2	2.42	0.46
2:B:16:PHE:HZ	2:B:25:PHE:CD2	2.33	0.46
2:B:103:GLN:NE2	2:B:315:SER:N	2.63	0.46
1:C:189:GLU:C	1:C:191:THR:N	2.71	0.46
1:C:204:PHE:HA	1:C:255:PRO:HD2	1.97	0.46
1:C:262:ALA:HB3	1:C:360:LEU:H	1.79	0.46
1:C:305:ASN:ND2	1:C:307:ARG:HE	2.13	0.46
2:D:382:ASP:C	2:D:384:LYS:N	2.73	0.46
1:E:270:PHE:HE2	1:E:294:PHE:HB2	1.75	0.46
1:E:366:ALA:O	1:E:368:LYS:N	2.48	0.46
2:F:276:LEU:C	2:F:278:GLY:N	2.72	0.46
1:G:91:ASP:C	1:G:93:LEU:N	2.72	0.46
1:G:243:ARG:HH21	1:G:287:LEU:HD22	1.76	0.46
1:G:387:TYR:N	1:G:387:TYR:HD2	2.13	0.46
2:H:506:PHE:CD2	2:H:507:LYS:N	2.83	0.46
2:B:146:ILE:HG12	2:B:147:ASP:N	2.29	0.46
1:C:192:PRO:HG3	1:C:240:ALA:HB1	1.97	0.46
2:D:500:GLU:CA	2:D:503:GLU:HB3	2.36	0.46
1:E:209:GLU:CB	1:E:260:THR:HG22	2.44	0.46
1:E:263:ASP:HB2	1:E:264:PRO:HD2	1.96	0.46
1:E:270:PHE:O	1:E:271:SER:C	2.56	0.46
2:F:97:SER:O	2:F:98:LYS:C	2.57	0.46
2:F:127:ILE:HD12	2:F:174:ILE:HG23	1.97	0.46
2:F:474:TYR:N	2:F:474:TYR:CD1	2.82	0.46
1:G:21:LEU:C	1:G:21:LEU:HD13	2.40	0.46
2:H:322:ILE:HG23	2:H:412:MET:HE2	1.96	0.46
1:A:115:LYS:HB3	1:A:115:LYS:HZ3	1.79	0.46
1:A:371:LYS:CD	1:A:371:LYS:H	2.27	0.46
1:C:85:MET:SD	1:C:104:LEU:HD23	2.55	0.46
1:E:245:VAL:HG12	1:E:289:THR:HG21	1.96	0.46
2:F:219:THR:HG23	2:F:220:ASN:H	1.78	0.46
2:F:397:TRP:O	2:F:402:ILE:HB	2.16	0.46
2:F:506:PHE:C	2:F:508:LEU:N	2.72	0.46
1:G:138:VAL:O	1:G:142:ILE:HG13	2.15	0.46
1:G:379:PRO:O	1:G:383:THR:CG2	2.63	0.46
2:H:16:PHE:CE1	2:H:23:ALA:HB3	2.51	0.46
1:A:150:ARG:NH2	1:A:150:ARG:HB3	2.29	0.46
2:B:276:LEU:HB3	2:B:299:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:PHE:C	2:B:508:LEU:H	2.22	0.46
1:C:91:ASP:C	1:C:93:LEU:H	2.23	0.46
1:C:309:LYS:HB2	1:C:309:LYS:NZ	2.30	0.46
2:D:45:ASP:OD1	2:D:105:ARG:HD2	2.15	0.46
1:E:150:ARG:NH2	1:E:150:ARG:HB3	2.30	0.46
1:E:368:LYS:CB	1:E:372:PHE:HD2	2.28	0.46
2:F:130:GLU:HG2	2:F:141:THR:HG22	1.97	0.46
1:A:21:LEU:HD12	1:A:93:LEU:CG	2.45	0.46
1:A:100:THR:O	1:A:103:ASP:HB2	2.16	0.46
1:A:170:ARG:HG3	1:A:196:ASP:HB2	1.97	0.46
2:B:314:LEU:HD21	2:B:417:SER:HA	1.98	0.46
2:B:384:LYS:HD3	2:B:384:LYS:N	2.31	0.46
1:C:73:LEU:HD21	2:D:467:LYS:HE3	1.97	0.46
2:D:314:LEU:HD21	2:D:417:SER:HA	1.97	0.46
1:E:90:TYR:CD2	1:E:90:TYR:C	2.92	0.46
1:E:371:LYS:H	1:E:371:LYS:CD	2.28	0.46
1:G:200:VAL:HG11	1:G:252:LEU:CD2	2.43	0.46
1:G:208:VAL:HG22	1:G:209:GLU:N	2.29	0.46
1:G:350:ILE:O	1:G:353:PHE:HB3	2.16	0.46
1:G:368:LYS:HB3	1:G:372:PHE:HD2	1.81	0.46
1:A:153:MET:HB2	1:A:155:ILE:HD13	1.97	0.46
1:A:183:HIS:CD2	1:C:189:GLU:OE2	2.69	0.46
1:A:238:ASP:C	1:A:242:ARG:NH2	2.73	0.46
1:A:350:ILE:O	1:A:353:PHE:HB3	2.15	0.46
2:B:97:SER:O	2:B:98:LYS:C	2.58	0.46
2:B:103:GLN:NE2	2:B:315:SER:H	2.13	0.46
1:C:12:GLU:HG3	1:C:13:ALA:H	1.80	0.46
2:F:285:VAL:CG1	2:F:286:LYS:N	2.78	0.46
1:G:12:GLU:CG	1:G:13:ALA:N	2.79	0.46
1:G:131:GLU:O	1:G:132:GLN:C	2.59	0.46
1:G:189:GLU:C	1:G:191:THR:H	2.23	0.46
2:H:455:LEU:HD13	2:H:459:ARG:CZ	2.46	0.46
2:B:263:GLN:O	2:B:264:SER:HB2	2.15	0.46
2:B:400:TYR:O	2:B:402:ILE:N	2.48	0.46
2:B:506:PHE:CD2	2:B:507:LYS:N	2.83	0.46
1:C:238:ASP:O	1:C:242:ARG:NH2	2.49	0.46
2:D:330:PHE:O	2:D:361:SER:HB2	2.15	0.46
2:D:412:MET:HE3	2:D:412:MET:HB3	1.83	0.46
2:D:496:LYS:O	2:D:500:GLU:HG3	2.15	0.46
1:E:84:LEU:O	1:E:85:MET:C	2.57	0.46
1:G:41:GLU:O	1:G:43:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:LEU:C	2:H:46:ALA:N	2.74	0.46
1:A:189:GLU:C	1:A:191:THR:H	2.24	0.46
1:A:216:GLN:HG2	1:A:370:LEU:HD11	1.97	0.46
2:B:240:GLU:O	2:B:243:ILE:N	2.49	0.46
1:C:240:ALA:C	1:C:242:ARG:N	2.70	0.46
1:C:335:ILE:O	1:C:338:TYR:N	2.41	0.46
1:E:12:GLU:C	1:E:12:GLU:CD	2.83	0.46
1:E:307:ARG:C	1:E:308:LYS:CD	2.87	0.46
1:E:317:ARG:O	1:E:321:ILE:HG13	2.16	0.46
2:F:322:ILE:HG23	2:F:412:MET:HE2	1.98	0.46
2:H:44:LEU:O	2:H:46:ALA:N	2.49	0.46
2:H:276:LEU:HB3	2:H:299:THR:HG21	1.98	0.46
1:A:14:ARG:CZ	1:C:183:HIS:CG	2.96	0.46
2:B:322:ILE:HG21	2:B:412:MET:HE2	1.97	0.46
2:B:500:GLU:CA	2:B:503:GLU:HB3	2.37	0.46
1:E:274:ARG:O	1:E:275:ILE:HG23	2.15	0.46
1:E:335:ILE:O	1:E:336:LYS:C	2.58	0.46
2:F:86:VAL:CB	2:F:87:PRO:HD3	2.45	0.46
2:F:197:ILE:HG12	2:F:373:TYR:CE1	2.51	0.46
2:F:207:ASP:HB2	2:F:208:PRO:CD	2.45	0.46
1:G:79:PHE:O	1:G:82:THR:N	2.49	0.46
2:H:198:THR:O	2:H:198:THR:CG2	2.44	0.46
1:A:68:ARG:NH1	1:A:78:ARG:O	2.49	0.46
1:C:374:ALA:HB3	1:C:375:PHE:CD1	2.50	0.46
2:D:506:PHE:C	2:D:508:LEU:N	2.72	0.46
1:E:21:LEU:O	1:E:22:ARG:C	2.58	0.46
2:F:420:ILE:HB	2:F:422:TYR:HE2	1.80	0.46
1:G:21:LEU:HD12	1:G:93:LEU:CG	2.45	0.46
1:G:73:LEU:HD21	2:H:467:LYS:CG	2.45	0.46
1:G:150:ARG:C	1:G:152:GLU:H	2.23	0.46
1:A:108:GLY:O	1:A:109:LYS:HB2	2.16	0.45
1:A:370:LEU:N	1:A:370:LEU:CD2	2.76	0.45
2:B:77:ASN:N	2:B:77:ASN:OD1	2.49	0.45
2:B:499:ASN:C	2:B:499:ASN:ND2	2.70	0.45
1:C:153:MET:HB2	1:C:155:ILE:HD13	1.98	0.45
1:C:188:ILE:O	1:C:188:ILE:HD12	2.16	0.45
1:E:83:VAL:O	2:F:481:SER:HB3	2.15	0.45
2:F:77:ASN:OD1	2:F:77:ASN:N	2.48	0.45
2:F:195:TYR:CE2	2:F:215:TYR:HB3	2.51	0.45
1:G:102:ARG:O	1:G:103:ASP:C	2.60	0.45
1:G:348:GLU:O	1:G:352:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:395:LEU:HD12	2:H:396:ASP:N	2.30	0.45
2:H:467:LYS:C	2:H:469:LEU:N	2.73	0.45
1:A:259:LEU:O	1:A:259:LEU:HD13	2.15	0.45
1:C:317:ARG:O	1:C:321:ILE:HG13	2.17	0.45
1:E:74:ASN:OD1	1:E:74:ASN:N	2.49	0.45
1:E:207:VAL:HB	1:E:258:ILE:HB	1.98	0.45
1:E:262:ALA:HB3	1:E:360:LEU:H	1.81	0.45
1:E:351:ASN:O	1:E:352:THR:C	2.59	0.45
2:H:322:ILE:HG21	2:H:412:MET:HE2	1.99	0.45
1:A:368:LYS:CB	1:A:372:PHE:HD2	2.29	0.45
1:C:74:ASN:OD1	1:C:74:ASN:N	2.49	0.45
2:D:276:LEU:HB3	2:D:299:THR:HG21	1.99	0.45
2:D:369:ILE:HB	2:D:410:VAL:HG13	1.99	0.45
1:E:189:GLU:OE2	1:G:183:HIS:CD2	2.69	0.45
1:E:259:LEU:HD12	1:E:259:LEU:O	2.16	0.45
1:G:19:ASN:C	1:G:21:LEU:N	2.72	0.45
1:G:285:GLU:HB3	1:G:286:ARG:H	1.56	0.45
1:G:309:LYS:HB2	1:G:309:LYS:NZ	2.31	0.45
1:A:192:PRO:HG3	1:A:240:ALA:HB1	1.99	0.45
2:B:29:ALA:HB2	2:B:179:ASP:HB3	1.97	0.45
1:C:159:GLU:HG2	1:C:240:ALA:HB3	1.98	0.45
2:F:506:PHE:CD2	2:F:507:LYS:N	2.84	0.45
1:G:37:PRO:N	2:H:507:LYS:HZ1	2.15	0.45
1:G:305:ASN:ND2	1:G:307:ARG:HE	2.15	0.45
1:A:102:ARG:C	1:A:104:LEU:N	2.72	0.45
2:B:397:TRP:CE2	2:B:409:MET:HE1	2.52	0.45
2:D:506:PHE:CD2	2:D:507:LYS:N	2.85	0.45
1:E:102:ARG:O	1:E:103:ASP:C	2.59	0.45
2:F:496:LYS:O	2:F:500:GLU:HG3	2.16	0.45
1:G:102:ARG:C	1:G:104:LEU:N	2.73	0.45
1:G:222:PHE:CZ	1:G:378:ILE:HG21	2.51	0.45
2:H:314:LEU:HD21	2:H:417:SER:HA	1.98	0.45
1:A:245:VAL:HG12	1:A:289:THR:HG21	1.99	0.45
1:A:344:LYS:C	1:A:346:TRP:H	2.25	0.45
2:B:382:ASP:C	2:B:384:LYS:N	2.74	0.45
2:B:441:LYS:O	2:B:444:LEU:N	2.45	0.45
1:C:31:GLN:HG2	1:C:32:LEU:N	2.31	0.45
1:C:154:LEU:O	1:C:155:ILE:C	2.59	0.45
1:C:286:ARG:C	1:C:287:LEU:HG	2.41	0.45
1:E:12:GLU:O	1:E:14:ARG:N	2.50	0.45
1:G:251:GLU:C	1:G:252:LEU:HD12	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:ARG:C	1:G:308:LYS:CD	2.90	0.45
1:G:336:LYS:O	1:G:336:LYS:HG2	2.15	0.45
2:H:84:GLN:HE21	2:H:85:GLU:HG3	1.82	0.45
2:H:398:LYS:C	2:H:400:TYR:N	2.73	0.45
1:A:67:ARG:H	1:A:67:ARG:HG2	1.59	0.45
1:A:294:PHE:O	1:A:387:TYR:HB2	2.17	0.45
1:A:335:ILE:O	1:A:338:TYR:N	2.43	0.45
1:C:82:THR:HA	1:C:138:VAL:CG1	2.46	0.45
1:C:270:PHE:HD2	1:C:294:PHE:HD1	1.65	0.45
2:D:214:TYR:CE2	2:D:216:PRO:HB3	2.51	0.45
1:E:86:ALA:O	1:E:89:ILE:HB	2.17	0.45
1:E:242:ARG:O	1:E:245:VAL:N	2.49	0.45
2:F:436:ILE:HG22	2:F:437:GLU:N	2.31	0.45
2:F:496:LYS:O	2:F:497:TYR:C	2.60	0.45
1:G:150:ARG:O	1:G:153:MET:N	2.45	0.45
1:G:153:MET:HB2	1:G:155:ILE:HD13	1.99	0.45
1:G:270:PHE:HD2	1:G:294:PHE:HD1	1.65	0.45
1:A:243:ARG:HD2	1:A:243:ARG:HA	1.65	0.45
1:A:330:LYS:O	1:A:331:ARG:C	2.60	0.45
2:B:44:LEU:O	2:B:46:ALA:N	2.50	0.45
2:B:465:LYS:NZ	2:B:465:LYS:HB3	2.32	0.45
2:B:497:TYR:HB3	2:B:498:GLN:H	1.68	0.45
1:C:34:LYS:HD2	1:C:34:LYS:HA	1.86	0.45
1:C:85:MET:HE1	1:C:104:LEU:CD2	2.41	0.45
1:C:85:MET:HG2	1:C:129:TRP:CH2	2.51	0.45
1:C:208:VAL:HG22	1:C:209:GLU:N	2.32	0.45
1:C:260:THR:HB	1:C:261:ASP:H	1.53	0.45
1:C:372:PHE:C	1:C:372:PHE:HD1	2.20	0.45
2:D:190:TYR:O	2:D:191:ILE:C	2.59	0.45
2:D:398:LYS:C	2:D:400:TYR:N	2.74	0.45
1:E:19:ASN:C	1:E:21:LEU:N	2.71	0.45
1:A:102:ARG:O	1:A:103:ASP:C	2.57	0.45
1:A:219:ARG:NE	1:C:14:ARG:NH2	2.64	0.45
1:A:379:PRO:O	1:A:383:THR:CG2	2.63	0.45
2:B:285:VAL:C	2:B:287:ASN:H	2.23	0.45
2:B:362:ILE:HA	2:B:363:PRO:HD3	1.79	0.45
1:C:21:LEU:HD22	1:C:21:LEU:HA	1.67	0.45
1:C:176:ILE:HG21	1:C:186:TYR:CE1	2.52	0.45
1:C:251:GLU:C	1:C:252:LEU:HD12	2.42	0.45
2:D:374:ALA:O	2:D:377:ILE:HG13	2.17	0.45
2:D:444:LEU:O	2:D:447:VAL:CG2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ASP:C	1:E:177:ASP:OD1	2.60	0.45
1:E:263:ASP:HB2	1:E:264:PRO:CD	2.47	0.45
2:F:362:ILE:O	2:F:408:GLN:HG2	2.17	0.45
1:G:159:GLU:HG2	1:G:238:ASP:HB2	1.98	0.45
2:H:240:GLU:O	2:H:243:ILE:N	2.50	0.45
1:A:19:ASN:C	1:A:21:LEU:N	2.73	0.45
1:A:21:LEU:O	1:A:22:ARG:C	2.59	0.45
1:A:39:VAL:HG13	1:A:68:ARG:C	2.41	0.45
1:A:232:THR:OG1	1:A:233:SER:O	2.21	0.45
2:B:45:ASP:OD1	2:B:105:ARG:HD2	2.17	0.45
2:B:474:TYR:N	2:B:474:TYR:CD1	2.84	0.45
1:C:12:GLU:O	1:C:14:ARG:N	2.50	0.45
1:C:214:PHE:C	1:C:214:PHE:CD2	2.94	0.45
1:C:302:ILE:HG22	1:C:317:ARG:CD	2.38	0.45
1:E:214:PHE:CD1	1:E:230:LEU:HD21	2.52	0.45
1:E:386:ASP:O	1:E:387:TYR:HB3	2.17	0.45
2:F:382:ASP:O	2:F:384:LYS:N	2.50	0.45
1:G:108:GLY:O	1:G:109:LYS:HB2	2.17	0.45
1:A:154:LEU:HD13	1:A:154:LEU:HA	1.76	0.44
2:B:191:ILE:O	2:B:192:LYS:C	2.60	0.44
1:C:25:PHE:O	1:C:26:LEU:C	2.59	0.44
1:C:33:LYS:HA	1:C:33:LYS:HD2	1.80	0.44
1:C:214:PHE:CE1	1:C:230:LEU:CD2	3.00	0.44
1:C:387:TYR:CD2	1:C:387:TYR:N	2.85	0.44
2:D:322:ILE:HG23	2:D:412:MET:HE2	1.99	0.44
1:E:252:LEU:HD12	1:E:252:LEU:N	2.31	0.44
1:E:285:GLU:HB3	1:E:286:ARG:H	1.51	0.44
1:E:330:LYS:O	1:E:331:ARG:C	2.57	0.44
2:F:312:ASP:OD2	2:F:312:ASP:N	2.50	0.44
1:G:79:PHE:C	1:G:81:GLN:N	2.74	0.44
1:G:170:ARG:HG3	1:G:196:ASP:HB2	1.99	0.44
2:H:103:GLN:HE21	2:H:315:SER:N	2.15	0.44
2:H:398:LYS:C	2:H:400:TYR:H	2.25	0.44
1:A:14:ARG:CZ	1:C:183:HIS:ND1	2.81	0.44
2:B:506:PHE:C	2:B:508:LEU:N	2.73	0.44
1:C:335:ILE:O	1:C:336:LYS:C	2.59	0.44
1:C:372:PHE:O	1:C:372:PHE:HD1	2.00	0.44
2:D:16:PHE:HZ	2:D:25:PHE:CD2	2.35	0.44
2:D:219:THR:CG2	2:D:220:ASN:N	2.60	0.44
2:D:240:GLU:O	2:D:243:ILE:N	2.50	0.44
1:E:259:LEU:O	1:E:259:LEU:CD1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:ARG:HH11	1:E:308:LYS:NZ	2.15	0.44
1:G:39:VAL:CG1	1:G:40:MET:N	2.79	0.44
1:G:261:ASP:OD1	1:G:361:GLU:CA	2.57	0.44
1:A:39:VAL:CG1	1:A:40:MET:N	2.80	0.44
2:B:474:TYR:N	2:B:474:TYR:HD1	2.15	0.44
1:E:160:LYS:H	1:E:160:LYS:HG2	1.59	0.44
1:E:176:ILE:HG21	1:E:186:TYR:CE1	2.52	0.44
1:E:208:VAL:HG22	1:E:209:GLU:N	2.32	0.44
1:E:261:ASP:OD1	1:E:361:GLU:CA	2.56	0.44
2:H:219:THR:HG23	2:H:220:ASN:H	1.77	0.44
1:A:14:ARG:HH22	1:C:183:HIS:CB	2.30	0.44
1:A:131:GLU:O	1:A:132:GLN:C	2.61	0.44
1:A:316:GLU:C	1:A:319:ASN:ND2	2.74	0.44
2:B:472:LEU:HD23	2:B:472:LEU:HA	1.64	0.44
2:B:504:GLY:O	2:B:505:LEU:C	2.61	0.44
1:C:111:SER:HB2	2:D:480:ARG:HH22	1.83	0.44
1:C:335:ILE:HG12	1:C:335:ILE:H	1.61	0.44
1:E:160:LYS:CB	1:E:160:LYS:HZ2	2.27	0.44
1:E:372:PHE:HD1	1:E:376:GLN:HB2	1.82	0.44
2:F:229:VAL:HG12	2:F:313:SER:HB3	2.00	0.44
1:G:330:LYS:O	1:G:331:ARG:C	2.59	0.44
1:A:14:ARG:HH22	1:C:183:HIS:HB3	1.83	0.44
1:A:372:PHE:CD1	1:A:372:PHE:O	2.70	0.44
1:C:150:ARG:O	1:C:153:MET:N	2.47	0.44
1:C:336:LYS:HB2	1:C:350:ILE:HG21	2.00	0.44
1:C:379:PRO:O	1:C:383:THR:HG22	2.18	0.44
2:D:127:ILE:HD12	2:D:174:ILE:HG23	1.97	0.44
2:D:142:PHE:HB3	2:D:144:LEU:HD13	1.99	0.44
2:D:146:ILE:HG12	2:D:147:ASP:N	2.33	0.44
2:D:395:LEU:HD12	2:D:396:ASP:H	1.81	0.44
2:F:83:PRO:O	2:F:86:VAL:HG23	2.18	0.44
2:F:465:LYS:NZ	2:F:465:LYS:HB3	2.33	0.44
2:F:508:LEU:HD13	2:F:508:LEU:HA	1.71	0.44
1:G:67:ARG:H	1:G:67:ARG:HG2	1.56	0.44
1:G:336:LYS:HB2	1:G:350:ILE:HG21	1.99	0.44
2:B:97:SER:OG	2:B:109:GLY:HA3	2.18	0.44
2:D:16:PHE:CE1	2:D:23:ALA:HB3	2.53	0.44
1:E:362:ILE:H	1:E:362:ILE:HG13	1.64	0.44
2:F:191:ILE:H	2:F:191:ILE:CD1	2.24	0.44
2:F:318:GLY:C	2:F:320:ASP:N	2.73	0.44
1:G:12:GLU:O	1:G:14:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PHE:O	1:A:376:GLN:HB2	2.18	0.44
1:C:262:ALA:CB	1:C:360:LEU:H	2.30	0.44
2:D:276:LEU:HD23	2:D:276:LEU:HA	1.84	0.44
1:E:173:ASN:HD22	1:E:173:ASN:HA	1.54	0.44
2:F:305:ASP:O	2:F:305:ASP:CG	2.60	0.44
1:G:21:LEU:HD22	1:G:21:LEU:HA	1.64	0.44
1:G:42:ILE:HD11	1:G:68:ARG:HG3	2.00	0.44
1:G:167:LEU:HG	1:G:168:ARG:N	2.32	0.44
1:G:340:TRP:HZ3	1:G:341:PHE:CE1	2.35	0.44
2:H:130:GLU:HG2	2:H:141:THR:HG22	2.00	0.44
1:A:97:GLU:O	1:A:98:TYR:CD1	2.71	0.44
1:A:286:ARG:C	1:A:287:LEU:HG	2.42	0.44
2:D:103:GLN:HE22	2:D:315:SER:H	1.66	0.44
2:D:349:PRO:O	2:D:417:SER:OG	2.33	0.44
2:F:58:ILE:O	2:F:205:PHE:HA	2.17	0.44
2:F:221:LYS:O	2:F:221:LYS:HD3	2.17	0.44
2:F:345:TYR:O	2:F:346:GLN:C	2.59	0.44
1:G:80:MET:HE3	2:H:477:GLU:CB	2.47	0.44
1:G:85:MET:HE1	1:G:104:LEU:CD2	2.45	0.44
1:G:100:THR:O	1:G:103:ASP:HB2	2.18	0.44
2:H:330:PHE:O	2:H:361:SER:HB2	2.18	0.44
2:H:441:LYS:O	2:H:443:ALA:N	2.50	0.44
1:A:21:LEU:HD22	1:A:21:LEU:HA	1.70	0.44
1:C:263:ASP:HB2	1:C:264:PRO:CD	2.47	0.44
2:D:30:ARG:HE	2:D:30:ARG:HB3	1.42	0.44
1:G:184:GLY:O	1:G:185:ALA:HB2	2.17	0.44
1:G:216:GLN:HG2	1:G:370:LEU:HD11	2.00	0.44
1:G:230:LEU:HD23	1:G:231:ILE:N	2.32	0.44
2:H:127:ILE:HD12	2:H:174:ILE:HG23	1.99	0.44
2:H:195:TYR:CE2	2:H:215:TYR:HB3	2.53	0.44
1:A:262:ALA:HB3	1:A:360:LEU:H	1.83	0.43
1:A:340:TRP:CZ3	1:A:341:PHE:CZ	2.99	0.43
2:B:127:ILE:HD12	2:B:174:ILE:HG23	1.99	0.43
1:C:21:LEU:O	1:C:22:ARG:C	2.61	0.43
1:C:85:MET:HE1	1:C:104:LEU:CB	2.47	0.43
2:D:103:GLN:NE2	2:D:315:SER:N	2.66	0.43
2:D:355:GLY:N	2:D:412:MET:HE3	2.33	0.43
1:E:189:GLU:C	1:E:191:THR:N	2.76	0.43
1:E:214:PHE:C	1:E:214:PHE:CD2	2.95	0.43
1:E:270:PHE:C	1:E:270:PHE:HD1	2.25	0.43
1:G:39:VAL:HG12	1:G:40:MET:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:MET:HE2	1:G:80:MET:HB2	1.74	0.43
1:G:335:ILE:O	1:G:336:LYS:C	2.59	0.43
2:H:504:GLY:O	2:H:505:LEU:C	2.59	0.43
1:A:31:GLN:HG2	1:A:32:LEU:N	2.33	0.43
1:A:226:TYR:O	1:A:227:LYS:C	2.58	0.43
1:A:368:LYS:HB3	1:A:372:PHE:HD2	1.83	0.43
2:B:358:PHE:HD1	2:B:408:GLN:O	2.01	0.43
1:C:79:PHE:O	1:C:82:THR:N	2.51	0.43
1:C:254:LEU:HA	1:C:255:PRO:HD3	1.78	0.43
2:D:396:ASP:HB3	2:D:399:ARG:HH11	1.82	0.43
1:E:31:GLN:HG2	1:E:32:LEU:N	2.32	0.43
1:E:154:LEU:HA	1:E:154:LEU:HD13	1.77	0.43
1:E:243:ARG:HH22	1:E:287:LEU:HD22	1.81	0.43
2:F:464:ALA:C	2:F:466:LYS:N	2.75	0.43
1:G:74:ASN:OD1	1:G:74:ASN:N	2.50	0.43
1:G:88:ILE:H	1:G:88:ILE:HG12	1.69	0.43
1:G:378:ILE:HB	1:G:379:PRO:CD	2.48	0.43
2:H:345:TYR:O	2:H:346:GLN:C	2.61	0.43
2:H:473:LYS:C	2:H:474:TYR:HD1	2.26	0.43
1:A:79:PHE:C	1:A:81:GLN:N	2.74	0.43
1:A:160:LYS:CB	1:A:160:LYS:HZ2	2.29	0.43
1:A:263:ASP:HB2	1:A:264:PRO:CD	2.48	0.43
1:A:302:ILE:H	1:A:302:ILE:HG13	1.69	0.43
2:B:374:ALA:O	2:B:377:ILE:HG13	2.18	0.43
1:C:21:LEU:HD13	1:C:21:LEU:C	2.43	0.43
2:D:309:PRO:O	2:D:349:PRO:HB3	2.18	0.43
2:D:473:LYS:C	2:D:474:TYR:HD1	2.27	0.43
1:E:189:GLU:O	1:E:191:THR:N	2.52	0.43
1:G:25:PHE:O	1:G:26:LEU:C	2.61	0.43
2:H:276:LEU:C	2:H:278:GLY:N	2.75	0.43
2:H:464:ALA:C	2:H:466:LYS:H	2.26	0.43
1:A:351:ASN:O	1:A:352:THR:C	2.61	0.43
2:B:47:THR:HG22	2:B:78:GLY:CA	2.48	0.43
2:B:276:LEU:C	2:B:278:GLY:N	2.74	0.43
1:C:79:PHE:C	1:C:81:GLN:N	2.74	0.43
1:C:100:THR:O	1:C:103:ASP:HB2	2.18	0.43
2:D:362:ILE:O	2:D:408:GLN:HG2	2.18	0.43
2:D:387:VAL:HG12	2:D:430:ILE:HB	1.99	0.43
1:E:39:VAL:HG13	1:E:68:ARG:C	2.43	0.43
1:E:154:LEU:O	1:E:155:ILE:C	2.59	0.43
1:A:176:ILE:HG21	1:A:186:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:LEU:HA	2:D:508:LEU:HD13	1.70	0.43
1:E:260:THR:HB	1:E:261:ASP:H	1.55	0.43
1:E:335:ILE:HG12	1:E:335:ILE:H	1.62	0.43
1:E:355:GLN:HE21	1:E:355:GLN:HB3	1.63	0.43
1:G:19:ASN:C	1:G:21:LEU:H	2.26	0.43
1:G:154:LEU:HD13	1:G:154:LEU:HA	1.76	0.43
1:G:294:PHE:O	1:G:387:TYR:HB2	2.18	0.43
2:H:464:ALA:C	2:H:466:LYS:N	2.76	0.43
1:A:79:PHE:O	1:A:80:MET:C	2.59	0.43
1:C:177:ASP:OD1	1:C:178:LEU:N	2.51	0.43
1:C:371:LYS:CD	1:C:371:LYS:H	2.29	0.43
2:D:276:LEU:C	2:D:278:GLY:N	2.75	0.43
1:E:33:LYS:HA	1:E:33:LYS:HD2	1.78	0.43
1:E:39:VAL:HG12	1:E:40:MET:O	2.18	0.43
1:E:98:TYR:HB3	1:E:156:LEU:HD23	2.01	0.43
2:F:499:ASN:C	2:F:499:ASN:ND2	2.69	0.43
1:G:79:PHE:O	1:G:81:GLN:N	2.51	0.43
1:G:91:ASP:C	1:G:93:LEU:H	2.26	0.43
2:H:465:LYS:HB3	2:H:465:LYS:NZ	2.34	0.43
1:A:167:LEU:HG	1:A:168:ARG:N	2.33	0.43
1:A:252:LEU:O	1:A:254:LEU:HD12	2.18	0.43
1:A:387:TYR:N	1:A:387:TYR:HD2	2.17	0.43
2:B:398:LYS:C	2:B:400:TYR:H	2.25	0.43
1:C:28:LEU:HD23	1:C:28:LEU:HA	1.90	0.43
1:C:189:GLU:C	1:C:191:THR:H	2.25	0.43
1:C:330:LYS:O	1:C:331:ARG:C	2.61	0.43
1:C:372:PHE:HD1	1:C:376:GLN:HB2	1.83	0.43
2:D:465:LYS:NZ	2:D:465:LYS:HB3	2.34	0.43
1:E:85:MET:SD	1:E:104:LEU:HD23	2.58	0.43
1:E:172:GLY:N	1:G:183:HIS:CE1	2.85	0.43
2:F:430:ILE:HG22	2:F:431:ALA:N	2.33	0.43
1:G:90:TYR:CD2	1:G:90:TYR:C	2.96	0.43
1:G:261:ASP:OD1	1:G:362:ILE:HG13	2.19	0.43
2:H:496:LYS:O	2:H:497:TYR:C	2.61	0.43
1:A:189:GLU:OE2	1:C:183:HIS:CD2	2.72	0.43
1:A:270:PHE:HD2	1:A:294:PHE:HD1	1.67	0.43
1:A:378:ILE:N	1:A:378:ILE:CD1	2.82	0.43
2:B:207:ASP:HB2	2:B:208:PRO:CD	2.48	0.43
2:B:338:ILE:O	2:B:338:ILE:HG23	2.18	0.43
2:B:382:ASP:O	2:B:384:LYS:N	2.52	0.43
2:B:396:ASP:HB3	2:B:399:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:O	1:C:132:GLN:C	2.61	0.43
1:C:159:GLU:CG	1:C:240:ALA:HB3	2.49	0.43
1:C:307:ARG:HG3	1:C:308:LYS:N	2.33	0.43
1:C:350:ILE:O	1:C:353:PHE:HB3	2.19	0.43
1:E:238:ASP:C	1:E:242:ARG:NH2	2.77	0.43
1:E:254:LEU:HA	1:E:255:PRO:HD3	1.74	0.43
2:F:16:PHE:HZ	2:F:25:PHE:CD2	2.37	0.43
2:F:142:PHE:HB3	2:F:144:LEU:HD13	2.01	0.43
2:F:204:ILE:HG12	2:F:214:TYR:HD1	1.83	0.43
1:G:262:ALA:HB3	1:G:360:LEU:H	1.84	0.43
1:G:270:PHE:C	1:G:270:PHE:HD1	2.24	0.43
2:H:219:THR:CG2	2:H:220:ASN:N	2.60	0.43
2:H:340:ARG:HH22	2:H:442:ASN:HB3	1.82	0.43
1:A:80:MET:CE	2:B:477:GLU:CB	2.97	0.43
2:D:504:GLY:O	2:D:505:LEU:C	2.62	0.43
1:G:175:VAL:O	1:G:175:VAL:CG2	2.65	0.43
2:H:99:TYR:HE2	2:H:348:HIS:CE1	2.37	0.43
1:A:39:VAL:HG12	1:A:40:MET:O	2.19	0.43
1:A:88:ILE:H	1:A:88:ILE:HG12	1.68	0.43
1:A:214:PHE:CD1	1:A:230:LEU:HD21	2.54	0.43
1:A:219:ARG:NH2	1:C:14:ARG:HH21	2.16	0.43
1:A:245:VAL:HG12	1:A:246:ARG:N	2.30	0.43
2:B:62:LEU:HD13	2:B:70:TYR:CE1	2.54	0.43
1:C:79:PHE:O	1:C:81:GLN:N	2.52	0.43
1:C:80:MET:HE2	1:C:80:MET:HB2	1.73	0.43
1:C:243:ARG:NH2	1:C:287:LEU:CD2	2.77	0.43
1:C:307:ARG:CB	1:C:308:LYS:HD3	2.49	0.43
1:C:344:LYS:C	1:C:346:TRP:H	2.27	0.43
2:D:398:LYS:C	2:D:400:TYR:H	2.26	0.43
1:E:21:LEU:HD22	1:E:21:LEU:HA	1.71	0.43
2:F:519:GLU:CD	2:F:519:GLU:N	2.76	0.43
1:A:278:ILE:O	1:A:279:SER:C	2.61	0.42
1:A:305:ASN:ND2	1:A:307:ARG:HE	2.17	0.42
1:A:335:ILE:O	1:A:336:LYS:C	2.59	0.42
2:B:197:ILE:HB	2:B:317:ILE:CD1	2.47	0.42
2:B:420:ILE:HB	2:B:422:TYR:CE2	2.51	0.42
1:C:68:ARG:NH1	1:C:78:ARG:O	2.52	0.42
1:C:372:PHE:CE1	1:C:377:TYR:HB2	2.54	0.42
1:E:28:LEU:HD23	1:E:28:LEU:HA	1.92	0.42
2:F:195:TYR:OH	2:F:216:PRO:HD2	2.18	0.42
2:F:263:GLN:O	2:F:264:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG12	1:A:335:ILE:H	1.54	0.42
1:C:379:PRO:O	1:C:383:THR:CG2	2.67	0.42
2:D:324:LEU:O	2:D:325:GLY:C	2.63	0.42
2:D:383:GLU:O	2:D:389:TRP:HB2	2.20	0.42
1:E:19:ASN:C	1:E:21:LEU:H	2.27	0.42
1:G:351:ASN:O	1:G:352:THR:C	2.60	0.42
2:H:472:LEU:HD23	2:H:472:LEU:HA	1.64	0.42
2:H:499:ASN:C	2:H:499:ASN:ND2	2.70	0.42
1:A:21:LEU:O	1:A:22:ARG:O	2.37	0.42
1:A:302:ILE:HB	1:A:303:PHE:HD2	1.77	0.42
1:A:387:TYR:N	1:A:387:TYR:CD2	2.87	0.42
2:B:395:LEU:HD12	2:B:396:ASP:N	2.33	0.42
2:B:496:LYS:O	2:B:497:TYR:C	2.61	0.42
1:C:87:SER:O	1:C:88:ILE:C	2.62	0.42
1:C:270:PHE:O	1:C:271:SER:C	2.61	0.42
2:D:29:ALA:HB2	2:D:179:ASP:HB3	2.01	0.42
2:D:82:PRO:HA	2:D:83:PRO:HD2	1.72	0.42
2:D:260:ASN:HD21	2:H:214:TYR:H	1.68	0.42
2:D:382:ASP:O	2:D:384:LYS:N	2.52	0.42
1:E:98:TYR:HA	1:E:99:PRO:HD3	1.76	0.42
1:E:381:LYS:HE2	1:E:386:ASP:HB3	2.00	0.42
2:F:187:ILE:O	2:F:190:TYR:N	2.52	0.42
1:G:150:ARG:C	1:G:152:GLU:N	2.76	0.42
2:H:191:ILE:O	2:H:192:LYS:C	2.63	0.42
2:H:214:TYR:CE2	2:H:216:PRO:HB3	2.54	0.42
2:H:420:ILE:HB	2:H:422:TYR:CE2	2.54	0.42
2:B:190:TYR:O	2:B:191:ILE:C	2.62	0.42
2:B:309:PRO:O	2:B:349:PRO:HB3	2.19	0.42
1:C:39:VAL:HG12	1:C:40:MET:O	2.19	0.42
1:C:43:PRO:O	1:C:144:VAL:HG11	2.19	0.42
1:C:270:PHE:HE2	1:C:294:PHE:HB2	1.82	0.42
2:D:197:ILE:C	2:D:197:ILE:HD12	2.44	0.42
2:D:464:ALA:C	2:D:466:LYS:N	2.77	0.42
1:E:41:GLU:O	1:E:43:PRO:HD3	2.20	0.42
1:E:79:PHE:C	1:E:81:GLN:N	2.75	0.42
1:E:243:ARG:HH21	1:E:287:LEU:HD22	1.81	0.42
1:E:298:SER:C	1:E:301:ASP:HB2	2.38	0.42
2:F:44:LEU:HD23	2:F:44:LEU:HA	1.87	0.42
1:G:77:LYS:HA	2:H:474:TYR:CE2	2.54	0.42
1:G:79:PHE:O	1:G:80:MET:C	2.62	0.42
1:G:370:LEU:N	1:G:370:LEU:CD2	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HD2	1:C:363:GLU:CG	2.45	0.42
2:B:305:ASP:CG	2:B:305:ASP:O	2.62	0.42
1:C:187:ALA:O	1:C:188:ILE:O	2.37	0.42
1:C:302:ILE:HB	1:C:303:PHE:CE2	2.55	0.42
1:C:366:ALA:O	1:C:368:LYS:N	2.52	0.42
2:D:450:LYS:O	2:D:453:GLN:HB3	2.19	0.42
1:E:91:ASP:C	1:E:93:LEU:H	2.27	0.42
1:G:324:ALA:HB3	1:G:357:LYS:HB3	2.01	0.42
2:H:98:LYS:O	2:H:99:TYR:C	2.62	0.42
2:H:305:ASP:O	2:H:305:ASP:CG	2.62	0.42
1:A:26:LEU:C	1:A:26:LEU:HD23	2.44	0.42
1:A:91:ASP:C	1:A:93:LEU:H	2.27	0.42
2:B:221:LYS:O	2:B:221:LYS:HD3	2.20	0.42
2:D:318:GLY:C	2:D:320:ASP:N	2.77	0.42
1:E:79:PHE:O	1:E:80:MET:C	2.61	0.42
1:E:79:PHE:O	1:E:81:GLN:N	2.53	0.42
1:E:210:LYS:O	1:E:211:ASP:C	2.61	0.42
2:F:227:GLN:O	2:F:313:SER:HA	2.20	0.42
2:F:264:SER:C	2:F:265:ILE:CG1	2.89	0.42
1:G:208:VAL:CG2	1:G:209:GLU:N	2.82	0.42
2:H:142:PHE:HB3	2:H:144:LEU:HD13	2.01	0.42
2:H:221:LYS:HD2	2:H:321:LEU:HD21	2.01	0.42
2:H:387:VAL:HG12	2:H:430:ILE:HB	2.01	0.42
1:A:214:PHE:CE1	1:A:230:LEU:HD22	2.54	0.42
1:A:307:ARG:HG3	1:A:308:LYS:N	2.35	0.42
1:A:372:PHE:HD1	1:A:372:PHE:O	2.02	0.42
1:E:21:LEU:CD1	1:E:93:LEU:HG	2.50	0.42
2:F:29:ALA:HB2	2:F:179:ASP:HB3	2.02	0.42
2:F:47:THR:HG22	2:F:78:GLY:CA	2.49	0.42
2:F:197:ILE:C	2:F:197:ILE:HD12	2.45	0.42
1:G:270:PHE:O	1:G:271:SER:C	2.62	0.42
2:H:362:ILE:O	2:H:408:GLN:HG2	2.20	0.42
1:A:14:ARG:HH21	1:C:219:ARG:NH2	2.15	0.42
1:A:243:ARG:O	1:A:244:PHE:C	2.62	0.42
1:A:271:SER:HB3	1:A:340:TRP:HH2	1.78	0.42
2:B:233:PRO:HD3	2:B:262:PHE:HB3	2.01	0.42
2:B:397:TRP:CD2	2:B:409:MET:HE1	2.55	0.42
1:C:132:GLN:HE21	1:C:132:GLN:HB2	1.62	0.42
1:C:316:GLU:HA	1:C:319:ASN:HD21	1.85	0.42
1:E:67:ARG:H	1:E:67:ARG:HG2	1.56	0.42
1:G:159:GLU:HG3	1:G:238:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:PRO:HD3	2:H:262:PHE:HB3	2.01	0.42
2:H:382:ASP:C	2:H:384:LYS:N	2.74	0.42
2:H:397:TRP:O	2:H:402:ILE:HB	2.18	0.42
2:B:464:ALA:C	2:B:466:LYS:N	2.77	0.42
1:C:378:ILE:HB	1:C:379:PRO:CD	2.50	0.42
1:E:21:LEU:HD12	1:E:93:LEU:HD11	2.02	0.42
1:E:132:GLN:O	1:E:133:LYS:C	2.62	0.42
1:E:159:GLU:OE1	1:E:190:PRO:HA	2.20	0.42
1:E:214:PHE:CE1	1:E:230:LEU:CD2	3.03	0.42
2:F:82:PRO:HA	2:F:83:PRO:HD2	1.71	0.42
2:F:98:LYS:O	2:F:99:TYR:C	2.62	0.42
2:F:386:ASP:OD1	2:F:388:ILE:HB	2.19	0.42
1:G:243:ARG:O	1:G:244:PHE:C	2.63	0.42
1:G:321:ILE:HG21	1:G:358:ALA:HB1	2.02	0.42
2:H:436:ILE:HG22	2:H:437:GLU:N	2.35	0.42
1:A:259:LEU:O	1:A:259:LEU:HD12	2.19	0.42
1:A:302:ILE:HB	1:A:303:PHE:CE2	2.54	0.42
2:B:16:PHE:CE1	2:B:23:ALA:HB3	2.55	0.42
3:B:531:RDC:H182	3:B:531:RDC:H15	1.96	0.42
1:E:85:MET:HG2	1:E:129:TRP:CH2	2.55	0.42
1:E:113:LEU:CD2	1:E:115:LYS:O	2.68	0.42
2:F:464:ALA:C	2:F:466:LYS:H	2.27	0.42
1:G:132:GLN:O	1:G:133:LYS:C	2.63	0.42
1:G:154:LEU:O	1:G:155:ILE:C	2.61	0.42
1:G:278:ILE:O	1:G:279:SER:C	2.63	0.42
2:H:110:LEU:O	2:H:111:GLY:C	2.63	0.42
2:H:318:GLY:C	2:H:320:ASP:N	2.76	0.42
2:H:430:ILE:HG22	2:H:431:ALA:N	2.35	0.42
2:H:459:ARG:O	2:H:463:GLU:HB2	2.20	0.42
1:A:21:LEU:HD13	1:A:21:LEU:C	2.45	0.41
1:A:274:ARG:HE	1:A:274:ARG:HB2	1.46	0.41
2:B:464:ALA:C	2:B:466:LYS:H	2.28	0.41
1:C:11:LYS:H	1:C:11:LYS:HG2	1.58	0.41
1:C:150:ARG:C	1:C:152:GLU:H	2.27	0.41
1:C:167:LEU:HG	1:C:168:ARG:N	2.34	0.41
1:E:218:HIS:CD2	1:E:223:TRP:NE1	2.78	0.41
2:F:276:LEU:C	2:F:278:GLY:H	2.27	0.41
2:H:86:VAL:CB	2:H:87:PRO:HD3	2.46	0.41
1:A:79:PHE:O	1:A:81:GLN:N	2.53	0.41
1:A:170:ARG:HB3	1:A:175:VAL:HG12	2.02	0.41
1:A:252:LEU:HB3	1:A:254:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:HA	1:A:319:ASN:HD21	1.84	0.41
2:B:322:ILE:O	2:B:323:GLU:C	2.62	0.41
1:C:216:GLN:HE21	1:C:216:GLN:HB2	1.60	0.41
2:F:355:GLY:N	2:F:412:MET:HE3	2.34	0.41
1:G:150:ARG:NH2	1:G:150:ARG:HB3	2.34	0.41
1:G:262:ALA:CB	1:G:360:LEU:H	2.33	0.41
2:H:146:ILE:HG12	2:H:147:ASP:N	2.34	0.41
1:A:132:GLN:O	1:A:133:LYS:C	2.64	0.41
1:A:173:ASN:HD22	1:A:173:ASN:HA	1.54	0.41
1:A:183:HIS:ND1	1:C:14:ARG:CZ	2.84	0.41
1:A:324:ALA:HB3	1:A:357:LYS:HB3	2.02	0.41
1:C:166:ASN:HB3	1:C:201:ASP:HB3	2.02	0.41
1:C:184:GLY:O	1:C:185:ALA:HB2	2.20	0.41
1:E:21:LEU:O	1:E:22:ARG:O	2.37	0.41
1:E:205:VAL:CG1	1:E:256:VAL:HG22	2.50	0.41
2:F:103:GLN:HE22	2:F:315:SER:H	1.67	0.41
2:F:374:ALA:O	2:F:377:ILE:HG13	2.21	0.41
1:G:188:ILE:O	1:G:188:ILE:CD1	2.68	0.41
1:G:382:ILE:O	1:G:383:THR:C	2.62	0.41
2:H:16:PHE:HZ	2:H:25:PHE:CD2	2.38	0.41
1:A:80:MET:HE2	1:A:80:MET:HB2	1.79	0.41
2:B:86:VAL:CB	2:B:87:PRO:HD3	2.47	0.41
2:B:322:ILE:HG23	2:B:412:MET:HE2	2.01	0.41
2:B:377:ILE:HA	2:B:378:PRO:HD3	1.94	0.41
2:B:508:LEU:O	2:B:510:SER:N	2.53	0.41
1:C:79:PHE:O	1:C:80:MET:C	2.63	0.41
1:C:351:ASN:O	1:C:352:THR:C	2.62	0.41
2:D:195:TYR:OH	2:D:216:PRO:HD2	2.21	0.41
2:D:222:ILE:HA	2:D:223:PRO:HD3	1.91	0.41
1:E:85:MET:HE3	1:E:104:LEU:HB3	1.99	0.41
2:F:500:GLU:CA	2:F:503:GLU:HB3	2.37	0.41
1:G:335:ILE:O	1:G:338:TYR:N	2.46	0.41
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.75	0.41
2:B:476:PRO:O	2:B:479:SER:HB2	2.20	0.41
1:C:265:TYR:O	1:C:268:TYR:HB3	2.19	0.41
2:D:397:TRP:O	2:D:402:ILE:HB	2.19	0.41
2:D:496:LYS:O	2:D:497:TYR:C	2.63	0.41
1:E:21:LEU:C	1:E:21:LEU:HD13	2.45	0.41
1:E:226:TYR:O	1:E:227:LYS:C	2.63	0.41
2:F:84:GLN:HE21	2:F:85:GLU:HG3	1.85	0.41
2:F:497:TYR:O	2:F:500:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:PRO:O	1:G:380:GLU:C	2.60	0.41
2:H:55:ASN:OD1	2:H:217:ARG:NH2	2.54	0.41
2:H:197:ILE:C	2:H:197:ILE:HD12	2.46	0.41
2:H:462:GLN:O	2:H:466:LYS:HB2	2.21	0.41
1:A:12:GLU:HG3	1:A:13:ALA:N	2.35	0.41
2:B:82:PRO:HA	2:B:83:PRO:HD2	1.73	0.41
1:C:21:LEU:O	1:C:22:ARG:O	2.39	0.41
1:C:84:LEU:O	1:C:85:MET:C	2.63	0.41
2:D:62:LEU:HD13	2:D:70:TYR:CE1	2.56	0.41
1:E:85:MET:HE1	1:E:104:LEU:CB	2.50	0.41
1:G:39:VAL:HG13	1:G:68:ARG:C	2.46	0.41
1:G:252:LEU:HB3	1:G:254:LEU:HD13	2.02	0.41
1:G:319:ASN:HD22	1:G:319:ASN:N	1.94	0.41
1:A:270:PHE:O	1:A:271:SER:C	2.64	0.41
1:A:285:GLU:HB3	1:A:286:ARG:H	1.53	0.41
1:C:232:THR:OG1	1:C:233:SER:O	2.33	0.41
2:D:340:ARG:HH22	2:D:442:ASN:HB3	1.85	0.41
1:E:12:GLU:CG	1:E:13:ALA:N	2.83	0.41
2:F:294:THR:C	2:F:296:LEU:N	2.78	0.41
2:H:414:HIS:NE2	2:H:416:CYS:HB3	2.34	0.41
1:A:110:HIS:HD2	2:B:480:ARG:NH1	2.19	0.41
2:B:142:PHE:HB3	2:B:144:LEU:HD13	2.02	0.41
2:B:471:TYR:C	2:B:473:LYS:N	2.79	0.41
1:C:245:VAL:HG12	1:C:289:THR:HG21	2.02	0.41
2:D:358:PHE:CB	2:D:451:LEU:HD11	2.51	0.41
1:E:167:LEU:HG	1:E:168:ARG:N	2.35	0.41
2:F:62:LEU:HD13	2:F:70:TYR:CE1	2.56	0.41
1:G:245:VAL:HG12	1:G:289:THR:HG21	2.03	0.41
1:G:307:ARG:CG	1:G:308:LYS:HD3	2.50	0.41
2:H:497:TYR:O	2:H:500:GLU:OE2	2.38	0.41
2:D:414:HIS:NE2	2:D:416:CYS:HB3	2.36	0.41
2:D:464:ALA:C	2:D:466:LYS:H	2.29	0.41
1:E:102:ARG:HD3	1:G:361:GLU:OE1	2.20	0.41
1:E:378:ILE:N	1:E:379:PRO:HD2	2.36	0.41
1:E:387:TYR:N	1:E:387:TYR:CD2	2.89	0.41
2:F:285:VAL:C	2:F:287:ASN:H	2.28	0.41
2:F:322:ILE:HG21	2:F:412:MET:HE2	2.03	0.41
2:F:398:LYS:C	2:F:400:TYR:N	2.78	0.41
3:F:531:RDC:H182	3:F:531:RDC:H15	2.00	0.41
1:G:11:LYS:H	1:G:11:LYS:HG2	1.60	0.41
1:G:21:LEU:O	1:G:22:ARG:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:VAL:HB	1:G:258:ILE:HB	2.03	0.41
1:G:252:LEU:HD12	1:G:252:LEU:N	2.35	0.41
1:G:344:LYS:C	1:G:346:TRP:H	2.29	0.41
2:H:322:ILE:O	2:H:323:GLU:C	2.63	0.41
2:H:383:GLU:O	2:H:389:TRP:HB2	2.21	0.41
1:A:208:VAL:CG2	1:A:209:GLU:N	2.83	0.41
1:A:260:THR:HB	1:A:261:ASP:H	1.49	0.41
1:A:372:PHE:HD1	1:A:376:GLN:HB2	1.86	0.41
2:B:214:TYR:CE2	2:B:216:PRO:HB3	2.56	0.41
1:C:324:ALA:HB3	1:C:357:LYS:HB3	2.02	0.41
1:C:355:GLN:HE21	1:C:355:GLN:HB3	1.60	0.41
2:D:374:ALA:O	2:D:377:ILE:CG1	2.69	0.41
1:E:270:PHE:HD2	1:E:294:PHE:HD1	1.67	0.41
1:E:335:ILE:O	1:E:338:TYR:N	2.46	0.41
1:E:385:LYS:HA	1:E:387:TYR:CE2	2.56	0.41
2:F:110:LEU:O	2:F:111:GLY:C	2.64	0.41
2:F:362:ILE:HA	2:F:363:PRO:HD3	1.82	0.41
2:F:508:LEU:O	2:F:510:SER:N	2.54	0.41
1:G:362:ILE:HG13	1:G:362:ILE:H	1.66	0.41
2:B:471:TYR:HB3	2:B:475:ILE:HD11	2.03	0.40
2:D:338:ILE:O	2:D:338:ILE:HG23	2.20	0.40
2:F:224:LYS:CG	2:F:225:PRO:HD2	2.42	0.40
2:H:251:ASP:OD2	2:H:251:ASP:N	2.53	0.40
2:H:374:ALA:O	2:H:377:ILE:CG1	2.69	0.40
2:H:377:ILE:HA	2:H:378:PRO:HD3	1.95	0.40
1:A:31:GLN:O	1:A:33:LYS:HB2	2.20	0.40
1:A:87:SER:O	1:A:88:ILE:C	2.62	0.40
1:A:265:TYR:O	1:A:268:TYR:HB3	2.20	0.40
1:A:307:ARG:HH11	1:A:308:LYS:NZ	2.20	0.40
2:B:316:VAL:HG13	2:B:351:ILE:HD12	2.04	0.40
2:B:497:TYR:O	2:B:500:GLU:OE2	2.39	0.40
2:D:305:ASP:CG	2:D:305:ASP:O	2.64	0.40
1:E:87:SER:O	1:E:88:ILE:C	2.65	0.40
2:F:387:VAL:HG12	2:F:430:ILE:HB	2.02	0.40
1:G:176:ILE:HG21	1:G:186:TYR:CE1	2.56	0.40
1:G:205:VAL:CG1	1:G:256:VAL:HG22	2.51	0.40
2:H:99:TYR:HH	2:H:348:HIS:HE2	1.69	0.40
2:H:227:GLN:O	2:H:313:SER:HA	2.21	0.40
1:A:41:GLU:O	1:A:43:PRO:HD3	2.21	0.40
1:A:207:VAL:HB	1:A:258:ILE:HB	2.04	0.40
1:A:261:ASP:OD1	1:A:362:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PRO:O	2:B:86:VAL:HG23	2.21	0.40
2:B:388:ILE:O	2:B:392:VAL:HG13	2.22	0.40
2:B:480:ARG:O	2:B:481:SER:C	2.64	0.40
1:C:139:ILE:O	1:C:140:VAL:C	2.63	0.40
1:C:150:ARG:C	1:C:152:GLU:N	2.80	0.40
1:C:150:ARG:NH2	1:C:150:ARG:HB3	2.36	0.40
1:C:387:TYR:N	1:C:387:TYR:HD2	2.18	0.40
1:E:374:ALA:HB3	1:E:375:PHE:CD1	2.56	0.40
2:F:191:ILE:O	2:F:192:LYS:C	2.63	0.40
1:G:252:LEU:O	1:G:254:LEU:HD12	2.20	0.40
2:H:62:LEU:HD13	2:H:70:TYR:CE1	2.57	0.40
1:A:154:LEU:O	1:A:155:ILE:C	2.62	0.40
1:A:189:GLU:HA	1:A:190:PRO:HD3	1.97	0.40
1:A:262:ALA:CB	1:A:360:LEU:H	2.34	0.40
1:A:353:PHE:O	1:A:354:LEU:C	2.65	0.40
2:B:107:MET:O	2:B:108:TYR:O	2.38	0.40
2:B:251:ASP:OD2	2:B:251:ASP:N	2.53	0.40
2:B:354:ALA:HA	2:B:412:MET:O	2.21	0.40
1:C:153:MET:O	1:C:154:LEU:CB	2.56	0.40
1:C:348:GLU:O	1:C:352:THR:HG23	2.21	0.40
2:D:187:ILE:O	2:D:190:TYR:N	2.50	0.40
1:E:336:LYS:HB2	1:E:350:ILE:HG21	2.04	0.40
2:F:87:PRO:C	2:F:89:ALA:H	2.30	0.40
2:F:437:GLU:O	2:F:437:GLU:HG3	2.22	0.40
2:F:473:LYS:C	2:F:474:TYR:HD1	2.29	0.40
1:G:173:ASN:HD22	1:G:173:ASN:HA	1.54	0.40
1:G:178:LEU:HD23	1:G:178:LEU:HA	1.79	0.40
1:G:224:LYS:C	1:G:224:LYS:CD	2.94	0.40
2:H:285:VAL:C	2:H:287:ASN:H	2.28	0.40
1:A:85:MET:HE1	1:A:104:LEU:CB	2.49	0.40
1:A:170:ARG:HG2	1:A:196:ASP:HB2	2.03	0.40
1:A:183:HIS:CE1	1:C:172:GLY:N	2.89	0.40
1:A:209:GLU:CB	1:A:260:THR:HG22	2.50	0.40
1:A:348:GLU:O	1:A:352:THR:HG23	2.21	0.40
1:A:370:LEU:H	1:A:370:LEU:CD2	2.17	0.40
2:B:383:GLU:O	2:B:389:TRP:HB2	2.21	0.40
1:C:159:GLU:HB2	1:C:190:PRO:HG3	2.04	0.40
1:C:302:ILE:H	1:C:302:ILE:HG13	1.71	0.40
1:C:311:TYR:CE1	1:C:377:TYR:CD2	3.10	0.40
2:D:322:ILE:O	2:D:323:GLU:C	2.64	0.40
1:E:140:VAL:CG1	1:E:141:ASP:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLN:O	1:G:33:LYS:HB2	2.21	0.40
2:H:27:ASN:O	2:H:28:PRO:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/389 (87%)	235 (69%)	76 (22%)	28 (8%)	0	8
1	C	339/389 (87%)	238 (70%)	73 (22%)	28 (8%)	0	8
1	E	339/389 (87%)	232 (68%)	78 (23%)	29 (9%)	0	7
1	G	339/389 (87%)	235 (69%)	76 (22%)	28 (8%)	0	8
2	B	504/530 (95%)	385 (76%)	88 (18%)	31 (6%)	1	12
2	D	504/530 (95%)	391 (78%)	87 (17%)	26 (5%)	1	15
2	F	504/530 (95%)	387 (77%)	90 (18%)	27 (5%)	1	14
2	H	504/530 (95%)	389 (77%)	91 (18%)	24 (5%)	2	16
All	All	3372/3676 (92%)	2492 (74%)	659 (20%)	221 (7%)	1	12

All (221) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	32	LEU
1	A	151	GLU
1	A	188	ILE
1	A	275	ILE
1	A	277	SER
2	B	107	MET
2	B	108	TYR

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Mol	Chain	Res	Type
2	B	165	ARG
2	B	264	SER
2	B	319	GLU
2	B	441	LYS
2	B	442	ASN
2	B	486	LEU
2	B	497	TYR
1	C	22	ARG
1	C	32	LEU
1	C	151	GLU
1	C	188	ILE
1	C	275	ILE
1	C	277	SER
2	D	107	MET
2	D	108	TYR
2	D	165	ARG
2	D	264	SER
2	D	319	GLU
2	D	442	ASN
2	D	486	LEU
2	D	497	TYR
1	E	22	ARG
1	E	32	LEU
1	E	151	GLU
1	E	188	ILE
1	E	275	ILE
1	E	277	SER
2	F	107	MET
2	F	108	TYR
2	F	165	ARG
2	F	264	SER
2	F	319	GLU
2	F	441	LYS
2	F	442	ASN
2	F	486	LEU
2	F	497	TYR
1	G	22	ARG
1	G	32	LEU
1	G	151	GLU
1	G	188	ILE
1	G	275	ILE
1	G	277	SER

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Mol	Chain	Res	Type
2	H	107	MET
2	H	108	TYR
2	H	165	ARG
2	H	264	SER
2	H	319	GLU
2	H	486	LEU
2	H	497	TYR
1	A	13	ALA
1	A	33	LYS
1	A	85	MET
1	A	155	ILE
1	A	336	LYS
1	A	354	LEU
1	A	370	LEU
2	B	255	LYS
2	B	346	GLN
2	B	402	ILE
2	B	468	LEU
2	B	509	ILE
1	C	13	ALA
1	C	18	ALA
1	C	33	LYS
1	C	85	MET
1	C	155	ILE
1	C	336	LYS
1	C	354	LEU
2	D	45	ASP
2	D	255	LYS
2	D	402	ILE
2	D	441	LYS
2	D	468	LEU
2	D	509	ILE
1	E	33	LYS
1	E	85	MET
1	E	147	SER
1	E	155	ILE
1	E	336	LYS
1	E	354	LEU
1	E	370	LEU
2	F	45	ASP
2	F	255	LYS
2	F	402	ILE

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Mol	Chain	Res	Type
2	F	468	LEU
2	F	509	ILE
1	G	33	LYS
1	G	85	MET
1	G	155	ILE
1	G	336	LYS
1	G	354	LEU
2	H	45	ASP
2	H	255	LYS
2	H	402	ILE
2	H	441	LYS
2	H	442	ASN
2	H	468	LEU
2	H	509	ILE
1	A	18	ALA
1	A	117	ILE
1	A	147	SER
1	A	150	ARG
1	A	357	LYS
2	B	45	ASP
2	B	98	LYS
2	B	99	TYR
2	B	151	ASN
2	B	401	GLY
1	C	147	SER
1	C	150	ARG
1	C	357	LYS
1	C	370	LEU
2	D	98	LYS
2	D	99	TYR
2	D	151	ASN
2	D	220	ASN
1	E	18	ALA
1	E	117	ILE
1	E	150	ARG
1	E	357	LYS
1	E	367	SER
1	E	387	TYR
2	F	98	LYS
2	F	99	TYR
2	F	220	ASN
1	G	117	ILE

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Mol	Chain	Res	Type
1	G	147	SER
1	G	150	ARG
1	G	357	LYS
1	G	370	LEU
2	H	98	LYS
2	H	99	TYR
2	H	151	ASN
2	H	220	ASN
1	A	185	ALA
2	B	95	TYR
2	B	191	ILE
2	B	347	GLY
2	B	383	GLU
1	C	117	ILE
1	C	240	ALA
1	E	13	ALA
1	E	185	ALA
2	F	95	TYR
2	F	111	GLY
2	F	151	ASN
2	F	383	GLU
1	G	13	ALA
1	G	18	ALA
1	G	161	GLY
1	G	382	ILE
1	A	103	ASP
1	A	263	ASP
1	A	278	ILE
2	B	276	LEU
1	C	154	LEU
1	C	185	ALA
1	C	278	ILE
2	D	95	TYR
2	D	111	GLY
2	D	383	GLU
1	E	263	ASP
1	E	278	ILE
2	F	346	GLN
1	G	11	LYS
1	G	106	TYR
1	G	263	ASP
1	G	278	ILE

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Mol	Chain	Res	Type
1	G	367	SER
2	H	95	TYR
1	A	106	TYR
1	A	139	ILE
1	A	240	ALA
2	B	329	ILE
2	B	382	ASP
1	C	233	SER
1	C	263	ASP
1	C	387	TYR
1	E	240	ALA
1	G	154	LEU
1	G	185	ALA
1	A	269	ILE
2	B	28	PRO
2	B	111	GLY
2	D	191	ILE
2	D	329	ILE
1	E	139	ILE
2	F	28	PRO
2	F	191	ILE
2	F	329	ILE
2	F	401	GLY
1	G	269	ILE
2	H	28	PRO
2	H	111	GLY
2	H	191	ILE
2	H	329	ILE
1	C	139	ILE
1	C	269	ILE
2	D	28	PRO
2	D	401	GLY
1	E	269	ILE
2	D	309	PRO
1	E	161	GLY
1	E	382	ILE
2	H	309	PRO
1	A	198	ILE
1	A	382	ILE
2	B	317	ILE
1	E	192	PRO
2	B	281	PRO

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Mol	Chain	Res	Type
2	B	309	PRO
1	C	198	ILE
2	F	281	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/345 (89%)	209 (68%)	97 (32%)	0	2
1	C	306/345 (89%)	208 (68%)	98 (32%)	0	2
1	E	306/345 (89%)	211 (69%)	95 (31%)	0	2
1	G	306/345 (89%)	210 (69%)	96 (31%)	0	2
2	B	451/473 (95%)	396 (88%)	55 (12%)	5	23
2	D	451/473 (95%)	397 (88%)	54 (12%)	5	24
2	F	451/473 (95%)	399 (88%)	52 (12%)	5	25
2	H	451/473 (95%)	395 (88%)	56 (12%)	4	23
All	All	3028/3272 (92%)	2425 (80%)	603 (20%)	1	8

All (603) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	11	LYS
1	A	15	ARG
1	A	21	LEU
1	A	25	PHE
1	A	29	VAL
1	A	30	GLU
1	A	31	GLN
1	A	34	LYS
1	A	38	LEU
1	A	41	GLU
1	A	69	ASN

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	75	GLU
1	A	80	MET
1	A	82	THR
1	A	83	VAL
1	A	85	MET
1	A	93	LEU
1	A	94	VAL
1	A	100	THR
1	A	101	ILE
1	A	113	LEU
1	A	115	LYS
1	A	116	SER
1	A	117	ILE
1	A	128	THR
1	A	140	VAL
1	A	146	THR
1	A	148	LEU
1	A	149	LEU
1	A	150	ARG
1	A	155	ILE
1	A	158	LYS
1	A	159	GLU
1	A	160	LYS
1	A	162	LYS
1	A	164	VAL
1	A	169	ILE
1	A	173	ASN
1	A	176	ILE
1	A	179	SER
1	A	180	LYS
1	A	183	HIS
1	A	188	ILE
1	A	189	GLU
1	A	194	LEU
1	A	195	ILE
1	A	200	VAL
1	A	205	VAL
1	A	213	VAL
1	A	216	GLN
1	A	230	LEU
1	A	231	ILE

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Mol	Chain	Res	Type
1	A	236	GLN
1	A	241	THR
1	A	242	ARG
1	A	243	ARG
1	A	250	GLU
1	A	258	ILE
1	A	259	LEU
1	A	273	PHE
1	A	275	ILE
1	A	285	GLU
1	A	289	THR
1	A	291	ASP
1	A	295	LEU
1	A	298	SER
1	A	302	ILE
1	A	308	LYS
1	A	309	LYS
1	A	311	TYR
1	A	312	LEU
1	A	313	SER
1	A	314	GLU
1	A	317	ARG
1	A	319	ASN
1	A	321	ILE
1	A	335	ILE
1	A	343	THR
1	A	344	LYS
1	A	346	TRP
1	A	349	GLU
1	A	351	ASN
1	A	355	GLN
1	A	360	LEU
1	A	362	ILE
1	A	370	LEU
1	A	371	LYS
1	A	373	LEU
1	A	375	PHE
1	A	378	ILE
1	A	380	GLU
1	A	383	THR
1	A	385	LYS
1	A	387	TYR

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Mol	Chain	Res	Type
1	A	388	ILE
2	B	30	ARG
2	B	41	GLU
2	B	52	ILE
2	B	74	VAL
2	B	81	ILE
2	B	113	LYS
2	B	120	GLN
2	B	135	ASN
2	B	137	LYS
2	B	154	ILE
2	B	170	THR
2	B	186	ARG
2	B	189	GLU
2	B	191	ILE
2	B	211	ASN
2	B	215	TYR
2	B	222	ILE
2	B	227	GLN
2	B	246	ASN
2	B	253	THR
2	B	254	ILE
2	B	264	SER
2	B	265	ILE
2	B	271	ASP
2	B	272	LYS
2	B	284	LYS
2	B	316	VAL
2	B	326	LEU
2	B	327	LYS
2	B	341	LYS
2	B	351	ILE
2	B	366	GLU
2	B	371	LEU
2	B	380	ILE
2	B	384	LYS
2	B	392	VAL
2	B	402	ILE
2	B	408	GLN
2	B	410	VAL
2	B	418	THR
2	B	435	ASN

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Mol	Chain	Res	Type
2	B	436	ILE
2	B	444	LEU
2	B	447	VAL
2	B	461	GLU
2	B	482	LEU
2	B	488	SER
2	B	499	ASN
2	B	501	ILE
2	B	506	PHE
2	B	508	LEU
2	B	510	SER
2	B	511	LYS
2	B	516	ILE
2	B	519	GLU
1	C	10	ASP
1	C	11	LYS
1	C	15	ARG
1	C	21	LEU
1	C	25	PHE
1	C	29	VAL
1	C	30	GLU
1	C	31	GLN
1	C	34	LYS
1	C	38	LEU
1	C	41	GLU
1	C	69	ASN
1	C	74	ASN
1	C	75	GLU
1	C	82	THR
1	C	83	VAL
1	C	85	MET
1	C	93	LEU
1	C	94	VAL
1	C	100	THR
1	C	101	ILE
1	C	113	LEU
1	C	115	LYS
1	C	116	SER
1	C	117	ILE
1	C	128	THR
1	C	140	VAL
1	C	146	THR

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Mol	Chain	Res	Type
1	C	148	LEU
1	C	149	LEU
1	C	150	ARG
1	C	155	ILE
1	C	158	LYS
1	C	159	GLU
1	C	160	LYS
1	C	162	LYS
1	C	164	VAL
1	C	167	LEU
1	C	173	ASN
1	C	176	ILE
1	C	179	SER
1	C	180	LYS
1	C	183	HIS
1	C	188	ILE
1	C	189	GLU
1	C	194	LEU
1	C	195	ILE
1	C	200	VAL
1	C	205	VAL
1	C	213	VAL
1	C	216	GLN
1	C	230	LEU
1	C	231	ILE
1	C	236	GLN
1	C	241	THR
1	C	242	ARG
1	C	243	ARG
1	C	250	GLU
1	C	258	ILE
1	C	259	LEU
1	C	271	SER
1	C	273	PHE
1	C	275	ILE
1	C	285	GLU
1	C	289	THR
1	C	291	ASP
1	C	295	LEU
1	C	298	SER
1	C	302	ILE
1	C	308	LYS

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Mol	Chain	Res	Type
1	C	309	LYS
1	C	311	TYR
1	C	312	LEU
1	C	313	SER
1	C	314	GLU
1	C	317	ARG
1	C	319	ASN
1	C	321	ILE
1	C	335	ILE
1	C	343	THR
1	C	344	LYS
1	C	346	TRP
1	C	349	GLU
1	C	351	ASN
1	C	355	GLN
1	C	360	LEU
1	C	362	ILE
1	C	370	LEU
1	C	371	LYS
1	C	372	PHE
1	C	373	LEU
1	C	375	PHE
1	C	378	ILE
1	C	380	GLU
1	C	383	THR
1	C	385	LYS
1	C	387	TYR
1	C	388	ILE
2	D	30	ARG
2	D	41	GLU
2	D	52	ILE
2	D	81	ILE
2	D	113	LYS
2	D	120	GLN
2	D	135	ASN
2	D	137	LYS
2	D	154	ILE
2	D	170	THR
2	D	186	ARG
2	D	189	GLU
2	D	191	ILE
2	D	211	ASN

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Mol	Chain	Res	Type
2	D	215	TYR
2	D	222	ILE
2	D	227	GLN
2	D	246	ASN
2	D	253	THR
2	D	254	ILE
2	D	265	ILE
2	D	271	ASP
2	D	272	LYS
2	D	284	LYS
2	D	316	VAL
2	D	326	LEU
2	D	327	LYS
2	D	341	LYS
2	D	351	ILE
2	D	366	GLU
2	D	371	LEU
2	D	380	ILE
2	D	384	LYS
2	D	392	VAL
2	D	402	ILE
2	D	408	GLN
2	D	410	VAL
2	D	418	THR
2	D	435	ASN
2	D	436	ILE
2	D	444	LEU
2	D	446	GLU
2	D	447	VAL
2	D	461	GLU
2	D	482	LEU
2	D	488	SER
2	D	499	ASN
2	D	501	ILE
2	D	506	PHE
2	D	508	LEU
2	D	510	SER
2	D	511	LYS
2	D	516	ILE
2	D	519	GLU
1	E	10	ASP
1	E	11	LYS

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Mol	Chain	Res	Type
1	E	15	ARG
1	E	21	LEU
1	E	25	PHE
1	E	29	VAL
1	E	30	GLU
1	E	31	GLN
1	E	34	LYS
1	E	38	LEU
1	E	41	GLU
1	E	69	ASN
1	E	74	ASN
1	E	75	GLU
1	E	82	THR
1	E	83	VAL
1	E	85	MET
1	E	93	LEU
1	E	94	VAL
1	E	100	THR
1	E	101	ILE
1	E	113	LEU
1	E	115	LYS
1	E	116	SER
1	E	117	ILE
1	E	128	THR
1	E	140	VAL
1	E	146	THR
1	E	148	LEU
1	E	149	LEU
1	E	150	ARG
1	E	155	ILE
1	E	158	LYS
1	E	160	LYS
1	E	162	LYS
1	E	164	VAL
1	E	167	LEU
1	E	173	ASN
1	E	176	ILE
1	E	179	SER
1	E	180	LYS
1	E	183	HIS
1	E	188	ILE
1	E	189	GLU

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Mol	Chain	Res	Type
1	E	194	LEU
1	E	195	ILE
1	E	200	VAL
1	E	205	VAL
1	E	213	VAL
1	E	216	GLN
1	E	229	ILE
1	E	230	LEU
1	E	231	ILE
1	E	236	GLN
1	E	241	THR
1	E	242	ARG
1	E	243	ARG
1	E	250	GLU
1	E	258	ILE
1	E	259	LEU
1	E	273	PHE
1	E	275	ILE
1	E	285	GLU
1	E	289	THR
1	E	291	ASP
1	E	295	LEU
1	E	298	SER
1	E	302	ILE
1	E	308	LYS
1	E	309	LYS
1	E	312	LEU
1	E	313	SER
1	E	314	GLU
1	E	319	ASN
1	E	321	ILE
1	E	335	ILE
1	E	343	THR
1	E	344	LYS
1	E	346	TRP
1	E	349	GLU
1	E	351	ASN
1	E	355	GLN
1	E	360	LEU
1	E	362	ILE
1	E	365	MET
1	E	370	LEU

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Mol	Chain	Res	Type
1	E	371	LYS
1	E	373	LEU
1	E	375	PHE
1	E	378	ILE
1	E	380	GLU
1	E	383	THR
1	E	385	LYS
1	E	387	TYR
1	E	388	ILE
2	F	30	ARG
2	F	41	GLU
2	F	81	ILE
2	F	113	LYS
2	F	120	GLN
2	F	135	ASN
2	F	137	LYS
2	F	154	ILE
2	F	170	THR
2	F	186	ARG
2	F	189	GLU
2	F	191	ILE
2	F	211	ASN
2	F	215	TYR
2	F	222	ILE
2	F	227	GLN
2	F	246	ASN
2	F	247	ASN
2	F	253	THR
2	F	254	ILE
2	F	265	ILE
2	F	271	ASP
2	F	272	LYS
2	F	284	LYS
2	F	316	VAL
2	F	326	LEU
2	F	327	LYS
2	F	341	LYS
2	F	351	ILE
2	F	366	GLU
2	F	371	LEU
2	F	380	ILE
2	F	384	LYS

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Mol	Chain	Res	Type
2	F	392	VAL
2	F	402	ILE
2	F	408	GLN
2	F	410	VAL
2	F	435	ASN
2	F	436	ILE
2	F	444	LEU
2	F	447	VAL
2	F	461	GLU
2	F	482	LEU
2	F	488	SER
2	F	499	ASN
2	F	501	ILE
2	F	506	PHE
2	F	508	LEU
2	F	510	SER
2	F	511	LYS
2	F	516	ILE
2	F	519	GLU
1	G	10	ASP
1	G	11	LYS
1	G	15	ARG
1	G	21	LEU
1	G	25	PHE
1	G	29	VAL
1	G	30	GLU
1	G	31	GLN
1	G	34	LYS
1	G	38	LEU
1	G	41	GLU
1	G	69	ASN
1	G	74	ASN
1	G	75	GLU
1	G	82	THR
1	G	83	VAL
1	G	85	MET
1	G	93	LEU
1	G	94	VAL
1	G	100	THR
1	G	101	ILE
1	G	113	LEU
1	G	115	LYS

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Mol	Chain	Res	Type
1	G	116	SER
1	G	117	ILE
1	G	128	THR
1	G	140	VAL
1	G	146	THR
1	G	148	LEU
1	G	149	LEU
1	G	150	ARG
1	G	155	ILE
1	G	158	LYS
1	G	160	LYS
1	G	162	LYS
1	G	164	VAL
1	G	167	LEU
1	G	173	ASN
1	G	176	ILE
1	G	179	SER
1	G	180	LYS
1	G	183	HIS
1	G	188	ILE
1	G	189	GLU
1	G	194	LEU
1	G	195	ILE
1	G	200	VAL
1	G	205	VAL
1	G	213	VAL
1	G	216	GLN
1	G	229	ILE
1	G	230	LEU
1	G	231	ILE
1	G	236	GLN
1	G	241	THR
1	G	242	ARG
1	G	243	ARG
1	G	250	GLU
1	G	258	ILE
1	G	259	LEU
1	G	273	PHE
1	G	275	ILE
1	G	285	GLU
1	G	289	THR
1	G	291	ASP

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Mol	Chain	Res	Type
1	G	295	LEU
1	G	298	SER
1	G	302	ILE
1	G	308	LYS
1	G	309	LYS
1	G	312	LEU
1	G	313	SER
1	G	314	GLU
1	G	316	GLU
1	G	317	ARG
1	G	319	ASN
1	G	321	ILE
1	G	335	ILE
1	G	343	THR
1	G	344	LYS
1	G	346	TRP
1	G	349	GLU
1	G	351	ASN
1	G	355	GLN
1	G	360	LEU
1	G	362	ILE
1	G	370	LEU
1	G	371	LYS
1	G	373	LEU
1	G	375	PHE
1	G	378	ILE
1	G	380	GLU
1	G	383	THR
1	G	385	LYS
1	G	387	TYR
1	G	388	ILE
2	H	30	ARG
2	H	41	GLU
2	H	52	ILE
2	H	81	ILE
2	H	113	LYS
2	H	120	GLN
2	H	135	ASN
2	H	137	LYS
2	H	154	ILE
2	H	170	THR
2	H	186	ARG

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Mol	Chain	Res	Type
2	H	189	GLU
2	H	191	ILE
2	H	211	ASN
2	H	215	TYR
2	H	222	ILE
2	H	227	GLN
2	H	246	ASN
2	H	247	ASN
2	H	251	ASP
2	H	253	THR
2	H	254	ILE
2	H	265	ILE
2	H	271	ASP
2	H	272	LYS
2	H	284	LYS
2	H	316	VAL
2	H	326	LEU
2	H	327	LYS
2	H	341	LYS
2	H	351	ILE
2	H	366	GLU
2	H	371	LEU
2	H	380	ILE
2	H	384	LYS
2	H	392	VAL
2	H	402	ILE
2	H	408	GLN
2	H	410	VAL
2	H	418	THR
2	H	435	ASN
2	H	436	ILE
2	H	444	LEU
2	H	446	GLU
2	H	447	VAL
2	H	461	GLU
2	H	482	LEU
2	H	488	SER
2	H	499	ASN
2	H	501	ILE
2	H	506	PHE
2	H	508	LEU
2	H	510	SER

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Mol	Chain	Res	Type
2	H	511	LYS
2	H	516	ILE
2	H	519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	81	GLN
1	A	110	HIS
1	A	132	GLN
1	A	173	ASN
1	A	183	HIS
1	A	215	GLN
1	A	216	GLN
1	A	218	HIS
1	A	225	GLN
1	A	236	GLN
1	A	305	ASN
1	A	319	ASN
1	A	347	GLN
1	A	355	GLN
2	B	27	ASN
2	B	34	GLN
2	B	84	GLN
2	B	103	GLN
2	B	149	ASN
2	B	227	GLN
2	B	246	ASN
2	B	247	ASN
2	B	287	ASN
2	B	414	HIS
2	B	435	ASN
2	B	442	ASN
2	B	490	ASN
2	B	498	GLN
2	B	499	ASN
1	C	81	GLN
1	C	110	HIS
1	C	132	GLN
1	C	173	ASN
1	C	183	HIS

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Mol	Chain	Res	Type
1	C	215	GLN
1	C	216	GLN
1	C	218	HIS
1	C	225	GLN
1	C	236	GLN
1	C	305	ASN
1	C	319	ASN
1	C	347	GLN
1	C	355	GLN
2	D	27	ASN
2	D	34	GLN
2	D	68	GLN
2	D	84	GLN
2	D	103	GLN
2	D	149	ASN
2	D	227	GLN
2	D	246	ASN
2	D	247	ASN
2	D	287	ASN
2	D	331	ASN
2	D	414	HIS
2	D	435	ASN
2	D	442	ASN
2	D	490	ASN
2	D	498	GLN
2	D	499	ASN
1	E	31	GLN
1	E	81	GLN
1	E	110	HIS
1	E	132	GLN
1	E	173	ASN
1	E	183	HIS
1	E	215	GLN
1	E	216	GLN
1	E	218	HIS
1	E	225	GLN
1	E	236	GLN
1	E	305	ASN
1	E	319	ASN
1	E	347	GLN
1	E	355	GLN
2	F	27	ASN

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Mol	Chain	Res	Type
2	F	34	GLN
2	F	68	GLN
2	F	84	GLN
2	F	103	GLN
2	F	149	ASN
2	F	227	GLN
2	F	246	ASN
2	F	247	ASN
2	F	287	ASN
2	F	414	HIS
2	F	435	ASN
2	F	442	ASN
2	F	490	ASN
2	F	498	GLN
2	F	499	ASN
1	G	31	GLN
1	G	81	GLN
1	G	110	HIS
1	G	132	GLN
1	G	173	ASN
1	G	183	HIS
1	G	215	GLN
1	G	216	GLN
1	G	218	HIS
1	G	225	GLN
1	G	236	GLN
1	G	305	ASN
1	G	319	ASN
1	G	355	GLN
2	H	27	ASN
2	H	34	GLN
2	H	68	GLN
2	H	84	GLN
2	H	103	GLN
2	H	149	ASN
2	H	227	GLN
2	H	246	ASN
2	H	247	ASN
2	H	287	ASN
2	H	414	HIS
2	H	435	ASN
2	H	442	ASN

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Mol	Chain	Res	Type
2	H	490	ASN
2	H	498	GLN
2	H	499	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	RDC	H	531	-	26,27,27	3.24	7 (26%)	33,39,39	2.00	11 (33%)
3	RDC	D	531	-	26,27,27	3.08	7 (26%)	33,39,39	1.91	12 (36%)
3	RDC	F	531	-	26,27,27	3.17	6 (23%)	33,39,39	1.98	11 (33%)
3	RDC	B	531	-	26,27,27	3.13	7 (26%)	33,39,39	1.94	11 (33%)

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	RDC	H	531	-	-	5/23/28/28	0/2/3/3
3	RDC	D	531	-	-	5/23/28/28	0/2/3/3
3	RDC	F	531	-	-	5/23/28/28	0/2/3/3
3	RDC	B	531	-	-	6/23/28/28	0/2/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	531	RDC	C6-CL1	-10.62	1.50	1.72
3	B	531	RDC	C6-CL1	-10.48	1.50	1.72
3	H	531	RDC	C6-CL1	-10.42	1.51	1.72
3	F	531	RDC	C6-CL1	-10.24	1.51	1.72
3	H	531	RDC	C5-C6	7.51	1.49	1.40
3	F	531	RDC	C5-C6	7.34	1.49	1.40
3	B	531	RDC	C5-C6	7.00	1.49	1.40
3	D	531	RDC	C5-C6	6.17	1.47	1.40
3	F	531	RDC	O1-C1	5.78	1.46	1.34
3	H	531	RDC	O1-C1	5.54	1.45	1.34
3	B	531	RDC	O1-C1	5.48	1.45	1.34
3	D	531	RDC	O1-C1	5.36	1.45	1.34
3	H	531	RDC	C2-C3	4.93	1.49	1.41
3	D	531	RDC	C2-C3	4.66	1.48	1.41
3	H	531	RDC	C6-C7	4.64	1.50	1.39
3	F	531	RDC	C2-C3	4.63	1.48	1.41
3	B	531	RDC	C2-C3	4.58	1.48	1.41
3	F	531	RDC	C2-C7	4.52	1.48	1.40
3	H	531	RDC	C2-C7	4.48	1.48	1.40
3	D	531	RDC	C2-C7	4.39	1.48	1.40
3	F	531	RDC	C6-C7	4.34	1.49	1.39
3	B	531	RDC	C2-C7	4.28	1.48	1.40
3	B	531	RDC	C6-C7	4.25	1.49	1.39
3	D	531	RDC	C6-C7	4.20	1.49	1.39
3	H	531	RDC	O1-C17	-2.26	1.43	1.47
3	D	531	RDC	O1-C17	-2.19	1.43	1.47
3	B	531	RDC	O1-C17	-2.17	1.43	1.47

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	531	RDC	C5-C6-C7	-4.99	118.32	122.06
3	H	531	RDC	C5-C6-C7	-4.60	118.61	122.06
3	D	531	RDC	C5-C6-C7	-4.09	119.00	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	531	RDC	C5-C6-C7	-4.04	119.03	122.06
3	H	531	RDC	C15-C14-C13	-3.84	111.39	122.45
3	B	531	RDC	C15-C14-C13	-3.83	111.42	122.45
3	F	531	RDC	C15-C14-C13	-3.66	111.90	122.45
3	B	531	RDC	O6-C15-C16	-3.66	108.69	116.34
3	D	531	RDC	C15-C14-C13	-3.52	112.31	122.45
3	H	531	RDC	C17-O1-C1	-3.40	111.33	117.67
3	F	531	RDC	C4-C5-C6	3.27	121.82	119.14
3	H	531	RDC	C8-C7-C2	-3.27	118.70	122.83
3	B	531	RDC	C17-O1-C1	-3.25	111.61	117.67
3	H	531	RDC	C12-C11-C10	-3.22	117.04	124.65
3	B	531	RDC	C12-C11-C10	-3.20	117.09	124.65
3	F	531	RDC	C8-C7-C6	3.18	123.69	118.67
3	H	531	RDC	C8-C7-C6	3.18	123.68	118.67
3	D	531	RDC	C12-C11-C10	-3.16	117.16	124.65
3	F	531	RDC	O6-C15-C16	-3.12	109.82	116.34
3	F	531	RDC	C8-C7-C2	-3.07	118.95	122.83
3	D	531	RDC	O6-C15-C16	-3.07	109.92	116.34
3	D	531	RDC	C17-O1-C1	-3.05	111.97	117.67
3	F	531	RDC	C12-C11-C10	-3.03	117.48	124.65
3	D	531	RDC	C8-C7-C2	-2.98	119.06	122.83
3	B	531	RDC	C8-C7-C6	2.96	123.34	118.67
3	D	531	RDC	C8-C7-C6	2.95	123.32	118.67
3	H	531	RDC	O1-C1-C2	2.89	120.80	113.53
3	D	531	RDC	O1-C1-O2	-2.84	118.93	123.55
3	H	531	RDC	O6-C15-C16	-2.80	110.49	116.34
3	F	531	RDC	C17-O1-C1	-2.77	112.51	117.67
3	H	531	RDC	O6-C14-C13	-2.73	108.86	115.43
3	B	531	RDC	C8-C7-C2	-2.72	119.39	122.83
3	B	531	RDC	C4-C5-C6	2.69	121.34	119.14
3	F	531	RDC	O6-C14-C13	-2.68	108.97	115.43
3	B	531	RDC	O6-C14-C13	-2.68	108.99	115.43
3	H	531	RDC	C4-C5-C6	2.66	121.32	119.14
3	B	531	RDC	O1-C1-O2	-2.64	119.25	123.55
3	D	531	RDC	O6-C14-C13	-2.63	109.10	115.43
3	B	531	RDC	O1-C1-C2	2.56	119.97	113.53
3	D	531	RDC	C4-C5-C6	2.56	121.24	119.14
3	F	531	RDC	O1-C1-C2	2.51	119.84	113.53
3	H	531	RDC	O1-C1-O2	-2.46	119.55	123.55
3	D	531	RDC	O1-C1-C2	2.45	119.69	113.53
3	F	531	RDC	O1-C1-O2	-2.07	120.18	123.55
3	D	531	RDC	C5-C4-C3	2.05	122.28	120.17

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	531	RDC	C6-C7-C8-C9
3	D	531	RDC	C6-C7-C8-C9
3	F	531	RDC	C6-C7-C8-C9
3	H	531	RDC	C6-C7-C8-C9
3	B	531	RDC	C2-C7-C8-C9
3	D	531	RDC	C2-C7-C8-C9
3	F	531	RDC	C2-C7-C8-C9
3	H	531	RDC	C2-C7-C8-C9
3	F	531	RDC	O2-C1-C2-C3
3	B	531	RDC	O2-C1-C2-C3
3	D	531	RDC	O2-C1-C2-C3
3	H	531	RDC	O2-C1-C2-C7
3	H	531	RDC	O2-C1-C2-C3
3	D	531	RDC	O2-C1-C2-C7
3	B	531	RDC	O2-C1-C2-C7
3	F	531	RDC	O2-C1-C2-C7
3	H	531	RDC	O1-C1-C2-C7
3	B	531	RDC	O1-C1-C2-C3
3	D	531	RDC	O1-C1-C2-C3
3	F	531	RDC	O1-C1-C2-C3
3	B	531	RDC	O1-C1-C2-C7

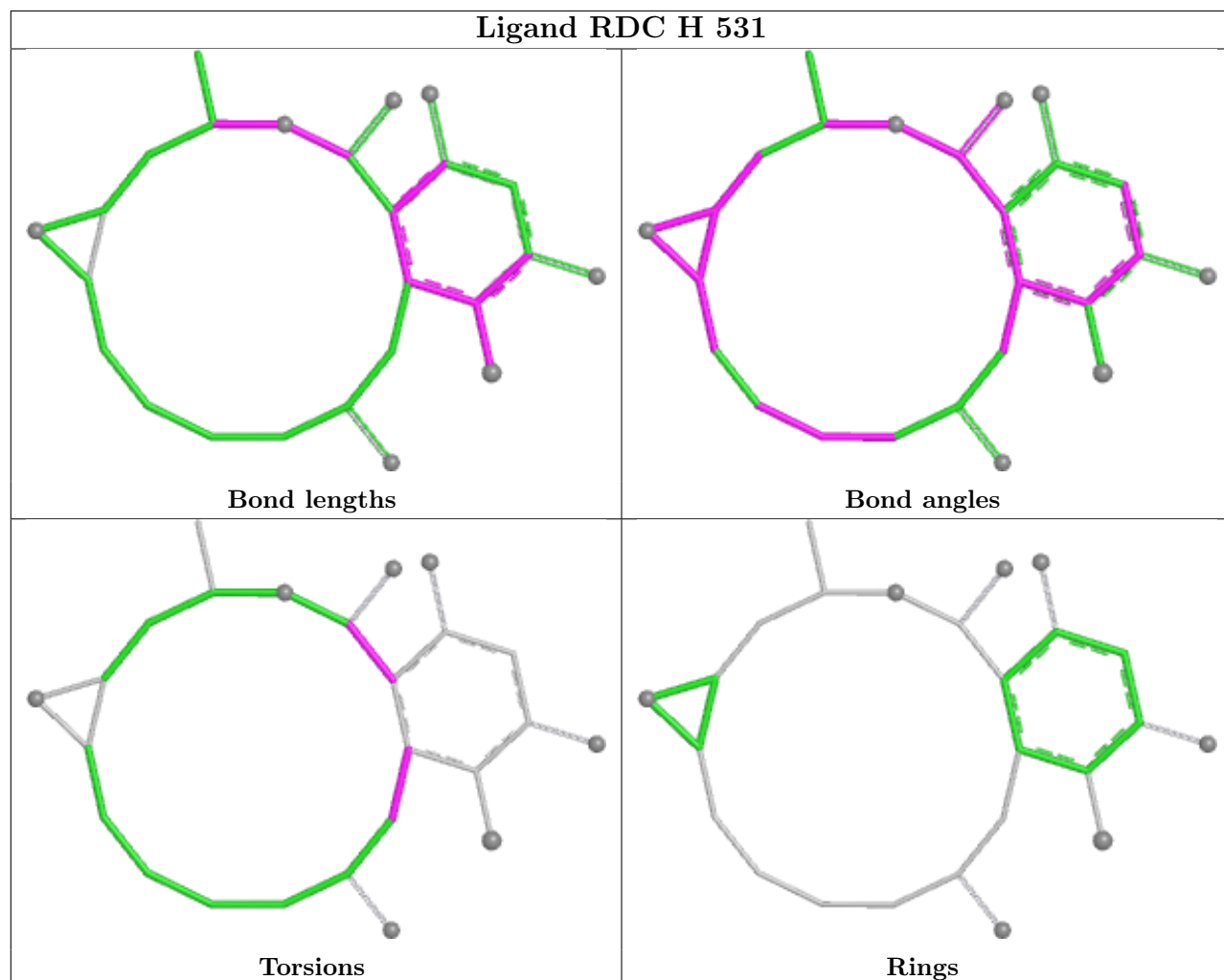
There are no ring outliers.

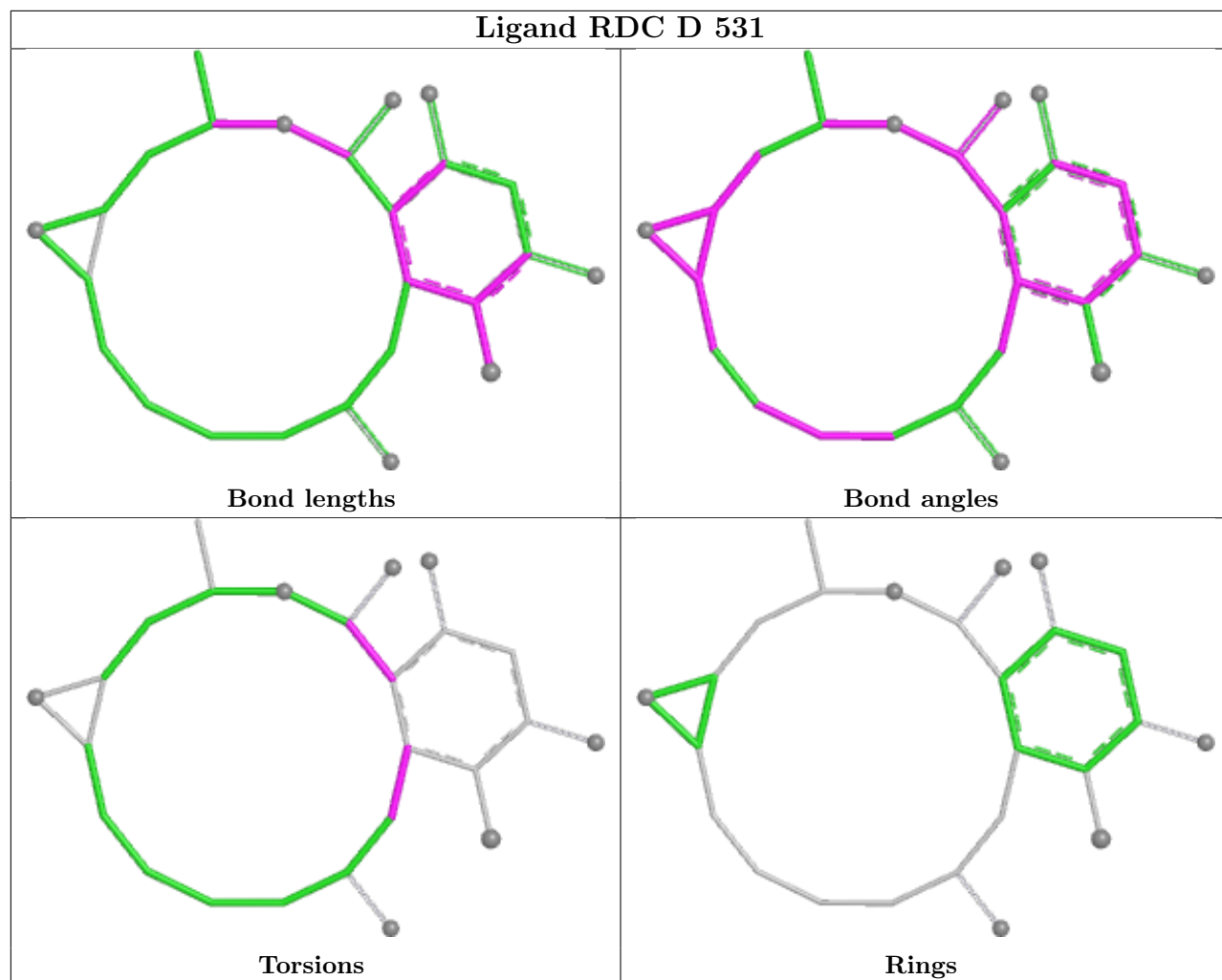
4 monomers are involved in 21 short contacts:

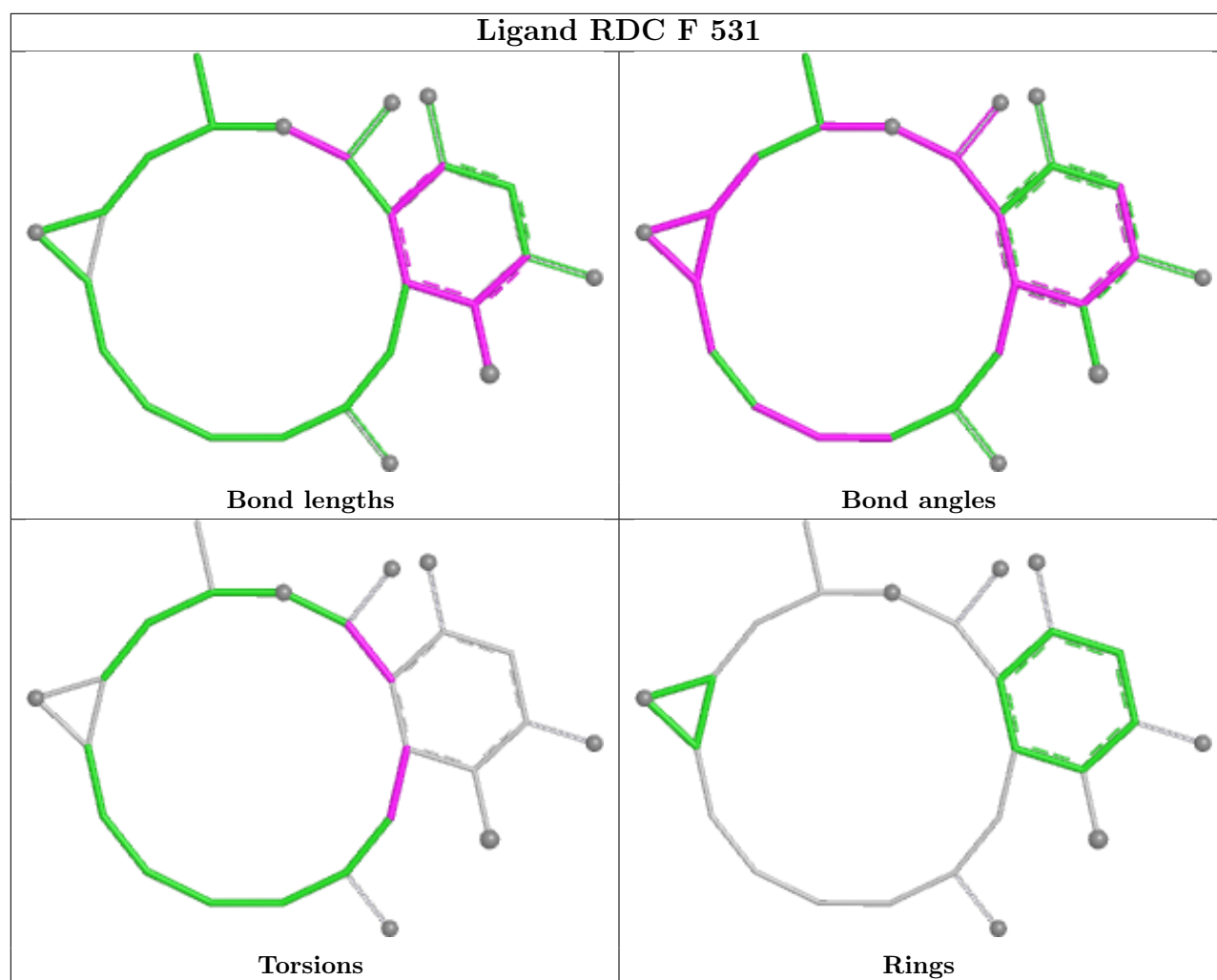
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	531	RDC	4	0
3	D	531	RDC	7	0
3	F	531	RDC	5	0
3	B	531	RDC	5	0

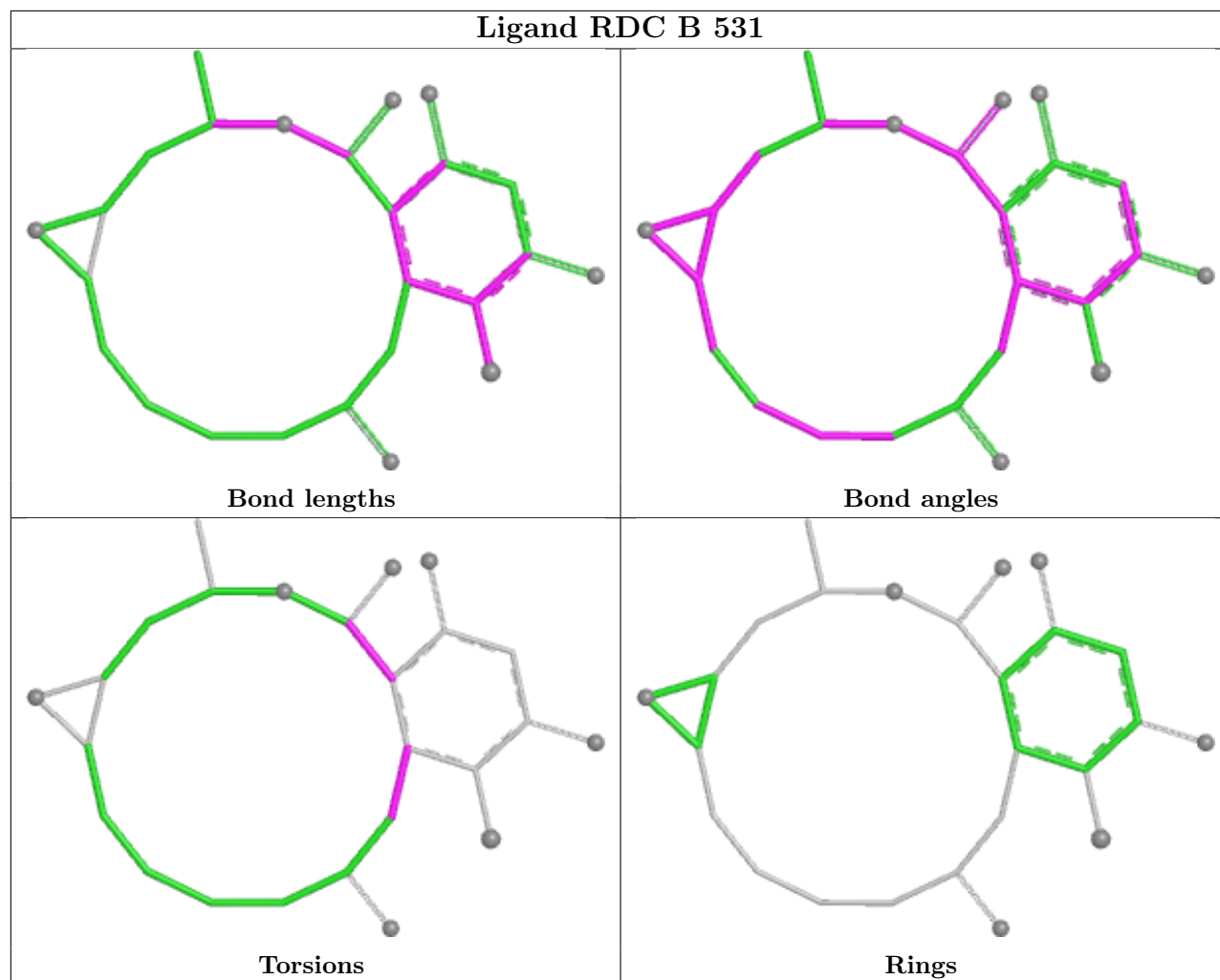
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	347/389 (89%)	0.72	27 (7%)	19	12	20, 72, 83, 85	0
1	C	347/389 (89%)	0.70	26 (7%)	20	13	20, 72, 83, 85	0
1	E	347/389 (89%)	0.68	23 (6%)	24	14	20, 72, 83, 85	0
1	G	347/389 (89%)	0.65	18 (5%)	33	18	20, 72, 83, 85	0
2	B	506/530 (95%)	0.47	19 (3%)	44	24	23, 71, 78, 86	0
2	D	506/530 (95%)	0.48	20 (3%)	42	23	23, 71, 78, 87	0
2	F	506/530 (95%)	0.44	17 (3%)	48	26	23, 71, 78, 90	0
2	H	506/530 (95%)	0.59	31 (6%)	27	15	23, 71, 78, 86	0
All	All	3412/3676 (92%)	0.57	181 (5%)	32	18	20, 71, 80, 90	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	GLU	8.7
1	E	159	GLU	8.3
1	A	159	GLU	7.7
1	G	159	GLU	7.6
2	F	166	GLY	6.3
2	B	165	ARG	5.9
2	B	166	GLY	5.6
2	D	165	ARG	5.3
2	H	347	GLY	4.9
1	G	111	SER	4.8
2	F	108	TYR	4.7
1	C	111	SER	4.7
1	G	36	GLU	4.6
1	E	43	PRO	4.6
1	E	36	GLU	4.2
2	D	108	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	22	ARG	4.2
1	G	110	HIS	4.1
2	F	90	PHE	4.1
2	B	108	TYR	3.9
1	G	343	THR	3.8
1	A	128	THR	3.6
1	G	306	SER	3.6
1	G	115	LYS	3.6
2	B	96	SER	3.5
1	A	110	HIS	3.5
1	C	19	ASN	3.5
2	D	347	GLY	3.5
1	C	343	THR	3.4
2	F	95	TYR	3.4
1	A	36	GLU	3.4
1	A	115	LYS	3.4
2	B	95	TYR	3.3
2	H	166	GLY	3.2
1	A	224	LYS	3.2
1	A	343	THR	3.2
1	C	13	ALA	3.2
2	H	131	THR	3.1
2	F	163	ASN	3.1
1	C	36	GLU	3.1
1	E	316	GLU	3.1
1	G	41	GLU	3.1
1	E	18	ALA	3.0
2	B	140	TYR	3.0
1	C	158	LYS	3.0
1	E	224	LYS	3.0
2	D	63	ILE	3.0
1	E	276	GLY	3.0
2	B	267	ASP	3.0
2	F	483	ALA	2.9
1	C	306	SER	2.9
1	E	111	SER	2.9
2	F	165	ARG	2.9
1	A	157	SER	2.9
2	D	166	GLY	2.9
2	H	108	TYR	2.9
2	H	488	SER	2.8
2	F	427	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	224	LYS	2.8
2	D	64	ASP	2.7
2	H	63	ILE	2.7
1	C	160	LYS	2.7
1	C	345	ALA	2.7
1	C	41	GLU	2.7
2	D	433	VAL	2.7
1	A	10	ASP	2.7
2	F	23	ALA	2.7
1	C	115	LYS	2.6
2	B	132	SER	2.6
1	A	18	ALA	2.6
1	C	316	GLU	2.6
1	A	286	ARG	2.6
2	H	336	ALA	2.6
1	A	129	TRP	2.6
1	C	105	TYR	2.6
1	E	129	TRP	2.6
2	H	277	ALA	2.6
2	F	89	ALA	2.6
2	D	168	HIS	2.5
1	C	224	LYS	2.5
1	G	10	ASP	2.5
2	D	366	GLU	2.5
2	D	392	VAL	2.5
1	G	162	LYS	2.5
1	E	162	LYS	2.5
1	C	74	ASN	2.5
1	G	18	ALA	2.5
1	C	317	ARG	2.5
1	A	29	VAL	2.5
2	F	265	ILE	2.4
1	C	331	ARG	2.4
1	G	363	GLU	2.4
1	A	200	VAL	2.4
1	E	343	THR	2.4
2	H	399	ARG	2.4
2	F	409	MET	2.4
2	B	16	PHE	2.4
2	F	267	ASP	2.4
1	C	286	ARG	2.4
1	A	190	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	505	LEU	2.4
2	H	248	LEU	2.4
2	H	366	GLU	2.4
1	A	344	LYS	2.4
2	B	448	ALA	2.3
1	E	78	ARG	2.3
1	A	106	TYR	2.3
1	C	42	ILE	2.3
2	B	347	GLY	2.3
1	A	158	LYS	2.3
1	A	345	ALA	2.3
2	B	229	VAL	2.3
2	F	212	VAL	2.3
2	H	505	LEU	2.3
2	H	293	ILE	2.3
2	D	126	PRO	2.3
2	H	297	VAL	2.3
1	A	287	LEU	2.3
2	F	451	LEU	2.3
1	E	192	PRO	2.3
1	E	110	HIS	2.2
2	H	348	HIS	2.2
1	G	109	LYS	2.2
1	E	118	GLU	2.2
1	G	286	ARG	2.2
2	B	251	ASP	2.2
1	C	162	LYS	2.2
2	B	130	GLU	2.2
2	H	165	ARG	2.2
2	B	22	LEU	2.2
2	H	300	PHE	2.2
1	C	129	TRP	2.2
2	H	140	TYR	2.2
1	A	30	GLU	2.2
1	A	237	PRO	2.2
1	C	161	GLY	2.2
2	F	63	ILE	2.2
2	D	279	LEU	2.2
2	D	131	THR	2.2
2	F	107	MET	2.2
2	B	139	ILE	2.2
2	B	231	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	160	LYS	2.2
2	D	336	ALA	2.1
2	H	94	LEU	2.2
1	E	160	LYS	2.1
2	D	91	GLY	2.1
2	H	199	PRO	2.1
1	E	185	ALA	2.1
2	H	139	ILE	2.1
2	D	33	TYR	2.1
2	D	107	MET	2.1
1	C	185	ALA	2.1
1	E	19	ASN	2.1
2	D	16	PHE	2.1
2	H	232	HIS	2.1
2	H	76	ASP	2.1
1	E	128	THR	2.1
2	H	315	SER	2.1
2	H	72	VAL	2.1
2	H	282	ASN	2.1
2	H	107	MET	2.1
1	C	106	TYR	2.0
2	D	140	TYR	2.0
1	A	267	TRP	2.0
2	B	164	THR	2.0
1	A	109	LYS	2.0
1	E	155	ILE	2.0
1	A	185	ALA	2.0
1	C	18	ALA	2.0
1	E	113	LEU	2.0
2	B	84	GLN	2.0
2	H	296	LEU	2.0
2	H	75	VAL	2.0
1	A	105	TYR	2.0
1	E	226	TYR	2.0
1	A	363	GLU	2.0
2	H	64	ASP	2.0
1	G	287	LEU	2.0
1	G	185	ALA	2.0
2	H	132	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

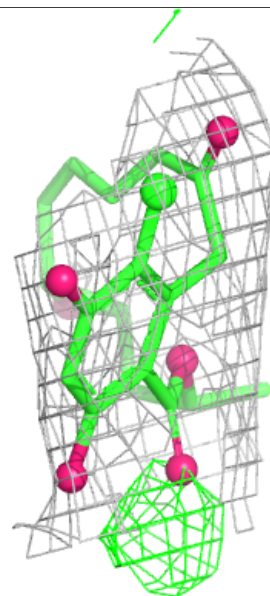
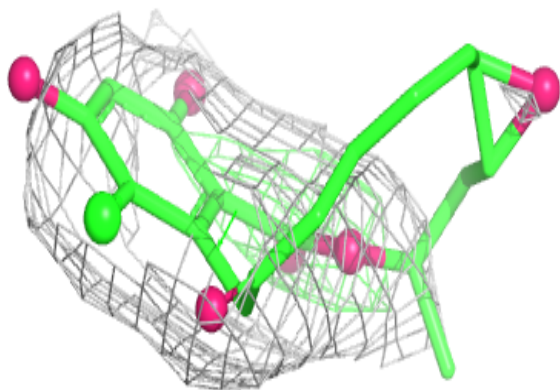
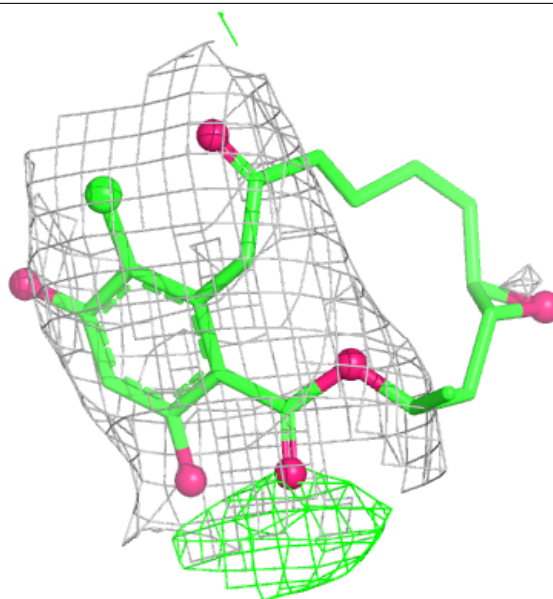
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RDC	D	531	25/25	0.74	0.20	92,93,94,94	0
3	RDC	H	531	25/25	0.78	0.18	92,93,94,94	0
3	RDC	B	531	25/25	0.81	0.18	92,93,94,94	0
3	RDC	F	531	25/25	0.86	0.15	92,93,94,94	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.

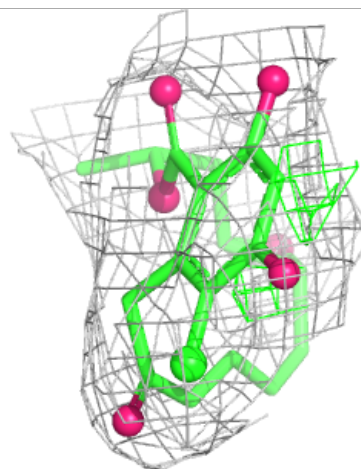
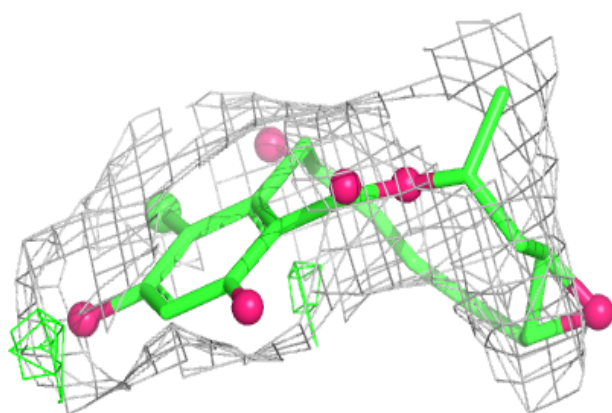
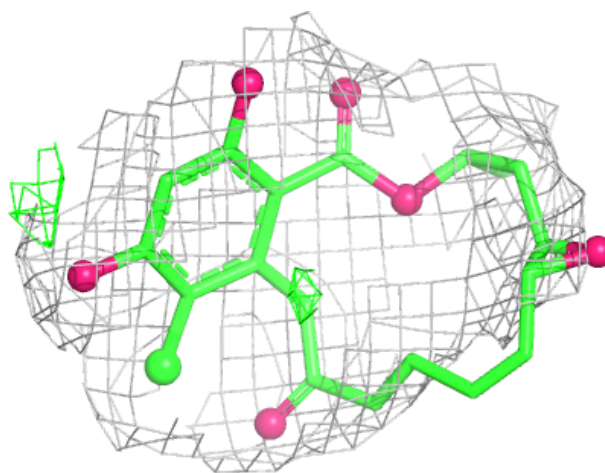
Electron density around RDC D 531:

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



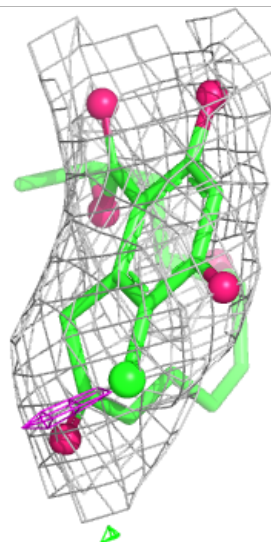
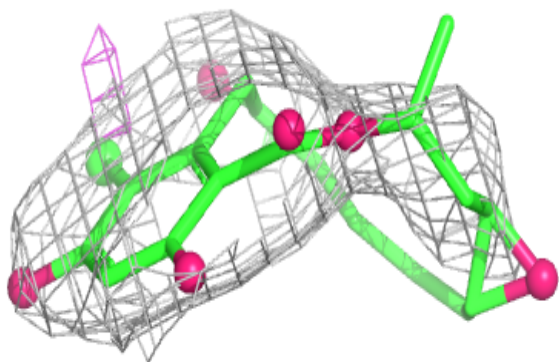
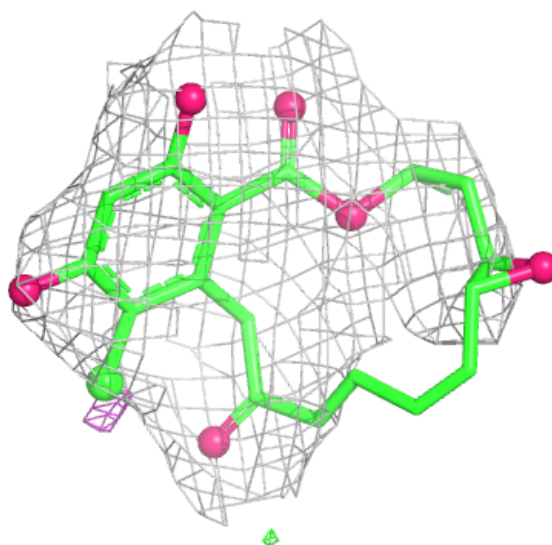
Electron density around RDC H 531:

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



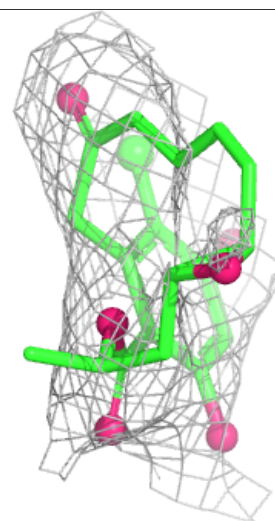
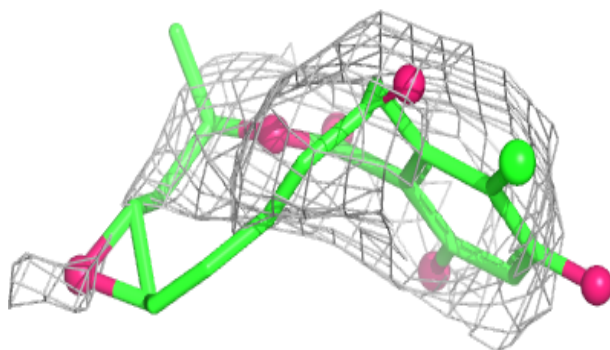
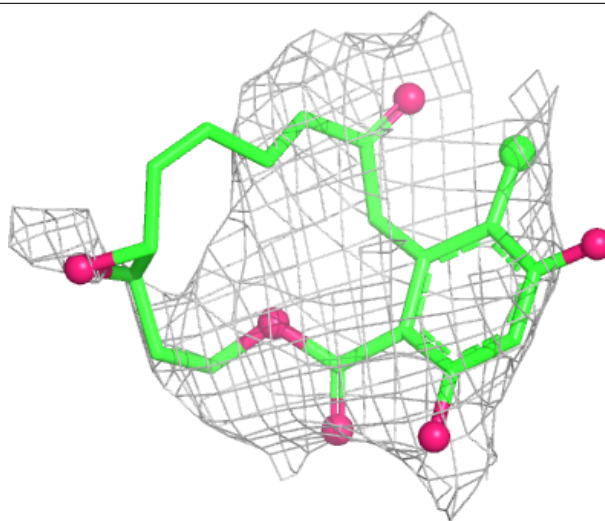
Electron density around RDC B 531:

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



Electron density around RDC F 531:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.