Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2025 – 04:22 PM JST

PDB ID	:	9IQB
Title	:	Crystal structure of beta-glucosidase from Acetivibrio thermocellus
Authors	:	Kamale, C.; Bhaumik, P.
Deposited on	:	2024-07-12
Resolution	:	3.00 Å(reported)

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

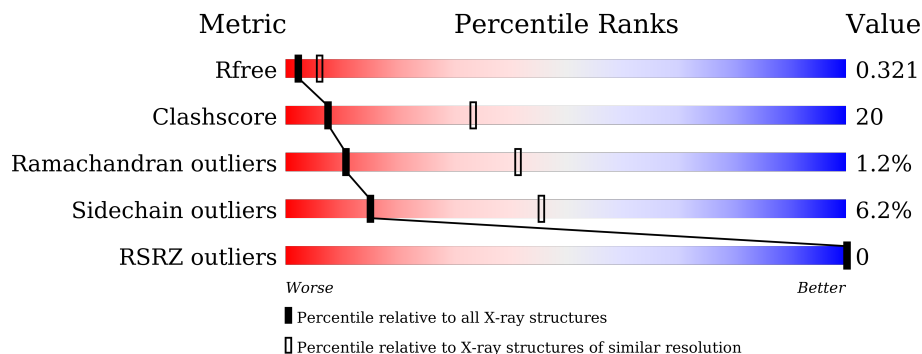|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.321
Clashscore		20
Ramachandran outliers		1.2%
Sidechain outliers		6.2%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	456	69% 26% • •
1	B	456	69% 27% • •
1	C	456	72% 24% • •
1	D	456	73% 23% • •
1	E	456	70% 27% • •
1	F	456	70% 25% • •

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	G	456	64% · 30% · 5% ·
1	H	456	65% · 30% · · ·
1	I	456	62% · 32% · 5% ·
1	J	456	66% · 28% · 5% ·
1	K	456	59% · 34% · 6% ·
1	L	456	53% · 38% · 7% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 44214 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 Beta-glucosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	B	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	C	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	D	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	E	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	F	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	G	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	H	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	I	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	J	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	K	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			
1	L	449	Total	C	N	O	S	0	0	0
			3658	2369	601	682	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	LEU	-	expression tag	UNP P26208
A	450	GLU	-	expression tag	UNP P26208
A	451	HIS	-	expression tag	UNP P26208
A	452	HIS	-	expression tag	UNP P26208
A	453	HIS	-	expression tag	UNP P26208

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Chain	Residue	Modelled	Actual	Comment	Reference
A	454	HIS	-	expression tag	UNP P26208
A	455	HIS	-	expression tag	UNP P26208
A	456	HIS	-	expression tag	UNP P26208
B	449	LEU	-	expression tag	UNP P26208
B	450	GLU	-	expression tag	UNP P26208
B	451	HIS	-	expression tag	UNP P26208
B	452	HIS	-	expression tag	UNP P26208
B	453	HIS	-	expression tag	UNP P26208
B	454	HIS	-	expression tag	UNP P26208
B	455	HIS	-	expression tag	UNP P26208
B	456	HIS	-	expression tag	UNP P26208
C	449	LEU	-	expression tag	UNP P26208
C	450	GLU	-	expression tag	UNP P26208
C	451	HIS	-	expression tag	UNP P26208
C	452	HIS	-	expression tag	UNP P26208
C	453	HIS	-	expression tag	UNP P26208
C	454	HIS	-	expression tag	UNP P26208
C	455	HIS	-	expression tag	UNP P26208
C	456	HIS	-	expression tag	UNP P26208
D	449	LEU	-	expression tag	UNP P26208
D	450	GLU	-	expression tag	UNP P26208
D	451	HIS	-	expression tag	UNP P26208
D	452	HIS	-	expression tag	UNP P26208
D	453	HIS	-	expression tag	UNP P26208
D	454	HIS	-	expression tag	UNP P26208
D	455	HIS	-	expression tag	UNP P26208
D	456	HIS	-	expression tag	UNP P26208
E	449	LEU	-	expression tag	UNP P26208
E	450	GLU	-	expression tag	UNP P26208
E	451	HIS	-	expression tag	UNP P26208
E	452	HIS	-	expression tag	UNP P26208
E	453	HIS	-	expression tag	UNP P26208
E	454	HIS	-	expression tag	UNP P26208
E	455	HIS	-	expression tag	UNP P26208
E	456	HIS	-	expression tag	UNP P26208
F	449	LEU	-	expression tag	UNP P26208
F	450	GLU	-	expression tag	UNP P26208
F	451	HIS	-	expression tag	UNP P26208
F	452	HIS	-	expression tag	UNP P26208
F	453	HIS	-	expression tag	UNP P26208
F	454	HIS	-	expression tag	UNP P26208
F	455	HIS	-	expression tag	UNP P26208

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Chain	Residue	Modelled	Actual	Comment	Reference
F	456	HIS	-	expression tag	UNP P26208
G	449	LEU	-	expression tag	UNP P26208
G	450	GLU	-	expression tag	UNP P26208
G	451	HIS	-	expression tag	UNP P26208
G	452	HIS	-	expression tag	UNP P26208
G	453	HIS	-	expression tag	UNP P26208
G	454	HIS	-	expression tag	UNP P26208
G	455	HIS	-	expression tag	UNP P26208
G	456	HIS	-	expression tag	UNP P26208
H	449	LEU	-	expression tag	UNP P26208
H	450	GLU	-	expression tag	UNP P26208
H	451	HIS	-	expression tag	UNP P26208
H	452	HIS	-	expression tag	UNP P26208
H	453	HIS	-	expression tag	UNP P26208
H	454	HIS	-	expression tag	UNP P26208
H	455	HIS	-	expression tag	UNP P26208
H	456	HIS	-	expression tag	UNP P26208
I	449	LEU	-	expression tag	UNP P26208
I	450	GLU	-	expression tag	UNP P26208
I	451	HIS	-	expression tag	UNP P26208
I	452	HIS	-	expression tag	UNP P26208
I	453	HIS	-	expression tag	UNP P26208
I	454	HIS	-	expression tag	UNP P26208
I	455	HIS	-	expression tag	UNP P26208
I	456	HIS	-	expression tag	UNP P26208
J	449	LEU	-	expression tag	UNP P26208
J	450	GLU	-	expression tag	UNP P26208
J	451	HIS	-	expression tag	UNP P26208
J	452	HIS	-	expression tag	UNP P26208
J	453	HIS	-	expression tag	UNP P26208
J	454	HIS	-	expression tag	UNP P26208
J	455	HIS	-	expression tag	UNP P26208
J	456	HIS	-	expression tag	UNP P26208
K	449	LEU	-	expression tag	UNP P26208
K	450	GLU	-	expression tag	UNP P26208
K	451	HIS	-	expression tag	UNP P26208
K	452	HIS	-	expression tag	UNP P26208
K	453	HIS	-	expression tag	UNP P26208
K	454	HIS	-	expression tag	UNP P26208
K	455	HIS	-	expression tag	UNP P26208
K	456	HIS	-	expression tag	UNP P26208
L	449	LEU	-	expression tag	UNP P26208

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Chain	Residue	Modelled	Actual	Comment	Reference
L	450	GLU	-	expression tag	UNP P26208
L	451	HIS	-	expression tag	UNP P26208
L	452	HIS	-	expression tag	UNP P26208
L	453	HIS	-	expression tag	UNP P26208
L	454	HIS	-	expression tag	UNP P26208
L	455	HIS	-	expression tag	UNP P26208
L	456	HIS	-	expression tag	UNP P26208

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).
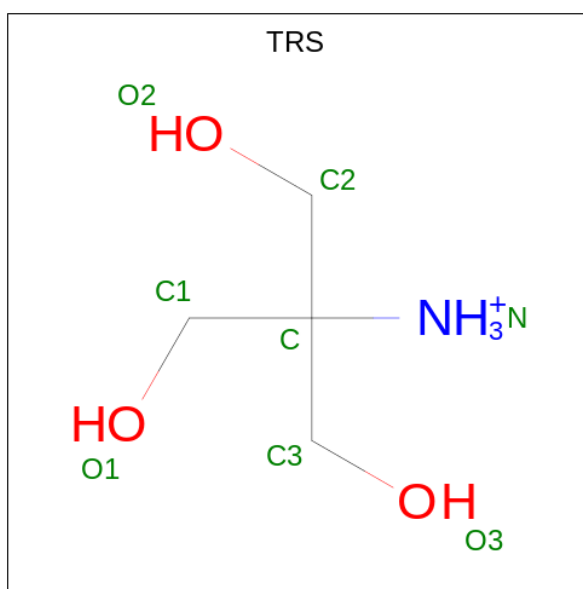
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	38	Total	O	0	0
			38	38		
3	C	27	Total	O	0	0
			27	27		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	29	Total 29	O 29	0	0
3	E	26	Total 26	O 26	0	0
3	F	24	Total 24	O 24	0	0
3	G	23	Total 23	O 23	0	0
3	H	17	Total 17	O 17	0	0
3	I	25	Total 25	O 25	0	0
3	J	25	Total 25	O 25	0	0
3	K	27	Total 27	O 27	0	0
3	L	17	Total 17	O 17	0	0

# 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.
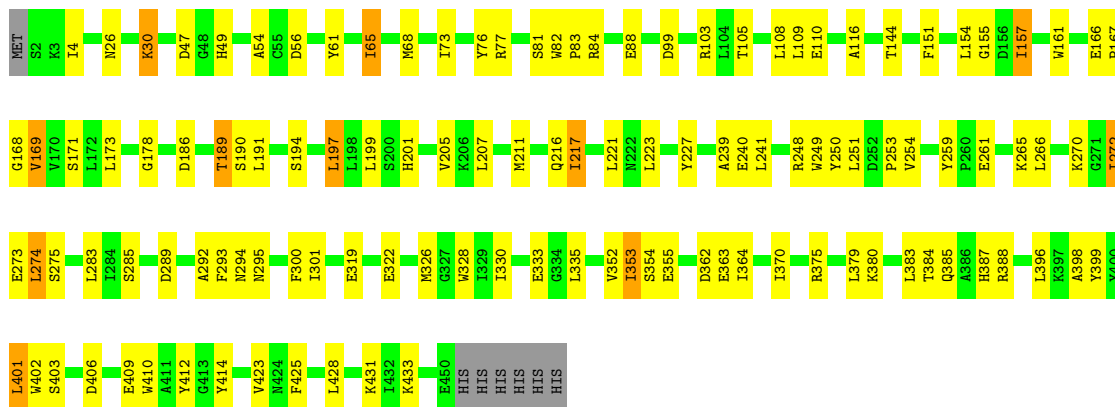
• Molecule 1: Beta-glucosidase A
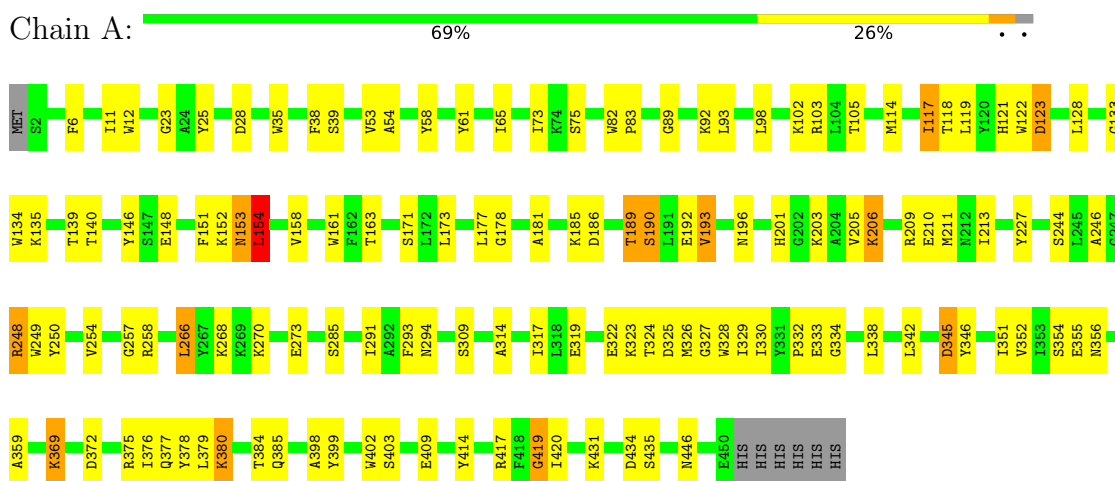
Chain A:

• Molecule 1: Beta-glucosidase A
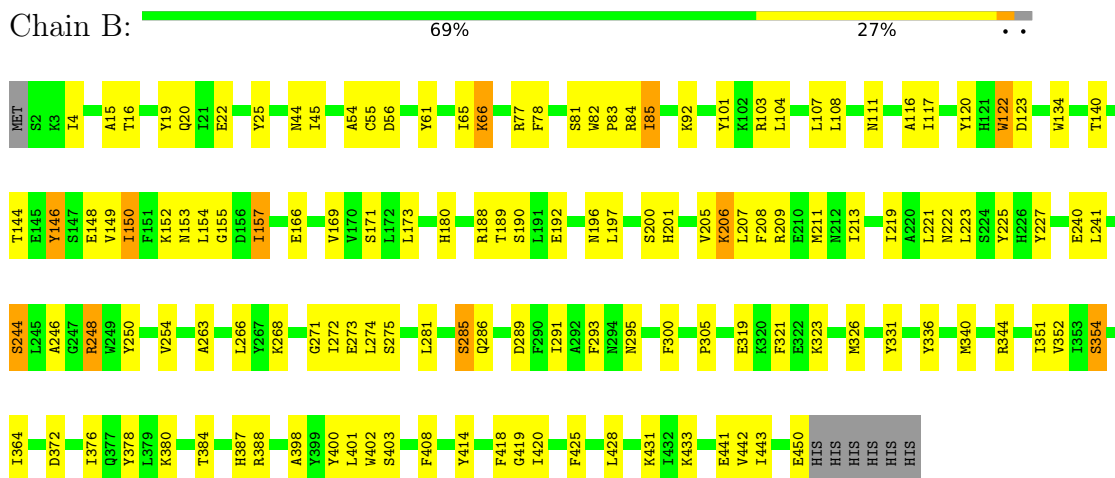
Chain B:

• Molecule 1: Beta-glucosidase A

Chain C:

● Molecule 1: Beta-glucosidase A

Chain D:

● Molecule 1: Beta-glucosidase A

Chain E:

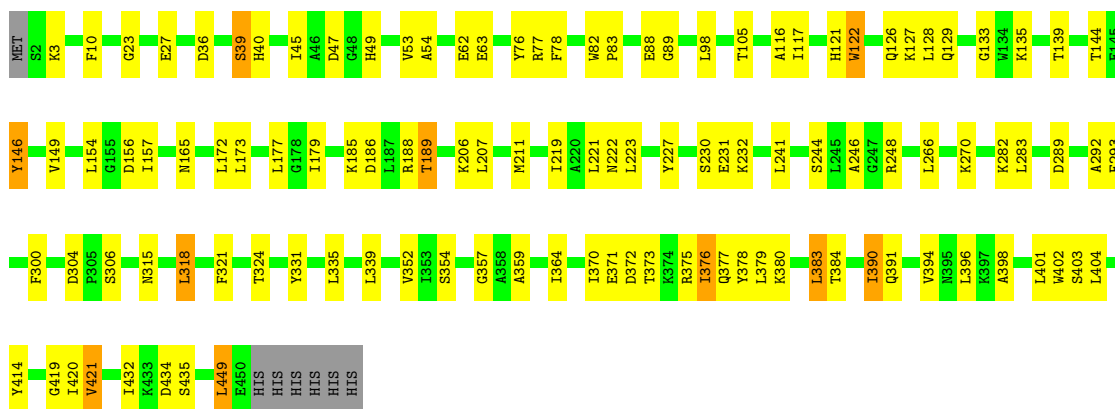● Molecule 1: Beta-glucosidase A

Chain F:

• Molecule 1: Beta-glucosidase A

Chain G:

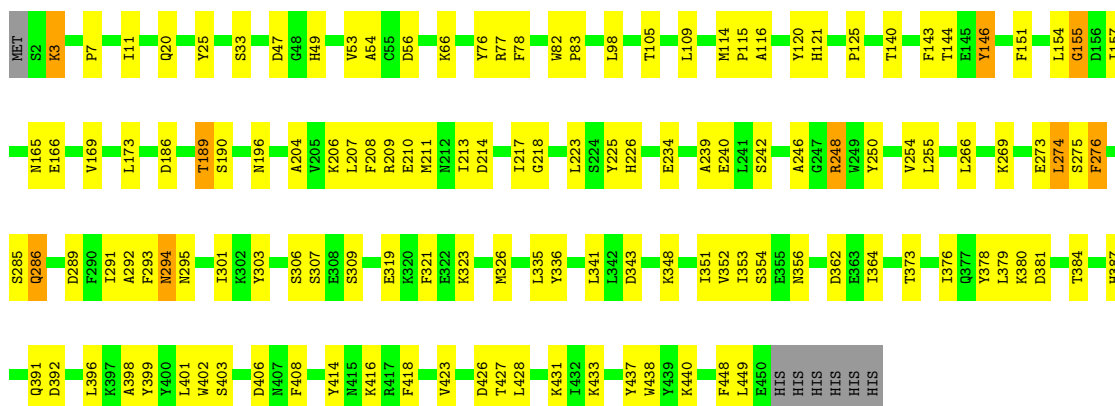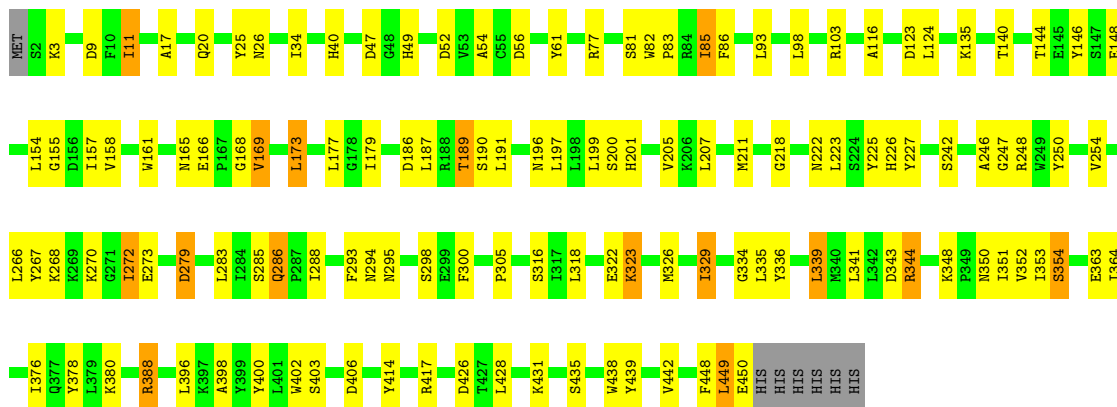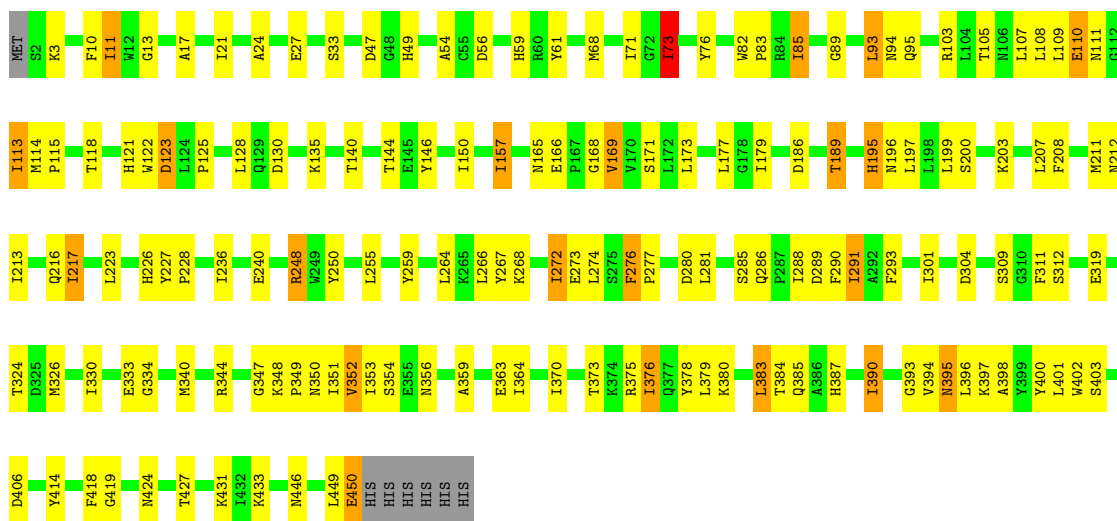• Molecule 1: Beta-glucosidase A

Chain H:

• Molecule 1: Beta-glucosidase A

Chain I:

62%   32%   5%

• Molecule 1: Beta-glucosidase A

Chain J:

66%   28%   5%

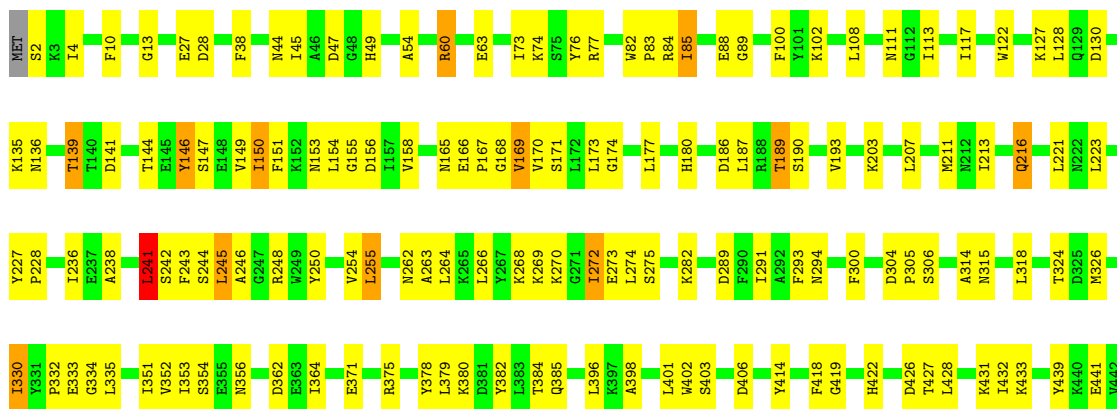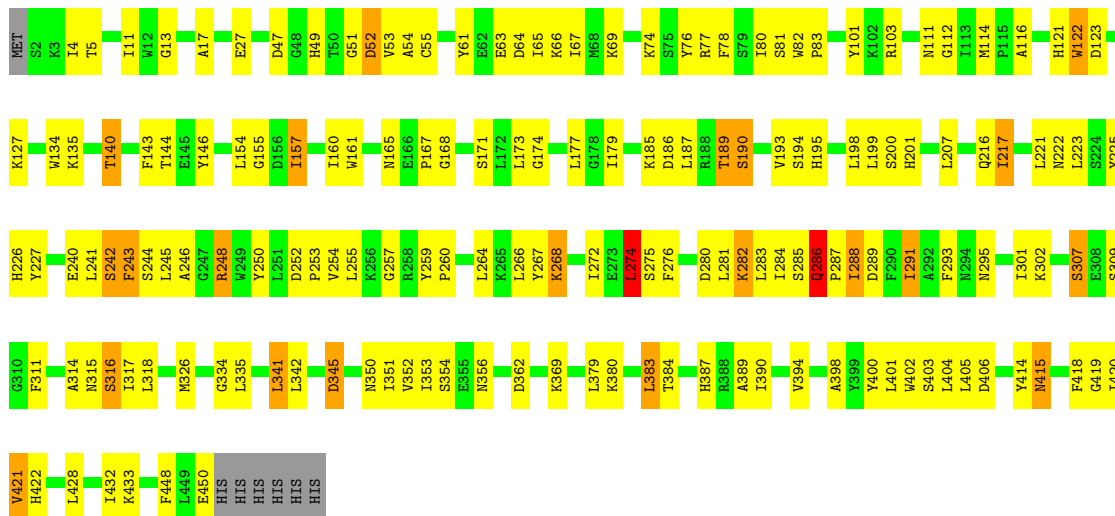• Molecule 1: Beta-glucosidase A

Chain K:

59%   34%   6%

• Molecule 1: Beta-glucosidase A

Chain L:
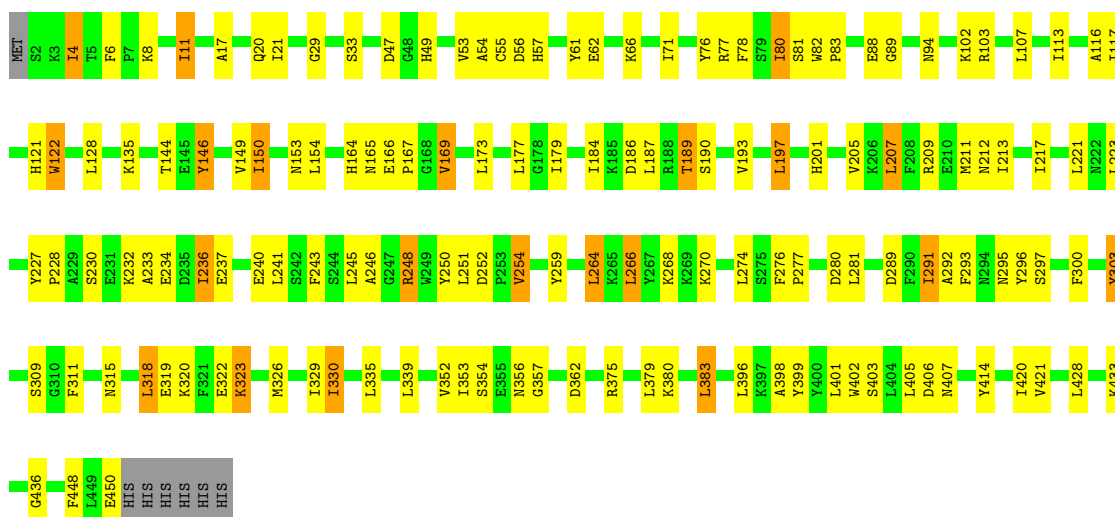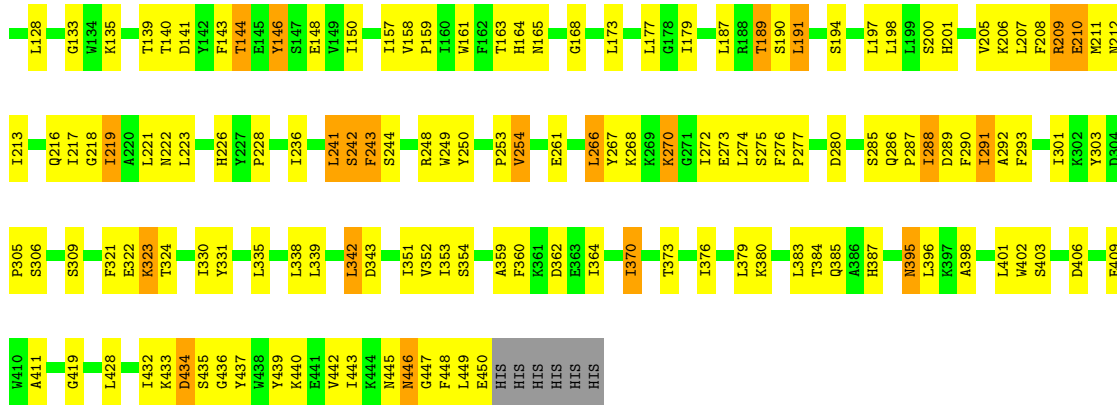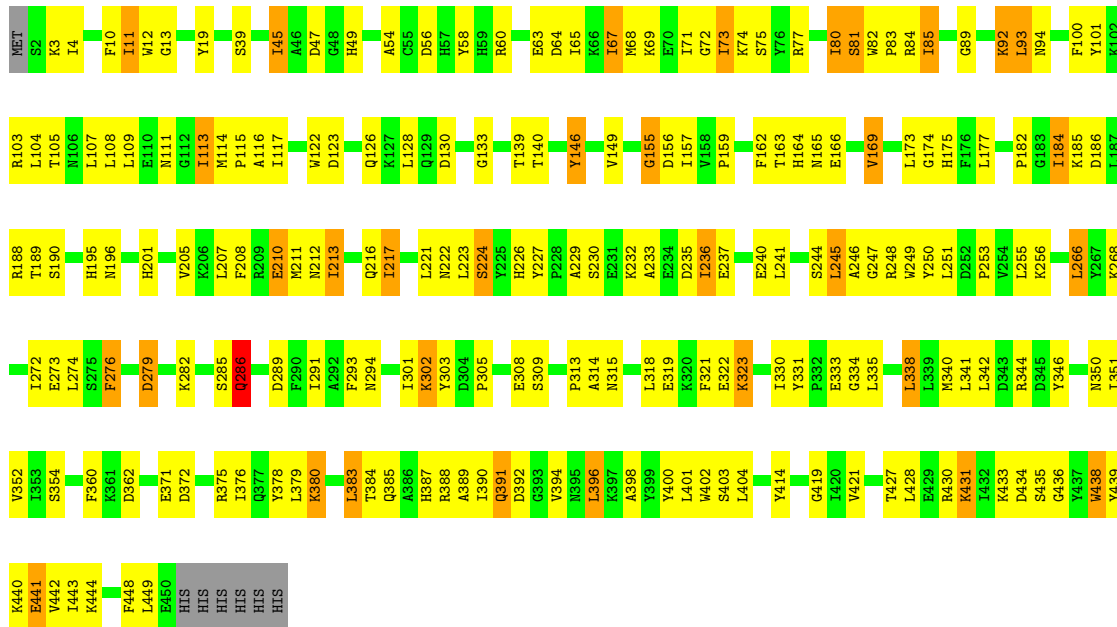
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	109.93Å　158.62Å　158.91Å 60.12°　88.19°　87.48°	Depositor
Resolution (Å)	34.99　–　3.00 34.99　–　3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (34.99-3.00) 82.1 (34.99-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.300　,　0.350 0.311　,　0.321	Depositor DCC
R_{free} test set	8755 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 12.9	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.075 for h,l,-k+l 0.075 for h,k-l,k 0.045 for h,-k+l,-k 0.045 for h,-l,k-l 0.094 for h,-k,-l 0.028 for -h,k,k-l 0.009 for -h,-k+l,l 0.009 for -h,l,k 0.012 for -h,-l,-k 0.030 for -h,-k,-k+l 0.011 for -h,k-l,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	44214	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9141e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.65	0/3760	0.79	0/5088
1	B	0.65	0/3760	0.78	0/5088
1	C	0.65	0/3760	0.77	0/5088
1	D	0.65	0/3760	0.79	0/5088
1	E	0.65	0/3760	0.81	0/5088
1	F	0.65	0/3760	0.80	0/5088
1	G	0.65	0/3760	0.78	0/5088
1	H	0.65	0/3760	0.79	0/5088
1	I	0.65	0/3760	0.78	0/5088
1	J	0.65	0/3760	0.78	0/5088
1	K	0.65	0/3760	0.78	0/5088
1	L	0.66	0/3760	0.80	0/5088
All	All	0.65	0/45120	0.79	0/61056

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	A	0	1
1	D	0	1
1	H	0	2
1	I	0	3
1	L	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	ASP	Peptide
1	D	419	GLY	Peptide
1	H	241	LEU	Peptide
1	H	449	LEU	Peptide
1	I	112	GLY	Peptide
1	I	316	SER	Peptide
1	I	419	GLY	Peptide
1	L	230	SER	Peptide

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	3658	0	3558	117	0
1	B	3658	0	3558	111	0
1	C	3658	0	3558	111	0
1	D	3658	0	3558	95	0
1	E	3658	0	3558	103	0
1	F	3658	0	3558	123	0
1	G	3658	0	3558	168	0
1	H	3658	0	3558	155	0
1	I	3658	0	3558	158	0
1	J	3658	0	3558	141	0
1	K	3658	0	3558	220	0
1	L	3658	0	3558	238	0
2	A	8	0	12	1	0
2	B	8	0	12	1	0
3	A	24	0	0	8	0
3	B	38	0	0	28	0
3	C	27	0	0	6	0
3	D	29	0	0	5	0
3	E	26	0	0	8	0
3	F	24	0	0	8	0
3	G	23	0	0	9	0
3	H	17	0	0	5	0
3	I	25	0	0	9	0
3	J	25	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	27	0	0	10	0
3	L	17	0	0	6	0
All	All	44214	0	42720	1724	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 20.

All (1724) 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:82:TRP:CH2	1:E:146:TYR:HB3	1.37	1.29
1:J:315:ASN:HA	1:J:318:LEU:CD1	1.69	1.23
1:A:403:SER:O	1:A:419:GLY:O	1.58	1.20
1:K:339:LEU:CA	1:K:342:LEU:HD21	1.73	1.19
1:I:199:LEU:HA	1:I:284:ILE:HD11	1.25	1.16
1:K:442:VAL:O	1:K:446:ASN:O	1.63	1.15
1:G:375:ARG:O	1:G:379:LEU:HD23	1.46	1.15
1:E:82:TRP:CZ2	1:E:146:TYR:HB3	1.82	1.15
1:E:82:TRP:CH2	1:E:146:TYR:CB	2.28	1.14
1:J:315:ASN:HA	1:J:318:LEU:HD11	1.16	1.14
1:K:338:LEU:O	1:K:342:LEU:HD22	1.46	1.14
1:K:85:ILE:O	1:K:93:LEU:O	1.65	1.12
1:K:339:LEU:HA	1:K:342:LEU:HD21	1.21	1.12
1:F:226:HIS:HB3	3:F:509:HOH:O	1.48	1.12
1:L:80:ILE:HD11	1:L:146:TYR:CE1	1.86	1.10
1:K:288:ILE:CD1	1:K:290:PHE:O	2.00	1.09
1:D:135:LYS:CE	1:D:189:THR:HG23	1.82	1.09
1:G:208:PHE:CD1	1:G:217:ILE:HD11	1.89	1.08
1:C:353:ILE:CD1	1:C:396:LEU:HD11	1.84	1.07
1:L:390:ILE:HD11	1:L:396:LEU:HB3	1.31	1.07
1:L:438:TRP:HZ3	1:L:442:VAL:HB	1.15	1.06
1:H:147:SER:HA	1:H:150:ILE:HD11	1.36	1.05
1:H:242:SER:O	1:H:244:SER:N	1.90	1.05
1:J:250:TYR:O	1:J:254:VAL:HG23	1.58	1.04
1:G:195:HIS:CG	1:G:276:PHE:CZ	2.44	1.04
1:D:135:LYS:HE2	1:D:189:THR:HG23	1.36	1.04
1:F:343:ASP:OD1	1:F:348:LYS:HD2	1.58	1.04
1:L:438:TRP:CE3	1:L:439:TYR:HA	1.93	1.03
1:L:438:TRP:CZ3	1:L:442:VAL:HB	1.96	1.01
1:L:438:TRP:CZ3	1:L:439:TYR:HA	1.94	1.01
1:K:209:ARG:O	1:K:212:ASN:N	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ASN:HA	1:D:318:LEU:CD1	1.92	1.00
1:K:250:TYR:O	1:K:254:VAL:HG23	1.57	1.00
1:I:404:LEU:O	1:I:420:ILE:O	1.78	0.99
1:L:438:TRP:CZ3	1:L:442:VAL:CG2	2.46	0.99
1:L:162:PHE:HB3	3:L:501:HOH:O	1.60	0.98
1:H:254:VAL:HG23	1:H:255:LEU:HD12	1.44	0.97
1:K:148:GLU:HG3	1:K:207:LEU:HD11	1.43	0.97
1:E:423:VAL:HB	3:E:502:HOH:O	1.62	0.97
1:K:370:ILE:HG13	1:K:433:LYS:HA	1.46	0.97
1:L:80:ILE:HD11	1:L:146:TYR:HE1	1.23	0.96
1:I:63:GLU:O	1:I:67:ILE:HD12	1.62	0.96
1:C:353:ILE:HD13	1:C:396:LEU:HD11	1.46	0.95
1:F:439:TYR:O	1:F:442:VAL:HG22	1.67	0.95
1:K:70:GLU:O	1:K:440:LYS:NZ	2.00	0.95
1:L:438:TRP:HE3	1:L:438:TRP:C	1.70	0.95
1:H:60:ARG:NH1	1:H:63:GLU:OE1	1.99	0.95
1:L:208:PHE:CE1	1:L:213:ILE:HG21	2.02	0.95
1:L:163:THR:HG21	1:L:201:HIS:ND1	1.81	0.94
1:L:390:ILE:CD1	1:L:396:LEU:HB3	1.97	0.94
1:A:61:TYR:O	1:A:65:ILE:HD13	1.68	0.94
1:K:339:LEU:C	1:K:342:LEU:HD21	1.86	0.94
1:K:242:SER:O	1:K:244:SER:N	2.00	0.94
1:L:438:TRP:CZ3	1:L:442:VAL:CB	2.52	0.93
1:I:260:PRO:HG3	3:I:501:HOH:O	1.67	0.93
1:C:30:LYS:NZ	1:C:81:SER:OG	2.01	0.93
1:J:315:ASN:CA	1:J:318:LEU:HD11	1.98	0.92
1:L:438:TRP:CE3	1:L:439:TYR:CA	2.53	0.92
1:J:420:ILE:C	3:J:501:HOH:O	2.07	0.92
1:C:169:VAL:HG12	1:C:173:LEU:HD13	1.52	0.91
1:K:370:ILE:CG1	1:K:433:LYS:HA	1.99	0.91
1:L:438:TRP:CZ3	1:L:442:VAL:HG21	2.03	0.91
1:K:148:GLU:CG	1:K:207:LEU:HD11	2.01	0.91
1:K:250:TYR:O	1:K:254:VAL:CG2	2.19	0.90
1:A:117:ILE:C	1:A:117:ILE:HD12	1.92	0.90
1:J:315:ASN:CA	1:J:318:LEU:CD1	2.50	0.90
1:K:135:LYS:HD2	1:K:189:THR:HG23	1.53	0.89
1:D:315:ASN:HA	1:D:318:LEU:HD12	1.55	0.89
1:F:298:SER:O	1:F:329:ILE:HD11	1.72	0.89
1:L:438:TRP:CE3	1:L:438:TRP:C	2.46	0.89
1:H:147:SER:HA	1:H:150:ILE:CD1	2.03	0.89
1:I:264:LEU:O	1:I:267:TYR:O	1.91	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:HIS:HD1	1:I:414:TYR:HD2	1.14	0.89
1:I:77:ARG:HH22	1:I:165:ASN:HD22	1.21	0.88
1:H:241:LEU:HD12	1:H:245:LEU:CD2	2.03	0.88
1:K:219:ILE:HD12	1:K:221:LEU:HD13	1.52	0.88
1:F:376:ILE:CD1	1:F:435:SER:HA	2.03	0.88
1:J:421:VAL:N	3:J:501:HOH:O	2.05	0.88
1:A:257:GLY:HA2	1:A:285:SER:OG	1.73	0.88
1:L:438:TRP:CE3	1:L:439:TYR:N	2.41	0.88
1:L:175:HIS:HA	1:L:184:ILE:HG23	1.56	0.87
1:K:288:ILE:HD12	1:K:290:PHE:O	1.72	0.87
1:A:117:ILE:HG23	1:A:158:VAL:HG11	1.54	0.87
1:L:109:LEU:HD11	1:L:157:ILE:CG2	2.04	0.87
1:L:175:HIS:HA	1:L:184:ILE:CG2	2.05	0.87
1:C:370:ILE:HD13	1:C:433:LYS:HA	1.54	0.86
1:H:241:LEU:HD12	1:H:245:LEU:HD21	1.57	0.86
1:C:406:ASP:HB2	1:C:423:VAL:HG12	1.56	0.86
1:F:148:GLU:HG3	1:F:211:MET:HE1	1.56	0.86
1:J:234:GLU:HB3	1:J:303:TYR:CZ	2.09	0.86
1:F:148:GLU:HG3	1:F:211:MET:CE	2.05	0.86
1:I:199:LEU:HA	1:I:284:ILE:CD1	2.05	0.86
1:A:210:GLU:O	1:B:305:PRO:HG2	1.76	0.85
1:G:264:LEU:O	1:G:268:LYS:HD3	1.76	0.85
1:I:195:HIS:CG	1:I:276:PHE:HE1	1.93	0.85
1:C:353:ILE:HD11	1:C:396:LEU:HD11	1.56	0.85
1:G:255:LEU:HD21	1:G:291:ILE:HD13	1.59	0.84
1:K:268:LYS:HD3	1:K:273:GLU:HG3	1.58	0.84
1:G:390:ILE:HA	1:G:394:VAL:HG12	1.59	0.84
1:G:424:ASN:HD22	1:G:427:THR:HG23	1.39	0.84
1:A:117:ILE:HG12	1:A:161:TRP:CZ3	2.12	0.84
1:I:404:LEU:HG	1:I:405:LEU:CD1	2.06	0.84
1:J:234:GLU:HB3	1:J:303:TYR:CE2	2.13	0.84
1:I:195:HIS:CG	1:I:276:PHE:CE1	2.66	0.83
1:K:219:ILE:HD12	1:K:221:LEU:CD1	2.08	0.83
1:K:339:LEU:C	1:K:342:LEU:CD2	2.46	0.83
1:A:39:SER:OG	3:A:601:HOH:O	1.94	0.83
1:E:82:TRP:CH2	1:E:143:PHE:HA	2.14	0.83
1:I:199:LEU:CA	1:I:284:ILE:HD11	2.07	0.83
1:H:136:ASN:O	1:H:139:THR:OG1	1.96	0.83
1:E:114:MET:SD	3:E:522:HOH:O	2.36	0.82
1:K:339:LEU:HA	1:K:342:LEU:CD2	2.08	0.82
1:D:135:LYS:HE2	1:D:189:THR:CG2	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:315:ASN:HA	1:J:318:LEU:HD12	1.62	0.81
1:I:257:GLY:HA2	1:I:285:SER:OG	1.80	0.81
1:I:154:LEU:HA	1:I:157:ILE:HD11	1.62	0.81
1:K:208:PHE:CD1	1:K:217:ILE:HD11	2.16	0.81
1:E:218:GLY:O	3:E:501:HOH:O	1.97	0.81
1:K:342:LEU:HD22	1:K:342:LEU:H	1.46	0.81
1:B:154:LEU:HA	1:B:157:ILE:HD11	1.63	0.81
1:L:165:ASN:HD21	1:L:294:ASN:HD21	1.28	0.81
1:C:272:ILE:O	1:C:273:GLU:HG2	1.81	0.80
1:E:255:LEU:HD11	1:E:291:ILE:HD13	1.63	0.80
1:A:189:THR:O	1:A:193:VAL:HG12	1.81	0.80
1:L:68:MET:HE2	1:L:73:ILE:HG21	1.63	0.80
1:L:188:ARG:HG2	1:L:272:ILE:HD12	1.64	0.80
1:L:380:LYS:HG2	1:L:448:PHE:CE2	2.17	0.80
1:K:433:LYS:O	1:K:435:SER:N	2.13	0.80
1:H:264:LEU:O	1:H:268:LYS:HD3	1.82	0.79
1:L:376:ILE:HG23	1:L:438:TRP:CD1	2.18	0.79
1:I:248:ARG:HB3	3:I:501:HOH:O	1.82	0.79
1:K:339:LEU:CA	1:K:342:LEU:CD2	2.59	0.79
1:A:93:LEU:HD11	1:A:98:LEU:HD11	1.63	0.79
1:H:441:GLU:OE1	1:H:444:LYS:HE3	1.83	0.79
1:H:268:LYS:HG3	1:H:273:GLU:HG2	1.64	0.79
1:J:89:GLY:HA3	1:J:128:LEU:HD21	1.64	0.79
1:D:372:ASP:OD2	1:D:435:SER:OG	1.98	0.78
1:K:117:ILE:HD11	3:K:501:HOH:O	1.82	0.78
1:A:148:GLU:OE2	1:A:152:LYS:NZ	2.13	0.78
1:K:353:ILE:CD1	1:K:396:LEU:HD11	2.14	0.78
1:D:379:LEU:O	1:D:383:LEU:HD12	1.83	0.78
1:L:3:LYS:HA	1:L:449:LEU:HD23	1.65	0.78
1:G:208:PHE:CE1	1:G:217:ILE:HD11	2.19	0.78
1:I:160:ILE:HD11	1:I:400:TYR:OH	1.83	0.78
1:A:117:ILE:HG12	1:A:161:TRP:CE3	2.19	0.78
1:K:75:SER:OG	1:K:114:MET:O	2.00	0.77
1:B:192:GLU:OE2	3:B:602:HOH:O	2.02	0.77
1:I:244:SER:HA	3:I:501:HOH:O	1.85	0.77
1:F:158:VAL:CG1	1:F:161:TRP:CZ2	2.67	0.77
1:I:254:VAL:HG13	1:I:255:LEU:HG	1.67	0.77
1:K:288:ILE:HD11	1:K:290:PHE:O	1.84	0.77
1:G:109:LEU:HD21	1:G:157:ILE:HG13	1.67	0.77
1:I:160:ILE:CD1	1:I:400:TYR:OH	2.33	0.77
1:I:116:ALA:HB2	1:I:160:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:352:VAL:HG13	1:J:398:ALA:HB3	1.67	0.76
1:J:211:MET:O	1:J:212:ASN:OD1	2.03	0.76
1:G:268:LYS:HG3	1:G:273:GLU:HG2	1.68	0.76
1:L:56:ASP:OD2	1:L:60:ARG:NH1	2.18	0.76
1:C:154:LEU:HA	1:C:157:ILE:HD11	1.67	0.76
1:J:433:LYS:HG3	3:J:501:HOH:O	1.85	0.76
1:L:315:ASN:HA	1:L:318:LEU:HD12	1.67	0.76
1:G:195:HIS:CE1	1:G:276:PHE:CE2	2.73	0.76
1:L:241:LEU:HD21	1:L:266:LEU:CD1	2.15	0.76
1:K:135:LYS:CD	1:K:189:THR:HG23	2.15	0.76
1:L:64:ASP:O	1:L:67:ILE:HG23	1.86	0.76
1:D:186:ASP:OD2	1:D:189:THR:OG1	2.04	0.75
1:H:241:LEU:O	1:H:242:SER:OG	2.04	0.75
1:I:195:HIS:HB2	1:I:276:PHE:CZ	2.21	0.75
1:I:242:SER:O	1:I:244:SER:N	2.19	0.75
1:A:257:GLY:CA	1:A:285:SER:OG	2.34	0.75
1:L:163:THR:HG1	1:L:164:HIS:CE1	2.03	0.75
1:B:200:SER:HB3	3:B:604:HOH:O	1.86	0.75
1:G:85:ILE:O	1:G:93:LEU:O	2.04	0.75
1:B:321:PHE:CE2	1:B:331:TYR:HD2	2.04	0.75
1:E:239:ALA:HA	1:E:301:ILE:HG12	1.67	0.75
1:I:134:TRP:CB	1:I:193:VAL:HG23	2.17	0.75
1:B:4:ILE:HG23	1:B:387:HIS:CD2	2.22	0.75
1:J:166:GLU:HB3	1:J:169:VAL:HG23	1.68	0.75
1:B:281:LEU:O	1:B:285:SER:OG	2.04	0.74
1:L:211:MET:O	1:L:212:ASN:OD1	2.04	0.74
1:A:380:LYS:O	1:A:384:THR:HG23	1.87	0.74
1:H:315:ASN:HA	1:H:318:LEU:CD1	2.16	0.74
1:K:241:LEU:O	1:K:242:SER:O	2.05	0.74
1:A:93:LEU:HD11	1:A:98:LEU:CD1	2.17	0.74
1:E:82:TRP:CZ2	1:E:146:TYR:CB	2.66	0.74
1:D:146:TYR:HA	3:D:517:HOH:O	1.88	0.73
1:G:135:LYS:HD3	1:G:189:THR:HG23	1.69	0.73
1:I:174:GLY:HA3	3:I:505:HOH:O	1.87	0.73
1:J:146:TYR:O	1:J:150:ILE:HD13	1.87	0.73
1:K:163:THR:OG1	1:K:219:ILE:HG22	1.88	0.73
1:K:353:ILE:HD12	1:K:396:LEU:HD11	1.71	0.73
1:H:13:GLY:C	1:H:73:ILE:HD11	2.09	0.73
1:B:291:ILE:HD12	1:B:291:ILE:O	1.88	0.73
1:J:241:LEU:HD22	1:J:311:PHE:CE1	2.24	0.73
1:E:274:LEU:N	1:E:274:LEU:HD23	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:241:LEU:HD21	1:L:266:LEU:HD13	1.69	0.72
1:D:315:ASN:HA	1:D:318:LEU:HD11	1.70	0.72
1:G:255:LEU:HD21	1:G:291:ILE:CD1	2.20	0.72
1:A:338:LEU:O	1:A:342:LEU:HD23	1.89	0.72
1:D:3:LYS:HA	1:D:449:LEU:HD22	1.71	0.72
1:J:362:ASP:OD2	1:J:433:LYS:HE2	1.89	0.72
1:F:376:ILE:HD11	1:F:435:SER:HA	1.70	0.72
1:A:314:ALA:O	1:A:317:ILE:HG22	1.89	0.71
1:D:40:HIS:HD2	3:D:509:HOH:O	1.72	0.71
1:E:82:TRP:HD1	1:E:125:PRO:CG	2.03	0.71
1:J:433:LYS:NZ	3:J:501:HOH:O	2.11	0.71
1:K:73:ILE:HD11	1:K:113:ILE:HD12	1.71	0.71
1:K:342:LEU:CD2	1:K:342:LEU:H	2.02	0.71
1:C:239:ALA:HA	1:C:301:ILE:HG12	1.72	0.71
1:D:39:SER:HA	1:D:45:ILE:HD11	1.73	0.71
1:D:89:GLY:HA3	1:D:128:LEU:HD11	1.73	0.71
1:A:154:LEU:HD23	1:A:154:LEU:H	1.56	0.71
1:L:302:LYS:HE2	1:L:314:ALA:HA	1.71	0.71
1:I:140:THR:HG23	1:I:200:SER:HB2	1.73	0.71
1:A:266:LEU:HB2	3:A:602:HOH:O	1.91	0.70
1:L:438:TRP:CE3	1:L:442:VAL:CG2	2.73	0.70
1:L:68:MET:HG2	1:L:404:LEU:HD11	1.71	0.70
1:H:47:ASP:HB2	1:H:49:HIS:CE1	2.26	0.70
1:C:30:LYS:NZ	1:C:81:SER:CB	2.54	0.70
1:B:401:LEU:HD21	1:B:420:ILE:HG21	1.73	0.70
1:H:147:SER:CA	1:H:150:ILE:HD11	2.16	0.70
1:L:438:TRP:O	1:L:441:GLU:HG3	1.92	0.70
1:B:197:LEU:CD1	3:B:616:HOH:O	2.39	0.70
1:B:197:LEU:HD12	3:B:616:HOH:O	1.92	0.69
1:H:254:VAL:CG2	1:H:255:LEU:HD12	2.20	0.69
1:L:109:LEU:CD1	1:L:157:ILE:CG2	2.69	0.69
1:D:244:SER:OG	1:D:248:ARG:NH1	2.24	0.69
1:K:370:ILE:HG13	1:K:433:LYS:CA	2.22	0.69
1:L:184:ILE:HD13	1:L:185:LYS:N	2.07	0.69
1:L:441:GLU:OE2	1:L:442:VAL:HG23	1.92	0.69
1:A:186:ASP:HB3	1:A:189:THR:CG2	2.23	0.69
1:I:134:TRP:HB3	1:I:193:VAL:HG23	1.75	0.69
1:D:188:ARG:NH1	3:D:502:HOH:O	2.24	0.69
1:D:321:PHE:CE2	1:D:331:TYR:HD2	2.10	0.69
1:K:288:ILE:HD13	1:K:290:PHE:H	1.56	0.69
1:L:195:HIS:CG	1:L:276:PHE:CE1	2.80	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:375:ARG:O	1:L:379:LEU:HD23	1.90	0.69
1:A:323:LYS:HE2	1:A:327:GLY:O	1.92	0.69
1:C:65:ILE:HD12	1:C:68:MET:HE2	1.73	0.69
1:I:51:GLY:O	1:I:53:VAL:N	2.25	0.69
1:C:76:TYR:HD2	1:C:108:LEU:HD21	1.55	0.69
1:L:68:MET:CE	1:L:73:ILE:HG21	2.23	0.69
1:L:166:GLU:HB3	1:L:169:VAL:HG22	1.73	0.69
1:A:173:LEU:HD23	1:A:177:LEU:HD12	1.74	0.69
1:A:186:ASP:OD2	1:A:189:THR:HG22	1.93	0.69
1:D:36:ASP:O	1:D:40:HIS:CD2	2.46	0.69
1:F:85:ILE:HG22	1:F:86:PHE:CD1	2.28	0.69
1:K:105:THR:OG1	3:K:501:HOH:O	2.10	0.69
1:G:364:ILE:HD13	1:G:370:ILE:HG12	1.75	0.69
1:C:292:ALA:HB1	1:C:354:SER:OG	1.92	0.69
1:F:158:VAL:HG11	1:F:161:TRP:CZ2	2.28	0.69
1:J:233:ALA:HA	1:J:236:ILE:CD1	2.23	0.69
1:G:208:PHE:CG	1:G:217:ILE:HD11	2.28	0.68
1:L:80:ILE:HD11	1:L:146:TYR:CZ	2.28	0.68
1:F:344:ARG:O	1:F:344:ARG:HG2	1.94	0.68
1:L:10:PHE:HE1	1:L:396:LEU:HD22	1.58	0.68
1:L:321:PHE:CE2	1:L:331:TYR:HD2	2.10	0.68
1:A:117:ILE:CG1	1:A:161:TRP:CE3	2.76	0.68
1:C:353:ILE:HD13	1:C:396:LEU:CD1	2.21	0.68
1:J:309:SER:OG	1:J:311:PHE:CE1	2.45	0.68
1:K:370:ILE:CD1	1:K:370:ILE:H	2.07	0.68
1:B:55:CYS:HA	3:B:620:HOH:O	1.94	0.68
1:L:338:LEU:C	1:L:338:LEU:HD13	2.13	0.68
1:D:156:ASP:OD2	3:D:501:HOH:O	2.12	0.68
1:H:2:SER:O	3:H:501:HOH:O	2.11	0.68
1:C:253:PRO:HG3	1:C:259:TYR:CD1	2.29	0.68
1:I:244:SER:O	3:I:501:HOH:O	2.09	0.68
1:D:77:ARG:HH22	1:D:165:ASN:HD22	1.42	0.68
1:H:364:ILE:HD11	1:H:431:LYS:HE2	1.75	0.68
1:J:322:GLU:O	1:J:330:ILE:HG23	1.92	0.68
1:E:406:ASP:O	3:E:502:HOH:O	2.12	0.68
1:C:99:ASP:O	1:C:103:ARG:HG3	1.94	0.67
1:C:169:VAL:HG12	1:C:173:LEU:CD1	2.24	0.67
1:G:195:HIS:CB	1:G:276:PHE:CZ	2.76	0.67
1:L:438:TRP:HE3	1:L:438:TRP:O	1.77	0.67
1:B:443:ILE:O	3:B:603:HOH:O	2.12	0.67
1:F:376:ILE:HD11	1:F:435:SER:CA	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:TYR:CE1	1:F:388:ARG:HG2	2.29	0.67
1:G:105:THR:O	1:G:109:LEU:HD13	1.94	0.67
1:L:186:ASP:OD2	1:L:189:THR:HG23	1.94	0.67
1:G:208:PHE:CE2	1:G:217:ILE:HG13	2.30	0.67
1:A:186:ASP:O	1:A:189:THR:HG23	1.94	0.67
1:C:385:GLN:HE22	1:C:388:ARG:HH11	1.42	0.67
1:I:282:LYS:HE2	1:I:282:LYS:HA	1.76	0.67
1:J:292:ALA:HB1	1:J:354:SER:OG	1.95	0.67
1:F:344:ARG:O	1:F:344:ARG:CG	2.43	0.67
1:K:121:HIS:HB3	3:K:511:HOH:O	1.94	0.67
1:L:388:ARG:O	1:L:391:GLN:O	2.13	0.67
1:C:168:GLY:O	3:C:501:HOH:O	2.13	0.67
1:D:77:ARG:HH22	1:D:165:ASN:ND2	1.92	0.67
1:E:225:TYR:HE1	1:E:341:LEU:HD12	1.60	0.67
1:K:173:LEU:HD23	1:K:177:LEU:HD12	1.77	0.67
1:L:93:LEU:HD22	1:L:94:ASN:N	2.10	0.67
1:B:154:LEU:O	1:B:157:ILE:HD13	1.94	0.67
1:E:381:ASP:O	1:E:384:THR:OG1	2.11	0.67
1:G:216:GLN:HA	1:G:289:ASP:OD2	1.95	0.67
1:H:216:GLN:HG2	1:H:289:ASP:CB	2.25	0.67
1:H:228:PRO:HG2	1:H:236:ILE:HD13	1.77	0.67
1:J:164:HIS:CE1	1:J:197:LEU:HD12	2.30	0.67
1:K:6:PHE:HE1	1:K:387:HIS:HB2	1.59	0.67
1:E:169:VAL:HG13	1:E:173:LEU:HD13	1.77	0.67
1:C:353:ILE:HG12	1:C:399:TYR:HA	1.75	0.66
1:K:89:GLY:HA3	1:K:128:LEU:HD11	1.75	0.66
1:B:101:TYR:HE2	3:B:605:HOH:O	1.79	0.66
1:L:63:GLU:O	1:L:67:ILE:HG22	1.94	0.66
1:K:187:LEU:HD22	1:K:272:ILE:HD13	1.76	0.66
1:G:166:GLU:HB3	1:G:169:VAL:HG22	1.76	0.66
1:H:166:GLU:HB3	1:H:169:VAL:HG22	1.76	0.66
1:B:61:TYR:O	1:B:65:ILE:HD13	1.96	0.66
1:C:380:LYS:O	1:C:384:THR:HG23	1.96	0.66
1:I:216:GLN:HA	1:I:289:ASP:OD2	1.95	0.66
1:B:196:ASN:O	3:B:604:HOH:O	2.13	0.66
1:E:291:ILE:HG22	1:E:351:ILE:HD13	1.77	0.66
1:B:169:VAL:HG13	1:B:173:LEU:HD13	1.78	0.66
1:K:73:ILE:CD1	1:K:113:ILE:HD12	2.26	0.66
1:B:81:SER:O	3:B:605:HOH:O	2.13	0.66
1:D:324:THR:HG22	1:D:359:ALA:O	1.96	0.66
1:K:208:PHE:CG	1:K:217:ILE:HD12	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HD11	1:A:119:LEU:HG	1.78	0.66
1:F:218:GLY:HA2	1:F:288:ILE:HG21	1.76	0.66
1:G:363:GLU:O	1:G:370:ILE:HD13	1.95	0.66
1:I:260:PRO:CG	3:I:501:HOH:O	2.34	0.66
1:L:376:ILE:HG23	1:L:438:TRP:HD1	1.59	0.66
1:F:9:ASP:O	1:F:11:ILE:CD1	2.44	0.65
1:H:147:SER:CA	1:H:150:ILE:CD1	2.74	0.65
1:K:219:ILE:CD1	1:K:221:LEU:CD1	2.73	0.65
1:A:178:GLY:HA3	1:A:185:LYS:HD2	1.77	0.65
1:C:30:LYS:HZ3	1:C:81:SER:CB	2.08	0.65
1:F:77:ARG:HH22	1:F:165:ASN:HD22	1.44	0.65
1:F:197:LEU:O	1:F:200:SER:OG	2.07	0.65
1:J:77:ARG:HH22	1:J:165:ASN:HD22	1.44	0.65
1:L:173:LEU:HD23	1:L:177:LEU:HD12	1.76	0.65
1:F:9:ASP:O	1:F:11:ILE:HD12	1.96	0.65
1:H:364:ILE:CD1	1:H:431:LYS:HE3	2.26	0.65
1:L:85:ILE:HG21	1:L:146:TYR:CD1	2.31	0.65
1:L:89:GLY:HA3	1:L:128:LEU:HD11	1.77	0.65
1:L:133:GLY:O	1:L:139:THR:OG1	2.13	0.65
1:D:207:LEU:HD21	1:D:211:MET:SD	2.37	0.65
1:D:241:LEU:HD21	1:D:266:LEU:HD22	1.78	0.65
1:J:71:ILE:HD12	1:J:436:GLY:O	1.96	0.65
1:K:201:HIS:CE1	1:K:219:ILE:HG23	2.31	0.65
1:K:228:PRO:HG2	1:K:236:ILE:HD13	1.79	0.65
1:L:216:GLN:HA	1:L:289:ASP:OD2	1.96	0.65
1:A:409:GLU:HB3	3:A:603:HOH:O	1.94	0.65
1:C:221:LEU:CD1	1:C:251:LEU:HD22	2.26	0.65
1:G:3:LYS:HA	1:G:449:LEU:HD13	1.78	0.65
1:I:257:GLY:CA	1:I:285:SER:OG	2.45	0.65
1:L:208:PHE:CD1	1:L:213:ILE:HG21	2.32	0.65
1:D:207:LEU:C	1:D:207:LEU:HD23	2.16	0.65
1:H:315:ASN:HA	1:H:318:LEU:HD12	1.78	0.65
1:I:116:ALA:CB	1:I:160:ILE:HD11	2.26	0.65
1:B:104:LEU:O	1:B:108:LEU:HD23	1.97	0.65
1:C:221:LEU:HD13	1:C:251:LEU:HD22	1.79	0.64
1:K:335:LEU:HD23	1:K:339:LEU:HD13	1.79	0.64
1:C:240:GLU:OE1	1:C:248:ARG:NH2	2.29	0.64
1:I:80:ILE:HD13	1:I:101:TYR:CD1	2.32	0.64
1:G:89:GLY:HA3	1:G:128:LEU:HD11	1.80	0.64
1:I:135:LYS:HD2	1:I:189:THR:HG23	1.80	0.64
1:E:82:TRP:CD1	1:E:125:PRO:CG	2.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:282:LYS:HA	1:I:282:LYS:CE	2.27	0.64
1:J:201:HIS:CE1	3:J:507:HOH:O	2.50	0.64
1:G:208:PHE:CD2	1:G:217:ILE:HG13	2.32	0.64
1:H:254:VAL:HG23	1:H:255:LEU:CD1	2.24	0.64
1:L:380:LYS:O	1:L:384:THR:HG23	1.98	0.64
1:B:408:PHE:HB3	3:B:613:HOH:O	1.96	0.64
1:J:207:LEU:O	1:J:207:LEU:HD23	1.97	0.64
1:L:208:PHE:CE1	1:L:213:ILE:CG2	2.79	0.64
1:G:195:HIS:HB2	1:G:276:PHE:CZ	2.33	0.64
1:K:6:PHE:CE1	1:K:387:HIS:HB2	2.32	0.64
1:A:135:LYS:CE	1:A:189:THR:HB	2.27	0.64
1:G:107:LEU:O	1:G:110:GLU:O	2.16	0.64
1:G:195:HIS:ND1	1:G:276:PHE:CE2	2.65	0.64
1:I:242:SER:O	1:I:245:LEU:N	2.30	0.64
1:G:240:GLU:OE1	1:G:248:ARG:NH2	2.25	0.64
1:K:324:THR:HG22	1:K:359:ALA:O	1.98	0.64
1:G:387:HIS:O	1:G:390:ILE:HG22	1.97	0.64
1:B:101:TYR:CE2	3:B:605:HOH:O	2.50	0.63
1:D:173:LEU:HD23	1:D:177:LEU:HD12	1.79	0.63
1:F:3:LYS:CA	1:F:449:LEU:HD22	2.28	0.63
1:F:3:LYS:HA	1:F:449:LEU:HD22	1.79	0.63
1:G:212:ASN:HD21	1:H:305:PRO:HG2	1.63	0.63
1:E:82:TRP:CD1	1:E:125:PRO:HG2	2.33	0.63
1:G:419:GLY:O	1:G:433:LYS:HE3	1.96	0.63
1:H:102:LYS:HE3	1:H:153:ASN:OD1	1.98	0.63
1:H:364:ILE:CD1	1:H:431:LYS:CE	2.76	0.63
1:L:233:ALA:HA	1:L:236:ILE:CD1	2.27	0.63
1:H:333:GLU:HA	1:H:385:GLN:HE21	1.63	0.63
1:I:362:ASP:OD2	1:I:433:LYS:HE2	1.98	0.63
1:B:153:ASN:CB	1:B:154:LEU:HD12	2.29	0.63
1:C:166:GLU:HB3	1:C:169:VAL:HG22	1.79	0.63
1:L:71:ILE:HD12	1:L:436:GLY:O	1.98	0.63
1:E:343:ASP:OD1	1:E:348:LYS:HG2	1.98	0.63
1:F:201:HIS:CE1	1:F:288:ILE:HD11	2.33	0.63
1:K:370:ILE:CD1	1:K:433:LYS:HA	2.28	0.63
1:H:76:TYR:HB2	1:H:113:ILE:HD11	1.81	0.63
1:H:173:LEU:HD23	1:H:177:LEU:HD12	1.80	0.63
1:H:216:GLN:HG2	1:H:289:ASP:HB3	1.80	0.63
1:K:76:TYR:HB2	1:K:113:ILE:HD11	1.79	0.63
1:B:206:LYS:HD2	1:B:207:LEU:N	2.13	0.63
1:L:208:PHE:CZ	1:L:213:ILE:CG2	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ILE:HG13	1:C:399:TYR:HD1	1.64	0.63
1:K:208:PHE:CG	1:K:217:ILE:CD1	2.81	0.63
1:L:255:LEU:HD11	1:L:291:ILE:HD13	1.80	0.63
1:C:403:SER:HB3	3:C:508:HOH:O	1.98	0.62
1:D:404:LEU:O	1:D:420:ILE:O	2.16	0.62
1:I:389:ALA:C	1:I:394:VAL:HG12	2.19	0.62
1:K:135:LYS:HD2	1:K:189:THR:CG2	2.28	0.62
1:C:239:ALA:N	1:C:301:ILE:HD11	2.14	0.62
1:C:353:ILE:CD1	1:C:396:LEU:CD1	2.71	0.62
1:E:239:ALA:N	1:E:301:ILE:HD11	2.14	0.62
1:H:10:PHE:HE1	1:H:396:LEU:HD13	1.64	0.62
1:I:61:TYR:HE2	1:I:103:ARG:NH1	1.97	0.62
1:F:165:ASN:HD21	1:F:294:ASN:HD21	1.47	0.62
1:G:165:ASN:N	3:G:505:HOH:O	2.30	0.62
1:I:134:TRP:HB2	1:I:193:VAL:HG23	1.80	0.62
1:L:77:ARG:HH22	1:L:165:ASN:HD22	1.47	0.62
1:L:80:ILE:HG13	1:L:146:TYR:OH	1.99	0.62
1:D:364:ILE:HD13	1:D:370:ILE:HG13	1.82	0.62
1:G:61:TYR:OH	1:G:103:ARG:CZ	2.48	0.62
1:J:187:LEU:O	1:J:187:LEU:HD23	2.00	0.62
1:C:154:LEU:HA	1:C:157:ILE:CD1	2.30	0.62
1:G:326:MET:HE2	1:G:418:PHE:CE1	2.35	0.62
1:H:241:LEU:CD1	1:H:245:LEU:CD2	2.76	0.62
1:A:377:GLN:NE2	1:A:380:LYS:HE3	2.14	0.62
1:C:30:LYS:HD3	1:C:84:ARG:HG3	1.82	0.62
1:I:143:PHE:CD2	1:I:200:SER:OG	2.53	0.62
1:G:165:ASN:CB	3:G:505:HOH:O	2.47	0.62
1:K:342:LEU:CD2	1:K:342:LEU:N	2.62	0.62
1:L:440:LYS:O	1:L:443:ILE:HG22	2.00	0.62
1:G:109:LEU:HD11	1:G:115:PRO:HG3	1.81	0.62
1:A:154:LEU:H	1:A:154:LEU:CD2	2.13	0.61
1:K:77:ARG:HH22	1:K:165:ASN:HD22	1.47	0.61
1:K:80:ILE:HD12	1:K:117:ILE:HG21	1.82	0.61
1:L:11:ILE:H	1:L:11:ILE:HD13	1.64	0.61
1:L:396:LEU:C	1:L:396:LEU:HD23	2.20	0.61
1:B:225:TYR:OH	3:B:601:HOH:O	1.85	0.61
1:E:353:ILE:HG13	1:E:396:LEU:HD11	1.83	0.61
1:G:212:ASN:HB3	1:H:306:SER:CB	2.30	0.61
1:G:226:HIS:HB3	1:G:301:ILE:HD13	1.82	0.61
1:G:424:ASN:ND2	1:G:427:THR:HG23	2.15	0.61
1:K:80:ILE:HD12	1:K:117:ILE:CG2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:MET:O	1:L:71:ILE:O	2.17	0.61
1:D:371:GLU:HA	1:D:434:ASP:OD2	2.01	0.61
1:G:259:TYR:OH	1:G:276:PHE:CZ	2.54	0.61
1:K:207:LEU:HD23	1:K:207:LEU:C	2.20	0.61
1:A:61:TYR:O	1:A:65:ILE:CD1	2.44	0.61
1:I:415:ASN:HD22	1:I:415:ASN:N	1.96	0.61
1:K:73:ILE:CD1	1:K:113:ILE:CD1	2.79	0.61
1:L:362:ASP:OD2	1:L:433:LYS:NZ	2.33	0.61
1:G:195:HIS:ND1	1:G:276:PHE:CZ	2.68	0.61
1:G:324:THR:HG22	1:G:359:ALA:O	2.01	0.61
1:K:395:ASN:OD1	1:K:395:ASN:N	2.33	0.61
1:L:45:ILE:HD12	1:L:45:ILE:N	2.15	0.61
1:A:291:ILE:HG22	1:A:351:ILE:HD13	1.82	0.61
1:K:47:ASP:HB2	1:K:49:HIS:CD2	2.35	0.61
1:L:39:SER:HA	1:L:45:ILE:HD11	1.83	0.61
1:B:401:LEU:CD2	1:B:420:ILE:HG21	2.31	0.61
1:J:89:GLY:HA3	1:J:128:LEU:CD2	2.31	0.61
1:J:232:LYS:O	1:J:236:ILE:HD12	2.00	0.61
1:K:161:TRP:HB2	1:K:217:ILE:HG12	1.83	0.61
1:L:39:SER:HA	1:L:45:ILE:CD1	2.30	0.61
1:L:438:TRP:CE3	1:L:442:VAL:HG23	2.36	0.61
1:H:364:ILE:HD11	1:H:431:LYS:CE	2.30	0.61
1:I:77:ARG:HH22	1:I:165:ASN:ND2	1.94	0.61
1:J:173:LEU:HD23	1:J:177:LEU:HD12	1.82	0.61
1:J:207:LEU:HD21	1:J:211:MET:SD	2.40	0.61
1:L:109:LEU:HD11	1:L:157:ILE:HG22	1.82	0.60
1:G:195:HIS:CG	1:G:276:PHE:CE2	2.89	0.60
1:G:290:PHE:CD1	1:G:352:VAL:CG1	2.85	0.60
1:H:47:ASP:OD2	1:H:49:HIS:HE1	1.85	0.60
1:H:102:LYS:CE	1:H:153:ASN:HB3	2.31	0.60
1:H:141:ASP:OD1	1:H:203:LYS:NZ	2.32	0.60
1:B:326:MET:HE2	1:B:418:PHE:CE1	2.37	0.60
1:G:268:LYS:HG3	1:G:273:GLU:CG	2.30	0.60
1:H:362:ASP:OD2	1:H:433:LYS:HE2	2.00	0.60
1:I:154:LEU:HA	1:I:157:ILE:CD1	2.31	0.60
1:I:195:HIS:ND1	1:I:276:PHE:HE1	1.98	0.60
1:J:375:ARG:O	1:J:379:LEU:HD23	2.01	0.60
1:K:211:MET:O	1:K:212:ASN:OD1	2.19	0.60
1:L:4:ILE:HG12	1:L:387:HIS:ND1	2.15	0.60
1:L:340:MET:O	1:L:344:ARG:HG2	2.01	0.60
1:F:279:ASP:OD1	1:F:279:ASP:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:353:ILE:HG13	1:J:396:LEU:HD11	1.84	0.60
1:K:335:LEU:O	1:K:339:LEU:HD13	2.01	0.60
1:I:186:ASP:OD2	1:I:189:THR:OG1	2.19	0.60
1:J:80:ILE:HD13	1:J:117:ILE:HG23	1.84	0.60
1:J:189:THR:HB	3:J:506:HOH:O	2.01	0.60
1:F:335:LEU:O	1:F:339:LEU:HD12	2.01	0.60
1:G:13:GLY:C	1:G:73:ILE:HD11	2.22	0.60
1:K:370:ILE:HG13	1:K:433:LYS:CG	2.32	0.60
1:C:355:GLU:OE1	3:C:502:HOH:O	2.16	0.60
1:G:109:LEU:HD21	1:G:157:ILE:CG1	2.32	0.60
1:G:197:LEU:O	1:G:200:SER:OG	2.15	0.60
1:H:241:LEU:CD1	1:H:245:LEU:HD21	2.31	0.60
1:L:350:ASN:C	1:L:351:ILE:HD12	2.21	0.60
1:A:431:LYS:HG2	3:A:604:HOH:O	2.01	0.60
1:D:390:ILE:HD13	1:D:394:VAL:O	2.01	0.60
1:E:25:TYR:OH	1:L:130:ASP:OD2	2.15	0.60
1:I:404:LEU:HG	1:I:405:LEU:HD13	1.82	0.60
1:L:67:ILE:HD11	1:L:421:VAL:CG2	2.31	0.60
1:C:105:THR:O	1:C:109:LEU:CD1	2.49	0.60
1:G:165:ASN:HB2	3:G:505:HOH:O	2.00	0.60
1:H:13:GLY:CA	1:H:73:ILE:HD11	2.31	0.60
1:L:208:PHE:CZ	1:L:213:ILE:HG23	2.37	0.60
1:A:117:ILE:C	1:A:117:ILE:CD1	2.64	0.60
1:F:336:TYR:CD1	1:F:388:ARG:HG2	2.37	0.60
1:J:193:VAL:HG23	3:J:502:HOH:O	2.02	0.60
1:B:171:SER:HB3	3:B:616:HOH:O	2.01	0.59
1:H:255:LEU:HD11	1:H:291:ILE:HD13	1.84	0.59
1:K:303:TYR:CZ	1:K:305:PRO:HD3	2.37	0.59
1:K:339:LEU:O	1:K:342:LEU:HD21	2.01	0.59
1:L:440:LYS:O	1:L:444:LYS:HD2	2.02	0.59
1:A:117:ILE:HD12	1:A:118:THR:N	2.16	0.59
1:E:336:TYR:OH	1:E:392:ASP:OD2	2.13	0.59
1:F:218:GLY:HA2	1:F:288:ILE:CG2	2.32	0.59
1:K:266:LEU:O	1:K:270:LYS:HE2	2.02	0.59
1:L:333:GLU:HA	1:L:385:GLN:HE21	1.67	0.59
1:A:322:GLU:HB2	1:A:330:ILE:HG12	1.85	0.59
1:C:65:ILE:HD12	1:C:68:MET:CE	2.31	0.59
1:F:166:GLU:HB3	1:F:169:VAL:HG22	1.84	0.59
1:K:141:ASP:O	1:K:144:THR:HG23	2.03	0.59
1:A:332:PRO:HB2	1:A:385:GLN:HE21	1.67	0.59
1:G:118:THR:CG2	3:G:505:HOH:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:ASP:HB2	1:I:49:HIS:CD2	2.37	0.59
1:I:384:THR:HG21	1:I:450:GLU:HG3	1.85	0.59
1:J:76:TYR:HB2	1:J:113:ILE:HD11	1.83	0.59
1:G:326:MET:CE	1:G:418:PHE:HE1	2.15	0.59
1:H:326:MET:HE2	1:H:418:PHE:CE1	2.38	0.59
1:I:173:LEU:HD23	1:I:177:LEU:HD12	1.83	0.59
1:J:212:ASN:CG	1:J:212:ASN:O	2.41	0.59
1:J:233:ALA:HA	1:J:236:ILE:HD11	1.83	0.59
1:K:339:LEU:O	1:K:342:LEU:CD2	2.51	0.59
1:L:255:LEU:HD11	1:L:291:ILE:CD1	2.32	0.59
1:I:259:TYR:HE1	1:I:281:LEU:HD21	1.68	0.59
1:F:266:LEU:O	1:F:266:LEU:HD13	2.02	0.59
1:K:288:ILE:HD13	1:K:288:ILE:C	2.23	0.59
1:K:342:LEU:HG	1:K:351:ILE:CD1	2.33	0.59
1:B:401:LEU:HD21	1:B:420:ILE:CG2	2.32	0.58
1:G:419:GLY:O	1:G:433:LYS:CE	2.51	0.58
1:A:102:LYS:O	1:A:105:THR:HG22	2.02	0.58
1:C:26:ASN:OD1	1:I:127:LYS:HE3	2.02	0.58
1:G:394:VAL:HG13	1:G:396:LEU:H	1.66	0.58
1:H:326:MET:CE	1:H:418:PHE:CE1	2.85	0.58
1:L:82:TRP:O	1:L:85:ILE:HG22	2.02	0.58
1:I:342:LEU:O	1:I:345:ASP:O	2.21	0.58
1:B:148:GLU:HG2	1:B:152:LYS:NZ	2.19	0.58
1:G:125:PRO:HB3	3:G:502:HOH:O	2.03	0.58
1:G:304:ASP:OD2	1:G:312:SER:OG	2.17	0.58
1:K:194:SER:O	1:K:198:LEU:HD12	2.04	0.58
1:K:338:LEU:O	1:K:342:LEU:CD2	2.36	0.58
1:B:146:TYR:O	1:B:150:ILE:HD13	2.04	0.58
1:B:241:LEU:HD21	1:B:266:LEU:HD22	1.84	0.58
1:B:326:MET:CE	1:B:418:PHE:CE1	2.87	0.58
1:G:109:LEU:CD2	1:G:157:ILE:HG13	2.33	0.58
1:L:208:PHE:CG	1:L:217:ILE:HD12	2.38	0.58
1:C:353:ILE:HG13	1:C:399:TYR:CD1	2.38	0.58
1:F:173:LEU:HD22	1:F:177:LEU:HD12	1.84	0.58
1:G:326:MET:CE	1:G:418:PHE:CE1	2.87	0.58
1:I:390:ILE:HA	1:I:394:VAL:HG12	1.85	0.58
1:K:75:SER:OG	1:K:114:MET:HB3	2.04	0.58
1:A:153:ASN:O	1:A:154:LEU:O	2.21	0.58
1:F:157:ILE:CD1	3:F:504:HOH:O	2.51	0.58
1:G:394:VAL:HG13	1:G:396:LEU:N	2.19	0.58
1:H:117:ILE:HD12	1:H:158:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:ASN:HA	1:H:318:LEU:HD13	1.86	0.58
1:J:11:ILE:HD11	1:J:398:ALA:HB2	1.86	0.58
1:J:233:ALA:C	1:J:236:ILE:CD1	2.72	0.58
1:L:67:ILE:HD11	1:L:421:VAL:HG21	1.86	0.58
1:B:425:PHE:CD1	3:B:620:HOH:O	2.52	0.58
1:G:259:TYR:HH	1:G:276:PHE:HZ	1.44	0.58
1:I:11:ILE:CD1	1:I:114:MET:CE	2.81	0.58
1:J:335:LEU:O	1:J:339:LEU:HD23	2.03	0.58
1:L:80:ILE:CG1	1:L:146:TYR:OH	2.52	0.58
1:K:206:LYS:O	1:K:210:GLU:HG3	2.04	0.58
1:C:4:ILE:HG23	1:C:387:HIS:CG	2.39	0.57
1:H:326:MET:CE	1:H:418:PHE:HE1	2.17	0.57
1:J:207:LEU:HD23	1:J:207:LEU:C	2.24	0.57
1:A:376:ILE:H	1:A:376:ILE:HD12	1.69	0.57
1:D:177:LEU:O	1:D:185:LYS:NZ	2.33	0.57
1:E:291:ILE:HG22	1:E:351:ILE:CD1	2.35	0.57
1:I:380:LYS:O	1:I:384:THR:HG23	2.03	0.57
1:G:173:LEU:HD23	1:G:177:LEU:HD12	1.86	0.57
1:H:380:LYS:O	1:H:384:THR:HG23	2.04	0.57
1:C:292:ALA:HA	1:C:352:VAL:O	2.04	0.57
1:C:295:ASN:HD22	1:C:335:LEU:HD13	1.70	0.57
1:I:226:HIS:HB3	1:I:301:ILE:HD13	1.87	0.57
1:J:291:ILE:HD12	1:J:292:ALA:O	2.05	0.57
1:L:165:ASN:ND2	1:L:294:ASN:HD21	2.00	0.57
1:B:408:PHE:CB	3:B:613:HOH:O	2.53	0.57
1:C:294:ASN:OD1	1:C:355:GLU:CG	2.53	0.57
1:H:146:TYR:O	1:H:149:VAL:HG12	2.05	0.57
1:I:286:GLN:NE2	1:I:287:PRO:O	2.37	0.57
1:L:64:ASP:HA	1:L:67:ILE:CG2	2.35	0.57
1:C:166:GLU:HB3	1:C:169:VAL:CG2	2.35	0.57
1:C:362:ASP:OD2	1:C:433:LYS:NZ	2.37	0.57
1:D:230:SER:OG	1:D:232:LYS:HE3	2.04	0.57
1:H:102:LYS:HE2	1:H:153:ASN:HB3	1.87	0.57
1:K:45:ILE:HD13	1:K:45:ILE:N	2.18	0.57
1:K:71:ILE:HG13	1:K:440:LYS:HB2	1.86	0.57
1:F:34:ILE:HG12	1:F:123:ASP:O	2.04	0.57
1:G:118:THR:HG21	3:G:505:HOH:O	2.05	0.57
1:K:208:PHE:CD1	1:K:217:ILE:CD1	2.87	0.57
1:L:438:TRP:CH2	1:L:442:VAL:HG21	2.39	0.57
1:A:323:LYS:CE	1:A:327:GLY:O	2.53	0.57
1:B:154:LEU:HA	1:B:157:ILE:CD1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:HIS:HB2	1:G:276:PHE:CE1	2.40	0.57
1:I:225:TYR:HE2	1:I:341:LEU:HD23	1.70	0.57
1:G:10:PHE:HB3	3:G:503:HOH:O	2.04	0.56
1:H:89:GLY:HA3	1:H:128:LEU:HD11	1.87	0.56
1:L:4:ILE:HG12	1:L:387:HIS:CE1	2.40	0.56
1:A:117:ILE:HD12	1:A:117:ILE:O	2.05	0.56
1:B:148:GLU:HG2	1:B:152:LYS:HZ2	1.70	0.56
1:D:396:LEU:C	1:D:396:LEU:HD23	2.25	0.56
1:I:314:ALA:HB1	1:I:317:ILE:HD13	1.86	0.56
1:K:226:HIS:HB3	1:K:301:ILE:HD13	1.86	0.56
1:L:146:TYR:O	1:L:149:VAL:HG12	2.04	0.56
1:A:324:THR:HG23	1:A:326:MET:O	2.06	0.56
1:F:267:TYR:O	1:F:272:ILE:HG23	2.06	0.56
1:F:318:LEU:HD22	1:F:329:ILE:HD12	1.87	0.56
1:I:255:LEU:HD11	1:I:291:ILE:HD13	1.87	0.56
1:I:404:LEU:HG	1:I:405:LEU:HD12	1.85	0.56
1:K:218:GLY:HA2	1:K:288:ILE:HG13	1.87	0.56
1:L:72:GLY:CA	1:L:444:LYS:HZ2	2.18	0.56
1:F:56:ASP:HB3	1:F:428:LEU:CD1	2.35	0.56
1:L:195:HIS:HB2	1:L:276:PHE:CE1	2.41	0.56
1:C:375:ARG:O	1:C:379:LEU:HG	2.06	0.56
1:F:17:ALA:HB3	1:F:20:GLN:HE21	1.70	0.56
1:F:77:ARG:HH22	1:F:165:ASN:ND2	2.03	0.56
1:G:54:ALA:HA	1:G:414:TYR:OH	2.05	0.56
1:J:233:ALA:HA	1:J:236:ILE:HD12	1.88	0.56
1:K:201:HIS:CE1	1:K:219:ILE:CG2	2.89	0.56
1:L:12:TRP:HB2	1:L:443:ILE:HD12	1.86	0.56
1:A:291:ILE:CG2	1:A:351:ILE:CD1	2.83	0.56
1:I:253:PRO:HB3	1:I:281:LEU:HD11	1.87	0.56
1:L:126:GLN:OE1	1:L:126:GLN:O	2.24	0.56
1:C:88:GLU:OE2	1:I:27:GLU:HA	2.05	0.56
1:F:85:ILE:HG22	1:F:86:PHE:CE1	2.41	0.56
1:G:109:LEU:CD2	1:G:157:ILE:CG1	2.83	0.56
1:I:241:LEU:O	1:I:242:SER:O	2.24	0.56
1:K:89:GLY:HA3	1:K:128:LEU:CD1	2.36	0.56
1:K:277:PRO:HG2	1:K:280:ASP:CG	2.24	0.56
1:L:77:ARG:HH22	1:L:165:ASN:ND2	2.04	0.56
1:G:350:ASN:C	1:G:351:ILE:HD12	2.26	0.56
1:K:67:ILE:HG12	1:K:432:ILE:HD11	1.87	0.56
1:L:233:ALA:HA	1:L:236:ILE:HD12	1.86	0.56
1:B:140:THR:HG22	3:B:604:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:LEU:O	1:F:191:LEU:CD2	2.54	0.56
1:F:376:ILE:CD1	1:F:435:SER:CA	2.78	0.56
1:F:376:ILE:HD13	1:F:435:SER:HA	1.88	0.56
1:L:247:GLY:HA2	3:L:511:HOH:O	2.06	0.56
1:J:241:LEU:C	1:J:241:LEU:HD23	2.26	0.56
1:L:69:LYS:CE	1:L:111:ASN:O	2.54	0.56
1:L:438:TRP:HZ3	1:L:442:VAL:CB	1.92	0.56
1:B:54:ALA:HA	1:B:414:TYR:OH	2.05	0.55
1:H:27:GLU:O	3:H:502:HOH:O	2.18	0.55
1:A:171:SER:HB3	1:A:193:VAL:HG22	1.87	0.55
1:E:82:TRP:HD1	1:E:125:PRO:HG2	1.68	0.55
1:G:228:PRO:HG3	1:G:236:ILE:HD13	1.89	0.55
1:H:28:ASP:C	3:H:503:HOH:O	2.45	0.55
1:J:166:GLU:HB3	1:J:169:VAL:CG2	2.36	0.55
1:J:296:TYR:HD1	1:J:357:GLY:O	1.89	0.55
1:K:148:GLU:HG2	1:K:207:LEU:HD11	1.85	0.55
1:L:375:ARG:O	1:L:379:LEU:CD2	2.54	0.55
1:F:295:ASN:HD22	1:F:335:LEU:HD13	1.71	0.55
1:G:11:ILE:HD13	1:G:11:ILE:H	1.71	0.55
1:G:356:ASN:O	1:G:401:LEU:HD12	2.07	0.55
1:K:207:LEU:HD21	1:K:211:MET:SD	2.46	0.55
1:A:89:GLY:HA3	1:A:128:LEU:HD11	1.88	0.55
1:E:186:ASP:OD2	1:E:189:THR:OG1	2.25	0.55
1:E:225:TYR:CE1	1:E:341:LEU:HD12	2.39	0.55
1:H:315:ASN:CA	1:H:318:LEU:HD12	2.35	0.55
1:J:233:ALA:CA	1:J:236:ILE:CD1	2.85	0.55
1:J:241:LEU:HD23	1:J:241:LEU:O	2.05	0.55
1:L:105:THR:O	1:L:108:LEU:CD1	2.54	0.55
1:C:30:LYS:HD2	1:C:83:PRO:HB2	1.89	0.55
1:D:321:PHE:HE2	1:D:331:TYR:HD2	1.53	0.55
1:H:165:ASN:HD21	1:H:294:ASN:HD21	1.54	0.55
1:I:314:ALA:O	1:I:316:SER:N	2.39	0.55
1:C:254:VAL:O	1:C:285:SER:HA	2.06	0.55
1:E:326:MET:CE	1:E:418:PHE:CE1	2.89	0.55
1:G:208:PHE:CG	1:G:217:ILE:CD1	2.90	0.55
1:I:422:HIS:HA	1:I:433:LYS:HZ1	1.71	0.55
1:J:186:ASP:HB3	3:J:506:HOH:O	2.05	0.55
1:J:383:LEU:HD21	1:J:399:TYR:CZ	2.42	0.55
1:K:197:LEU:O	1:K:200:SER:OG	2.19	0.55
1:K:370:ILE:CD1	1:K:370:ILE:N	2.70	0.55
1:B:153:ASN:HB3	1:B:154:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:VAL:HG12	1:J:217:ILE:HG21	1.89	0.55
1:L:226:HIS:HB3	1:L:301:ILE:HD13	1.87	0.55
1:D:89:GLY:HA3	1:D:128:LEU:CD1	2.37	0.55
1:J:56:ASP:OD1	1:J:56:ASP:O	2.25	0.55
1:B:240:GLU:OE1	1:B:248:ARG:NH2	2.37	0.55
1:K:241:LEU:O	1:K:244:SER:OG	2.24	0.55
1:L:379:LEU:O	1:L:383:LEU:HD12	2.07	0.55
1:C:105:THR:O	1:C:109:LEU:HD13	2.07	0.54
1:E:380:LYS:O	1:E:384:THR:HG23	2.07	0.54
1:I:248:ARG:HG2	1:I:252:ASP:OD1	2.07	0.54
1:J:330:ILE:O	1:J:330:ILE:HD13	2.06	0.54
1:K:370:ILE:CG1	1:K:433:LYS:CA	2.78	0.54
1:B:271:GLY:C	1:B:272:ILE:HD12	2.28	0.54
1:C:186:ASP:OD2	1:C:189:THR:OG1	2.26	0.54
1:C:272:ILE:O	1:C:273:GLU:CG	2.52	0.54
1:E:321:PHE:O	1:E:323:LYS:HD3	2.07	0.54
1:J:6:PHE:CZ	1:J:383:LEU:HD12	2.41	0.54
1:J:233:ALA:O	1:J:236:ILE:HD11	2.07	0.54
1:L:72:GLY:O	1:L:73:ILE:O	2.25	0.54
1:L:430:ARG:O	1:L:431:LYS:HE3	2.07	0.54
1:B:166:GLU:OE2	2:B:501:TRS:H32	2.08	0.54
1:E:291:ILE:CG2	1:E:351:ILE:CD1	2.85	0.54
1:G:113:ILE:HD13	1:G:113:ILE:C	2.27	0.54
1:H:10:PHE:HE1	1:H:396:LEU:CD1	2.20	0.54
1:H:403:SER:O	1:H:419:GLY:HA2	2.07	0.54
1:K:77:ARG:HA	1:K:116:ALA:O	2.07	0.54
1:L:380:LYS:CG	1:L:448:PHE:CE2	2.90	0.54
1:L:105:THR:O	1:L:108:LEU:HD12	2.07	0.54
1:L:321:PHE:HE2	1:L:331:TYR:HD2	1.51	0.54
1:B:321:PHE:HE2	1:B:331:TYR:HD2	1.52	0.54
1:D:380:LYS:O	1:D:384:THR:HG23	2.07	0.54
1:H:150:ILE:HD13	1:H:150:ILE:H	1.73	0.54
1:K:286:GLN:OE1	1:K:287:PRO:HD2	2.08	0.54
1:C:270:LYS:O	1:C:270:LYS:HD2	2.08	0.54
1:C:353:ILE:CG1	1:C:399:TYR:HA	2.37	0.54
1:F:154:LEU:O	1:F:158:VAL:HG12	2.08	0.54
1:G:340:MET:O	1:G:344:ARG:HG3	2.08	0.54
1:I:390:ILE:N	1:I:394:VAL:HG12	2.23	0.54
1:B:326:MET:CE	1:B:418:PHE:HE1	2.20	0.54
1:E:82:TRP:HB3	1:E:83:PRO:HD3	1.89	0.54
1:B:442:VAL:N	3:B:611:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:TYR:HB2	1:E:143:PHE:HE2	1.73	0.54
1:E:326:MET:CE	1:E:418:PHE:HE1	2.20	0.54
1:J:144:THR:HG22	1:J:207:LEU:HD12	1.89	0.54
1:K:64:ASP:HA	1:K:67:ILE:HG22	1.90	0.54
1:A:333:GLU:HA	1:A:385:GLN:HG2	1.90	0.54
1:B:149:VAL:HG23	1:B:150:ILE:HD13	1.90	0.54
1:D:315:ASN:CA	1:D:318:LEU:HD12	2.34	0.54
1:E:292:ALA:HA	1:E:352:VAL:O	2.08	0.54
1:F:3:LYS:HB2	1:F:449:LEU:CD2	2.38	0.54
1:B:211:MET:HB2	1:B:213:ILE:HD11	1.90	0.53
1:J:17:ALA:O	1:J:21:ILE:HG12	2.08	0.53
1:L:80:ILE:CD1	1:L:146:TYR:HE1	2.08	0.53
1:L:80:ILE:HG23	1:L:117:ILE:HG23	1.90	0.53
1:G:61:TYR:CZ	1:G:103:ARG:CZ	2.91	0.53
1:H:227:TYR:HB2	1:H:300:PHE:CD1	2.43	0.53
1:H:448:PHE:CD2	1:H:449:LEU:N	2.75	0.53
1:J:318:LEU:HD22	1:J:318:LEU:C	2.29	0.53
1:K:108:LEU:HD22	1:K:113:ILE:HD13	1.90	0.53
1:K:143:PHE:CE2	1:K:164:HIS:NE2	2.77	0.53
1:D:39:SER:HA	1:D:45:ILE:CD1	2.37	0.53
1:E:209:ARG:NH2	1:E:289:ASP:OD1	2.40	0.53
1:H:147:SER:O	1:H:150:ILE:CD1	2.55	0.53
1:I:177:LEU:O	1:I:185:LYS:NZ	2.39	0.53
1:B:154:LEU:HD12	1:B:154:LEU:N	2.24	0.53
1:D:207:LEU:HD23	1:D:207:LEU:O	2.09	0.53
1:D:364:ILE:CD1	1:D:370:ILE:HD11	2.38	0.53
1:F:250:TYR:O	1:F:254:VAL:HG23	2.08	0.53
1:K:84:ARG:O	1:K:94:ASN:ND2	2.42	0.53
1:L:166:GLU:HB3	1:L:169:VAL:CG2	2.37	0.53
1:L:403:SER:O	1:L:419:GLY:HA2	2.07	0.53
1:C:54:ALA:HA	1:C:414:TYR:OH	2.09	0.53
1:I:195:HIS:HB2	1:I:276:PHE:CE1	2.44	0.53
1:L:164:HIS:O	3:L:501:HOH:O	2.19	0.53
1:A:117:ILE:HD12	1:A:118:THR:CA	2.38	0.53
1:D:231:GLU:OE1	1:D:231:GLU:N	2.34	0.53
1:G:10:PHE:HE1	1:G:396:LEU:HD13	1.73	0.53
1:H:330:ILE:HD12	1:H:382:TYR:HE1	1.74	0.53
1:J:433:LYS:CG	3:J:501:HOH:O	2.48	0.53
1:K:219:ILE:CD1	1:K:221:LEU:HD13	2.32	0.53
1:K:434:ASP:HA	1:K:437:TYR:HD2	1.74	0.53
1:F:158:VAL:HG13	1:F:161:TRP:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:TYR:OH	1:G:103:ARG:NH1	2.41	0.53
1:I:11:ILE:CD1	1:I:114:MET:HE1	2.39	0.53
1:K:6:PHE:CZ	3:K:512:HOH:O	2.54	0.53
1:K:288:ILE:CD1	1:K:290:PHE:H	2.22	0.53
1:K:342:LEU:HG	1:K:351:ILE:HD13	1.91	0.53
1:L:244:SER:HB3	1:L:248:ARG:NH1	2.23	0.53
1:C:364:ILE:HD13	1:C:431:LYS:HD2	1.91	0.53
1:E:223:LEU:HD12	1:E:293:PHE:CB	2.39	0.53
1:F:3:LYS:H	1:F:449:LEU:HD13	1.73	0.53
1:H:439:TYR:O	1:H:443:ILE:HG13	2.08	0.53
1:K:80:ILE:CG2	1:K:85:ILE:HD11	2.39	0.53
1:K:370:ILE:HD11	1:K:433:LYS:HA	1.91	0.53
1:C:166:GLU:O	1:C:169:VAL:HG23	2.09	0.53
1:G:89:GLY:HA3	1:G:128:LEU:CD1	2.39	0.53
1:I:288:ILE:H	1:I:288:ILE:HD13	1.73	0.53
1:K:168:GLY:HA2	1:K:250:TYR:CZ	2.44	0.53
1:L:338:LEU:O	1:L:342:LEU:HD23	2.09	0.53
1:A:203:LYS:O	1:A:206:LYS:HG3	2.09	0.52
1:D:3:LYS:CA	1:D:449:LEU:HD22	2.39	0.52
1:E:206:LYS:HG2	3:E:509:HOH:O	2.09	0.52
1:G:113:ILE:HD13	1:G:114:MET:N	2.24	0.52
1:I:295:ASN:HD22	1:I:335:LEU:HD13	1.73	0.52
1:K:205:VAL:O	1:K:208:PHE:O	2.27	0.52
1:K:384:THR:HG21	1:K:450:GLU:HG3	1.91	0.52
1:L:341:LEU:O	1:L:341:LEU:HD23	2.08	0.52
1:H:84:ARG:NH1	3:H:502:HOH:O	2.43	0.52
1:I:160:ILE:HD13	1:I:400:TYR:OH	2.10	0.52
1:K:267:TYR:HA	1:K:270:LYS:HE3	1.91	0.52
1:K:380:LYS:O	1:K:384:THR:HG23	2.08	0.52
1:B:134:TRP:CZ3	3:B:604:HOH:O	2.54	0.52
1:C:326:MET:HE2	1:C:328:TRP:CZ2	2.44	0.52
1:G:11:ILE:HD13	1:G:397:LYS:O	2.10	0.52
1:K:218:GLY:HA2	1:K:288:ILE:CG1	2.39	0.52
1:L:72:GLY:HA3	1:L:443:ILE:HG21	1.90	0.52
1:L:89:GLY:HA3	1:L:128:LEU:CD1	2.40	0.52
1:D:3:LYS:HD3	1:D:449:LEU:HD22	1.91	0.52
1:I:54:ALA:HA	1:I:414:TYR:OH	2.08	0.52
1:A:73:ILE:HG13	1:A:73:ILE:O	2.09	0.52
1:C:409:GLU:C	3:C:503:HOH:O	2.47	0.52
1:D:23:GLY:HA3	1:D:53:VAL:O	2.08	0.52
1:J:29:GLY:HA3	1:J:94:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:HIS:HE1	1:F:52:ASP:OD1	1.93	0.52
1:G:121:HIS:HD2	3:G:508:HOH:O	1.92	0.52
1:I:223:LEU:HD12	1:I:293:PHE:CB	2.39	0.52
1:K:274:LEU:HD23	1:K:275:SER:N	2.25	0.52
1:A:211:MET:HB2	1:A:213:ILE:HD11	1.90	0.52
1:A:377:GLN:HE22	1:A:380:LYS:HE3	1.73	0.52
1:E:77:ARG:HH22	1:E:165:ASN:HD22	1.55	0.52
1:F:3:LYS:CB	1:F:449:LEU:HD22	2.39	0.52
1:H:186:ASP:OD2	1:H:189:THR:OG1	2.28	0.52
1:K:201:HIS:ND1	1:K:219:ILE:CG2	2.73	0.52
1:K:241:LEU:C	1:K:242:SER:O	2.46	0.52
1:K:380:LYS:HB2	1:K:448:PHE:CE2	2.44	0.52
1:L:223:LEU:O	1:L:224:SER:HB3	2.09	0.52
1:A:359:ALA:HA	1:A:417:ARG:O	2.10	0.52
1:B:208:PHE:O	1:B:211:MET:O	2.28	0.52
1:E:274:LEU:N	1:E:274:LEU:CD2	2.71	0.52
1:G:121:HIS:CE1	1:G:165:ASN:ND2	2.77	0.52
1:L:208:PHE:CE1	1:L:213:ILE:HD13	2.45	0.52
1:C:221:LEU:HD13	1:C:251:LEU:CD2	2.40	0.52
1:I:140:THR:HG22	1:I:200:SER:HA	1.92	0.52
1:I:326:MET:CE	1:I:418:PHE:CE1	2.93	0.52
1:K:242:SER:O	1:K:243:PHE:C	2.48	0.52
1:B:103:ARG:O	1:B:107:LEU:HD23	2.09	0.52
1:F:268:LYS:O	1:F:268:LYS:HD3	2.10	0.52
1:H:47:ASP:HB2	1:H:49:HIS:ND1	2.25	0.52
1:L:103:ARG:O	1:L:107:LEU:HD23	2.09	0.52
1:I:352:VAL:HG13	1:I:398:ALA:HB3	1.92	0.51
1:L:223:LEU:HD12	1:L:293:PHE:CB	2.40	0.51
1:A:266:LEU:N	3:A:602:HOH:O	2.43	0.51
1:D:10:PHE:HE1	1:D:396:LEU:CD2	2.23	0.51
1:E:306:SER:OG	1:E:307:SER:N	2.44	0.51
1:F:201:HIS:O	1:F:205:VAL:HG23	2.11	0.51
1:F:352:VAL:HG13	1:F:398:ALA:HB3	1.92	0.51
1:G:56:ASP:OD1	1:G:59:HIS:ND1	2.24	0.51
1:H:77:ARG:HH22	1:H:165:ASN:HD22	1.57	0.51
1:J:233:ALA:O	1:J:236:ILE:CD1	2.59	0.51
1:L:69:LYS:HE3	1:L:111:ASN:O	2.10	0.51
1:L:175:HIS:CA	1:L:184:ILE:HG23	2.37	0.51
1:C:353:ILE:HG12	1:C:398:ALA:O	2.10	0.51
1:E:144:THR:HG22	1:E:207:LEU:HD22	1.93	0.51
1:I:17:ALA:HB2	1:I:121:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:ASP:HB2	1:I:49:HIS:HD2	1.74	0.51
1:J:78:PHE:HE1	1:J:80:ILE:HD11	1.76	0.51
1:J:236:ILE:HD13	1:J:237:GLU:H	1.74	0.51
1:K:383:LEU:HB3	3:K:512:HOH:O	2.10	0.51
1:L:11:ILE:HD11	1:L:398:ALA:HB2	1.92	0.51
1:L:105:THR:HA	1:L:108:LEU:HG	1.92	0.51
1:A:293:PHE:C	1:A:294:ASN:HD22	2.14	0.51
1:K:370:ILE:H	1:K:370:ILE:HD12	1.74	0.51
1:L:385:GLN:HA	1:L:385:GLN:OE1	2.10	0.51
1:C:30:LYS:CE	1:C:84:ARG:HG3	2.41	0.51
1:E:82:TRP:HD1	1:E:125:PRO:HG3	1.74	0.51
1:K:39:SER:N	3:K:505:HOH:O	2.44	0.51
1:L:155:GLY:O	1:L:213:ILE:HD11	2.11	0.51
1:L:221:LEU:HD21	1:L:250:TYR:HB2	1.92	0.51
1:D:135:LYS:NZ	1:D:189:THR:HG23	2.25	0.51
1:K:56:ASP:HB3	1:K:428:LEU:CD1	2.40	0.51
1:K:370:ILE:HG13	1:K:433:LYS:HG3	1.92	0.51
1:G:166:GLU:HB3	1:G:169:VAL:CG2	2.41	0.51
1:I:293:PHE:CE1	1:I:353:ILE:HD13	2.46	0.51
1:I:350:ASN:C	1:I:351:ILE:HD12	2.32	0.51
1:K:288:ILE:HD13	1:K:290:PHE:N	2.23	0.51
1:C:68:MET:SD	1:C:73:ILE:HD11	2.51	0.51
1:D:54:ALA:HA	1:D:414:TYR:OH	2.10	0.51
1:E:47:ASP:HB2	1:E:49:HIS:CD2	2.46	0.51
1:F:157:ILE:HD13	3:F:504:HOH:O	2.09	0.51
1:G:446:ASN:ND2	3:G:503:HOH:O	2.27	0.51
1:H:211:MET:HB2	1:H:213:ILE:HD11	1.92	0.51
1:H:422:HIS:HA	1:H:433:LYS:HZ1	1.75	0.51
1:K:148:GLU:HG3	1:K:207:LEU:CD1	2.29	0.51
1:L:389:ALA:C	1:L:391:GLN:O	2.49	0.51
1:L:441:GLU:OE2	1:L:442:VAL:CG2	2.58	0.51
1:E:121:HIS:CE1	3:E:506:HOH:O	2.62	0.51
1:F:47:ASP:HB2	1:F:49:HIS:CD2	2.46	0.51
1:G:378:TYR:HD1	1:G:379:LEU:HD22	1.76	0.51
1:H:241:LEU:CD1	1:H:245:LEU:HD22	2.41	0.51
1:I:302:LYS:NZ	1:I:314:ALA:HA	2.26	0.51
1:I:326:MET:CE	1:I:418:PHE:HE1	2.24	0.51
1:K:322:GLU:O	1:K:330:ILE:HD12	2.11	0.51
1:A:102:LYS:HG2	1:A:154:LEU:HD21	1.92	0.50
1:B:85:ILE:N	1:B:85:ILE:CD1	2.74	0.50
1:I:195:HIS:HB2	1:I:276:PHE:HZ	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:PRO:HG2	1:J:280:ASP:CG	2.31	0.50
1:K:163:THR:HG1	1:K:219:ILE:HG22	1.76	0.50
1:L:155:GLY:C	1:L:213:ILE:HD11	2.31	0.50
1:B:441:GLU:C	3:B:611:HOH:O	2.49	0.50
1:C:406:ASP:HB2	1:C:423:VAL:CG1	2.37	0.50
1:B:321:PHE:HE2	1:B:331:TYR:CD2	2.28	0.50
1:B:372:ASP:O	1:B:376:ILE:HD12	2.12	0.50
1:B:378:TYR:CD1	1:B:378:TYR:C	2.85	0.50
1:F:158:VAL:HG13	1:F:161:TRP:CZ2	2.45	0.50
1:F:335:LEU:HG	1:F:339:LEU:HD11	1.92	0.50
1:G:47:ASP:HB2	1:G:49:HIS:CD2	2.47	0.50
1:G:288:ILE:HD11	1:G:291:ILE:CD1	2.42	0.50
1:I:76:TYR:CZ	1:I:78:PHE:HB3	2.46	0.50
1:K:6:PHE:HD2	1:K:10:PHE:CE2	2.29	0.50
1:L:73:ILE:O	1:L:113:ILE:HD13	2.11	0.50
1:L:175:HIS:HA	1:L:184:ILE:HG22	1.90	0.50
1:L:233:ALA:HA	1:L:236:ILE:HD11	1.92	0.50
1:L:440:LYS:O	1:L:444:LYS:CD	2.59	0.50
1:E:240:GLU:OE1	1:E:248:ARG:NH2	2.38	0.50
1:F:344:ARG:O	1:F:344:ARG:HD2	2.12	0.50
1:G:272:ILE:C	1:G:272:ILE:HD13	2.32	0.50
1:J:405:LEU:HB2	3:J:515:HOH:O	2.10	0.50
1:K:291:ILE:HD13	1:K:292:ALA:N	2.26	0.50
1:K:353:ILE:HD11	1:K:396:LEU:HD11	1.92	0.50
1:L:379:LEU:HD11	1:L:401:LEU:HD11	1.92	0.50
1:C:248:ARG:HA	1:C:251:LEU:HB2	1.92	0.50
1:E:295:ASN:HD22	1:E:335:LEU:HD13	1.77	0.50
1:J:207:LEU:C	1:J:207:LEU:CD2	2.79	0.50
1:K:209:ARG:O	1:K:212:ASN:CA	2.58	0.50
1:L:47:ASP:HB2	1:L:49:HIS:CD2	2.46	0.50
1:C:333:GLU:HA	1:C:385:GLN:HE21	1.76	0.50
1:D:376:ILE:HG13	1:D:377:GLN:N	2.26	0.50
1:F:363:GLU:HG3	3:F:511:HOH:O	2.11	0.50
1:H:379:LEU:HD11	1:H:401:LEU:HD11	1.94	0.50
1:I:390:ILE:CA	1:I:394:VAL:HG12	2.42	0.50
1:K:370:ILE:CG1	1:K:370:ILE:O	2.59	0.50
1:L:233:ALA:C	1:L:236:ILE:CD1	2.80	0.50
1:A:268:LYS:HD3	1:A:273:GLU:HB2	1.94	0.50
1:A:291:ILE:HG22	1:A:351:ILE:CD1	2.41	0.50
1:E:285:SER:O	1:E:286:GLN:C	2.50	0.50
1:F:339:LEU:HD21	1:F:396:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:208:PHE:CE2	1:K:217:ILE:HG13	2.46	0.50
1:A:153:ASN:O	1:A:154:LEU:C	2.51	0.50
1:C:61:TYR:O	1:C:65:ILE:HD13	2.12	0.50
1:C:223:LEU:HD12	1:C:293:PHE:CB	2.42	0.50
1:F:227:TYR:HB2	1:F:300:PHE:CD1	2.46	0.50
1:I:103:ARG:HG2	1:I:103:ARG:HH11	1.77	0.50
1:I:356:ASN:O	1:I:401:LEU:HD12	2.12	0.50
1:J:55:CYS:SG	1:J:406:ASP:O	2.70	0.50
1:L:10:PHE:HE1	1:L:396:LEU:CD2	2.25	0.50
1:A:38:PHE:HE1	3:A:609:HOH:O	1.94	0.50
1:A:205:VAL:O	1:A:209:ARG:HG2	2.12	0.50
1:C:161:TRP:CB	1:C:217:ILE:HD12	2.42	0.50
1:D:144:THR:HG22	1:D:207:LEU:HD12	1.94	0.50
1:F:85:ILE:N	1:F:85:ILE:CD1	2.75	0.50
1:G:348:LYS:HE2	1:G:393:GLY:O	2.12	0.50
1:I:421:VAL:HA	1:I:432:ILE:HA	1.94	0.50
1:L:195:HIS:CB	1:L:276:PHE:CE1	2.95	0.50
1:C:227:TYR:HB2	1:C:300:PHE:CD1	2.47	0.49
1:E:109:LEU:CD1	1:E:115:PRO:CG	2.90	0.49
1:F:77:ARG:HA	1:F:116:ALA:O	2.12	0.49
1:G:351:ILE:HD12	1:G:351:ILE:N	2.27	0.49
1:I:187:LEU:HD13	1:I:187:LEU:C	2.32	0.49
1:L:85:ILE:HD13	1:L:93:LEU:HD23	1.94	0.49
1:D:88:GLU:OE1	1:D:127:LYS:HE3	2.11	0.49
1:D:304:ASP:OD1	1:D:306:SER:HB3	2.12	0.49
1:D:364:ILE:HD13	1:D:370:ILE:CG1	2.43	0.49
1:E:211:MET:HB2	1:E:213:ILE:HD11	1.93	0.49
1:E:379:LEU:HD11	1:E:401:LEU:HD11	1.94	0.49
1:H:85:ILE:N	1:H:85:ILE:CD1	2.75	0.49
1:H:168:GLY:HA2	1:H:250:TYR:CZ	2.47	0.49
1:I:80:ILE:CD1	1:I:101:TYR:CD1	2.95	0.49
1:K:141:ASP:HA	1:K:144:THR:HG23	1.94	0.49
1:L:232:LYS:O	1:L:236:ILE:HD12	2.11	0.49
1:C:105:THR:O	1:C:109:LEU:HD12	2.12	0.49
1:F:364:ILE:HD13	1:F:431:LYS:HD2	1.94	0.49
1:K:211:MET:HB2	1:K:213:ILE:HD11	1.93	0.49
1:L:73:ILE:HG22	1:L:113:ILE:HG23	1.94	0.49
1:L:396:LEU:C	1:L:396:LEU:CD2	2.80	0.49
1:B:188:ARG:HD2	3:B:602:HOH:O	2.11	0.49
1:G:267:TYR:O	1:G:272:ILE:HG22	2.13	0.49
1:J:205:VAL:O	1:J:209:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:ALA:O	1:L:236:ILE:HD11	2.12	0.49
1:F:380:LYS:HB3	1:F:438:TRP:CZ2	2.48	0.49
1:I:240:GLU:OE1	1:I:248:ARG:NH2	2.35	0.49
1:B:425:PHE:HD1	3:B:620:HOH:O	1.91	0.49
1:E:226:HIS:CD2	1:E:242:SER:OG	2.65	0.49
1:H:216:GLN:HA	1:H:289:ASP:OD2	2.13	0.49
1:K:209:ARG:O	1:K:210:GLU:C	2.49	0.49
1:A:250:TYR:O	1:A:254:VAL:HG23	2.12	0.49
1:B:84:ARG:HB2	3:B:605:HOH:O	2.13	0.49
1:B:107:LEU:O	1:B:111:ASN:ND2	2.40	0.49
1:C:322:GLU:O	1:C:330:ILE:HD12	2.12	0.49
1:G:195:HIS:CG	1:G:276:PHE:HZ	2.24	0.49
1:G:195:HIS:CD2	1:G:276:PHE:CZ	3.00	0.49
1:J:164:HIS:HE1	1:J:197:LEU:HD12	1.73	0.49
1:L:232:LYS:HB2	1:L:235:ASP:OD1	2.13	0.49
1:L:379:LEU:C	1:L:383:LEU:HD12	2.33	0.49
1:A:35:TRP:HE3	3:A:601:HOH:O	1.96	0.49
1:B:354:SER:O	1:B:400:TYR:HB2	2.13	0.49
1:C:30:LYS:HE2	1:C:84:ARG:CZ	2.43	0.49
1:F:201:HIS:NE2	1:F:288:ILE:CD1	2.76	0.49
1:J:241:LEU:HD21	1:J:245:LEU:HD11	1.94	0.49
1:K:198:LEU:O	1:K:201:HIS:HB3	2.13	0.49
1:L:109:LEU:CD1	1:L:157:ILE:HG23	2.43	0.49
1:L:303:TYR:CE1	1:L:305:PRO:HD3	2.48	0.49
1:A:355:GLU:OE1	2:A:501:TRS:N	2.46	0.49
1:C:423:VAL:HG13	1:C:425:PHE:CZ	2.48	0.49
1:F:247:GLY:HA2	3:F:517:HOH:O	2.13	0.49
1:F:351:ILE:HD12	1:F:351:ILE:N	2.28	0.49
1:H:227:TYR:OH	1:H:334:GLY:HA2	2.13	0.49
1:I:326:MET:HE2	1:I:418:PHE:CE1	2.48	0.49
1:L:13:GLY:HA2	1:L:73:ILE:HD12	1.93	0.49
1:L:352:VAL:HG13	1:L:398:ALA:HB3	1.95	0.49
1:B:4:ILE:CG2	1:B:387:HIS:CG	2.96	0.48
1:B:352:VAL:HG13	1:B:398:ALA:HB3	1.95	0.48
1:I:61:TYR:CE2	1:I:103:ARG:NH1	2.80	0.48
1:I:194:SER:O	1:I:198:LEU:HD12	2.12	0.48
1:K:81:SER:OG	1:K:83:PRO:HD2	2.11	0.48
1:G:103:ARG:HD2	1:G:107:LEU:HD13	1.94	0.48
1:J:128:LEU:N	1:J:128:LEU:HD22	2.27	0.48
1:B:403:SER:O	1:B:419:GLY:HA2	2.14	0.48
1:H:146:TYR:O	1:H:150:ILE:CD1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:380:LYS:HB2	1:H:448:PHE:CE2	2.48	0.48
1:I:80:ILE:CD1	1:I:101:TYR:CG	2.96	0.48
1:E:352:VAL:HG13	1:E:398:ALA:HB3	1.96	0.48
1:F:376:ILE:HD11	1:F:435:SER:N	2.27	0.48
1:H:314:ALA:O	1:H:318:LEU:HD12	2.13	0.48
1:I:161:TRP:CB	1:I:217:ILE:HD12	2.43	0.48
1:K:44:ASN:C	1:K:45:ILE:HD13	2.33	0.48
1:K:288:ILE:HD13	1:K:289:ASP:N	2.28	0.48
1:L:241:LEU:O	1:L:245:LEU:HD22	2.13	0.48
1:B:16:THR:O	3:B:606:HOH:O	2.20	0.48
1:C:47:ASP:HB2	1:C:49:HIS:CD2	2.49	0.48
1:C:144:THR:HG22	1:C:207:LEU:HD22	1.95	0.48
1:F:187:LEU:O	1:F:191:LEU:HD23	2.14	0.48
1:F:242:SER:HB3	3:F:509:HOH:O	2.12	0.48
1:G:379:LEU:O	1:G:383:LEU:HD12	2.13	0.48
1:H:324:THR:HG23	1:H:326:MET:H	1.78	0.48
1:K:276:PHE:HB3	3:K:517:HOH:O	2.13	0.48
1:L:236:ILE:HD13	1:L:237:GLU:H	1.78	0.48
1:L:335:LEU:C	1:L:335:LEU:HD13	2.34	0.48
1:C:191:LEU:O	1:C:194:SER:OG	2.29	0.48
1:E:109:LEU:HD11	1:E:115:PRO:CG	2.44	0.48
1:G:268:LYS:CG	1:G:273:GLU:HG2	2.41	0.48
1:H:108:LEU:HA	1:H:111:ASN:OD1	2.14	0.48
1:I:428:LEU:HD12	1:I:428:LEU:N	2.28	0.48
1:L:321:PHE:HE2	1:L:331:TYR:CD2	2.29	0.48
1:L:351:ILE:HD12	1:L:351:ILE:N	2.28	0.48
1:A:154:LEU:HD23	1:A:154:LEU:N	2.26	0.48
1:G:208:PHE:CE2	1:G:217:ILE:CG1	2.97	0.48
1:J:326:MET:HA	1:J:326:MET:HE3	1.96	0.48
1:K:80:ILE:HG23	1:K:85:ILE:HD11	1.95	0.48
1:L:13:GLY:HA3	1:L:400:TYR:CD1	2.49	0.48
1:F:165:ASN:ND2	1:F:294:ASN:HD21	2.11	0.48
1:H:223:LEU:HD12	1:H:293:PHE:CB	2.43	0.48
1:D:105:THR:HG21	1:D:154:LEU:CD2	2.44	0.48
1:F:61:TYR:OH	1:F:103:ARG:NE	2.41	0.48
1:G:277:PRO:HG2	1:G:280:ASP:CG	2.34	0.48
1:H:315:ASN:CA	1:H:318:LEU:CD1	2.90	0.48
1:I:65:ILE:HG21	1:I:111:ASN:ND2	2.29	0.48
1:I:255:LEU:HD23	1:I:288:ILE:HD11	1.95	0.48
1:I:379:LEU:O	1:I:383:LEU:HD12	2.14	0.48
1:L:54:ALA:HA	1:L:414:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLY:O	1:A:139:THR:OG1	2.22	0.48
1:E:54:ALA:HA	1:E:414:TYR:OH	2.14	0.48
1:E:82:TRP:CH2	1:E:143:PHE:CA	2.93	0.48
1:G:212:ASN:HB3	1:H:306:SER:HA	1.96	0.48
1:H:241:LEU:CD2	1:H:262:ASN:HB2	2.44	0.48
1:J:56:ASP:HB3	1:J:428:LEU:CD1	2.44	0.48
1:K:266:LEU:O	1:K:266:LEU:HD13	2.14	0.48
1:B:4:ILE:CG2	1:B:387:HIS:CD2	2.95	0.47
1:C:274:LEU:HD12	1:C:275:SER:N	2.29	0.47
1:G:348:LYS:CE	1:G:393:GLY:O	2.61	0.47
1:G:406:ASP:OD1	1:G:419:GLY:HA3	2.13	0.47
1:K:219:ILE:CD1	1:K:221:LEU:HD11	2.43	0.47
1:L:165:ASN:HD21	1:L:294:ASN:ND2	2.05	0.47
1:L:201:HIS:O	1:L:205:VAL:HG23	2.13	0.47
1:F:40:HIS:CE1	1:F:52:ASP:OD1	2.67	0.47
1:F:322:GLU:CG	3:F:520:HOH:O	2.62	0.47
1:G:267:TYR:HB3	1:G:272:ILE:HG23	1.95	0.47
1:K:226:HIS:CD2	1:K:242:SER:OG	2.67	0.47
1:K:445:ASN:OD1	1:K:447:GLY:O	2.32	0.47
1:A:154:LEU:CD2	1:A:154:LEU:N	2.76	0.47
1:B:45:ILE:HD13	1:B:45:ILE:N	2.29	0.47
1:B:223:LEU:HD12	1:B:293:PHE:CB	2.43	0.47
1:D:335:LEU:HD21	1:D:339:LEU:HD11	1.96	0.47
1:F:54:ALA:HA	1:F:414:TYR:OH	2.13	0.47
1:H:216:GLN:CG	1:H:289:ASP:HB3	2.44	0.47
1:C:82:TRP:HB3	1:C:83:PRO:HD3	1.96	0.47
1:E:378:TYR:CD1	1:E:378:TYR:C	2.88	0.47
1:G:68:MET:O	1:G:71:ILE:O	2.33	0.47
1:H:111:ASN:OD1	1:H:113:ILE:HG22	2.13	0.47
1:H:432:ILE:H	1:H:432:ILE:HD12	1.79	0.47
1:I:259:TYR:CE1	1:I:281:LEU:HD21	2.46	0.47
1:K:219:ILE:HD13	1:K:221:LEU:HD11	1.96	0.47
1:B:56:ASP:HB3	1:B:428:LEU:CD1	2.44	0.47
1:B:274:LEU:HD23	1:B:275:SER:N	2.30	0.47
1:C:151:PHE:HB2	1:C:211:MET:HE1	1.96	0.47
1:D:223:LEU:HD12	1:D:293:PHE:CB	2.45	0.47
1:L:56:ASP:HB3	1:L:428:LEU:CD1	2.44	0.47
1:A:189:THR:O	1:A:193:VAL:CG1	2.60	0.47
1:E:326:MET:HE2	1:E:418:PHE:CE1	2.50	0.47
1:E:326:MET:HE3	1:E:418:PHE:CE1	2.50	0.47
1:F:93:LEU:HD11	1:F:98:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:TYR:OH	1:G:334:GLY:HA2	2.15	0.47
1:I:64:ASP:OD1	1:I:405:LEU:HD21	2.15	0.47
1:I:242:SER:O	1:I:243:PHE:C	2.52	0.47
1:J:103:ARG:O	1:J:107:LEU:HG	2.15	0.47
1:K:55:CYS:SG	1:K:406:ASP:O	2.73	0.47
1:L:207:LEU:O	1:L:207:LEU:HD22	2.15	0.47
1:F:123:ASP:OD1	3:F:501:HOH:O	2.20	0.47
1:G:394:VAL:O	1:G:395:ASN:HB2	2.15	0.47
1:H:241:LEU:HD22	1:H:262:ASN:HD22	1.79	0.47
1:J:187:LEU:C	1:J:187:LEU:CD2	2.83	0.47
1:J:233:ALA:CA	1:J:236:ILE:HD12	2.44	0.47
1:K:322:GLU:C	1:K:330:ILE:HD12	2.35	0.47
1:L:322:GLU:O	1:L:330:ILE:HD12	2.15	0.47
1:B:319:GLU:O	1:B:319:GLU:HG3	2.14	0.47
1:G:277:PRO:HG2	1:G:280:ASP:OD2	2.14	0.47
1:B:211:MET:HB2	1:B:213:ILE:CD1	2.44	0.47
1:C:401:LEU:HD12	1:C:402:TRP:N	2.30	0.47
1:D:352:VAL:HG13	1:D:398:ALA:HB3	1.95	0.47
1:H:216:GLN:HG2	1:H:289:ASP:HB2	1.95	0.47
1:I:116:ALA:CB	1:I:160:ILE:CD1	2.93	0.47
1:J:315:ASN:C	1:J:318:LEU:CD1	2.82	0.47
1:L:362:ASP:OD2	1:L:433:LYS:CE	2.63	0.47
1:A:134:TRP:O	1:A:196:ASN:ND2	2.48	0.47
1:B:15:ALA:O	1:B:403:SER:OG	2.23	0.47
1:B:319:GLU:HB2	3:B:615:HOH:O	2.14	0.47
1:C:30:LYS:CD	1:C:84:ARG:HG3	2.44	0.47
1:G:85:ILE:N	1:G:85:ILE:CD1	2.78	0.47
1:H:335:LEU:HD13	1:H:335:LEU:C	2.35	0.47
1:J:54:ALA:HA	1:J:414:TYR:OH	2.15	0.47
1:J:187:LEU:HD23	1:J:187:LEU:C	2.34	0.47
1:L:240:GLU:OE1	1:L:248:ARG:NH2	2.47	0.47
1:L:279:ASP:N	1:L:279:ASP:OD1	2.47	0.47
1:C:410:TRP:N	3:C:503:HOH:O	2.48	0.46
1:D:149:VAL:HB	3:D:517:HOH:O	2.15	0.46
1:E:239:ALA:CA	1:E:301:ILE:HG12	2.43	0.46
1:H:356:ASN:O	1:H:401:LEU:HD12	2.15	0.46
1:J:240:GLU:OE1	1:J:248:ARG:NH2	2.41	0.46
1:J:375:ARG:O	1:J:379:LEU:CD2	2.62	0.46
1:K:76:TYR:CZ	1:K:78:PHE:HB3	2.50	0.46
1:L:19:TYR:OH	3:L:502:HOH:O	2.20	0.46
1:L:233:ALA:CA	1:L:236:ILE:CD1	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:PHE:CE2	1:B:331:TYR:CD2	2.94	0.46
1:C:154:LEU:O	1:C:157:ILE:HD13	2.15	0.46
1:G:195:HIS:CE1	1:G:276:PHE:HE2	2.28	0.46
1:H:73:ILE:CG2	1:H:113:ILE:HD12	2.45	0.46
1:I:195:HIS:CB	1:I:276:PHE:CE1	2.98	0.46
1:L:3:LYS:CA	1:L:449:LEU:HD23	2.42	0.46
1:L:229:ALA:HB3	1:L:302:LYS:HB3	1.98	0.46
1:A:82:TRP:HB3	1:A:83:PRO:HD3	1.97	0.46
1:G:226:HIS:HB3	1:G:301:ILE:CD1	2.44	0.46
1:K:208:PHE:CE1	1:K:213:ILE:HB	2.50	0.46
1:L:378:TYR:CD1	1:L:378:TYR:C	2.89	0.46
1:A:375:ARG:O	1:A:379:LEU:HD23	2.15	0.46
1:C:301:ILE:C	1:C:301:ILE:HD12	2.36	0.46
1:G:61:TYR:OH	1:G:103:ARG:NH2	2.48	0.46
1:L:4:ILE:HG23	1:L:387:HIS:CG	2.50	0.46
1:C:294:ASN:OD1	1:C:355:GLU:CD	2.53	0.46
1:C:319:GLU:HG3	1:C:319:GLU:O	2.16	0.46
1:F:144:THR:HG22	1:F:207:LEU:HD22	1.97	0.46
1:I:168:GLY:HA2	1:I:250:TYR:CZ	2.50	0.46
1:J:223:LEU:HD12	1:J:293:PHE:CB	2.45	0.46
1:K:73:ILE:HD11	1:K:113:ILE:CD1	2.43	0.46
1:K:342:LEU:HG	1:K:351:ILE:HD11	1.97	0.46
1:E:211:MET:HB2	1:E:213:ILE:CD1	2.46	0.46
1:E:214:ASP:HB3	1:F:316:SER:HB3	1.96	0.46
1:F:364:ILE:CD1	1:F:431:LYS:HD2	2.45	0.46
1:I:11:ILE:CD1	1:I:114:MET:HE2	2.44	0.46
1:J:252:ASP:O	1:J:254:VAL:O	2.34	0.46
1:K:402:TRP:HA	1:K:403:SER:HA	1.66	0.46
1:C:197:LEU:HD13	1:C:197:LEU:HA	1.84	0.46
1:D:27:GLU:HA	1:J:88:GLU:OE2	2.15	0.46
1:D:62:GLU:HG2	1:D:63:GLU:N	2.31	0.46
1:F:166:GLU:HB3	1:F:169:VAL:CG2	2.46	0.46
1:H:45:ILE:HD13	1:H:45:ILE:N	2.30	0.46
1:H:216:GLN:CG	1:H:289:ASP:CB	2.93	0.46
1:H:332:PRO:O	1:H:385:GLN:HG3	2.15	0.46
1:K:217:ILE:O	1:K:288:ILE:HG12	2.16	0.46
1:L:302:LYS:HE3	1:L:313:PRO:O	2.15	0.46
1:L:341:LEU:HD23	3:L:512:HOH:O	2.16	0.46
1:C:201:HIS:O	1:C:205:VAL:HG23	2.16	0.46
1:D:135:LYS:HE3	1:D:189:THR:HG23	1.88	0.46
1:D:321:PHE:HE2	1:D:331:TYR:CD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:LEU:HD11	1:E:115:PRO:HG2	1.98	0.46
1:H:238:ALA:O	1:H:241:LEU:O	2.33	0.46
1:L:341:LEU:CD2	3:L:512:HOH:O	2.63	0.46
1:A:54:ALA:HA	1:A:414:TYR:OH	2.16	0.46
1:A:117:ILE:CG2	1:A:158:VAL:HG11	2.36	0.46
1:A:123:ASP:OD1	1:A:123:ASP:N	2.40	0.46
1:A:376:ILE:HG13	1:A:435:SER:HA	1.97	0.46
1:D:133:GLY:O	1:D:139:THR:OG1	2.23	0.46
1:H:147:SER:O	1:H:150:ILE:HD13	2.16	0.46
1:H:274:LEU:HD23	1:H:275:SER:N	2.30	0.46
1:H:406:ASP:OD1	1:H:419:GLY:HA3	2.16	0.46
1:I:267:TYR:O	1:I:268:LYS:HB2	2.16	0.46
1:L:360:PHE:O	1:L:362:ASP:OD1	2.34	0.46
1:A:324:THR:CG2	1:A:326:MET:O	2.63	0.46
1:A:356:ASN:HB3	1:A:399:TYR:CE1	2.51	0.46
1:B:66:LYS:HD2	1:B:66:LYS:C	2.36	0.46
1:C:73:ILE:HG13	1:C:73:ILE:O	2.15	0.46
1:F:135:LYS:HE2	1:F:189:THR:HG23	1.98	0.46
1:F:223:LEU:HD12	1:F:293:PHE:CB	2.45	0.46
1:G:110:GLU:O	1:G:111:ASN:HB2	2.16	0.46
1:I:77:ARG:HA	1:I:116:ALA:HB3	1.98	0.46
1:I:80:ILE:HD12	1:I:101:TYR:CG	2.51	0.46
1:K:187:LEU:HD23	1:K:191:LEU:CD2	2.46	0.46
1:L:438:TRP:HE3	1:L:439:TYR:N	1.96	0.46
1:D:105:THR:HG21	1:D:154:LEU:HD22	1.97	0.45
1:E:76:TYR:CD2	1:E:78:PHE:HD2	2.35	0.45
1:E:234:GLU:HB2	1:E:303:TYR:CD2	2.51	0.45
1:F:350:ASN:C	1:F:351:ILE:HD12	2.36	0.45
1:F:378:TYR:CD1	1:F:378:TYR:C	2.90	0.45
1:G:61:TYR:CZ	1:G:103:ARG:NH2	2.84	0.45
1:K:80:ILE:CD1	1:K:117:ILE:HG21	2.46	0.45
1:K:173:LEU:HD22	1:K:179:ILE:HD11	1.98	0.45
1:K:306:SER:HA	1:L:212:ASN:ND2	2.31	0.45
1:L:10:PHE:CE1	1:L:396:LEU:HD22	2.46	0.45
1:E:234:GLU:O	1:E:303:TYR:HD2	1.99	0.45
1:F:82:TRP:N	1:F:83:PRO:CD	2.80	0.45
1:F:169:VAL:O	1:F:173:LEU:HB2	2.16	0.45
1:G:353:ILE:HG13	1:G:396:LEU:HD21	1.99	0.45
1:I:82:TRP:HB3	1:I:83:PRO:HD3	1.97	0.45
1:I:116:ALA:HA	1:I:160:ILE:HG13	1.97	0.45
1:I:288:ILE:HD13	1:I:288:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:249:TRP:O	1:K:253:PRO:HG2	2.16	0.45
1:E:56:ASP:HB3	1:E:428:LEU:CD1	2.47	0.45
1:I:379:LEU:HD21	1:I:401:LEU:HD11	1.99	0.45
1:J:11:ILE:O	1:J:11:ILE:HG12	2.16	0.45
1:J:433:LYS:CD	3:J:501:HOH:O	2.64	0.45
1:L:108:LEU:HD12	1:L:109:LEU:HG	1.98	0.45
1:B:197:LEU:HD11	3:B:616:HOH:O	2.13	0.45
1:F:82:TRP:HB3	1:F:83:PRO:HD3	1.98	0.45
1:F:285:SER:O	1:F:286:GLN:C	2.54	0.45
1:G:211:MET:HB3	1:G:213:ILE:HD11	1.99	0.45
1:G:290:PHE:CD1	1:G:352:VAL:HG11	2.51	0.45
1:H:144:THR:HG22	1:H:207:LEU:HD22	1.97	0.45
1:I:274:LEU:HD13	1:I:275:SER:N	2.32	0.45
1:K:370:ILE:CG1	1:K:433:LYS:CG	2.94	0.45
1:K:370:ILE:O	1:K:370:ILE:HG12	2.17	0.45
1:C:216:GLN:HA	1:C:289:ASP:OD2	2.16	0.45
1:D:324:THR:CG2	1:D:359:ALA:O	2.63	0.45
1:H:146:TYR:O	1:H:150:ILE:HD13	2.16	0.45
1:H:149:VAL:O	1:H:153:ASN:ND2	2.46	0.45
1:I:227:TYR:OH	1:I:334:GLY:HA2	2.17	0.45
1:I:285:SER:O	1:I:286:GLN:C	2.54	0.45
1:J:212:ASN:O	1:J:212:ASN:ND2	2.50	0.45
1:A:446:ASN:ND2	1:A:446:ASN:O	2.50	0.45
1:C:261:GLU:OE2	1:C:265:LYS:HE3	2.16	0.45
1:F:227:TYR:OH	1:F:334:GLY:HA2	2.17	0.45
1:G:93:LEU:HD23	1:G:95:GLN:N	2.31	0.45
1:G:394:VAL:HG13	1:G:395:ASN:N	2.31	0.45
1:G:402:TRP:HA	1:G:403:SER:HA	1.69	0.45
1:I:190:SER:O	1:I:193:VAL:HG12	2.17	0.45
1:I:415:ASN:N	1:I:415:ASN:ND2	2.64	0.45
1:J:77:ARG:HA	1:J:116:ALA:O	2.16	0.45
1:J:173:LEU:HD22	1:J:179:ILE:HD11	1.97	0.45
1:J:295:ASN:O	1:J:356:ASN:OD1	2.34	0.45
1:K:64:ASP:O	1:K:67:ILE:HG23	2.17	0.45
1:L:85:ILE:HD13	1:L:93:LEU:CD2	2.45	0.45
1:A:227:TYR:OH	1:A:334:GLY:HA2	2.16	0.45
1:C:167:PRO:HD2	1:C:221:LEU:HD23	1.98	0.45
1:E:77:ARG:HA	1:E:116:ALA:O	2.17	0.45
1:G:373:THR:O	1:G:376:ILE:HG12	2.16	0.45
1:I:74:LYS:CG	3:I:511:HOH:O	2.64	0.45
1:I:241:LEU:HD13	1:I:241:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:189:THR:CB	3:J:506:HOH:O	2.60	0.45
1:K:64:ASP:O	1:K:67:ILE:CG2	2.64	0.45
1:K:342:LEU:HD23	1:K:343:ASP:H	1.82	0.45
1:L:45:ILE:N	1:L:45:ILE:CD1	2.79	0.45
1:D:227:TYR:HB2	1:D:300:PHE:CD1	2.52	0.45
1:G:82:TRP:HB3	1:G:83:PRO:HD3	1.99	0.45
1:I:309:SER:HB3	1:I:311:PHE:CE2	2.52	0.45
1:I:345:ASP:OD1	1:I:345:ASP:N	2.50	0.45
1:I:402:TRP:HA	1:I:403:SER:HA	1.67	0.45
1:K:379:LEU:HD21	1:K:401:LEU:HD11	1.99	0.45
1:L:73:ILE:HD13	1:L:73:ILE:HA	1.85	0.45
1:L:226:HIS:HB3	1:L:301:ILE:CD1	2.47	0.45
1:A:211:MET:HB2	1:A:213:ILE:CD1	2.47	0.45
1:B:4:ILE:HG21	1:B:387:HIS:CG	2.52	0.45
1:B:78:PHE:CE1	1:B:117:ILE:HG12	2.52	0.45
1:E:151:PHE:HB2	1:E:211:MET:HE1	1.99	0.45
1:G:105:THR:O	1:G:109:LEU:CD1	2.65	0.45
1:G:351:ILE:HG22	1:G:396:LEU:HD23	1.99	0.45
1:I:259:TYR:CZ	1:I:276:PHE:CZ	3.05	0.45
1:J:47:ASP:HB2	1:J:49:HIS:CD2	2.52	0.45
1:L:338:LEU:C	1:L:338:LEU:CD1	2.84	0.45
1:A:356:ASN:HB3	1:A:399:TYR:OH	2.17	0.45
1:B:146:TYR:O	1:B:149:VAL:HG22	2.16	0.45
1:B:419:GLY:O	1:B:433:LYS:HE2	2.16	0.45
1:E:387:HIS:CE1	1:E:391:GLN:NE2	2.85	0.45
1:F:186:ASP:OD2	1:F:189:THR:OG1	2.35	0.45
1:B:219:ILE:HG12	1:B:221:LEU:CD1	2.47	0.44
1:C:294:ASN:OD1	1:C:355:GLU:HG3	2.18	0.44
1:D:76:TYR:CD2	1:D:78:PHE:HD2	2.34	0.44
1:D:76:TYR:CZ	1:D:78:PHE:HB3	2.52	0.44
1:F:158:VAL:HG13	1:F:158:VAL:O	2.16	0.44
1:I:244:SER:CA	3:I:501:HOH:O	2.52	0.44
1:J:402:TRP:HA	1:J:403:SER:HA	1.72	0.44
1:K:163:THR:HG1	1:K:219:ILE:CG2	2.28	0.44
1:K:370:ILE:N	1:K:370:ILE:HD13	2.31	0.44
1:L:140:THR:HG21	1:L:196:ASN:HD22	1.82	0.44
1:E:105:THR:HG21	1:E:157:ILE:HD11	1.98	0.44
1:E:217:ILE:HG12	3:E:501:HOH:O	2.16	0.44
1:F:148:GLU:CG	1:F:211:MET:HE1	2.38	0.44
1:G:76:TYR:H	1:G:113:ILE:HD11	1.82	0.44
1:J:318:LEU:HD13	1:J:318:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:288:ILE:HA	3:K:508:HOH:O	2.16	0.44
1:B:44:ASN:C	1:B:45:ILE:HD13	2.38	0.44
1:F:3:LYS:HB2	1:F:449:LEU:HD22	1.99	0.44
1:G:103:ARG:CD	1:G:107:LEU:HD13	2.47	0.44
1:G:419:GLY:C	1:G:433:LYS:HE2	2.37	0.44
1:B:25:TYR:OH	1:H:130:ASP:OD2	2.32	0.44
1:B:340:MET:O	1:B:344:ARG:HG3	2.17	0.44
1:D:82:TRP:HB3	1:D:83:PRO:HD3	2.00	0.44
1:D:135:LYS:HZ1	1:D:189:THR:HA	1.83	0.44
1:F:11:ILE:CD1	1:F:11:ILE:N	2.80	0.44
1:H:60:ARG:HG2	3:H:515:HOH:O	2.16	0.44
1:H:82:TRP:N	1:H:83:PRO:CD	2.80	0.44
1:H:375:ARG:O	1:H:378:TYR:HB3	2.17	0.44
1:H:428:LEU:N	1:H:428:LEU:HD12	2.33	0.44
1:K:403:SER:O	1:K:419:GLY:HA2	2.17	0.44
1:L:233:ALA:O	1:L:236:ILE:CD1	2.65	0.44
1:L:340:MET:CE	1:L:394:VAL:HG23	2.47	0.44
1:C:227:TYR:HB2	1:C:300:PHE:CE1	2.52	0.44
1:D:173:LEU:HD22	1:D:179:ILE:HD11	1.99	0.44
1:H:44:ASN:C	1:H:45:ILE:HD13	2.38	0.44
1:H:304:ASP:OD1	1:H:306:SER:OG	2.33	0.44
1:J:379:LEU:HD11	1:J:401:LEU:HD11	1.99	0.44
1:L:249:TRP:O	1:L:253:PRO:HG2	2.17	0.44
1:A:105:THR:HG21	1:A:154:LEU:HD13	1.99	0.44
1:B:291:ILE:HD11	1:B:351:ILE:HG12	1.98	0.44
1:G:93:LEU:HD23	1:G:94:ASN:N	2.33	0.44
1:H:379:LEU:HD11	1:H:401:LEU:CD1	2.48	0.44
1:K:140:THR:O	1:K:144:THR:HG22	2.17	0.44
1:K:370:ILE:O	1:K:370:ILE:HD13	2.17	0.44
1:L:77:ARG:HA	1:L:116:ALA:O	2.18	0.44
1:F:402:TRP:HA	1:F:403:SER:HA	1.67	0.44
1:G:76:TYR:HB3	1:G:113:ILE:HD11	2.00	0.44
1:J:211:MET:HB2	1:J:213:ILE:HD11	1.99	0.44
1:K:119:LEU:HD21	1:K:161:TRP:HE3	1.82	0.44
1:B:77:ARG:HA	1:B:116:ALA:O	2.17	0.44
1:B:268:LYS:HD3	1:B:273:GLU:HB2	2.00	0.44
1:D:372:ASP:OD1	1:D:375:ARG:NH1	2.50	0.44
1:G:390:ILE:HD13	1:G:390:ILE:O	2.17	0.44
1:G:431:LYS:HE2	1:G:431:LYS:HA	2.00	0.44
1:H:449:LEU:O	1:H:450:GLU:HB3	2.18	0.44
1:J:264:LEU:HD21	1:J:276:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:GLY:O	1:K:73:ILE:O	2.36	0.44
1:K:163:THR:OG1	1:K:219:ILE:CG2	2.63	0.44
1:L:380:LYS:HG2	1:L:448:PHE:HE2	1.76	0.44
1:B:20:GLN:HA	3:B:613:HOH:O	2.17	0.44
1:F:354:SER:O	1:F:400:TYR:HB2	2.18	0.44
1:G:3:LYS:CA	1:G:449:LEU:HD13	2.45	0.44
1:H:351:ILE:HG22	1:H:396:LEU:HD23	1.99	0.44
1:I:198:LEU:O	1:I:284:ILE:HD12	2.18	0.44
1:J:266:LEU:O	1:J:266:LEU:HD22	2.18	0.44
1:K:82:TRP:HB3	1:K:83:PRO:HD3	2.00	0.44
1:K:360:PHE:O	1:K:362:ASP:OD1	2.35	0.44
1:L:174:GLY:O	1:L:182:PRO:O	2.36	0.44
1:B:171:SER:CB	3:B:616:HOH:O	2.63	0.43
1:B:227:TYR:HB2	1:B:300:PHE:CD1	2.53	0.43
1:G:324:THR:CG2	1:G:359:ALA:O	2.65	0.43
1:G:349:PRO:O	1:G:351:ILE:CD1	2.66	0.43
1:H:166:GLU:HB3	1:H:169:VAL:CG2	2.45	0.43
1:H:353:ILE:HG13	1:H:396:LEU:HD21	1.99	0.43
1:H:375:ARG:O	1:H:379:LEU:HD23	2.18	0.43
1:I:351:ILE:HD12	1:I:351:ILE:N	2.33	0.43
1:L:4:ILE:CG1	1:L:387:HIS:ND1	2.80	0.43
1:L:108:LEU:O	1:L:113:ILE:O	2.35	0.43
1:C:77:ARG:HA	1:C:116:ALA:O	2.16	0.43
1:D:206:LYS:HD2	1:D:283:LEU:HD11	2.00	0.43
1:D:357:GLY:HA3	1:D:402:TRP:O	2.18	0.43
1:H:89:GLY:HA3	1:H:128:LEU:CD1	2.47	0.43
1:J:81:SER:OG	1:J:83:PRO:HD2	2.18	0.43
1:J:318:LEU:HD22	1:J:319:GLU:N	2.33	0.43
1:K:411:ALA:HB3	3:K:521:HOH:O	2.18	0.43
1:L:114:MET:CG	1:L:159:PRO:HG3	2.48	0.43
1:L:302:LYS:CE	1:L:314:ALA:HA	2.44	0.43
1:A:345:ASP:HB2	1:A:346:TYR:CD2	2.53	0.43
1:E:437:TYR:O	1:E:440:LYS:HB3	2.18	0.43
1:F:329:ILE:H	1:F:329:ILE:HD13	1.82	0.43
1:G:13:GLY:O	1:G:400:TYR:HA	2.17	0.43
1:G:223:LEU:HD12	1:G:293:PHE:CB	2.47	0.43
1:G:309:SER:HB3	1:G:311:PHE:CE1	2.54	0.43
1:H:47:ASP:OD2	1:H:49:HIS:CE1	2.70	0.43
1:H:73:ILE:HG23	1:H:113:ILE:HD12	2.00	0.43
1:H:227:TYR:HB2	1:H:300:PHE:CE1	2.53	0.43
1:I:318:LEU:HD22	1:I:318:LEU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:71:ILE:HD11	1:K:436:GLY:O	2.18	0.43
1:C:56:ASP:HB3	1:C:428:LEU:CD1	2.48	0.43
1:D:77:ARG:HA	1:D:116:ALA:O	2.18	0.43
1:E:285:SER:O	1:E:286:GLN:O	2.37	0.43
1:F:201:HIS:CE1	1:F:288:ILE:CD1	3.02	0.43
1:G:10:PHE:HE1	1:G:396:LEU:CD1	2.31	0.43
1:G:144:THR:HG22	1:G:207:LEU:HD22	1.99	0.43
1:J:78:PHE:CE1	1:J:80:ILE:HD11	2.53	0.43
1:A:82:TRP:N	1:A:83:PRO:CD	2.81	0.43
1:A:151:PHE:HB2	1:A:211:MET:HE1	2.01	0.43
1:A:402:TRP:HA	1:A:403:SER:HA	1.70	0.43
1:B:206:LYS:HD2	1:B:206:LYS:C	2.38	0.43
1:B:213:ILE:H	1:B:213:ILE:HD12	1.84	0.43
1:B:291:ILE:HD12	1:B:291:ILE:C	2.38	0.43
1:C:250:TYR:O	1:C:254:VAL:HG23	2.19	0.43
1:E:165:ASN:O	1:E:166:GLU:C	2.57	0.43
1:E:356:ASN:HB3	1:E:399:TYR:CE1	2.53	0.43
1:I:280:ASP:O	1:I:283:LEU:HB3	2.17	0.43
1:J:11:ILE:CG1	1:J:398:ALA:HB2	2.49	0.43
1:J:62:GLU:O	1:J:66:LYS:HG2	2.18	0.43
1:K:364:ILE:HD13	1:K:370:ILE:HG23	2.00	0.43
1:L:256:LYS:HD2	1:L:346:TYR:CE2	2.53	0.43
1:A:326:MET:C	1:A:328:TRP:H	2.22	0.43
1:F:353:ILE:HG13	1:F:396:LEU:HD11	1.99	0.43
1:I:281:LEU:HD13	1:I:281:LEU:HA	1.84	0.43
1:K:56:ASP:CB	1:K:428:LEU:CD1	2.96	0.43
1:K:119:LEU:O	1:K:146:TYR:OH	2.32	0.43
1:A:323:LYS:HD2	1:A:329:ILE:HA	2.00	0.43
1:D:47:ASP:HB2	1:D:49:HIS:CD2	2.54	0.43
1:H:88:GLU:OE2	1:H:127:LYS:NZ	2.49	0.43
1:J:259:TYR:CE1	1:J:281:LEU:HD11	2.54	0.43
1:K:223:LEU:HD12	1:K:293:PHE:CB	2.48	0.43
1:K:226:HIS:HB3	1:K:301:ILE:CD1	2.49	0.43
1:K:342:LEU:HD23	1:K:343:ASP:N	2.33	0.43
1:L:163:THR:OG1	1:L:164:HIS:CE1	2.67	0.43
1:A:6:PHE:CE2	1:A:12:TRP:HH2	2.37	0.43
1:C:249:TRP:O	1:C:253:PRO:HG2	2.18	0.43
1:D:3:LYS:HB2	1:D:449:LEU:CD2	2.49	0.43
1:E:154:LEU:O	1:E:157:ILE:HG13	2.18	0.43
1:E:210:GLU:O	1:F:305:PRO:HD2	2.19	0.43
1:G:173:LEU:HD22	1:G:179:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:228:PRO:HB3	1:J:236:ILE:HA	1.99	0.43
1:K:133:GLY:O	1:K:139:THR:HG21	2.19	0.43
1:K:208:PHE:CD1	1:K:213:ILE:HD13	2.53	0.43
1:K:335:LEU:CD2	1:K:339:LEU:HD13	2.48	0.43
1:L:109:LEU:CD1	1:L:157:ILE:HG21	2.48	0.43
1:L:248:ARG:HA	1:L:251:LEU:HB2	2.00	0.43
1:L:379:LEU:HD11	1:L:401:LEU:CD1	2.47	0.43
1:B:82:TRP:HB3	1:B:83:PRO:HD3	2.01	0.43
1:B:244:SER:HB3	1:B:263:ALA:HB2	2.00	0.43
1:D:78:PHE:CE1	1:D:117:ILE:HG12	2.53	0.43
1:D:378:TYR:C	1:D:378:TYR:CD1	2.92	0.43
1:K:321:PHE:CE1	1:K:331:TYR:HD2	2.37	0.43
1:A:102:LYS:HG2	1:A:154:LEU:CD2	2.49	0.43
1:A:186:ASP:HB3	1:A:189:THR:HG21	1.99	0.43
1:B:149:VAL:HG23	1:B:150:ILE:CD1	2.49	0.43
1:C:4:ILE:CG2	1:C:387:HIS:CG	3.01	0.43
1:F:17:ALA:HB3	1:F:20:GLN:NE2	2.34	0.43
1:F:25:TYR:CZ	1:F:26:ASN:ND2	2.87	0.43
1:G:17:ALA:O	1:G:21:ILE:HG12	2.18	0.43
1:G:199:LEU:HG	1:G:203:LYS:HD2	2.01	0.43
1:H:147:SER:C	1:H:150:ILE:CD1	2.87	0.43
1:H:167:PRO:HD2	1:H:221:LEU:HD23	2.00	0.43
1:H:314:ALA:C	1:H:318:LEU:HD12	2.40	0.43
1:I:74:LYS:HG3	3:I:511:HOH:O	2.18	0.43
1:I:140:THR:HG23	1:I:200:SER:CB	2.47	0.43
1:J:187:LEU:O	1:J:190:SER:OG	2.24	0.43
1:J:448:PHE:HB3	3:J:510:HOH:O	2.19	0.43
1:L:319:GLU:OE1	1:L:323:LYS:HE2	2.19	0.43
1:A:121:HIS:CD2	3:A:608:HOH:O	2.72	0.42
1:A:135:LYS:HZ1	1:A:189:THR:HA	1.84	0.42
1:G:212:ASN:HB3	1:H:306:SER:CA	2.49	0.42
1:H:10:PHE:CE1	1:H:396:LEU:CD1	3.02	0.42
1:I:55:CYS:SG	1:I:406:ASP:O	2.76	0.42
1:I:173:LEU:HD22	1:I:179:ILE:HD11	2.01	0.42
1:J:243:PHE:HD1	1:J:248:ARG:HB2	1.84	0.42
1:H:245:LEU:HD13	1:H:263:ALA:HB1	2.00	0.42
1:J:80:ILE:CD1	1:J:80:ILE:N	2.82	0.42
1:J:166:GLU:OE1	1:J:169:VAL:HG21	2.18	0.42
1:K:209:ARG:O	1:K:211:MET:N	2.52	0.42
1:B:285:SER:O	1:B:286:GLN:C	2.57	0.42
1:C:363:GLU:HG3	3:C:514:HOH:O	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:LEU:O	1:E:155:GLY:C	2.57	0.42
1:F:268:LYS:CE	1:F:273:GLU:HB3	2.49	0.42
1:G:384:THR:HG21	1:G:450:GLU:OE1	2.19	0.42
1:J:356:ASN:O	1:J:401:LEU:HD12	2.19	0.42
1:L:319:GLU:OE1	1:L:319:GLU:HA	2.19	0.42
1:A:244:SER:O	1:A:249:TRP:HB2	2.19	0.42
1:A:352:VAL:HG13	1:A:398:ALA:HB3	2.01	0.42
1:B:336:TYR:CE2	1:B:388:ARG:HG2	2.54	0.42
1:B:364:ILE:HD13	1:B:431:LYS:HD2	2.02	0.42
1:H:102:LYS:HE3	1:H:153:ASN:HB3	2.00	0.42
1:H:174:GLY:HA2	1:H:180:HIS:O	2.19	0.42
1:J:297:SER:OG	1:J:329:ILE:HG13	2.19	0.42
1:K:353:ILE:HD11	1:K:396:LEU:HD21	2.02	0.42
1:L:81:SER:OG	1:L:84:ARG:HG3	2.19	0.42
1:L:291:ILE:O	1:L:291:ILE:HG23	2.19	0.42
1:L:319:GLU:HG3	1:L:319:GLU:O	2.20	0.42
1:D:219:ILE:HG23	1:D:221:LEU:CD1	2.49	0.42
1:F:187:LEU:O	1:F:191:LEU:HD22	2.19	0.42
1:G:140:THR:HG22	1:G:196:ASN:O	2.20	0.42
1:G:347:GLY:O	1:G:348:LYS:C	2.58	0.42
1:H:38:PHE:O	1:H:44:ASN:ND2	2.37	0.42
1:H:187:LEU:O	1:H:190:SER:HB3	2.19	0.42
1:K:291:ILE:HD13	1:K:292:ALA:O	2.19	0.42
1:A:28:ASP:OD2	1:A:58:TYR:OH	2.24	0.42
1:A:378:TYR:CD1	1:A:378:TYR:C	2.92	0.42
1:C:352:VAL:HG13	1:C:398:ALA:HB3	2.01	0.42
1:E:3:LYS:HA	1:E:449:LEU:HA	2.01	0.42
1:F:81:SER:O	1:F:85:ILE:HD13	2.20	0.42
1:K:216:GLN:HA	1:K:289:ASP:OD2	2.19	0.42
1:K:322:GLU:OE1	3:K:502:HOH:O	2.22	0.42
1:L:211:MET:O	1:L:212:ASN:CG	2.58	0.42
1:L:302:LYS:HG3	1:L:314:ALA:HB2	2.01	0.42
1:A:23:GLY:HA3	1:A:53:VAL:O	2.20	0.42
1:A:89:GLY:HA3	1:A:128:LEU:CD1	2.48	0.42
1:A:201:HIS:O	1:A:205:VAL:HG23	2.19	0.42
1:F:168:GLY:HA2	1:F:250:TYR:CZ	2.54	0.42
1:F:199:LEU:HD12	1:F:283:LEU:HD23	2.01	0.42
1:F:380:LYS:HB2	1:F:448:PHE:CE2	2.55	0.42
1:G:76:TYR:N	1:G:113:ILE:HD11	2.35	0.42
1:G:186:ASP:OD2	1:G:189:THR:OG1	2.37	0.42
1:I:428:LEU:N	1:I:428:LEU:CD1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:318:LEU:CD1	1:J:318:LEU:H	2.33	0.42
1:J:383:LEU:CD2	1:J:399:TYR:CZ	3.02	0.42
1:K:187:LEU:HD23	1:K:187:LEU:C	2.40	0.42
1:K:323:LYS:HB2	1:K:323:LYS:HE2	1.78	0.42
1:A:190:SER:O	1:A:193:VAL:HG13	2.20	0.42
1:A:369:LYS:NZ	1:A:434:ASP:OD1	2.53	0.42
1:G:107:LEU:HA	1:G:110:GLU:HG3	2.02	0.42
1:H:82:TRP:HB3	1:H:83:PRO:HD3	2.02	0.42
1:H:272:ILE:H	1:H:272:ILE:HD12	1.84	0.42
1:K:306:SER:HA	1:L:212:ASN:CG	2.39	0.42
1:L:13:GLY:HA2	1:L:75:SER:O	2.20	0.42
1:L:371:GLU:HA	1:L:434:ASP:OD2	2.20	0.42
1:L:372:ASP:OD2	1:L:435:SER:OG	2.25	0.42
1:L:402:TRP:HA	1:L:403:SER:HA	1.70	0.42
1:A:25:TYR:OH	1:G:130:ASP:OD2	2.28	0.42
1:B:293:PHE:HE1	1:B:295:ASN:HB2	1.85	0.42
1:D:401:LEU:HD23	1:D:401:LEU:C	2.39	0.42
1:E:33:SER:HB3	1:E:83:PRO:HG2	2.00	0.42
1:E:140:THR:HG21	1:E:196:ASN:HD22	1.85	0.42
1:F:323:LYS:HE2	1:F:323:LYS:N	2.35	0.42
1:G:135:LYS:HD3	1:G:189:THR:CG2	2.45	0.42
1:H:211:MET:HB2	1:H:213:ILE:CD1	2.50	0.42
1:H:241:LEU:HD22	1:H:262:ASN:ND2	2.35	0.42
1:I:66:LYS:C	1:I:66:LYS:HD3	2.40	0.42
1:I:318:LEU:HD22	1:I:318:LEU:N	2.34	0.42
1:J:149:VAL:O	1:J:153:ASN:ND2	2.46	0.42
1:K:364:ILE:HD13	1:K:370:ILE:CG2	2.49	0.42
1:A:6:PHE:CD2	1:A:12:TRP:CH2	3.08	0.42
1:C:4:ILE:HG23	1:C:387:HIS:CD2	2.55	0.42
1:E:239:ALA:N	1:E:301:ILE:CD1	2.80	0.42
1:G:93:LEU:HD23	1:G:93:LEU:C	2.40	0.42
1:I:223:LEU:HD12	1:I:293:PHE:HB2	2.02	0.42
1:K:321:PHE:O	1:K:323:LYS:HD3	2.19	0.42
1:K:335:LEU:O	1:K:339:LEU:CD1	2.68	0.42
1:K:373:THR:HA	1:K:376:ILE:HD12	2.02	0.42
1:L:108:LEU:HD13	1:L:115:PRO:HD3	2.02	0.42
1:A:11:ILE:HD11	1:A:398:ALA:HB2	2.00	0.41
1:A:140:THR:HG22	1:A:196:ASN:O	2.20	0.41
1:B:120:TYR:CE1	1:B:122:TRP:HA	2.55	0.41
1:E:11:ILE:HG21	3:E:522:HOH:O	2.20	0.41
1:E:204:ALA:O	1:E:208:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:THR:HA	1:E:376:ILE:HD12	2.02	0.41
1:G:276:PHE:CD2	1:G:281:LEU:CD2	3.03	0.41
1:G:288:ILE:HG13	1:G:290:PHE:O	2.20	0.41
1:G:290:PHE:CE1	1:G:352:VAL:HG11	2.55	0.41
1:H:4:ILE:HD11	1:H:448:PHE:CZ	2.55	0.41
1:J:77:ARG:HH22	1:J:165:ASN:ND2	2.15	0.41
1:J:82:TRP:HB3	1:J:83:PRO:HD3	2.01	0.41
1:A:372:ASP:O	1:A:376:ILE:HD12	2.20	0.41
1:B:402:TRP:HA	1:B:403:SER:HA	1.61	0.41
1:C:161:TRP:HB2	1:C:217:ILE:HD12	2.03	0.41
1:E:53:VAL:HG23	1:E:54:ALA:N	2.34	0.41
1:E:250:TYR:O	1:E:254:VAL:HG23	2.20	0.41
1:E:402:TRP:HA	1:E:403:SER:HA	1.73	0.41
1:F:227:TYR:HB2	1:F:300:PHE:CE1	2.54	0.41
1:G:195:HIS:CD2	1:G:276:PHE:CE2	3.07	0.41
1:H:402:TRP:HA	1:H:403:SER:HA	1.67	0.41
1:J:233:ALA:CA	1:J:236:ILE:HD11	2.49	0.41
1:K:342:LEU:N	1:K:342:LEU:HD23	2.36	0.41
1:A:38:PHE:CB	1:A:181:ALA:HB2	2.50	0.41
1:A:135:LYS:NZ	1:A:189:THR:HA	2.35	0.41
1:B:144:THR:HG22	1:B:207:LEU:HD22	2.01	0.41
1:C:326:MET:HE1	1:C:412:TYR:CE2	2.56	0.41
1:D:126:GLN:NE2	1:D:129:GLN:HB3	2.35	0.41
1:D:207:LEU:C	1:D:207:LEU:CD2	2.88	0.41
1:E:109:LEU:CD1	1:E:115:PRO:HG3	2.50	0.41
1:E:275:SER:O	1:E:276:PHE:O	2.38	0.41
1:G:123:ASP:OD1	1:G:123:ASP:N	2.53	0.41
1:H:441:GLU:CD	1:H:444:LYS:HE3	2.41	0.41
1:J:250:TYR:O	1:J:254:VAL:CG2	2.47	0.41
1:J:315:ASN:CA	1:J:318:LEU:HD12	2.37	0.41
1:K:207:LEU:HD23	1:K:207:LEU:O	2.20	0.41
1:K:352:VAL:HG13	1:K:398:ALA:HB3	2.03	0.41
1:L:101:TYR:O	1:L:105:THR:HG23	2.20	0.41
1:L:104:LEU:C	1:L:104:LEU:HD23	2.40	0.41
1:A:163:THR:OG1	1:A:201:HIS:HD2	2.03	0.41
1:B:19:TYR:HE2	1:B:408:PHE:CE2	2.39	0.41
1:C:199:LEU:CD1	1:C:283:LEU:HD23	2.50	0.41
1:F:56:ASP:HB3	1:F:428:LEU:HD13	2.03	0.41
1:J:20:GLN:O	1:J:407:ASN:HB2	2.20	0.41
1:J:21:ILE:HD12	1:J:57:HIS:CD2	2.56	0.41
1:J:335:LEU:O	1:J:339:LEU:CD2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:76:TYR:CB	1:K:113:ILE:HD11	2.47	0.41
1:K:385:GLN:OE1	1:K:385:GLN:HA	2.20	0.41
1:L:285:SER:O	1:L:286:GLN:C	2.58	0.41
1:D:76:TYR:CE2	1:D:78:PHE:CD2	3.09	0.41
1:D:128:LEU:CD1	1:D:128:LEU:N	2.84	0.41
1:G:11:ILE:HD11	1:G:398:ALA:HB2	2.02	0.41
1:G:285:SER:O	1:G:286:GLN:C	2.59	0.41
1:H:147:SER:C	1:H:150:ILE:HD13	2.41	0.41
1:H:189:THR:O	1:H:193:VAL:HG13	2.19	0.41
1:I:13:GLY:O	1:I:400:TYR:HA	2.20	0.41
1:L:82:TRP:HB3	1:L:83:PRO:HD3	2.02	0.41
1:L:233:ALA:CA	1:L:236:ILE:HD12	2.49	0.41
1:L:438:TRP:CD2	1:L:439:TYR:N	2.87	0.41
1:A:93:LEU:HD11	1:A:98:LEU:HD13	1.99	0.41
1:E:319:GLU:O	1:E:319:GLU:HG3	2.21	0.41
1:E:364:ILE:CD1	1:E:431:LYS:HE3	2.50	0.41
1:F:173:LEU:HD13	1:F:179:ILE:CG1	2.50	0.41
1:G:108:LEU:HD22	1:G:113:ILE:HD12	2.01	0.41
1:G:195:HIS:CB	1:G:276:PHE:HZ	2.26	0.41
1:H:76:TYR:CB	1:H:113:ILE:HD11	2.50	0.41
1:H:241:LEU:HD13	1:H:241:LEU:HA	1.86	0.41
1:I:121:HIS:O	1:I:122:TRP:HB2	2.20	0.41
1:I:123:ASP:OD1	1:I:123:ASP:N	2.47	0.41
1:I:255:LEU:CD2	1:I:288:ILE:HD11	2.49	0.41
1:K:67:ILE:CG1	1:K:432:ILE:HD11	2.50	0.41
1:L:58:TYR:HD1	1:L:100:PHE:CE2	2.39	0.41
1:L:268:LYS:HD3	1:L:273:GLU:HB2	2.02	0.41
1:A:61:TYR:OH	1:A:103:ARG:NE	2.44	0.41
1:C:241:LEU:HD21	1:C:266:LEU:HD22	2.02	0.41
1:D:420:ILE:O	1:D:421:VAL:O	2.38	0.41
1:G:168:GLY:HA2	1:G:250:TYR:CZ	2.56	0.41
1:H:54:ALA:HA	1:H:414:TYR:OH	2.21	0.41
1:H:135:LYS:HD2	1:H:189:THR:HG23	2.02	0.41
1:H:154:LEU:N	1:H:154:LEU:CD1	2.84	0.41
1:K:339:LEU:O	1:K:342:LEU:HD23	2.20	0.41
1:L:438:TRP:CH2	1:L:439:TYR:HD1	2.39	0.41
1:A:258:ARG:NH2	1:I:369:LYS:HE2	2.35	0.41
1:C:370:ILE:HD12	1:C:370:ILE:N	2.35	0.41
1:D:379:LEU:C	1:D:383:LEU:HD12	2.41	0.41
1:H:147:SER:O	1:H:150:ILE:HD11	2.21	0.41
1:H:213:ILE:H	1:H:213:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:ILE:HB	1:I:387:HIS:ND1	2.36	0.41
1:I:51:GLY:O	1:I:52:ASP:C	2.59	0.41
1:I:154:LEU:O	1:I:157:ILE:HD13	2.21	0.41
1:J:227:TYR:CD2	1:J:300:PHE:CE1	3.09	0.41
1:J:380:LYS:HB2	1:J:448:PHE:CE2	2.55	0.41
1:K:3:LYS:HA	1:K:449:LEU:HA	2.03	0.41
1:A:244:SER:HA	1:A:248:ARG:HB3	2.02	0.41
1:B:22:GLU:CD	3:B:630:HOH:O	2.59	0.41
1:B:85:ILE:N	1:B:85:ILE:HD13	2.36	0.41
1:B:336:TYR:HE2	1:B:388:ARG:HG2	1.85	0.41
1:C:56:ASP:O	1:C:56:ASP:OD1	2.39	0.41
1:D:49:HIS:ND1	1:D:414:TYR:HD2	2.18	0.41
1:D:377:GLN:CD	1:D:380:LYS:HE2	2.42	0.41
1:E:66:LYS:C	1:E:66:LYS:HD3	2.41	0.41
1:E:362:ASP:OD2	1:E:433:LYS:NZ	2.50	0.41
1:F:225:TYR:CE1	1:F:341:LEU:HD12	2.55	0.41
1:G:319:GLU:HG3	1:G:319:GLU:O	2.21	0.41
1:G:333:GLU:HA	1:G:385:GLN:HE21	1.86	0.41
1:G:378:TYR:CD1	1:G:378:TYR:C	2.95	0.41
1:H:364:ILE:HD13	1:H:431:LYS:CE	2.49	0.41
1:I:198:LEU:O	1:I:201:HIS:HB3	2.21	0.41
1:I:293:PHE:CZ	1:I:353:ILE:CD1	3.04	0.41
1:J:102:LYS:HA	1:J:154:LEU:HD21	2.03	0.41
1:J:167:PRO:HD2	1:J:221:LEU:HD23	2.03	0.41
1:J:251:LEU:O	1:J:254:VAL:O	2.39	0.41
1:L:175:HIS:ND1	1:L:184:ILE:HG21	2.36	0.41
1:A:75:SER:HA	1:A:114:MET:O	2.21	0.41
1:C:239:ALA:N	1:C:301:ILE:CD1	2.82	0.41
1:D:377:GLN:OE1	1:D:380:LYS:HE2	2.21	0.41
1:E:20:GLN:NE2	1:E:408:PHE:O	2.52	0.41
1:E:326:MET:HE3	1:E:418:PHE:HE1	1.85	0.41
1:E:380:LYS:HB2	1:E:448:PHE:CE2	2.56	0.41
1:F:140:THR:HG22	1:F:196:ASN:O	2.21	0.41
1:F:406:ASP:OD2	1:F:417:ARG:HD3	2.21	0.41
1:J:11:ILE:CD1	1:J:398:ALA:HB2	2.51	0.41
1:J:186:ASP:OD2	1:J:189:THR:OG1	2.38	0.41
1:J:291:ILE:HD12	1:J:292:ALA:N	2.36	0.41
1:K:64:ASP:CA	1:K:67:ILE:HG22	2.51	0.41
1:K:211:MET:HB2	1:K:213:ILE:CD1	2.51	0.41
1:D:121:HIS:O	1:D:122:TRP:HB2	2.21	0.40
1:E:380:LYS:HB3	1:E:438:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:HIS:NE2	1:F:288:ILE:HD11	2.37	0.40
1:G:24:ALA:HB1	1:G:27:GLU:HB3	2.02	0.40
1:I:314:ALA:C	1:I:318:LEU:HD23	2.42	0.40
1:J:184:ILE:CG2	3:J:506:HOH:O	2.69	0.40
1:J:323:LYS:HB2	1:J:323:LYS:NZ	2.36	0.40
1:K:82:TRP:N	1:K:83:PRO:CD	2.84	0.40
1:K:292:ALA:HA	1:K:352:VAL:O	2.21	0.40
1:D:227:TYR:HB2	1:D:300:PHE:CE1	2.56	0.40
1:G:73:ILE:HD12	1:G:73:ILE:HA	1.80	0.40
1:H:364:ILE:HD13	1:H:431:LYS:HE3	2.03	0.40
1:K:115:PRO:O	1:K:159:PRO:HD2	2.21	0.40
1:A:135:LYS:NZ	1:A:192:GLU:OE1	2.55	0.40
1:C:173:LEU:O	1:C:178:GLY:N	2.54	0.40
1:F:85:ILE:N	1:F:85:ILE:HD13	2.37	0.40
1:F:93:LEU:HD11	1:F:98:LEU:CD2	2.51	0.40
1:G:211:MET:HB3	1:G:213:ILE:CD1	2.51	0.40
1:H:166:GLU:O	1:H:169:VAL:HG23	2.21	0.40
1:I:4:ILE:HD11	1:I:448:PHE:CZ	2.56	0.40
1:I:144:THR:HG22	1:I:207:LEU:HD22	2.04	0.40
1:L:82:TRP:N	1:L:83:PRO:CD	2.85	0.40
1:B:201:HIS:O	1:B:205:VAL:HG23	2.21	0.40
1:B:250:TYR:O	1:B:254:VAL:HG23	2.22	0.40
1:D:154:LEU:HD23	1:D:157:ILE:HD11	2.02	0.40
1:D:421:VAL:HA	1:D:432:ILE:HA	2.03	0.40
1:E:140:THR:HG22	1:E:196:ASN:O	2.21	0.40
1:F:11:ILE:HD12	1:F:11:ILE:N	2.35	0.40
1:G:259:TYR:CB	1:G:264:LEU:HD11	2.51	0.40
1:H:165:ASN:ND2	1:H:294:ASN:HD21	2.17	0.40
1:H:266:LEU:O	1:H:269:LYS:O	2.40	0.40
1:H:352:VAL:HG13	1:H:398:ALA:HB3	2.03	0.40
1:J:4:ILE:HD11	1:J:450:GLU:HB2	2.03	0.40
1:J:121:HIS:O	1:J:122:TRP:HB2	2.21	0.40
1:K:80:ILE:HD12	1:K:117:ILE:HG23	2.03	0.40
1:K:439:TYR:O	1:K:443:ILE:HG13	2.21	0.40
1:L:12:TRP:HB2	1:L:443:ILE:CD1	2.48	0.40
1:L:92:LYS:HA	1:L:92:LYS:HD3	1.89	0.40
1:L:227:TYR:OH	1:L:334:GLY:HA2	2.20	0.40
1:C:30:LYS:HZ1	1:C:84:ARG:NE	2.19	0.40
1:D:292:ALA:HA	1:D:352:VAL:O	2.22	0.40
1:D:402:TRP:HA	1:D:403:SER:HA	1.66	0.40
1:E:294:ASN:N	1:E:294:ASN:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ILE:C	1:E:301:ILE:HD12	2.41	0.40
1:F:103:ARG:HH11	1:F:103:ARG:HG3	1.87	0.40
1:F:344:ARG:O	1:F:344:ARG:CD	2.68	0.40
1:G:363:GLU:C	1:G:370:ILE:HD13	2.42	0.40
1:H:151:PHE:HA	1:H:154:LEU:O	2.21	0.40
1:I:167:PRO:HD2	1:I:221:LEU:HD23	2.04	0.40
1:J:61:TYR:OH	1:J:103:ARG:NE	2.35	0.40
1:J:241:LEU:CD2	1:J:245:LEU:HD11	2.51	0.40
1:K:254:VAL:O	1:K:285:SER:HA	2.22	0.40
1:K:267:TYR:HA	1:K:270:LYS:CE	2.52	0.40
1:L:80:ILE:HD11	1:L:146:TYR:OH	2.22	0.40
1:L:362:ASP:OD2	1:L:433:LYS:HE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/456 (98%)	415 (93%)	26 (6%)	6 (1%)	10	39
1	B	447/456 (98%)	418 (94%)	26 (6%)	3 (1%)	19	54
1	C	447/456 (98%)	410 (92%)	35 (8%)	2 (0%)	30	66
1	D	447/456 (98%)	417 (93%)	26 (6%)	4 (1%)	14	49
1	E	447/456 (98%)	412 (92%)	29 (6%)	6 (1%)	10	39
1	F	447/456 (98%)	420 (94%)	24 (5%)	3 (1%)	19	54
1	G	447/456 (98%)	407 (91%)	37 (8%)	3 (1%)	19	54
1	H	447/456 (98%)	409 (92%)	28 (6%)	10 (2%)	5	27
1	I	447/456 (98%)	405 (91%)	30 (7%)	12 (3%)	4	22
1	J	447/456 (98%)	414 (93%)	31 (7%)	2 (0%)	30	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	447/456 (98%)	400 (90%)	39 (9%)	8 (2%)	7	32
1	L	447/456 (98%)	406 (91%)	34 (8%)	7 (2%)	8	34
All	All	5364/5472 (98%)	4933 (92%)	365 (7%)	66 (1%)	11	41

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LEU
1	A	420	ILE
1	D	122	TRP
1	D	373	THR
1	E	276	PHE
1	F	124	LEU
1	H	243	PHE
1	I	52	ASP
1	I	122	TRP
1	I	242	SER
1	I	243	PHE
1	I	315	ASN
1	K	73	ILE
1	K	242	SER
1	K	243	PHE
1	K	434	ASP
1	L	73	ILE
1	L	246	ALA
1	L	276	PHE
1	A	246	ALA
1	B	246	ALA
1	D	246	ALA
1	E	155	GLY
1	E	246	ALA
1	F	246	ALA
1	G	73	ILE
1	G	395	ASN
1	H	270	LYS
1	I	268	LYS
1	I	274	LEU
1	J	122	TRP
1	J	246	ALA
1	L	155	GLY
1	A	122	TRP

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Mol	Chain	Res	Type
1	A	153	ASN
1	B	122	TRP
1	C	272	ILE
1	E	3	LYS
1	G	122	TRP
1	H	122	TRP
1	H	156	ASP
1	I	307	SER
1	K	122	TRP
1	K	209	ARG
1	K	210	GLU
1	D	421	VAL
1	E	286	GLN
1	H	272	ILE
1	H	448	PHE
1	I	246	ALA
1	L	122	TRP
1	A	419	GLY
1	F	155	GLY
1	H	246	ALA
1	H	371	GLU
1	K	158	VAL
1	L	210	GLU
1	B	155	GLY
1	E	7	PRO
1	H	155	GLY
1	I	286	GLN
1	I	421	VAL
1	L	286	GLN
1	I	155	GLY
1	C	155	GLY
1	H	170	VAL

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	388/395 (98%)	370 (95%)	18 (5%)	23	56
1	B	388/395 (98%)	366 (94%)	22 (6%)	17	49
1	C	388/395 (98%)	374 (96%)	14 (4%)	30	64
1	D	388/395 (98%)	372 (96%)	16 (4%)	26	60
1	E	388/395 (98%)	373 (96%)	15 (4%)	27	61
1	F	388/395 (98%)	365 (94%)	23 (6%)	16	47
1	G	388/395 (98%)	358 (92%)	30 (8%)	10	37
1	H	388/395 (98%)	366 (94%)	22 (6%)	17	49
1	I	388/395 (98%)	363 (94%)	25 (6%)	14	44
1	J	388/395 (98%)	358 (92%)	30 (8%)	10	37
1	K	388/395 (98%)	358 (92%)	30 (8%)	10	37
1	L	388/395 (98%)	344 (89%)	44 (11%)	4	21
All	All	4656/4740 (98%)	4367 (94%)	289 (6%)	15	45

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	117	ILE
1	A	123	ASP
1	A	146	TYR
1	A	154	LEU
1	A	189	THR
1	A	190	SER
1	A	193	VAL
1	A	206	LYS
1	A	248	ARG
1	A	266	LEU
1	A	270	LYS
1	A	309	SER
1	A	319	GLU
1	A	345	ASP
1	A	354	SER
1	A	369	LYS
1	A	380	LYS
1	B	66	LYS
1	B	85	ILE
1	B	92	LYS
1	B	123	ASP

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Mol	Chain	Res	Type
1	B	146	TYR
1	B	150	ILE
1	B	157	ILE
1	B	180	HIS
1	B	189	THR
1	B	190	SER
1	B	206	LYS
1	B	209	ARG
1	B	222	ASN
1	B	244	SER
1	B	248	ARG
1	B	285	SER
1	B	289	ASP
1	B	323	LYS
1	B	354	SER
1	B	380	LYS
1	B	384	THR
1	B	450	GLU
1	C	30	LYS
1	C	65	ILE
1	C	110	GLU
1	C	157	ILE
1	C	169	VAL
1	C	171	SER
1	C	189	THR
1	C	190	SER
1	C	197	LEU
1	C	217	ILE
1	C	274	LEU
1	C	353	ILE
1	C	383	LEU
1	C	401	LEU
1	D	39	SER
1	D	98	LEU
1	D	146	TYR
1	D	172	LEU
1	D	189	THR
1	D	222	ASN
1	D	270	LYS
1	D	282	LYS
1	D	289	ASP
1	D	318	LEU

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Mol	Chain	Res	Type
1	D	354	SER
1	D	376	ILE
1	D	383	LEU
1	D	390	ILE
1	D	391	GLN
1	D	449	LEU
1	E	98	LEU
1	E	146	TYR
1	E	189	THR
1	E	190	SER
1	E	248	ARG
1	E	266	LEU
1	E	269	LYS
1	E	273	GLU
1	E	274	LEU
1	E	294	ASN
1	E	309	SER
1	E	354	SER
1	E	416	LYS
1	E	426	ASP
1	E	427	THR
1	F	11	ILE
1	F	85	ILE
1	F	146	TYR
1	F	169	VAL
1	F	173	LEU
1	F	189	THR
1	F	190	SER
1	F	222	ASN
1	F	248	ARG
1	F	270	LYS
1	F	272	ILE
1	F	279	ASP
1	F	286	GLN
1	F	323	LYS
1	F	326	MET
1	F	329	ILE
1	F	339	LEU
1	F	344	ARG
1	F	354	SER
1	F	388	ARG
1	F	426	ASP

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Mol	Chain	Res	Type
1	F	449	LEU
1	F	450	GLU
1	G	11	ILE
1	G	33	SER
1	G	73	ILE
1	G	85	ILE
1	G	93	LEU
1	G	110	GLU
1	G	113	ILE
1	G	123	ASP
1	G	146	TYR
1	G	150	ILE
1	G	157	ILE
1	G	169	VAL
1	G	171	SER
1	G	189	THR
1	G	195	HIS
1	G	217	ILE
1	G	248	ARG
1	G	266	LEU
1	G	272	ILE
1	G	274	LEU
1	G	276	PHE
1	G	291	ILE
1	G	330	ILE
1	G	352	VAL
1	G	354	SER
1	G	376	ILE
1	G	380	LYS
1	G	383	LEU
1	G	390	ILE
1	G	450	GLU
1	H	60	ARG
1	H	74	LYS
1	H	85	ILE
1	H	100	PHE
1	H	139	THR
1	H	146	TYR
1	H	150	ILE
1	H	169	VAL
1	H	171	SER
1	H	189	THR

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Mol	Chain	Res	Type
1	H	216	GLN
1	H	241	LEU
1	H	245	LEU
1	H	248	ARG
1	H	255	LEU
1	H	282	LYS
1	H	330	ILE
1	H	354	SER
1	H	426	ASP
1	H	427	THR
1	H	444	LYS
1	H	450	GLU
1	I	5	THR
1	I	69	LYS
1	I	81	SER
1	I	140	THR
1	I	146	TYR
1	I	157	ILE
1	I	171	SER
1	I	189	THR
1	I	190	SER
1	I	217	ILE
1	I	222	ASN
1	I	248	ARG
1	I	266	LEU
1	I	272	ILE
1	I	274	LEU
1	I	282	LYS
1	I	286	GLN
1	I	288	ILE
1	I	291	ILE
1	I	307	SER
1	I	341	LEU
1	I	345	ASP
1	I	354	SER
1	I	383	LEU
1	I	415	ASN
1	J	4	ILE
1	J	8	LYS
1	J	11	ILE
1	J	33	SER
1	J	53	VAL

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Mol	Chain	Res	Type
1	J	80	ILE
1	J	135	LYS
1	J	146	TYR
1	J	150	ILE
1	J	169	VAL
1	J	189	THR
1	J	197	LEU
1	J	207	LEU
1	J	230	SER
1	J	236	ILE
1	J	248	ARG
1	J	254	VAL
1	J	264	LEU
1	J	266	LEU
1	J	268	LYS
1	J	270	LYS
1	J	274	LEU
1	J	289	ASP
1	J	291	ILE
1	J	303	TYR
1	J	318	LEU
1	J	320	LYS
1	J	323	LYS
1	J	330	ILE
1	J	383	LEU
1	K	67	ILE
1	K	74	LYS
1	K	75	SER
1	K	85	ILE
1	K	93	LEU
1	K	144	THR
1	K	146	TYR
1	K	150	ILE
1	K	157	ILE
1	K	189	THR
1	K	190	SER
1	K	191	LEU
1	K	219	ILE
1	K	222	ASN
1	K	241	LEU
1	K	248	ARG
1	K	254	VAL

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Mol	Chain	Res	Type
1	K	261	GLU
1	K	266	LEU
1	K	270	LYS
1	K	288	ILE
1	K	291	ILE
1	K	309	SER
1	K	323	LYS
1	K	342	LEU
1	K	354	SER
1	K	370	ILE
1	K	395	ASN
1	K	409	GLU
1	K	446	ASN
1	L	11	ILE
1	L	45	ILE
1	L	65	ILE
1	L	67	ILE
1	L	74	LYS
1	L	80	ILE
1	L	81	SER
1	L	85	ILE
1	L	92	LYS
1	L	93	LEU
1	L	113	ILE
1	L	123	ASP
1	L	146	TYR
1	L	156	ASP
1	L	169	VAL
1	L	184	ILE
1	L	190	SER
1	L	210	GLU
1	L	213	ILE
1	L	217	ILE
1	L	222	ASN
1	L	224	SER
1	L	236	ILE
1	L	245	LEU
1	L	266	LEU
1	L	274	LEU
1	L	279	ASP
1	L	282	LYS
1	L	286	GLN

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Mol	Chain	Res	Type
1	L	302	LYS
1	L	308	GLU
1	L	309	SER
1	L	323	LYS
1	L	338	LEU
1	L	354	SER
1	L	380	LYS
1	L	383	LEU
1	L	391	GLN
1	L	392	ASP
1	L	396	LEU
1	L	427	THR
1	L	431	LYS
1	L	438	TRP
1	L	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	165	ASN
1	A	201	HIS
1	A	294	ASN
1	A	377	GLN
1	A	385	GLN
1	A	391	GLN
1	A	407	ASN
1	B	126	GLN
1	B	356	ASN
1	C	121	HIS
1	C	201	HIS
1	C	295	ASN
1	C	385	GLN
1	C	387	HIS
1	D	40	HIS
1	D	44	ASN
1	D	126	GLN
1	D	165	ASN
1	D	294	ASN
1	D	295	ASN
1	D	356	ASN
1	D	387	HIS

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Mol	Chain	Res	Type
1	D	391	GLN
1	E	121	HIS
1	E	165	ASN
1	E	196	ASN
1	E	226	HIS
1	E	286	GLN
1	E	295	ASN
1	E	356	ASN
1	E	387	HIS
1	E	391	GLN
1	E	446	ASN
1	F	20	GLN
1	F	40	HIS
1	F	121	HIS
1	F	165	ASN
1	F	201	HIS
1	F	356	ASN
1	G	106	ASN
1	G	121	HIS
1	G	212	ASN
1	G	356	ASN
1	G	385	GLN
1	G	424	ASN
1	H	121	HIS
1	H	126	GLN
1	H	165	ASN
1	H	195	HIS
1	H	196	ASN
1	H	201	HIS
1	H	385	GLN
1	I	165	ASN
1	I	196	ASN
1	I	295	ASN
1	I	385	GLN
1	I	415	ASN
1	J	57	HIS
1	J	94	ASN
1	J	165	ASN
1	J	201	HIS
1	J	356	ASN
1	J	377	GLN
1	J	385	GLN

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Mol	Chain	Res	Type
1	J	387	HIS
1	J	445	ASN
1	J	446	ASN
1	K	165	ASN
1	K	175	HIS
1	K	226	HIS
1	K	356	ASN
1	K	415	ASN
1	L	121	HIS
1	L	165	ASN
1	L	196	ASN
1	L	295	ASN
1	L	385	GLN
1	L	446	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 ⓘ

2 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
2	TRS	B	501	-	7,7,7	0.21	0	9,9,9	0.53	0
2	TRS	A	501	-	7,7,7	0.12	0	9,9,9	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	B	501	-	-	3/9/9/9	-
2	TRS	A	501	-	-	9/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TRS	C2-C-C1-O1
2	A	501	TRS	C3-C-C1-O1
2	A	501	TRS	N-C-C1-O1
2	A	501	TRS	C1-C-C2-O2
2	A	501	TRS	C3-C-C2-O2
2	A	501	TRS	N-C-C2-O2
2	A	501	TRS	N-C-C3-O3
2	A	501	TRS	C2-C-C3-O3
2	B	501	TRS	C1-C-C2-O2
2	B	501	TRS	N-C-C2-O2
2	A	501	TRS	C1-C-C3-O3
2	B	501	TRS	C3-C-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	TRS	1	0
2	A	501	TRS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

Ligand TRS B 501

Ligand TRS A 501

Bond lengths

Bond angles

Torsions

Rings
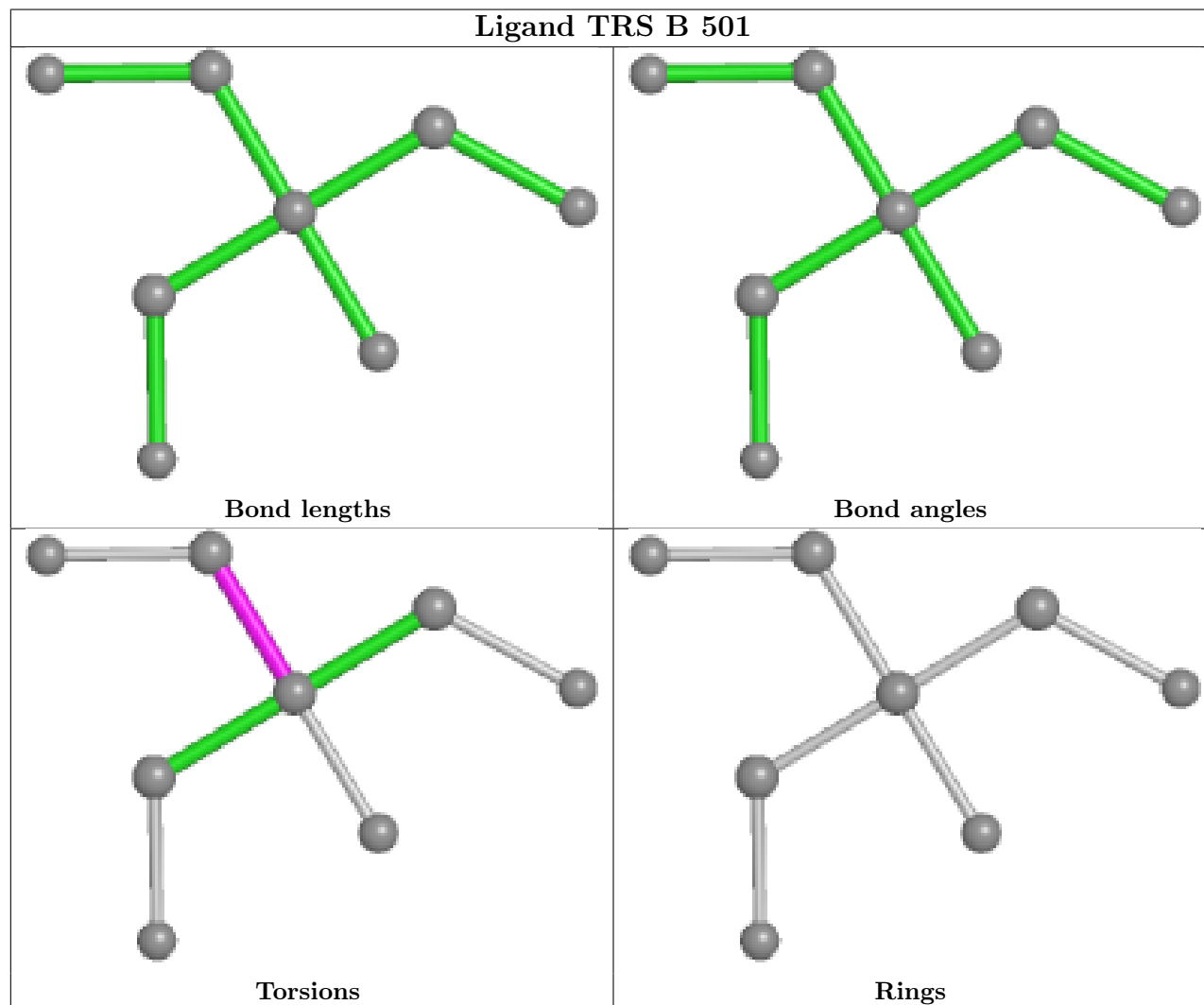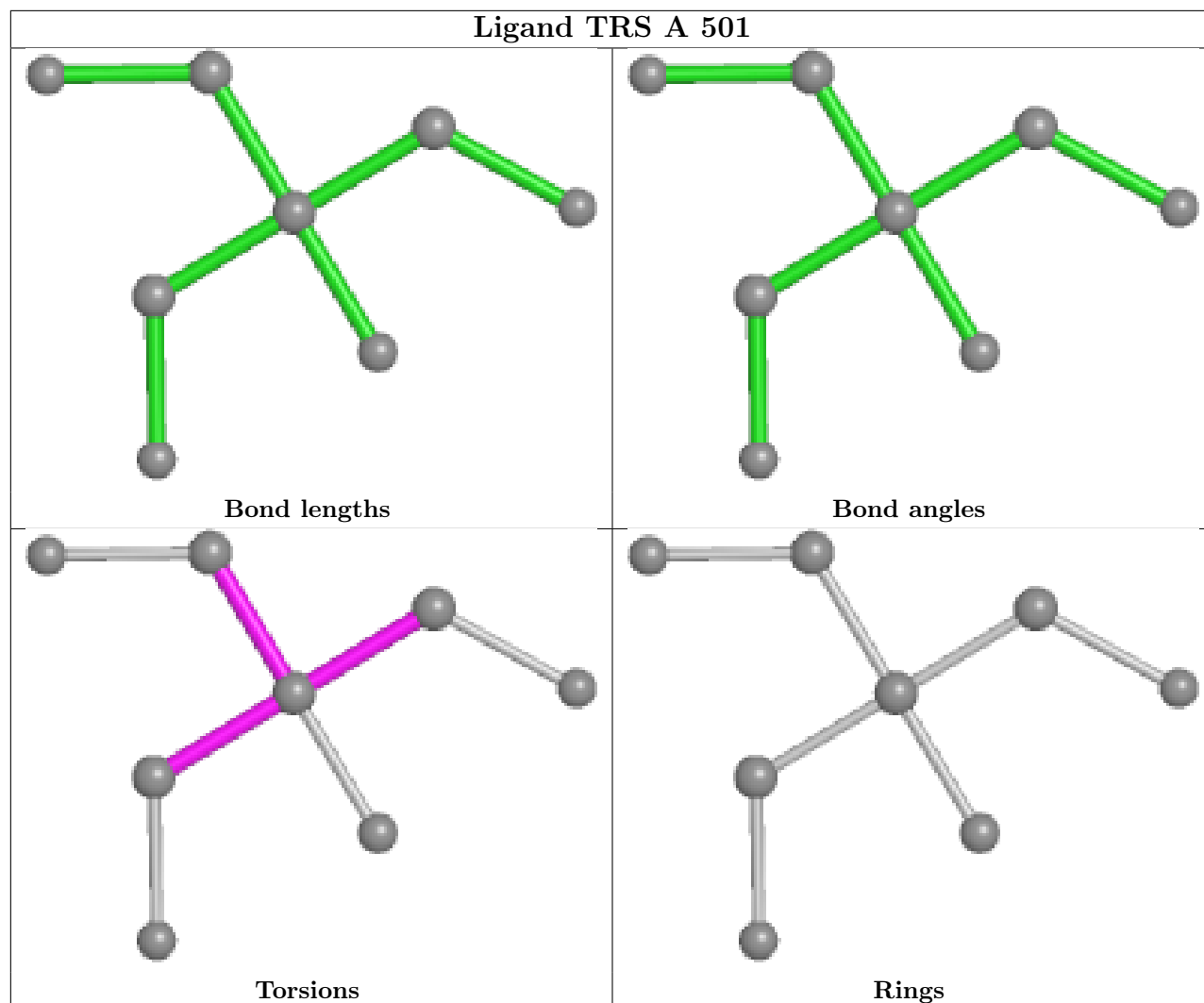
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	449/456 (98%)	-1.45	0	100	100	16, 35, 58, 80	0
1	B	449/456 (98%)	-1.43	0	100	100	16, 33, 57, 74	0
1	C	449/456 (98%)	-1.44	0	100	100	19, 37, 60, 93	0
1	D	449/456 (98%)	-1.44	0	100	100	18, 42, 66, 81	0
1	E	449/456 (98%)	-1.48	0	100	100	17, 29, 46, 70	0
1	F	449/456 (98%)	-1.44	0	100	100	17, 38, 57, 81	0
1	G	449/456 (98%)	-1.42	0	100	100	19, 42, 65, 75	0
1	H	449/456 (98%)	-1.42	0	100	100	17, 42, 67, 86	0
1	I	449/456 (98%)	-1.38	0	100	100	19, 47, 69, 82	0
1	J	449/456 (98%)	-1.36	0	100	100	19, 43, 73, 100	0
1	K	449/456 (98%)	-1.33	0	100	100	21, 54, 75, 92	0
1	L	449/456 (98%)	-1.34	0	100	100	21, 52, 79, 107	0
All	All	5388/5472 (98%)	-1.41	0	100	100	16, 40, 68, 107	0

There are no RSRZ outliers to report.

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

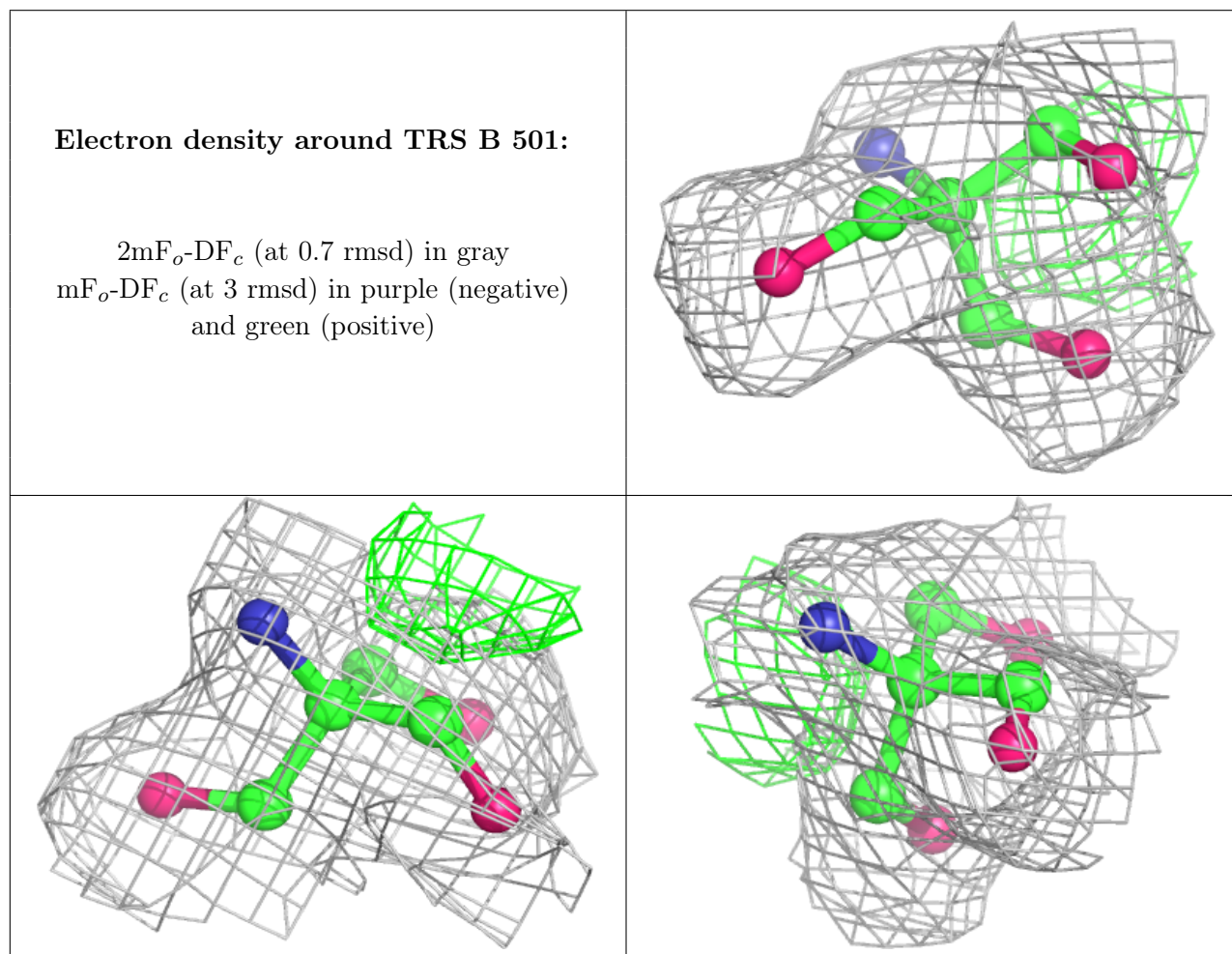There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

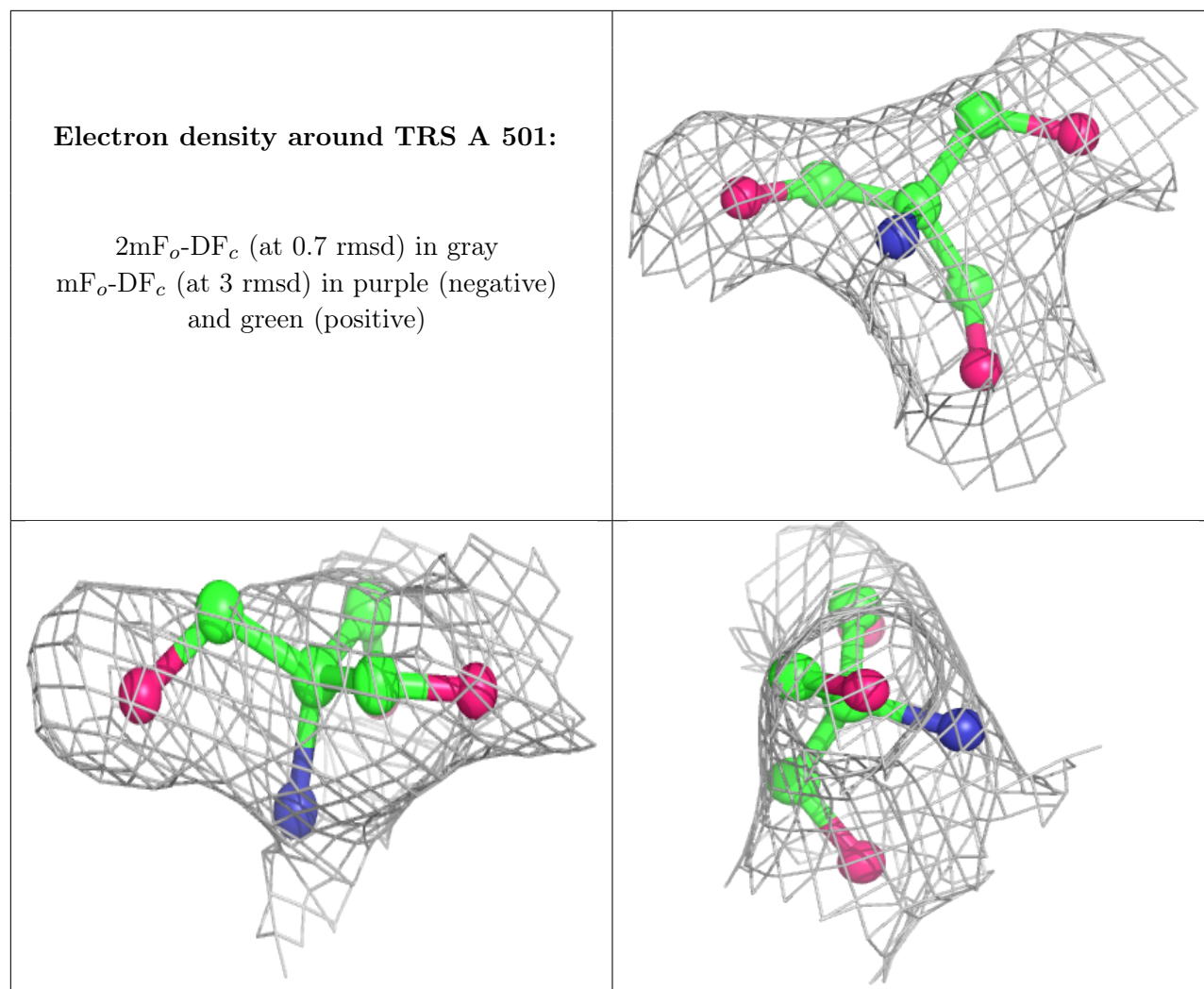There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

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($\mathring{A}^2$)	Q<0.9
2	TRS	B	501	8/8	0.98	0.05	21,23,24,24	0
2	TRS	A	501	8/8	0.99	0.04	19,20,20,21	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 TRS B 501:

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

Electron density around TRS A 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.