



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 12:06 PM EDT

PDB ID : 1LWU
Title : Crystal structure of fragment D from lamprey fibrinogen complexed with the peptide Gly-His-Arg-Pro-amide
Authors : Yang, Z.; Spraggon, G.; Pandi, L.; Everse, S.J.; Riley, M.; Doolittle, R.F.
Deposited on : 2002-06-03
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

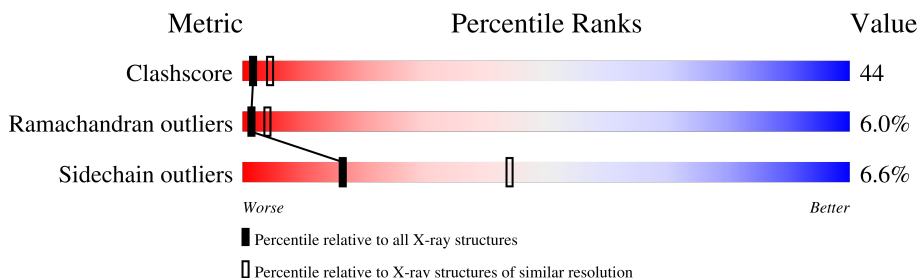
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)




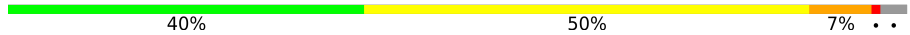
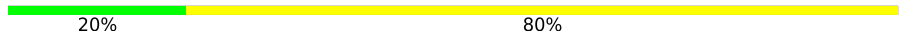
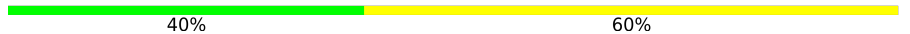



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	25% 48% 9% • 17%
1	D	119	27% 45% 11% • 17%
1	G	119	25% 50% 8% • 17%
1	J	119	27% 45% 10% • 17%
2	B	323	45% 44% 8% ••
2	E	323	45% 44% 8% ••
2	H	323	41% 49% 7% ••
2	K	323	43% 47% 7% ••

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Mol	Chain	Length	Quality of chain
3	C	323	
3	F	323	
3	I	323	
3	L	323	
4	M	5	
4	N	5	
4	O	5	
4	P	5	
5	Q	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BMA	E	502	-	-	X	-
11	GAL	H	507	-	-	X	-
6	NDG	D	301	-	-	X	-
6	NDG	H	506	-	-	X	-
6	NDG	K	501	-	-	X	-
6	NDG	N	101	-	-	X	-
7	MAN	E	503	-	-	X	-
7	MAN	H	503	-	-	X	-
7	MAN	H	505	-	-	X	-
7	MAN	P	101	-	-	X	-
9	NAG	C	501	-	-	X	-
9	NAG	C	502	-	-	X	-
9	NAG	E	501	-	-	X	-
9	NAG	F	502	-	-	X	-
9	NAG	I	502	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 24360 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 Fibrinogen alpha-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	99	833	523	155	152	3	0	0	0
1	D	99	833	523	155	152	3	0	0	0
1	G	99	833	523	155	152	3	0	0	0
1	J	99	833	523	155	152	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	THR	conflict	UNP P02674
D	153	ALA	THR	conflict	UNP P02674
G	153	ALA	THR	conflict	UNP P02674
J	153	ALA	THR	conflict	UNP P02674

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	315	2535	1579	453	482	21	0	0	0
2	E	315	2535	1579	453	482	21	0	0	0
2	H	315	2535	1579	453	482	21	0	0	0
2	K	315	2535	1579	453	482	21	0	0	0

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	317	2599	1642	451	493	13	0	0	0
3	F	317	2599	1642	451	493	13	0	0	0
3	I	313	2568	1625	444	486	13	0	0	0
3	L	313	2568	1625	444	486	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	PRO	SER	conflict	UNP P04115
F	137	PRO	SER	conflict	UNP P04115
I	137	PRO	SER	conflict	UNP P04115
L	137	PRO	SER	conflict	UNP P04115

- Molecule 4 is a protein called Peptide Ligand Gly-His-Arg-Pro-NH₂.

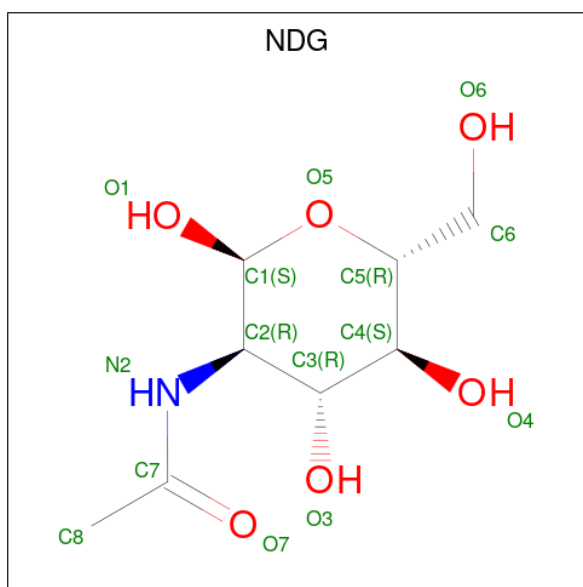
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	M	5	33	19	10	4	0	0	1
4	N	5	33	19	10	4	0	0	1
4	O	5	33	19	10	4	0	0	1
4	P	5	33	19	10	4	0	0	1

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	Q	2	28	16	2	10	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	Total 15	8	1	6	0	0
6	D	1	Total 15	8	1	6	0	0
6	H	1	Total 15	8	1	6	0	0
6	H	1	Total 15	8	1	6	0	0
6	H	1	Total 15	8	1	6	0	0
6	K	1	Total 15	8	1	6	0	0
6	M	1	Total 15	8	1	6	0	0
6	N	1	Total 15	8	1	6	0	0
6	O	1	Total 15	8	1	6	0	0

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 12 6 6	0	0
7	C	1	Total C O 11 6 5	0	0
7	E	1	Total C O 12 6 6	0	0
7	F	1	Total C O 11 6 5	0	0
7	H	1	Total C O 12 6 6	0	0
7	H	1	Total C O 12 6 6	0	0
7	J	1	Total C O 11 6 5	0	0
7	L	1	Total C O 11 6 5	0	0
7	N	1	Total C O 12 6 6	0	0
7	P	1	Total C O 12 6 6	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

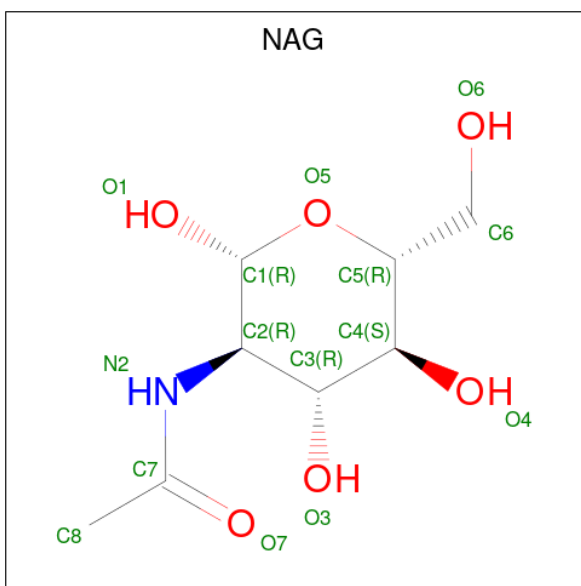
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Ca 1 1	0	0
8	F	1	Total Ca 1 1	0	0
8	H	1	Total Ca 1 1	0	0
8	I	1	Total Ca 1 1	0	0
8	K	1	Total Ca 1 1	0	0
8	L	1	Total Ca 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



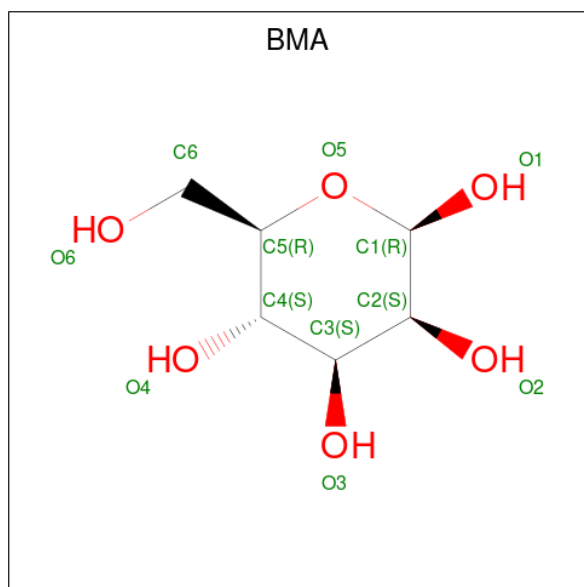
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	E	1	Total C N O 15 8 1 6	0	0
9	F	1	Total C N O 14 8 1 5	0	0
9	F	1	Total C N O 14 8 1 5	0	0

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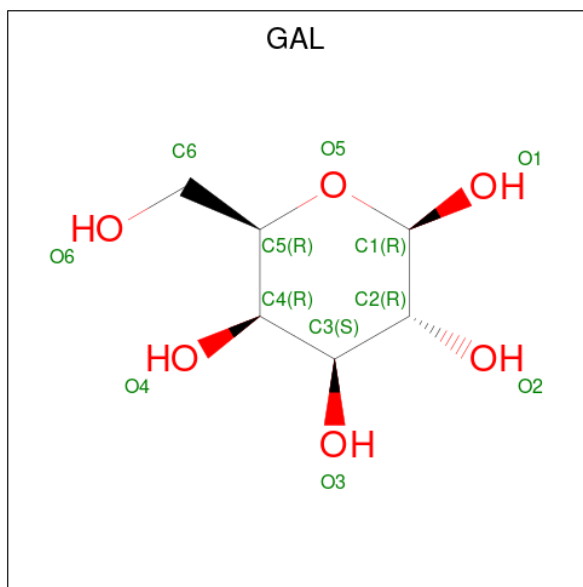
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			12	6	6		
10	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 11 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆).



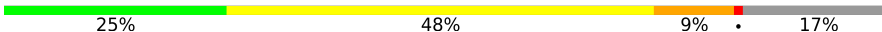
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	1	Total C O 12 6 6	0	0

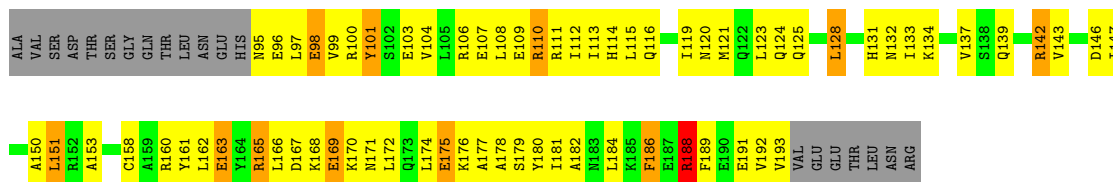
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

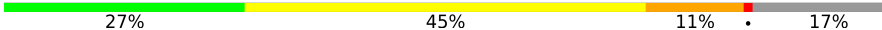
Note EDS was not executed.

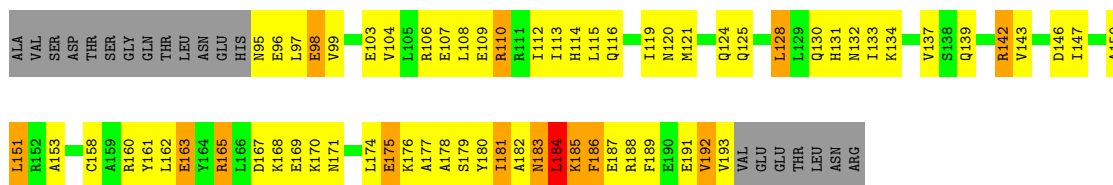
- Molecule 1: Fibrinogen alpha-1 chain

Chain A: 

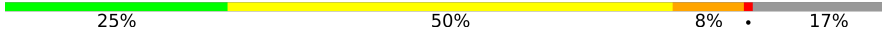


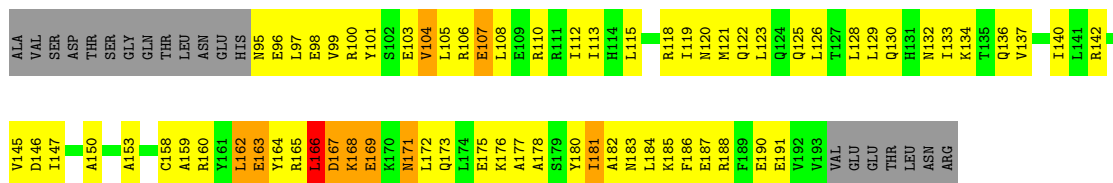
- Molecule 1: Fibrinogen alpha-1 chain

Chain D: 



- Molecule 1: Fibrinogen alpha-1 chain

Chain G: 



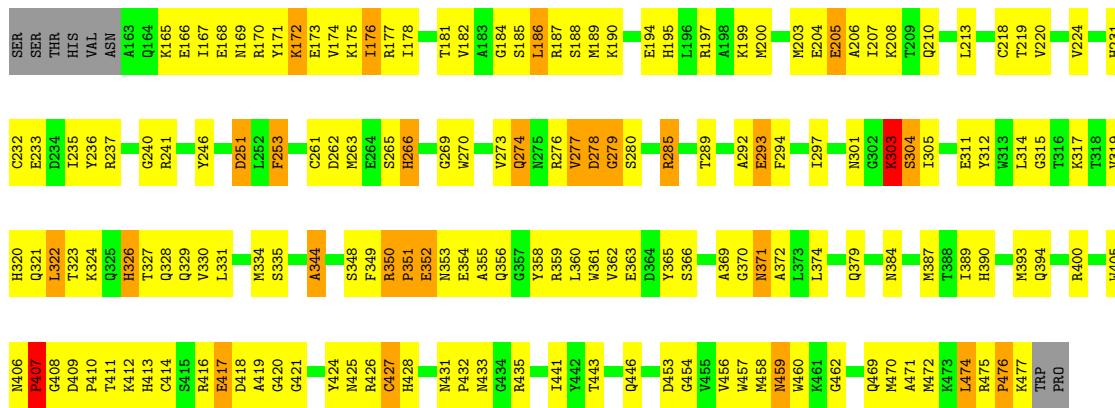
- Molecule 1: Fibrinogen alpha-1 chain

Chain J: 

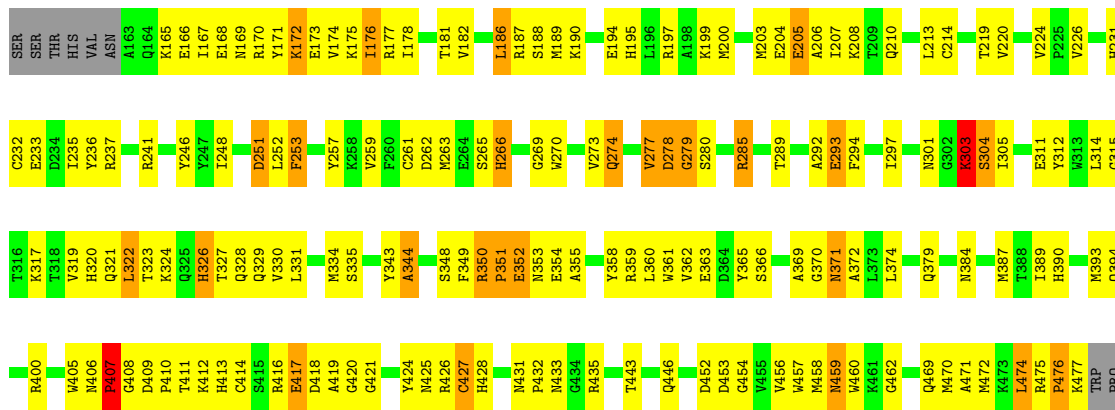




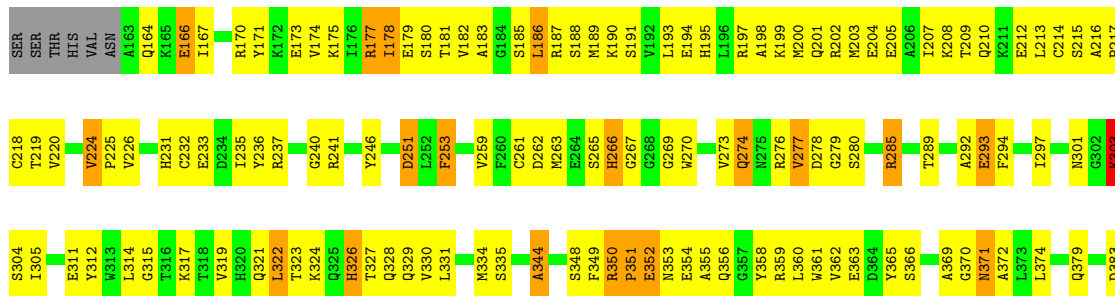
● Molecule 2: Fibrinogen beta chain

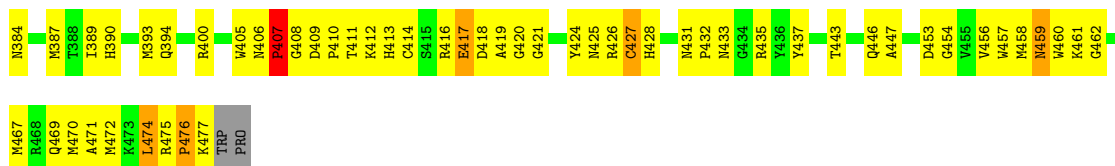


● Molecule 2: Fibrinogen beta chain

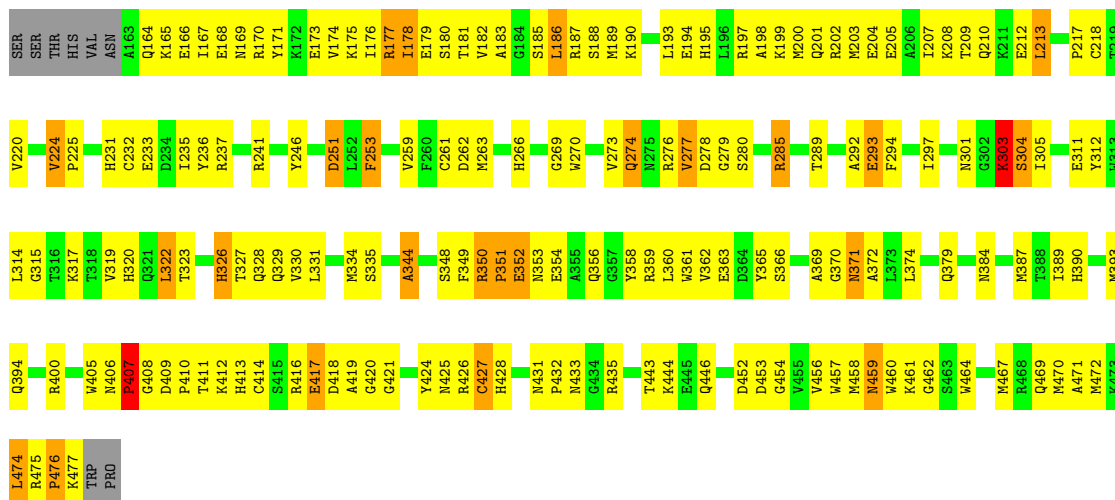


● Molecule 2: Fibrinogen beta chain

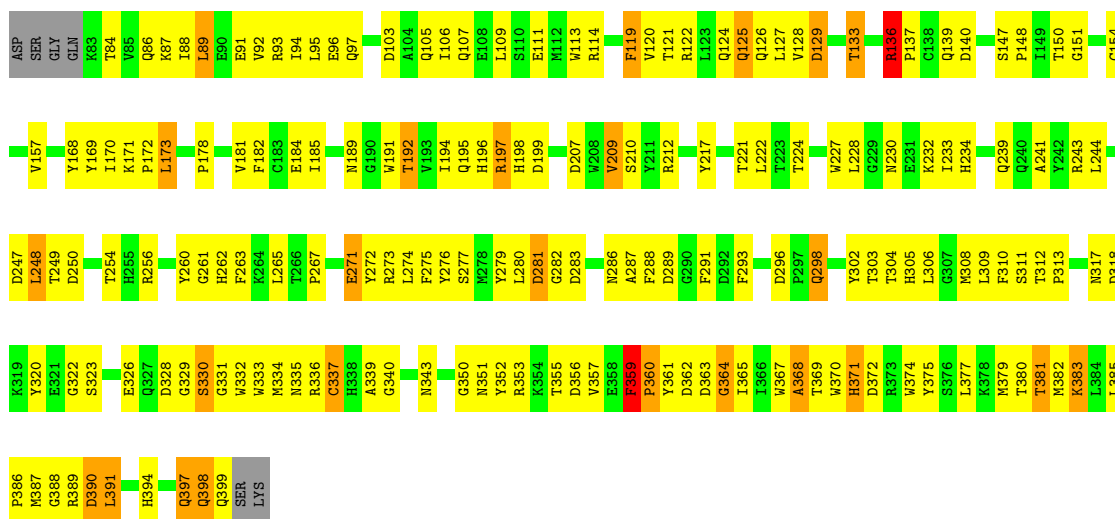




• Molecule 2: Fibrinogen beta chain

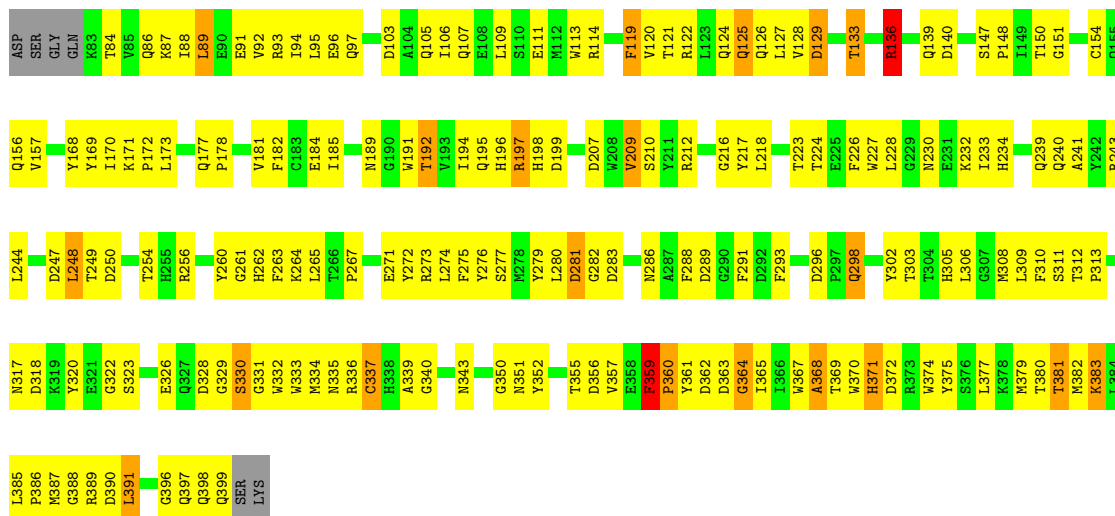


• Molecule 3: Fibrinogen gamma chain

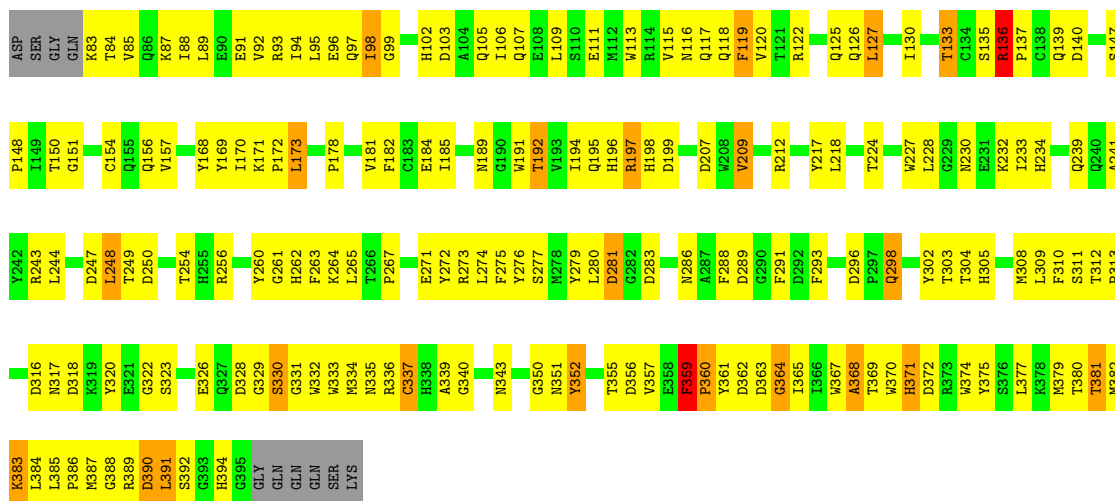


• Molecule 3: Fibrinogen gamma chain

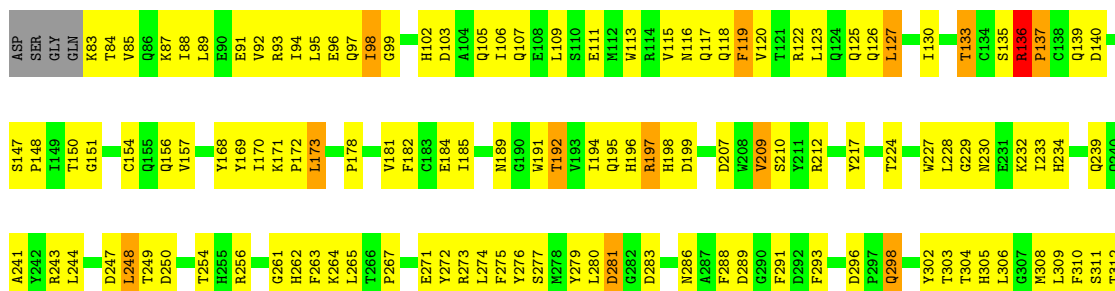


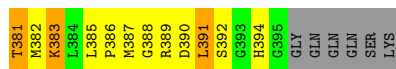
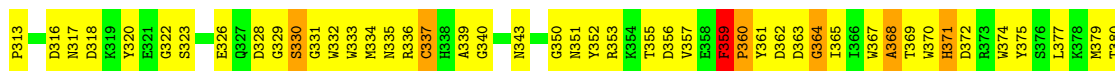


• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain





- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2



- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2



- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2



- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.73Å 47.65Å 244.65Å 88.81° 97.23° 86.17°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	87.9 (20.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	24360	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

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: CA, MAN, NAG, BMA, NH2, NDG, GAL

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	0.38	0/840	0.66	0/1126
1	D	0.36	0/840	0.67	0/1126
1	G	0.35	0/840	0.58	0/1126
1	J	0.35	0/840	0.59	0/1126
2	B	0.43	0/2602	0.69	1/3517 (0.0%)
2	E	0.46	0/2602	0.71	1/3517 (0.0%)
2	H	0.42	0/2602	0.69	1/3517 (0.0%)
2	K	0.43	0/2602	0.69	1/3517 (0.0%)
3	C	0.39	0/2671	0.64	2/3616 (0.1%)
3	F	0.39	0/2671	0.62	1/3616 (0.0%)
3	I	0.38	0/2640	0.64	1/3575 (0.0%)
3	L	0.39	0/2640	0.64	2/3575 (0.1%)
4	M	0.51	0/33	0.55	0/43
4	N	0.57	0/33	0.78	0/43
4	O	0.46	0/33	0.61	0/43
4	P	0.48	0/33	0.58	0/43
All	All	0.41	0/24522	0.66	10/33126 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	136	ARG	C-N-CD	-8.41	102.10	120.60
3	F	136	ARG	C-N-CD	-6.86	105.50	120.60
3	I	136	ARG	C-N-CD	-6.69	105.89	120.60
2	E	421	GLY	N-CA-C	-5.84	98.49	113.10
3	L	136	ARG	C-N-CD	-5.79	107.87	120.60
2	B	421	GLY	N-CA-C	-5.61	99.08	113.10
3	L	137	PRO	CA-N-CD	-5.46	103.85	111.50
2	H	421	GLY	N-CA-C	-5.40	99.61	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	421	GLY	N-CA-C	-5.18	100.14	113.10
3	C	390	ASP	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	833	0	864	126	0
1	D	833	0	864	94	0
1	G	833	0	864	114	0
1	J	833	0	864	137	0
2	B	2535	0	2364	206	0
2	E	2535	0	2364	202	0
2	H	2535	0	2364	248	0
2	K	2535	0	2364	230	0
3	C	2599	0	2427	209	0
3	F	2599	0	2428	205	0
3	I	2568	0	2401	226	0
3	L	2568	0	2401	232	0
4	M	33	0	32	7	0
4	N	33	0	32	5	0
4	O	33	0	32	4	0
4	P	33	0	32	4	0
5	Q	28	0	26	5	0
6	B	15	0	12	3	0
6	D	15	0	12	9	0
6	H	45	0	36	31	0
6	K	15	0	12	7	0
6	M	15	0	12	5	0
6	N	15	0	12	25	0
6	O	15	0	12	2	0
7	B	12	0	12	3	0
7	C	11	0	10	2	0
7	E	12	0	12	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	11	0	10	5	0
7	H	24	0	24	27	0
7	J	11	0	10	2	0
7	L	11	0	10	2	0
7	N	12	0	12	1	0
7	P	12	0	12	8	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
9	C	28	0	26	9	0
9	E	15	0	15	9	0
9	F	28	0	26	11	0
9	I	28	0	26	8	0
10	E	12	0	12	23	0
10	H	12	0	12	1	0
11	H	12	0	12	10	0
All	All	24360	0	23072	2079	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 44.

All (2079) 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)
10:E:502:BMA:C5	6:N:101:NDG:H8C1	1.68	1.21
9:I:502:NAG:O3	7:J:301:MAN:C1	1.91	1.18
1:A:188:ARG:H	1:A:188:ARG:HD2	1.07	1.18
7:H:503:MAN:O6	7:H:505:MAN:H62	1.39	1.18
10:E:502:BMA:H62	7:E:503:MAN:H62	1.16	1.15
7:H:505:MAN:O1	6:H:506:NDG:N2	1.79	1.13
3:L:390:ASP:CG	3:L:391:LEU:H	1.48	1.13
3:F:279:TYR:HB2	3:F:286:ASN:HD22	1.14	1.12
3:L:279:TYR:HB2	3:L:286:ASN:HD22	1.14	1.09
6:H:506:NDG:C1	11:H:507:GAL:H3	1.83	1.09
9:C:501:NAG:O4	9:C:502:NAG:C5	2.01	1.09
6:H:506:NDG:H2	11:H:507:GAL:C3	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:506:NDG:H2	11:H:507:GAL:O3	1.54	1.08
3:I:279:TYR:HB2	3:I:286:ASN:HD22	1.15	1.07
3:F:194:ILE:HD12	3:F:233:ILE:HG12	1.35	1.07
3:C:194:ILE:HD12	3:C:233:ILE:HG12	1.35	1.06
3:C:279:TYR:HB2	3:C:286:ASN:HD22	1.15	1.06
9:F:501:NAG:O4	9:F:502:NAG:C5	2.04	1.06
7:H:503:MAN:HO1	7:P:101:MAN:C1	1.68	1.06
9:I:501:NAG:O4	9:I:502:NAG:O5	1.73	1.06
3:L:150:THR:HG22	3:L:151:GLY:H	1.20	1.06
2:H:393:MET:HG3	2:H:425:ASN:HB2	1.39	1.05
2:E:393:MET:HG3	2:E:425:ASN:HB2	1.39	1.05
3:I:194:ILE:HD12	3:I:233:ILE:HG12	1.36	1.05
2:K:393:MET:HG3	2:K:425:ASN:HB2	1.38	1.05
1:A:188:ARG:HB3	1:A:188:ARG:HH11	1.18	1.04
10:E:502:BMA:H1	6:N:101:NDG:O3	1.56	1.04
7:B:502:MAN:H61	6:M:101:NDG:H3	1.35	1.03
2:H:267:GLY:N	6:H:506:NDG:O3	1.91	1.03
3:C:150:THR:HG22	3:C:151:GLY:H	1.18	1.03
3:F:150:THR:HG22	3:F:151:GLY:H	1.22	1.03
3:I:279:TYR:HB2	3:I:286:ASN:ND2	1.72	1.02
2:B:393:MET:HG3	2:B:425:ASN:HB2	1.40	1.02
1:A:97:LEU:HD21	1:J:108:LEU:HB2	1.42	1.01
3:L:194:ILE:HD12	3:L:233:ILE:HG12	1.38	1.01
3:L:351:ASN:HB3	3:L:375:TYR:HD1	1.24	1.01
3:L:279:TYR:HB2	3:L:286:ASN:ND2	1.74	1.00
3:C:279:TYR:HB2	3:C:286:ASN:ND2	1.75	1.00
10:E:502:BMA:O5	6:N:101:NDG:H8C1	1.62	1.00
3:F:279:TYR:HB2	3:F:286:ASN:ND2	1.75	1.00
3:F:351:ASN:HB3	3:F:375:TYR:HD1	1.22	1.00
3:C:303:THR:HB	3:C:339:ALA:HB2	1.43	1.00
1:D:142:ARG:HB2	1:D:142:ARG:HH11	1.24	1.00
9:F:501:NAG:O4	9:F:502:NAG:O5	1.78	0.99
3:I:351:ASN:HB3	3:I:375:TYR:HD1	1.23	0.99
3:I:303:THR:HB	3:I:339:ALA:HB2	1.43	0.99
9:C:502:NAG:O3	7:C:503:MAN:C1	2.09	0.99
3:F:303:THR:HB	3:F:339:ALA:HB2	1.44	0.99
7:H:503:MAN:O1	7:P:101:MAN:C1	2.10	0.98
3:C:351:ASN:HB3	3:C:375:TYR:HD1	1.24	0.98
3:L:303:THR:HB	3:L:339:ALA:HB2	1.44	0.98
3:I:391:LEU:HG	3:I:394:HIS:HB2	1.45	0.98
9:I:501:NAG:O4	9:I:502:NAG:C5	2.12	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:502:BMA:H62	7:E:503:MAN:C6	1.94	0.97
3:I:150:THR:HG22	3:I:151:GLY:H	1.25	0.96
1:A:142:ARG:HB2	1:A:142:ARG:HH11	1.30	0.96
2:B:172:LYS:HE2	2:B:172:LYS:HA	1.48	0.95
9:C:501:NAG:O4	9:C:502:NAG:H5	1.62	0.95
1:J:126:LEU:HB3	1:J:184:LEU:HD13	1.49	0.95
3:C:136:ARG:HB3	3:C:136:ARG:HH11	1.31	0.94
2:H:164:GLN:HB2	3:I:84:THR:HG23	1.46	0.94
3:F:136:ARG:HB3	3:F:136:ARG:HH11	1.32	0.94
9:F:502:NAG:O3	7:F:503:MAN:C1	2.15	0.94
2:E:172:LYS:HE2	2:E:172:LYS:HA	1.50	0.94
10:E:502:BMA:H61	6:N:101:NDG:H8C2	1.50	0.94
7:H:505:MAN:H1	6:H:506:NDG:O1	1.66	0.93
2:K:393:MET:CG	2:K:425:ASN:HB2	1.99	0.91
2:H:393:MET:CG	2:H:425:ASN:HB2	1.99	0.91
2:K:167:ILE:HG21	3:L:88:ILE:HG23	1.53	0.91
9:F:501:NAG:HO4	9:F:502:NAG:C5	1.84	0.90
1:J:187:GLU:HG2	1:J:188:ARG:H	1.37	0.90
7:H:503:MAN:HO6	7:H:505:MAN:H62	1.16	0.89
2:E:393:MET:CG	2:E:425:ASN:HB2	2.01	0.89
3:F:398:GLN:HE21	3:F:399:GLN:HG3	1.35	0.89
3:L:390:ASP:CG	3:L:391:LEU:N	2.26	0.89
10:E:502:BMA:H5	6:N:101:NDG:H8C1	1.54	0.88
10:E:502:BMA:C5	6:N:101:NDG:C8	2.52	0.88
2:B:393:MET:CG	2:B:425:ASN:HB2	2.04	0.88
3:I:279:TYR:CB	3:I:286:ASN:HD22	1.86	0.88
10:E:502:BMA:C6	6:N:101:NDG:C8	2.52	0.88
7:L:501:MAN:C1	5:Q:2:NAG:O3	2.21	0.88
2:E:231:HIS:HD2	2:E:233:GLU:H	1.21	0.87
3:I:351:ASN:HB3	3:I:375:TYR:CD1	2.10	0.86
9:I:502:NAG:HO3	7:J:301:MAN:C1	1.84	0.86
3:F:351:ASN:HB3	3:F:375:TYR:CD1	2.09	0.86
2:B:231:HIS:HD2	2:B:233:GLU:H	1.20	0.86
2:B:273:VAL:HG21	2:B:474:LEU:HD22	1.58	0.86
3:F:279:TYR:CB	3:F:286:ASN:HD22	1.88	0.86
3:L:279:TYR:CB	3:L:286:ASN:HD22	1.87	0.86
2:H:371:ASN:HD21	2:H:374:LEU:HD11	1.41	0.85
6:H:502:NDG:H6C2	6:K:501:NDG:H3	1.56	0.85
9:I:501:NAG:O4	9:I:502:NAG:H62	1.75	0.85
3:C:279:TYR:CB	3:C:286:ASN:HD22	1.88	0.85
6:D:301:NDG:N2	7:E:503:MAN:O1	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:231:HIS:HD2	2:K:233:GLU:H	1.24	0.85
2:B:208:LYS:HE2	2:B:208:LYS:HA	1.58	0.85
2:E:208:LYS:HE2	2:E:208:LYS:HA	1.58	0.85
1:J:162:LEU:H	2:K:210:GLN:HE22	1.24	0.85
2:E:273:VAL:HG21	2:E:474:LEU:HD22	1.57	0.85
3:C:351:ASN:HB3	3:C:375:TYR:CD1	2.11	0.85
1:G:126:LEU:HB3	1:G:184:LEU:HD13	1.59	0.85
1:D:142:ARG:HB2	1:D:142:ARG:NH1	1.91	0.85
7:H:505:MAN:C1	6:H:506:NDG:O1	2.24	0.85
1:A:188:ARG:HB3	1:A:188:ARG:NH1	1.91	0.84
1:G:162:LEU:H	2:H:210:GLN:HE22	1.25	0.84
3:I:385:LEU:HD23	3:I:386:PRO:HD2	1.60	0.84
3:F:207:ASP:OD2	3:F:209:VAL:HG13	1.78	0.84
6:H:506:NDG:C2	11:H:507:GAL:H3	2.06	0.84
2:K:273:VAL:HG21	2:K:474:LEU:HD22	1.58	0.84
1:A:188:ARG:HD2	1:A:188:ARG:N	1.92	0.84
2:H:231:HIS:HD2	2:H:233:GLU:H	1.22	0.84
1:A:97:LEU:HD23	1:J:108:LEU:HD13	1.59	0.83
6:H:506:NDG:H4	11:H:507:GAL:H4	1.59	0.83
1:J:162:LEU:HD22	1:J:163:GLU:O	1.78	0.83
2:H:220:VAL:HG23	3:I:140:ASP:HA	1.60	0.83
2:E:379:GLN:HE22	2:E:462:GLY:HA2	1.42	0.83
10:E:502:BMA:H3	6:N:101:NDG:O3	1.78	0.83
2:H:273:VAL:HG21	2:H:474:LEU:HD22	1.59	0.83
2:K:177:ARG:HH22	2:K:181:THR:HG21	1.43	0.83
2:K:371:ASN:HD21	2:K:374:LEU:HD11	1.44	0.83
6:D:301:NDG:O1	7:E:503:MAN:H1	1.79	0.83
1:D:103:GLU:HA	1:D:106:ARG:HG2	1.61	0.83
2:E:293:GLU:HB2	2:E:315:GLY:H	1.42	0.83
3:F:385:LEU:HD23	3:F:386:PRO:HD2	1.58	0.83
3:L:351:ASN:HB3	3:L:375:TYR:CD1	2.11	0.83
2:H:379:GLN:HE22	2:H:462:GLY:HA2	1.43	0.82
2:B:371:ASN:HD21	2:B:374:LEU:HD11	1.44	0.82
3:L:385:LEU:HD23	3:L:386:PRO:HD2	1.61	0.82
1:A:115:LEU:O	1:A:119:ILE:HG12	1.78	0.82
3:C:136:ARG:HB3	3:C:136:ARG:NH1	1.94	0.82
10:E:502:BMA:C1	6:N:101:NDG:O3	2.28	0.82
3:F:136:ARG:HB3	3:F:136:ARG:NH1	1.95	0.82
3:C:351:ASN:HB2	3:C:374:TRP:O	1.80	0.82
3:I:207:ASP:OD2	3:I:209:VAL:HG13	1.80	0.82
2:B:379:GLN:HE22	2:B:462:GLY:HA2	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:GLU:O	2:H:215:SER:N	2.13	0.82
6:H:506:NDG:C2	11:H:507:GAL:C3	2.58	0.82
2:K:293:GLU:HB2	2:K:315:GLY:H	1.43	0.82
9:C:501:NAG:O4	9:C:502:NAG:C6	2.28	0.81
2:H:177:ARG:HH22	2:H:181:THR:HG21	1.44	0.81
6:H:502:NDG:H8C2	7:H:503:MAN:H62	1.63	0.81
2:H:194:GLU:HA	2:H:197:ARG:NH1	1.96	0.81
1:A:103:GLU:HA	1:A:106:ARG:HG2	1.60	0.81
7:H:503:MAN:O1	7:P:101:MAN:H1	1.79	0.81
2:K:393:MET:SD	2:K:425:ASN:HB2	2.20	0.81
2:H:393:MET:SD	2:H:425:ASN:HB2	2.21	0.81
3:L:351:ASN:HB2	3:L:374:TRP:O	1.81	0.81
2:B:293:GLU:HB2	2:B:315:GLY:H	1.45	0.80
2:H:323:THR:OG1	2:H:351:PRO:HD2	1.81	0.80
2:K:379:GLN:HE22	2:K:462:GLY:HA2	1.43	0.80
1:J:146:ASP:HB3	3:L:127:LEU:HD11	1.63	0.80
1:A:142:ARG:HB2	1:A:142:ARG:NH1	1.96	0.80
9:F:501:NAG:O4	9:F:502:NAG:H5	1.82	0.80
2:K:293:GLU:HG3	2:K:314:LEU:HA	1.64	0.80
3:F:390:ASP:CG	3:F:391:LEU:H	1.84	0.80
2:E:371:ASN:HD21	2:E:374:LEU:HD11	1.45	0.80
3:I:197:ARG:HB2	3:I:380:THR:HB	1.63	0.80
3:F:197:ARG:HB2	3:F:380:THR:HB	1.63	0.79
3:I:391:LEU:HA	3:I:394:HIS:HD2	1.44	0.79
3:L:250:ASP:HB2	3:L:375:TYR:OH	1.82	0.79
3:C:194:ILE:HG23	3:C:233:ILE:HD11	1.64	0.79
10:E:502:BMA:H61	6:N:101:NDG:C8	2.11	0.79
1:A:104:VAL:HG22	1:J:100:ARG:HD2	1.63	0.79
1:D:115:LEU:O	1:D:119:ILE:HG12	1.81	0.79
2:K:194:GLU:HA	2:K:197:ARG:NH1	1.97	0.79
3:C:197:ARG:HB2	3:C:380:THR:HB	1.64	0.79
3:F:250:ASP:HB2	3:F:375:TYR:OH	1.81	0.79
3:L:293:PHE:HE2	3:L:303:THR:HG21	1.47	0.79
3:C:256:ARG:HD3	3:C:283:ASP:O	1.83	0.79
9:E:501:NAG:H4	6:N:101:NDG:O5	1.82	0.79
3:C:293:PHE:HE2	3:C:303:THR:HG21	1.47	0.79
2:E:323:THR:OG1	2:E:351:PRO:HD2	1.83	0.79
2:K:323:THR:OG1	2:K:351:PRO:HD2	1.83	0.79
3:I:351:ASN:HB2	3:I:374:TRP:O	1.82	0.79
5:Q:1:NAG:O4	5:Q:2:NAG:O5	1.96	0.79
1:A:111:ARG:HH12	1:J:96:GLU:HB2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:GLU:HG3	1:G:176:LYS:N	1.98	0.78
6:H:506:NDG:H2	11:H:507:GAL:H3	1.64	0.78
3:I:247:ASP:HB2	3:I:381:THR:HG23	1.65	0.78
1:A:188:ARG:H	1:A:188:ARG:CD	1.91	0.78
2:B:323:THR:OG1	2:B:351:PRO:HD2	1.83	0.78
3:C:385:LEU:HD23	3:C:386:PRO:HD2	1.64	0.78
2:E:293:GLU:HG3	2:E:314:LEU:HA	1.64	0.78
1:G:162:LEU:HD22	1:G:163:GLU:O	1.83	0.78
3:L:391:LEU:HG	3:L:394:HIS:HB2	1.64	0.78
1:J:188:ARG:HG3	1:J:190:GLU:HG2	1.66	0.78
1:G:160:ARG:HG2	1:G:160:ARG:HH11	1.49	0.78
3:I:250:ASP:HB2	3:I:375:TYR:OH	1.84	0.78
3:C:250:ASP:HB2	3:C:375:TYR:OH	1.84	0.78
2:H:293:GLU:HB2	2:H:315:GLY:H	1.47	0.78
3:L:197:ARG:HB2	3:L:380:THR:HB	1.65	0.78
1:D:139:GLN:O	1:D:143:VAL:HG23	1.84	0.77
2:B:393:MET:SD	2:B:425:ASN:HB2	2.25	0.77
2:H:212:GLU:O	2:H:215:SER:HB2	1.83	0.77
3:I:293:PHE:HE2	3:I:303:THR:HG21	1.48	0.77
3:L:247:ASP:HB2	3:L:381:THR:HG23	1.65	0.77
9:F:502:NAG:O3	7:F:503:MAN:O5	2.01	0.77
9:I:501:NAG:O4	9:I:502:NAG:C6	2.30	0.77
2:K:263:MET:HE2	2:K:269:GLY:H	1.48	0.77
3:C:207:ASP:OD2	3:C:209:VAL:HG13	1.84	0.77
3:L:207:ASP:OD2	3:L:209:VAL:HG13	1.84	0.77
3:F:293:PHE:HE2	3:F:303:THR:HG21	1.48	0.77
2:H:167:ILE:HG21	3:I:88:ILE:HG23	1.65	0.77
3:L:117:GLN:O	3:L:120:VAL:HG12	1.84	0.77
1:A:168:LYS:HD3	1:A:170:LYS:HE2	1.67	0.77
2:B:293:GLU:HG3	2:B:314:LEU:HA	1.66	0.77
3:F:351:ASN:HB2	3:F:374:TRP:O	1.83	0.77
3:C:150:THR:HG22	3:C:151:GLY:N	1.98	0.77
2:E:393:MET:SD	2:E:425:ASN:HB2	2.25	0.77
2:H:179:GLU:HG3	2:H:180:SER:H	1.49	0.77
2:H:194:GLU:HA	2:H:197:ARG:HH12	1.49	0.77
2:K:194:GLU:HA	2:K:197:ARG:HH12	1.50	0.77
1:J:175:GLU:HG3	1:J:176:LYS:N	1.99	0.76
3:L:256:ARG:HD3	3:L:283:ASP:O	1.85	0.76
3:F:256:ARG:HD3	3:F:283:ASP:O	1.85	0.76
3:I:194:ILE:HG23	3:I:233:ILE:HD11	1.68	0.76
9:F:501:NAG:O4	9:F:502:NAG:C1	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:293:GLU:HG3	2:H:314:LEU:HA	1.67	0.76
3:F:247:ASP:HB2	3:F:381:THR:HG23	1.68	0.76
2:E:384:ASN:ND2	4:N:2:HIS:NE2	2.34	0.76
1:G:118:ARG:O	1:G:122:GLN:HG3	1.86	0.76
1:J:118:ARG:O	1:J:122:GLN:HG3	1.86	0.76
2:K:179:GLU:HG3	2:K:180:SER:H	1.50	0.76
3:F:194:ILE:HG23	3:F:233:ILE:HD11	1.68	0.76
1:G:146:ASP:HB3	3:I:127:LEU:HD11	1.66	0.76
3:I:298:GLN:NE2	3:I:298:GLN:H	1.84	0.76
2:K:167:ILE:CG2	3:L:88:ILE:HG23	2.15	0.75
6:D:301:NDG:O1	7:E:503:MAN:C1	2.33	0.75
3:I:256:ARG:HD3	3:I:283:ASP:O	1.86	0.75
3:F:150:THR:HG23	3:F:169:TYR:O	1.86	0.75
3:F:385:LEU:HD23	3:F:386:PRO:CD	2.15	0.75
2:E:417:GLU:O	2:E:418:ASP:HB2	1.85	0.75
3:L:130:ILE:HA	3:L:133:THR:HG23	1.67	0.75
1:D:168:LYS:HD3	1:D:170:LYS:HE2	1.69	0.75
3:I:130:ILE:HA	3:I:133:THR:HG23	1.67	0.75
1:A:103:GLU:HA	1:A:106:ARG:HH11	1.51	0.75
7:H:503:MAN:O6	7:H:505:MAN:C6	2.29	0.75
9:C:502:NAG:HO3	7:C:503:MAN:C1	2.00	0.74
2:H:263:MET:HE2	2:H:269:GLY:H	1.52	0.74
3:L:298:GLN:NE2	3:L:298:GLN:H	1.85	0.74
2:H:219:THR:HG22	3:I:139:GLN:HB2	1.69	0.74
1:J:160:ARG:HH11	1:J:160:ARG:HG2	1.52	0.74
3:L:194:ILE:HG23	3:L:233:ILE:HD11	1.69	0.74
2:B:199:LYS:HG2	2:B:203:MET:CE	2.17	0.74
1:D:103:GLU:HA	1:D:106:ARG:HH11	1.51	0.74
3:F:154:CYS:SG	3:F:192:THR:HB	2.27	0.74
2:B:417:GLU:O	2:B:418:ASP:HB2	1.86	0.74
3:L:385:LEU:HD23	3:L:386:PRO:CD	2.17	0.74
2:B:263:MET:HE2	2:B:269:GLY:H	1.52	0.74
1:A:139:GLN:O	1:A:143:VAL:HG23	1.88	0.74
10:E:502:BMA:H1	6:N:101:NDG:C3	2.18	0.74
3:F:298:GLN:NE2	3:F:298:GLN:H	1.86	0.74
1:G:175:GLU:HG3	1:G:176:LYS:HG3	1.70	0.73
3:L:150:THR:HG22	3:L:151:GLY:N	2.00	0.73
2:E:359:ARG:NH2	2:E:394:GLN:HE21	1.86	0.73
7:H:505:MAN:HO1	6:H:506:NDG:HA	1.34	0.73
3:I:117:GLN:O	3:I:120:VAL:HG12	1.87	0.73
3:I:385:LEU:HD23	3:I:386:PRO:CD	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:HG3	1:A:192:VAL:HG23	1.70	0.73
3:C:247:ASP:HB2	3:C:381:THR:HG23	1.70	0.73
2:K:217:PRO:HB2	3:L:136:ARG:NH1	2.03	0.73
3:L:85:VAL:HA	3:L:88:ILE:HD12	1.70	0.73
2:H:417:GLU:O	2:H:418:ASP:HB2	1.89	0.73
2:E:263:MET:HE2	2:E:269:GLY:H	1.52	0.72
1:A:111:ARG:HH22	1:J:96:GLU:HB3	1.55	0.72
3:C:129:ASP:O	3:C:133:THR:HG23	1.89	0.72
3:L:305:HIS:CE1	3:L:339:ALA:H	2.08	0.72
1:A:97:LEU:CD2	1:J:108:LEU:HD13	2.20	0.72
3:C:250:ASP:OD2	3:C:254:THR:HB	1.88	0.72
1:G:126:LEU:HD11	3:I:106:ILE:HG12	1.71	0.72
2:K:426:ARG:HH21	4:P:6:NH2:N	1.86	0.72
2:H:359:ARG:HH21	2:H:394:GLN:HE21	1.36	0.72
3:I:107:GLN:HA	3:I:107:GLN:HE21	1.54	0.72
3:C:385:LEU:HD23	3:C:386:PRO:CD	2.19	0.72
10:E:502:BMA:C6	7:E:503:MAN:H62	2.08	0.72
1:G:112:ILE:HD11	3:I:92:VAL:HG22	1.72	0.72
3:I:85:VAL:HA	3:I:88:ILE:HD12	1.70	0.72
1:J:126:LEU:HD11	3:L:106:ILE:HG12	1.71	0.72
1:J:175:GLU:HG3	1:J:176:LYS:HG3	1.72	0.72
3:L:107:GLN:HA	3:L:107:GLN:HE21	1.55	0.72
3:L:328:ASP:HA	3:L:363:ASP:HB3	1.71	0.72
2:B:208:LYS:HE2	2:B:208:LYS:CA	2.20	0.72
2:B:231:HIS:CD2	2:B:233:GLU:H	2.07	0.71
2:E:208:LYS:HE2	2:E:208:LYS:CA	2.19	0.71
3:C:298:GLN:NE2	3:C:298:GLN:H	1.86	0.71
2:E:359:ARG:HH21	2:E:394:GLN:HE21	1.38	0.71
2:H:261:CYS:HB3	2:H:263:MET:HE3	1.71	0.71
3:I:250:ASP:OD2	3:I:254:THR:HB	1.90	0.71
3:I:305:HIS:CE1	3:I:339:ALA:H	2.09	0.71
2:K:173:GLU:HA	2:K:176:ILE:HG13	1.72	0.71
3:L:150:THR:HG23	3:L:169:TYR:O	1.91	0.71
2:E:199:LYS:HG2	2:E:203:MET:CE	2.20	0.71
3:L:135:SER:O	3:L:137:PRO:HD3	1.90	0.71
2:H:170:ARG:HA	2:H:173:GLU:HG2	1.72	0.71
2:K:417:GLU:O	2:K:418:ASP:HB2	1.91	0.71
2:B:190:LYS:HB2	3:C:109:LEU:HD21	1.73	0.71
3:I:328:ASP:HA	3:I:363:ASP:HB3	1.71	0.71
3:C:328:ASP:HA	3:C:363:ASP:HB3	1.73	0.70
3:I:150:THR:HG23	3:I:169:TYR:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:CYS:HB3	2:B:263:MET:HE3	1.73	0.70
7:H:503:MAN:O1	7:P:101:MAN:O5	2.00	0.70
2:K:384:ASN:HD21	6:K:501:NDG:C2	2.03	0.70
3:C:390:ASP:CG	3:C:391:LEU:N	2.44	0.70
1:D:186:PHE:CE2	2:E:177:ARG:HG3	2.26	0.70
3:I:305:HIS:HE1	3:I:339:ALA:H	1.39	0.70
3:L:305:HIS:HE1	3:L:339:ALA:H	1.40	0.70
1:J:164:TYR:OH	2:K:203:MET:HG2	1.90	0.70
2:B:359:ARG:HH21	2:B:394:GLN:HE21	1.38	0.70
2:H:393:MET:HG3	2:H:425:ASN:CB	2.20	0.70
2:K:393:MET:HG3	2:K:425:ASN:CB	2.20	0.70
9:F:502:NAG:C3	7:F:503:MAN:C1	2.69	0.70
1:G:175:GLU:HG3	1:G:176:LYS:H	1.57	0.70
3:I:191:TRP:CE3	3:I:383:LYS:HG3	2.27	0.70
3:C:150:THR:HG23	3:C:169:TYR:O	1.92	0.69
9:C:501:NAG:HO4	9:C:502:NAG:C5	2.05	0.69
1:J:175:GLU:HG3	1:J:176:LYS:H	1.57	0.69
1:A:111:ARG:HH22	1:J:96:GLU:CB	2.05	0.69
3:C:154:CYS:SG	3:C:192:THR:HB	2.32	0.69
1:G:162:LEU:O	1:G:163:GLU:HB2	1.93	0.69
3:C:328:ASP:OD1	3:C:363:ASP:HA	1.91	0.69
9:C:501:NAG:O4	9:C:502:NAG:H62	1.93	0.69
3:F:250:ASP:OD2	3:F:254:THR:HB	1.92	0.69
3:F:328:ASP:HA	3:F:363:ASP:HB3	1.73	0.69
2:H:231:HIS:CD2	2:H:233:GLU:H	2.08	0.69
2:E:231:HIS:CD2	2:E:233:GLU:H	2.06	0.69
2:E:293:GLU:HB2	2:E:315:GLY:N	2.07	0.69
3:F:328:ASP:OD1	3:F:363:ASP:HA	1.93	0.69
3:F:305:HIS:CE1	3:F:339:ALA:H	2.10	0.69
2:H:432:PRO:O	2:H:433:ASN:HB2	1.93	0.69
3:I:150:THR:HG22	3:I:151:GLY:N	2.04	0.69
2:K:178:ILE:CG2	3:L:98:ILE:HG21	2.22	0.69
3:F:305:HIS:HE1	3:F:339:ALA:H	1.40	0.69
1:J:178:ALA:HB2	2:K:188:SER:OG	1.93	0.69
1:D:130:GLN:HE22	1:D:182:ALA:HA	1.57	0.69
2:E:261:CYS:HB3	2:E:263:MET:HE3	1.75	0.69
3:L:250:ASP:OD2	3:L:254:THR:HB	1.93	0.69
3:L:328:ASP:OD1	3:L:363:ASP:HA	1.93	0.69
3:F:150:THR:HG22	3:F:151:GLY:N	2.01	0.68
2:H:359:ARG:NH2	2:H:394:GLN:HE21	1.90	0.68
1:J:168:LYS:HB2	1:J:171:ASN:HD21	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:THR:CG2	3:L:151:GLY:H	2.03	0.68
3:C:305:HIS:CE1	3:C:339:ALA:H	2.10	0.68
2:E:220:VAL:HG23	3:F:140:ASP:HA	1.74	0.68
3:F:191:TRP:CE2	3:F:385:LEU:HD12	2.28	0.68
2:B:432:PRO:O	2:B:433:ASN:HB2	1.93	0.68
3:F:129:ASP:O	3:F:133:THR:HG23	1.92	0.68
1:A:107:GLU:HG2	1:J:100:ARG:NH1	2.08	0.68
2:B:428:HIS:O	4:M:1:GLY:N	2.24	0.68
2:H:178:ILE:CG2	3:I:98:ILE:HG21	2.23	0.68
2:H:371:ASN:HD21	2:H:374:LEU:CD1	2.07	0.68
3:I:328:ASP:OD1	3:I:363:ASP:HA	1.93	0.68
3:L:154:CYS:SG	3:L:192:THR:HB	2.33	0.68
3:L:335:ASN:C	3:L:337:CYS:H	1.95	0.68
2:B:413:HIS:ND1	2:B:416:ARG:HG3	2.08	0.68
10:E:502:BMA:C6	6:N:101:NDG:H8C2	2.18	0.68
10:E:502:BMA:C3	6:N:101:NDG:O3	2.42	0.68
2:K:231:HIS:CD2	2:K:233:GLU:H	2.10	0.68
1:J:112:ILE:HD11	3:L:92:VAL:HG22	1.74	0.68
3:F:150:THR:CG2	3:F:151:GLY:H	2.05	0.68
2:K:384:ASN:HD21	6:K:501:NDG:C1	2.06	0.68
3:C:390:ASP:CG	3:C:391:LEU:H	1.97	0.68
3:F:335:ASN:C	3:F:337:CYS:H	1.98	0.68
7:H:503:MAN:O1	7:P:101:MAN:O2	2.10	0.68
1:J:120:ASN:OD1	1:J:187:GLU:HG3	1.93	0.68
2:K:432:PRO:O	2:K:433:ASN:HB2	1.94	0.68
3:L:209:VAL:HB	3:L:212:ARG:HH12	1.59	0.68
2:B:359:ARG:NH2	2:B:394:GLN:HE21	1.91	0.67
3:C:305:HIS:HE1	3:C:339:ALA:H	1.41	0.67
3:L:191:TRP:CE3	3:L:383:LYS:HG3	2.30	0.67
1:G:168:LYS:HB2	1:G:171:ASN:HD21	1.59	0.67
3:I:191:TRP:CE2	3:I:385:LEU:HD12	2.29	0.67
1:A:119:ILE:HD11	2:B:178:ILE:HG12	1.77	0.67
1:D:107:GLU:HG3	1:G:97:LEU:HD11	1.76	0.67
1:D:119:ILE:HD11	2:E:178:ILE:HG12	1.77	0.67
3:I:209:VAL:HB	3:I:212:ARG:HH12	1.60	0.67
3:I:335:ASN:C	3:I:337:CYS:H	1.98	0.67
3:C:335:ASN:C	3:C:337:CYS:H	1.98	0.67
1:G:178:ALA:HB2	2:H:188:SER:OG	1.94	0.67
10:E:502:BMA:H2	7:N:102:MAN:O2	1.95	0.67
2:H:164:GLN:HB2	3:I:84:THR:CG2	2.24	0.67
6:H:502:NDG:C6	6:K:501:NDG:H3	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:HB3	1:J:111:ARG:HH22	1.58	0.67
1:A:97:LEU:HD21	1:J:108:LEU:CB	2.23	0.67
3:C:209:VAL:HB	3:C:212:ARG:HH12	1.59	0.67
3:I:154:CYS:SG	3:I:192:THR:HB	2.35	0.67
1:J:122:GLN:NE2	3:L:103:ASP:HB2	2.10	0.67
3:L:390:ASP:C	3:L:392:SER:H	1.98	0.67
3:L:367:TRP:H	3:L:371:HIS:CE1	2.13	0.66
3:C:191:TRP:CE2	3:C:385:LEU:HD12	2.30	0.66
1:J:162:LEU:HD12	2:K:210:GLN:HB2	1.77	0.66
1:G:188:ARG:HE	1:G:190:GLU:HG2	1.61	0.66
1:G:188:ARG:HG3	1:G:190:GLU:HG2	1.75	0.66
1:J:172:LEU:O	1:J:172:LEU:HD23	1.95	0.66
2:K:335:SER:HB2	2:K:469:GLN:HB2	1.78	0.66
1:D:170:LYS:O	1:D:174:LEU:HG	1.95	0.66
1:J:162:LEU:O	1:J:163:GLU:HB2	1.96	0.66
2:B:371:ASN:HD21	2:B:374:LEU:CD1	2.08	0.66
3:F:191:TRP:CE3	3:F:383:LYS:HG3	2.30	0.66
1:G:172:LEU:O	1:G:172:LEU:HD23	1.95	0.66
1:A:170:LYS:O	1:A:174:LEU:HG	1.96	0.66
1:A:188:ARG:HH11	1:A:188:ARG:CB	2.02	0.66
1:J:181:ILE:HD12	2:K:185:SER:HB2	1.77	0.66
2:K:371:ASN:HD21	2:K:374:LEU:CD1	2.08	0.66
3:C:194:ILE:CD1	3:C:233:ILE:HG12	2.19	0.65
3:C:367:TRP:H	3:C:371:HIS:CE1	2.14	0.65
2:E:293:GLU:HG2	2:E:294:PHE:N	2.11	0.65
2:E:393:MET:HG3	2:E:425:ASN:CB	2.21	0.65
3:F:209:VAL:HB	3:F:212:ARG:HH12	1.61	0.65
3:F:248:LEU:HB3	3:F:377:LEU:HD13	1.78	0.65
2:K:293:GLU:HB2	2:K:315:GLY:N	2.10	0.65
3:C:191:TRP:CE3	3:C:383:LYS:HG3	2.30	0.65
2:H:413:HIS:ND1	2:H:416:ARG:HG3	2.12	0.65
3:I:392:SER:C	3:I:394:HIS:H	2.00	0.65
3:I:367:TRP:H	3:I:371:HIS:CE1	2.14	0.65
3:L:191:TRP:CE2	3:L:385:LEU:HD12	2.31	0.65
1:G:181:ILE:HD12	2:H:185:SER:HB2	1.77	0.65
2:B:293:GLU:HB2	2:B:315:GLY:N	2.10	0.65
1:A:161:TYR:HA	2:B:210:GLN:HE22	1.61	0.65
1:A:146:ASP:HB3	3:C:127:LEU:HD21	1.77	0.65
1:A:184:LEU:HD21	2:B:185:SER:OG	1.97	0.65
2:E:219:THR:HG22	3:F:139:GLN:HB2	1.78	0.65
3:L:391:LEU:HD12	3:L:394:HIS:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:TYR:HA	2:E:210:GLN:HE22	1.61	0.65
2:E:190:LYS:HB2	3:F:109:LEU:HD21	1.78	0.65
3:F:367:TRP:H	3:F:371:HIS:CE1	2.15	0.65
3:L:336:ARG:O	3:L:337:CYS:HB2	1.97	0.65
1:G:182:ALA:C	1:G:184:LEU:H	2.00	0.65
2:K:293:GLU:HG2	2:K:294:PHE:N	2.12	0.65
6:D:301:NDG:O1	7:E:503:MAN:O1	2.15	0.64
2:H:293:GLU:HB2	2:H:315:GLY:N	2.12	0.64
3:C:209:VAL:HA	3:C:212:ARG:HH11	1.62	0.64
3:C:227:TRP:HE1	3:C:230:ASN:ND2	1.94	0.64
1:G:122:GLN:NE2	3:I:103:ASP:HB2	2.11	0.64
1:G:162:LEU:HD12	2:H:210:GLN:HB2	1.79	0.64
2:H:293:GLU:HG2	2:H:294:PHE:N	2.11	0.64
2:K:179:GLU:HA	2:K:183:ALA:CB	2.28	0.64
1:A:160:ARG:HG2	1:A:160:ARG:HH11	1.62	0.64
1:A:170:LYS:HD3	1:A:174:LEU:HD11	1.80	0.64
1:J:115:LEU:HD12	1:J:118:ARG:HD2	1.80	0.64
2:K:232:CYS:HB3	2:K:263:MET:HE1	1.78	0.64
3:F:390:ASP:CG	3:F:391:LEU:N	2.50	0.64
3:I:391:LEU:HD12	3:I:394:HIS:CD2	2.32	0.64
2:K:360:LEU:HD11	2:K:362:VAL:HG13	1.80	0.64
2:E:232:CYS:HB3	2:E:263:MET:HE1	1.79	0.64
2:B:393:MET:HG3	2:B:425:ASN:CB	2.23	0.64
1:G:169:GLU:C	1:G:171:ASN:H	1.99	0.64
3:I:136:ARG:HH22	3:I:139:GLN:NE2	1.96	0.64
3:I:209:VAL:HA	3:I:212:ARG:HH11	1.62	0.64
2:K:359:ARG:HH21	2:K:394:GLN:HE21	1.43	0.64
3:F:308:MET:HG3	3:F:335:ASN:HB2	1.80	0.64
3:C:122:ARG:HG2	3:C:126:GLN:HE21	1.63	0.64
2:H:387:MET:HB2	2:H:426:ARG:HG2	1.79	0.64
3:I:184:GLU:HB3	3:I:191:TRP:HB2	1.78	0.64
2:K:261:CYS:HB3	2:K:263:MET:HE3	1.80	0.64
5:Q:1:NAG:HO4	5:Q:2:NAG:C5	2.10	0.64
1:G:115:LEU:HD12	1:G:118:ARG:HD2	1.81	0.63
1:G:164:TYR:OH	2:H:203:MET:HG2	1.98	0.63
2:K:359:ARG:NH2	2:K:394:GLN:HE21	1.96	0.63
5:Q:1:NAG:O4	5:Q:2:NAG:C5	2.46	0.63
1:A:96:GLU:HB2	1:J:111:ARG:HH12	1.62	0.63
2:B:293:GLU:HG2	2:B:294:PHE:N	2.13	0.63
3:I:261:GLY:H	3:I:280:LEU:HD23	1.62	0.63
3:C:308:MET:HG3	3:C:335:ASN:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:O	1:D:163:GLU:CB	2.46	0.63
3:F:261:GLY:H	3:F:280:LEU:HD23	1.64	0.63
2:H:414:CYS:SG	2:H:427:CYS:N	2.72	0.63
2:H:232:CYS:HB3	2:H:263:MET:HE1	1.79	0.63
2:E:405:TRP:HB2	2:E:426:ARG:HA	1.81	0.63
2:H:179:GLU:HA	2:H:183:ALA:CB	2.28	0.63
3:C:335:ASN:CG	3:C:336:ARG:H	2.02	0.63
3:C:385:LEU:HD23	3:C:386:PRO:N	2.14	0.63
2:E:432:PRO:O	2:E:433:ASN:HB2	1.97	0.63
2:H:171:TYR:HA	2:H:174:VAL:HG12	1.81	0.63
3:C:184:GLU:HB3	3:C:191:TRP:HB2	1.80	0.63
1:D:170:LYS:HD3	1:D:174:LEU:HD11	1.81	0.63
3:L:227:TRP:HE1	3:L:230:ASN:ND2	1.97	0.63
2:E:413:HIS:ND1	2:E:416:ARG:HG3	2.14	0.63
3:F:122:ARG:HG2	3:F:126:GLN:HE21	1.64	0.63
2:H:178:ILE:HG23	3:I:98:ILE:HG21	1.80	0.63
1:J:123:LEU:HB3	1:J:184:LEU:O	1.98	0.63
1:J:169:GLU:C	1:J:171:ASN:H	2.01	0.63
2:B:387:MET:HB2	2:B:426:ARG:HG2	1.81	0.62
2:E:371:ASN:HD21	2:E:374:LEU:CD1	2.11	0.62
3:L:209:VAL:HA	3:L:212:ARG:HH11	1.63	0.62
1:A:98:GLU:CB	3:L:89:LEU:HD11	2.29	0.62
2:B:173:GLU:HA	2:B:176:ILE:HD12	1.81	0.62
3:C:397:GLN:O	3:C:398:GLN:HB3	1.99	0.62
2:H:301:ASN:HD21	2:H:305:ILE:HD11	1.64	0.62
3:I:335:ASN:CG	3:I:336:ARG:H	2.01	0.62
3:C:336:ARG:O	3:C:337:CYS:HB2	1.98	0.62
3:F:261:GLY:N	3:F:280:LEU:HD23	2.14	0.62
3:I:135:SER:O	3:I:137:PRO:HD3	1.98	0.62
2:B:278:ASP:O	2:B:280:SER:N	2.30	0.62
2:K:405:TRP:HB2	2:K:426:ARG:HA	1.81	0.62
3:F:279:TYR:CD2	3:F:286:ASN:HB2	2.35	0.62
1:J:121:MET:O	1:J:125:GLN:HG3	1.99	0.62
1:A:147:ILE:HG23	2:B:207:ILE:HD11	1.82	0.62
2:B:232:CYS:HB3	2:B:263:MET:HE1	1.80	0.62
2:B:405:TRP:HB2	2:B:426:ARG:HA	1.81	0.62
10:E:502:BMA:H3	6:N:101:NDG:HB	1.64	0.62
1:A:100:ARG:HH12	1:J:107:GLU:HG3	1.64	0.62
1:G:160:ARG:HG2	1:G:160:ARG:NH1	2.15	0.62
3:L:385:LEU:HD23	3:L:386:PRO:N	2.14	0.62
3:I:308:MET:HG3	3:I:335:ASN:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:VAL:O	1:G:103:GLU:HG3	2.00	0.62
1:G:129:LEU:HB3	2:H:189:MET:HE1	1.82	0.62
1:G:158:CYS:HB3	2:H:214:CYS:HA	1.81	0.62
1:G:168:LYS:CB	1:G:171:ASN:HD21	2.13	0.62
3:L:184:GLU:HB3	3:L:191:TRP:HB2	1.80	0.62
3:F:209:VAL:HA	3:F:212:ARG:HH11	1.64	0.61
1:J:168:LYS:CB	1:J:171:ASN:HD21	2.12	0.61
1:J:182:ALA:C	1:J:184:LEU:H	2.02	0.61
1:A:97:LEU:O	3:L:89:LEU:HD21	2.00	0.61
3:F:170:ILE:HD13	3:F:181:VAL:HG21	1.82	0.61
3:F:196:HIS:HE1	3:F:198:HIS:ND1	1.98	0.61
2:B:186:LEU:HD11	3:C:105:GLN:HB3	1.83	0.61
2:B:205:GLU:HG3	2:B:206:ALA:N	2.15	0.61
3:C:261:GLY:N	3:C:280:LEU:HD23	2.14	0.61
1:G:172:LEU:C	1:G:175:GLU:HG2	2.20	0.61
6:H:502:NDG:H8C2	7:H:503:MAN:C6	2.30	0.61
1:J:123:LEU:HD22	1:J:184:LEU:HA	1.82	0.61
2:K:178:ILE:HG23	3:L:98:ILE:HG21	1.80	0.61
3:F:351:ASN:HB2	3:F:375:TYR:HA	1.82	0.61
1:G:126:LEU:HD21	2:H:186:LEU:HD21	1.82	0.61
3:I:136:ARG:HH12	3:I:139:GLN:HG2	1.64	0.61
1:J:99:VAL:O	1:J:103:GLU:HG3	1.99	0.61
1:J:172:LEU:C	1:J:175:GLU:HG2	2.20	0.61
2:K:167:ILE:HG21	3:L:88:ILE:CG2	2.29	0.61
1:A:143:VAL:HG22	3:C:124:GLN:NE2	2.16	0.61
3:C:351:ASN:HB2	3:C:375:TYR:HA	1.83	0.61
2:E:335:SER:HB2	2:E:469:GLN:HB2	1.83	0.61
10:E:502:BMA:H5	6:N:101:NDG:N2	2.16	0.61
2:K:413:HIS:ND1	2:K:416:ARG:HG3	2.16	0.61
2:B:365:TYR:CB	2:B:371:ASN:ND2	2.63	0.61
1:D:95:ASN:HB2	1:D:98:GLU:HG3	1.83	0.61
2:H:179:GLU:HA	2:H:183:ALA:HB2	1.82	0.61
3:L:305:HIS:CE1	3:L:340:GLY:H	2.19	0.61
3:C:261:GLY:H	3:C:280:LEU:HD23	1.65	0.61
3:F:184:GLU:HB3	3:F:191:TRP:HB2	1.83	0.61
2:H:365:TYR:CB	2:H:371:ASN:ND2	2.64	0.61
2:K:351:PRO:HA	2:K:359:ARG:O	2.00	0.61
2:B:335:SER:HB2	2:B:469:GLN:HB2	1.83	0.61
2:E:387:MET:HB2	2:E:426:ARG:HG2	1.83	0.61
2:H:278:ASP:O	2:H:280:SER:N	2.33	0.61
2:H:360:LEU:HD11	2:H:362:VAL:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:387:MET:HB2	2:K:426:ARG:HG2	1.81	0.61
2:K:406:ASN:O	2:K:408:GLY:N	2.34	0.61
1:A:95:ASN:HB2	1:A:98:GLU:HG3	1.83	0.61
2:B:251:ASP:OD2	2:B:253:PHE:HE1	1.84	0.61
3:C:194:ILE:HD12	3:C:233:ILE:CG1	2.22	0.61
2:E:231:HIS:NE2	2:E:475:ARG:HA	2.16	0.61
3:F:385:LEU:HD23	3:F:386:PRO:N	2.14	0.61
2:K:179:GLU:HA	2:K:183:ALA:HB2	1.81	0.61
2:K:231:HIS:NE2	2:K:475:ARG:HA	2.15	0.61
3:L:115:VAL:HA	3:L:118:GLN:OE1	2.00	0.61
3:C:351:ASN:CB	3:C:375:TYR:HA	2.31	0.60
1:D:180:TYR:O	1:D:182:ALA:N	2.29	0.60
1:A:162:LEU:O	1:A:163:GLU:CB	2.49	0.60
3:C:280:LEU:O	3:C:281:ASP:HB2	2.00	0.60
3:I:261:GLY:N	3:I:280:LEU:HD23	2.15	0.60
1:J:160:ARG:HG2	2:K:213:LEU:HD22	1.82	0.60
3:C:197:ARG:HG2	3:C:365:ILE:HD13	1.83	0.60
3:C:279:TYR:CD2	3:C:286:ASN:HB2	2.36	0.60
1:D:113:ILE:HG13	2:E:170:ARG:NH1	2.16	0.60
2:E:251:ASP:OD2	2:E:253:PHE:HE1	1.83	0.60
3:F:336:ARG:O	3:F:337:CYS:HB2	2.01	0.60
1:A:107:GLU:HG3	1:J:97:LEU:HD11	1.82	0.60
1:A:119:ILE:HD11	2:B:178:ILE:CG1	2.32	0.60
1:D:104:VAL:HG22	1:G:100:ARG:HD2	1.83	0.60
3:F:335:ASN:CG	3:F:336:ARG:H	2.04	0.60
2:H:189:MET:HB3	3:I:109:LEU:CD1	2.32	0.60
2:H:251:ASP:OD2	2:H:253:PHE:HE1	1.84	0.60
3:I:197:ARG:HG2	3:I:365:ILE:HD13	1.83	0.60
3:I:227:TRP:HE1	3:I:230:ASN:ND2	1.98	0.60
2:K:432:PRO:HB3	2:K:470:MET:HG2	1.84	0.60
3:L:308:MET:HG3	3:L:335:ASN:HB2	1.81	0.60
2:B:220:VAL:HG23	3:C:140:ASP:HA	1.82	0.60
1:D:108:LEU:HD21	3:F:89:LEU:HD12	1.82	0.60
3:F:194:ILE:CD1	3:F:233:ILE:HG12	2.22	0.60
3:F:197:ARG:HG2	3:F:365:ILE:HD13	1.82	0.60
2:K:233:GLU:O	2:K:237:ARG:HG3	2.02	0.60
2:K:251:ASP:OD2	2:K:253:PHE:HE1	1.85	0.60
2:E:414:CYS:SG	2:E:427:CYS:N	2.73	0.60
10:E:502:BMA:C2	6:N:101:NDG:O3	2.49	0.60
2:H:405:TRP:HB2	2:H:426:ARG:HA	1.83	0.60
2:K:173:GLU:HA	2:K:176:ILE:CG1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:197:ARG:HG2	3:L:365:ILE:HD13	1.82	0.60
2:B:414:CYS:SG	2:B:427:CYS:N	2.75	0.60
1:D:146:ASP:HB3	3:F:127:LEU:HD21	1.84	0.60
6:H:502:NDG:H8C2	7:H:503:MAN:H4	1.84	0.60
3:I:351:ASN:CB	3:I:375:TYR:HA	2.32	0.60
3:L:280:LEU:O	3:L:281:ASP:HB2	2.02	0.60
3:L:335:ASN:CG	3:L:336:ARG:H	2.04	0.60
2:H:266:HIS:C	6:H:506:NDG:O3	2.40	0.60
3:I:279:TYR:CD2	3:I:286:ASN:HB2	2.37	0.60
3:I:336:ARG:O	3:I:337:CYS:HB2	2.02	0.60
2:K:182:VAL:HG12	3:L:102:HIS:NE2	2.17	0.60
3:L:279:TYR:CD2	3:L:286:ASN:HB2	2.36	0.60
2:B:379:GLN:NE2	2:B:462:GLY:HA2	2.16	0.60
3:F:280:LEU:O	3:F:281:ASP:HB2	2.01	0.60
3:F:351:ASN:CB	3:F:375:TYR:HA	2.31	0.60
1:G:121:MET:O	1:G:125:GLN:HG3	2.02	0.60
2:H:231:HIS:NE2	2:H:475:ARG:HA	2.16	0.60
3:I:351:ASN:HB2	3:I:375:TYR:HA	1.84	0.60
3:I:385:LEU:HD23	3:I:386:PRO:N	2.16	0.60
2:K:189:MET:HB3	3:L:109:LEU:CD1	2.32	0.60
3:L:311:SER:O	3:L:331:GLY:HA2	2.01	0.60
3:C:170:ILE:HD13	3:C:181:VAL:HG21	1.84	0.60
2:H:236:TYR:CE1	2:H:241:ARG:HD2	2.37	0.60
3:I:320:TYR:HD1	3:I:322:GLY:H	1.49	0.60
3:L:391:LEU:HA	3:L:394:HIS:CD2	2.38	0.59
1:A:95:ASN:O	1:A:99:VAL:HG23	2.03	0.59
1:A:162:LEU:HD23	2:B:213:LEU:CD1	2.32	0.59
2:B:277:VAL:HG23	2:B:469:GLN:HG2	1.84	0.59
2:B:301:ASN:HD21	2:B:305:ILE:HD11	1.67	0.59
2:B:360:LEU:HD11	2:B:362:VAL:HG13	1.84	0.59
2:H:182:VAL:HG12	3:I:102:HIS:NE2	2.17	0.59
3:I:248:LEU:HB3	3:I:377:LEU:HD13	1.83	0.59
1:J:126:LEU:HD21	2:K:186:LEU:HD21	1.83	0.59
3:L:261:GLY:H	3:L:280:LEU:HD23	1.67	0.59
3:L:261:GLY:N	3:L:280:LEU:HD23	2.17	0.59
1:A:113:ILE:HG13	2:B:170:ARG:NH1	2.18	0.59
1:G:158:CYS:O	2:H:218:CYS:HB3	2.01	0.59
2:H:170:ARG:HA	2:H:173:GLU:CG	2.32	0.59
2:H:335:SER:HB2	2:H:469:GLN:HB2	1.84	0.59
2:B:231:HIS:NE2	2:B:475:ARG:HA	2.17	0.59
3:C:194:ILE:HG23	3:C:233:ILE:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:GLN:OE1	2:E:174:VAL:HG22	2.02	0.59
1:D:119:ILE:HD11	2:E:178:ILE:CG1	2.32	0.59
3:I:359:PHE:HB2	3:I:360:PRO:HD2	1.85	0.59
2:K:220:VAL:HG23	3:L:140:ASP:HA	1.83	0.59
2:K:352:GLU:O	2:K:358:TYR:HA	2.03	0.59
2:K:365:TYR:CG	2:K:366:SER:N	2.70	0.59
3:L:196:HIS:HE1	3:L:198:HIS:ND1	2.00	0.59
3:L:351:ASN:CB	3:L:375:TYR:HA	2.32	0.59
1:A:107:GLU:HG3	1:J:97:LEU:HD21	1.83	0.59
1:D:97:LEU:HD21	1:G:108:LEU:HB2	1.84	0.59
3:F:227:TRP:HE1	3:F:230:ASN:ND2	2.00	0.59
1:A:176:LYS:O	1:A:180:TYR:HB2	2.02	0.59
2:E:236:TYR:CE1	2:E:241:ARG:HD2	2.37	0.59
2:E:365:TYR:CG	2:E:366:SER:N	2.70	0.59
1:G:183:ASN:HB2	2:H:181:THR:HG23	1.84	0.59
2:K:168:GLU:HG3	2:K:168:GLU:O	2.02	0.59
2:K:370:GLY:HA3	2:K:459:ASN:HB3	1.84	0.59
3:L:351:ASN:HB2	3:L:375:TYR:HA	1.84	0.59
1:D:176:LYS:O	1:D:180:TYR:HB2	2.03	0.59
2:E:301:ASN:HD21	2:E:305:ILE:HD11	1.68	0.59
3:F:195:GLN:HG3	3:F:227:TRP:HE3	1.68	0.59
2:H:277:VAL:HG23	2:H:469:GLN:HG2	1.85	0.59
2:H:329:GLN:HG2	2:H:475:ARG:O	2.03	0.59
3:I:280:LEU:O	3:I:281:ASP:HB2	2.02	0.59
3:L:320:TYR:HD1	3:L:322:GLY:H	1.50	0.59
3:C:94:ILE:HD13	3:C:97:GLN:NE2	2.17	0.59
2:H:351:PRO:HA	2:H:359:ARG:O	2.03	0.59
2:K:405:TRP:CZ2	2:K:412:LYS:HD2	2.37	0.59
3:L:248:LEU:HB3	3:L:377:LEU:HD13	1.83	0.59
3:C:136:ARG:HH11	3:C:136:ARG:CB	2.12	0.59
2:E:292:ALA:O	2:E:293:GLU:CB	2.50	0.59
1:G:134:LYS:O	1:G:137:VAL:HG12	2.02	0.59
1:J:106:ARG:O	1:J:110:ARG:HG3	2.03	0.59
2:B:233:GLU:O	2:B:237:ARG:HG3	2.02	0.59
2:K:426:ARG:NH2	4:P:6:NH2:N	2.50	0.59
1:A:116:GLN:OE1	2:B:174:VAL:HG22	2.03	0.58
2:B:432:PRO:HB3	2:B:470:MET:HG2	1.85	0.58
3:C:303:THR:CB	3:C:339:ALA:HB2	2.27	0.58
1:D:184:LEU:O	1:D:186:PHE:N	2.36	0.58
1:D:186:PHE:HE2	2:E:177:ARG:HG3	1.65	0.58
2:E:351:PRO:HA	2:E:359:ARG:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:SER:C	2:H:187:ARG:H	2.06	0.58
2:H:213:LEU:C	2:H:215:SER:H	2.05	0.58
2:H:365:TYR:CG	2:H:366:SER:N	2.71	0.58
3:I:115:VAL:HA	3:I:118:GLN:OE1	2.03	0.58
2:K:185:SER:C	2:K:187:ARG:H	2.05	0.58
3:F:154:CYS:HB2	3:F:192:THR:HG22	1.86	0.58
1:J:129:LEU:HB3	2:K:189:MET:HE1	1.84	0.58
3:L:249:THR:HB	3:L:379:MET:HB2	1.85	0.58
3:I:98:ILE:O	3:I:102:HIS:HB2	2.04	0.58
9:E:501:NAG:H4	6:N:101:NDG:C5	2.34	0.58
3:I:311:SER:O	3:I:331:GLY:HA2	2.03	0.58
1:J:187:GLU:CG	1:J:188:ARG:H	2.12	0.58
2:K:189:MET:HB3	3:L:109:LEU:HD13	1.86	0.58
2:K:365:TYR:CB	2:K:371:ASN:ND2	2.67	0.58
3:L:170:ILE:HD13	3:L:181:VAL:HG21	1.86	0.58
1:A:120:ASN:O	1:A:124:GLN:HG2	2.03	0.58
2:B:292:ALA:O	2:B:293:GLU:CB	2.52	0.58
3:C:248:LEU:HB3	3:C:377:LEU:HD13	1.86	0.58
1:D:162:LEU:O	1:D:163:GLU:HB2	2.03	0.58
2:E:173:GLU:HA	2:E:176:ILE:HD12	1.85	0.58
2:E:359:ARG:NH2	2:E:394:GLN:NE2	2.51	0.58
3:F:94:ILE:HD13	3:F:97:GLN:NE2	2.17	0.58
2:H:212:GLU:O	2:H:215:SER:CB	2.51	0.58
3:I:305:HIS:CE1	3:I:340:GLY:H	2.21	0.58
1:J:147:ILE:HD13	2:K:207:ILE:HD11	1.84	0.58
2:K:278:ASP:O	2:K:280:SER:N	2.31	0.58
3:L:359:PHE:HB2	3:L:360:PRO:HD2	1.86	0.58
1:A:153:ALA:HA	2:B:279:GLY:O	2.04	0.58
2:E:365:TYR:CB	2:E:371:ASN:ND2	2.66	0.58
2:K:277:VAL:HG23	2:K:469:GLN:HG2	1.85	0.58
1:A:115:LEU:HD22	2:B:178:ILE:HD11	1.86	0.58
1:A:171:ASN:HB2	2:B:195:HIS:CE1	2.39	0.58
3:C:305:HIS:CE1	3:C:340:GLY:H	2.22	0.58
2:H:379:GLN:NE2	2:H:462:GLY:HA2	2.15	0.58
3:I:94:ILE:HG22	3:I:95:LEU:HD23	1.86	0.58
3:I:170:ILE:HD13	3:I:181:VAL:HG21	1.85	0.58
2:K:414:CYS:SG	2:K:427:CYS:N	2.77	0.58
2:B:365:TYR:CG	2:B:366:SER:N	2.72	0.58
2:B:365:TYR:HB3	2:B:371:ASN:HD22	1.68	0.58
2:E:390:HIS:CE1	2:E:428:HIS:HB2	2.39	0.58
7:H:505:MAN:O1	6:H:506:NDG:O1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:196:HIS:HE1	3:I:198:HIS:ND1	2.01	0.58
3:L:99:GLY:O	3:L:103:ASP:HB2	2.04	0.58
3:L:194:ILE:CD1	3:L:233:ILE:HG12	2.23	0.58
3:C:195:GLN:HG3	3:C:227:TRP:HE3	1.68	0.58
1:D:143:VAL:HG22	3:F:124:GLN:NE2	2.19	0.58
6:D:301:NDG:H3	7:E:503:MAN:O1	2.04	0.58
3:I:194:ILE:CD1	3:I:233:ILE:HG12	2.23	0.58
3:C:398:GLN:NE2	3:C:399:GLN:HG3	2.19	0.57
2:E:432:PRO:HB3	2:E:470:MET:HG2	1.86	0.57
3:F:359:PHE:HB2	3:F:360:PRO:HD2	1.85	0.57
2:H:267:GLY:N	6:H:506:NDG:HB	1.98	0.57
2:H:359:ARG:NH2	2:H:394:GLN:NE2	2.51	0.57
2:H:432:PRO:HB3	2:H:470:MET:HG2	1.86	0.57
2:K:301:ASN:HD21	2:K:305:ILE:HD11	1.68	0.57
2:H:166:GLU:HG3	2:H:167:ILE:HG13	1.86	0.57
1:A:186:PHE:CE2	2:B:177:ARG:HG3	2.39	0.57
1:D:162:LEU:HD23	2:E:213:LEU:CD1	2.34	0.57
3:F:320:TYR:HD1	3:F:322:GLY:H	1.50	0.57
2:H:350:ARG:HG3	2:H:350:ARG:HH11	1.69	0.57
3:I:107:GLN:HA	3:I:107:GLN:NE2	2.20	0.57
2:K:236:TYR:CE1	2:K:241:ARG:HD2	2.38	0.57
1:A:176:LYS:HE3	1:A:180:TYR:CE1	2.39	0.57
3:C:311:SER:O	3:C:331:GLY:HA2	2.03	0.57
2:E:173:GLU:HA	2:E:176:ILE:CD1	2.34	0.57
2:E:459:ASN:HD22	2:E:459:ASN:H	1.52	0.57
3:F:305:HIS:CE1	3:F:340:GLY:H	2.22	0.57
2:H:384:ASN:ND2	4:O:2:HIS:NE2	2.51	0.57
3:I:99:GLY:O	3:I:103:ASP:HB2	2.04	0.57
1:J:160:ARG:CG	2:K:213:LEU:HD22	2.34	0.57
2:K:292:ALA:O	2:K:293:GLU:CB	2.52	0.57
2:K:315:GLY:O	2:K:319:VAL:HG23	2.04	0.57
2:K:379:GLN:NE2	2:K:462:GLY:HA2	2.17	0.57
3:L:195:GLN:HG3	3:L:227:TRP:HE3	1.68	0.57
1:A:108:LEU:HD21	3:C:89:LEU:HD12	1.86	0.57
3:C:196:HIS:HE1	3:C:198:HIS:ND1	2.01	0.57
2:E:379:GLN:NE2	2:E:462:GLY:HA2	2.16	0.57
1:G:106:ARG:O	1:G:110:ARG:HG3	2.05	0.57
2:H:167:ILE:O	2:H:167:ILE:HG22	2.04	0.57
2:H:189:MET:HB3	3:I:109:LEU:HD13	1.87	0.57
2:B:236:TYR:CE1	2:B:241:ARG:HD2	2.39	0.57
2:B:329:GLN:HG2	2:B:475:ARG:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:ARG:NH2	2:B:394:GLN:NE2	2.52	0.57
2:B:426:ARG:HH21	4:M:6:NH2:N	2.02	0.57
1:G:147:ILE:HD13	2:H:207:ILE:HD11	1.85	0.57
1:G:168:LYS:HB3	1:G:171:ASN:OD1	2.05	0.57
1:G:183:ASN:C	1:G:185:LYS:H	2.08	0.57
2:H:175:LYS:HG2	2:H:179:GLU:OE2	2.05	0.57
3:I:249:THR:HB	3:I:379:MET:HB2	1.85	0.57
1:J:183:ASN:C	1:J:185:LYS:H	2.08	0.57
1:A:162:LEU:H	2:B:210:GLN:NE2	2.03	0.57
2:B:365:TYR:HB2	2:B:371:ASN:ND2	2.20	0.57
3:C:359:PHE:HB2	3:C:360:PRO:HD2	1.86	0.57
2:E:278:ASP:O	2:E:280:SER:N	2.37	0.57
3:F:89:LEU:HD21	1:G:97:LEU:HB2	1.87	0.57
3:F:311:SER:O	3:F:331:GLY:HA2	2.04	0.57
1:G:107:GLU:HG2	1:G:110:ARG:HH12	1.69	0.57
1:G:188:ARG:CG	1:G:190:GLU:HG2	2.33	0.57
3:I:154:CYS:HB2	3:I:192:THR:HG22	1.86	0.57
1:A:109:GLU:O	1:A:113:ILE:HG22	2.05	0.57
2:B:219:THR:HG22	3:C:139:GLN:HB2	1.87	0.57
1:D:95:ASN:O	1:D:99:VAL:HG23	2.04	0.57
1:D:120:ASN:ND2	1:D:191:GLU:OE1	2.38	0.57
2:E:197:ARG:HB3	2:E:197:ARG:CZ	2.35	0.57
2:E:233:GLU:O	2:E:237:ARG:HG3	2.05	0.57
3:I:320:TYR:HD1	3:I:322:GLY:N	2.03	0.57
3:C:125:GLN:HG2	3:C:126:GLN:N	2.19	0.57
3:C:320:TYR:CD1	3:C:322:GLY:N	2.73	0.57
2:E:405:TRP:CZ2	2:E:412:LYS:HD2	2.40	0.57
1:J:168:LYS:HB3	1:J:171:ASN:OD1	2.04	0.57
3:L:136:ARG:HH12	3:L:139:GLN:HG2	1.69	0.57
2:B:173:GLU:HA	2:B:176:ILE:CD1	2.35	0.56
3:F:92:VAL:O	3:F:96:GLU:HG3	2.05	0.56
3:F:249:THR:HB	3:F:379:MET:HB2	1.87	0.56
2:H:354:GLU:HB2	2:H:358:TYR:CZ	2.40	0.56
2:K:201:GLN:HE21	2:K:201:GLN:HA	1.70	0.56
2:K:475:ARG:HG3	2:K:476:PRO:HD2	1.87	0.56
2:B:190:LYS:O	2:B:190:LYS:HG2	2.04	0.56
3:C:249:THR:HB	3:C:379:MET:HB2	1.86	0.56
2:E:205:GLU:HG3	2:E:206:ALA:N	2.19	0.56
3:F:194:ILE:HD12	3:F:233:ILE:CG1	2.24	0.56
2:H:365:TYR:HB2	2:H:371:ASN:ND2	2.20	0.56
2:B:301:ASN:ND2	2:B:305:ILE:HD11	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:PRO:HA	2:B:359:ARG:O	2.06	0.56
2:B:417:GLU:OE1	4:M:3:ARG:NH1	2.39	0.56
3:C:191:TRP:CZ3	3:C:385:LEU:HB2	2.40	0.56
1:D:147:ILE:HG23	2:E:207:ILE:HD11	1.87	0.56
2:E:277:VAL:HG23	2:E:469:GLN:HG2	1.86	0.56
2:E:443:THR:OG1	2:E:446:GLN:HG3	2.04	0.56
1:G:180:TYR:C	1:G:182:ALA:H	2.08	0.56
1:G:182:ALA:C	1:G:184:LEU:N	2.56	0.56
2:H:201:GLN:HA	2:H:201:GLN:HE21	1.69	0.56
2:H:301:ASN:ND2	2:H:305:ILE:HD11	2.20	0.56
2:K:350:ARG:HH11	2:K:350:ARG:HG3	1.69	0.56
3:F:194:ILE:HG23	3:F:233:ILE:CD1	2.35	0.56
9:F:501:NAG:HO4	9:F:502:NAG:C1	2.11	0.56
3:I:195:GLN:HG3	3:I:227:TRP:HE3	1.71	0.56
3:L:94:ILE:HG22	3:L:95:LEU:HD23	1.87	0.56
1:A:107:GLU:HG2	1:J:100:ARG:HH12	1.69	0.56
2:B:197:ARG:HB3	2:B:197:ARG:CZ	2.35	0.56
3:C:154:CYS:HB2	3:C:192:THR:HG22	1.88	0.56
2:E:186:LEU:HD11	3:F:105:GLN:HB3	1.86	0.56
2:E:354:GLU:HB2	2:E:358:TYR:CZ	2.40	0.56
2:H:292:ALA:O	2:H:293:GLU:CB	2.53	0.56
2:H:370:GLY:HA3	2:H:459:ASN:HB3	1.86	0.56
10:H:504:BMA:H1	6:O:101:NDG:O3	2.06	0.56
3:I:248:LEU:HD22	3:I:248:LEU:N	2.20	0.56
1:J:160:ARG:HG2	1:J:160:ARG:NH1	2.17	0.56
2:B:405:TRP:CZ2	2:B:412:LYS:HD2	2.41	0.56
2:K:359:ARG:NH2	2:K:394:GLN:NE2	2.54	0.56
3:L:107:GLN:HA	3:L:107:GLN:NE2	2.21	0.56
3:C:320:TYR:HD1	3:C:322:GLY:N	2.03	0.56
1:D:165:ARG:HD3	1:D:165:ARG:N	2.20	0.56
2:E:328:GLN:O	2:E:349:PHE:N	2.37	0.56
2:B:190:LYS:O	2:B:194:GLU:HB2	2.05	0.56
6:B:501:NDG:H6C2	6:M:101:NDG:H4	1.88	0.56
2:E:190:LYS:O	2:E:190:LYS:HG2	2.04	0.56
3:I:302:TYR:HA	3:I:336:ARG:HB2	1.88	0.56
2:K:170:ARG:O	2:K:174:VAL:HG23	2.05	0.56
1:D:125:GLN:OE1	3:F:106:ILE:HG21	2.05	0.56
2:H:352:GLU:O	2:H:358:TYR:HA	2.05	0.56
1:J:107:GLU:HG2	1:J:110:ARG:HH12	1.69	0.56
1:J:134:LYS:O	1:J:137:VAL:HG12	2.05	0.56
2:B:387:MET:SD	2:B:426:ARG:HG2	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:248:LEU:HD22	3:F:248:LEU:N	2.20	0.56
2:H:315:GLY:O	2:H:319:VAL:HG23	2.05	0.56
6:H:502:NDG:C8	7:H:503:MAN:H4	2.36	0.56
3:L:111:GLU:O	3:L:115:VAL:HG23	2.05	0.56
3:L:320:TYR:HD1	3:L:322:GLY:N	2.04	0.56
3:F:303:THR:CB	3:F:339:ALA:HB2	2.28	0.55
2:H:365:TYR:HB3	2:H:371:ASN:HD22	1.69	0.55
2:E:476:PRO:O	2:E:477:LYS:HE3	2.06	0.55
2:H:418:ASP:HA	2:H:453:ASP:HB3	1.88	0.55
2:H:475:ARG:HG3	2:H:476:PRO:HD2	1.87	0.55
2:B:200:MET:CE	3:C:119:PHE:HB3	2.36	0.55
3:C:92:VAL:O	3:C:96:GLU:HG3	2.06	0.55
3:C:93:ARG:O	3:C:97:GLN:HG3	2.06	0.55
2:E:384:ASN:CG	9:E:501:NAG:O1	2.45	0.55
3:F:191:TRP:CZ3	3:F:385:LEU:HB2	2.42	0.55
1:G:169:GLU:C	1:G:171:ASN:N	2.59	0.55
3:I:191:TRP:CE3	3:I:385:LEU:HB2	2.42	0.55
3:I:194:ILE:HG23	3:I:233:ILE:CD1	2.36	0.55
3:L:98:ILE:O	3:L:102:HIS:HB2	2.05	0.55
2:B:475:ARG:HG3	2:B:476:PRO:HD2	1.88	0.55
3:C:248:LEU:HD22	3:C:248:LEU:N	2.21	0.55
1:D:153:ALA:HA	2:E:279:GLY:O	2.06	0.55
2:E:352:GLU:O	2:E:358:TYR:HA	2.06	0.55
1:G:133:ILE:HG12	2:H:193:LEU:HD21	1.89	0.55
2:K:329:GLN:HG2	2:K:475:ARG:O	2.07	0.55
3:L:191:TRP:CE3	3:L:385:LEU:HB2	2.41	0.55
3:L:302:TYR:HA	3:L:336:ARG:HB2	1.89	0.55
1:A:162:LEU:O	1:A:163:GLU:HB2	2.05	0.55
3:F:93:ARG:NH1	1:G:95:ASN:N	2.54	0.55
3:F:398:GLN:NE2	3:F:399:GLN:HG3	2.15	0.55
3:I:111:GLU:O	3:I:115:VAL:HG23	2.07	0.55
1:J:147:ILE:CD1	2:K:207:ILE:HD11	2.37	0.55
2:K:178:ILE:HG21	3:L:98:ILE:HG21	1.88	0.55
2:K:354:GLU:HB2	2:K:358:TYR:CZ	2.41	0.55
2:B:350:ARG:HH11	2:B:350:ARG:HG3	1.70	0.55
2:B:406:ASN:O	2:B:408:GLY:N	2.40	0.55
1:D:109:GLU:O	1:D:113:ILE:HG22	2.07	0.55
2:E:348:SER:HB3	2:E:363:GLU:HB3	1.89	0.55
1:G:162:LEU:O	1:G:163:GLU:CB	2.55	0.55
2:B:315:GLY:O	2:B:319:VAL:HG23	2.07	0.55
7:B:502:MAN:H61	6:M:101:NDG:C3	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:320:TYR:CD1	3:L:322:GLY:N	2.75	0.55
2:B:390:HIS:CE1	2:B:428:HIS:HB2	2.41	0.55
1:D:160:ARG:HG2	1:D:160:ARG:HH11	1.70	0.55
1:D:176:LYS:HE3	1:D:180:TYR:CE1	2.41	0.55
1:G:119:ILE:O	1:G:119:ILE:HG22	2.06	0.55
2:B:370:GLY:HA3	2:B:459:ASN:HB3	1.88	0.55
1:D:171:ASN:HB2	2:E:195:HIS:CE1	2.41	0.55
3:F:93:ARG:O	3:F:97:GLN:HG3	2.07	0.55
2:E:365:TYR:HB3	2:E:371:ASN:HD22	1.72	0.55
3:F:320:TYR:HD1	3:F:322:GLY:N	2.04	0.55
1:A:146:ASP:HB3	3:C:127:LEU:CD2	2.38	0.54
2:B:204:GLU:O	2:B:208:LYS:HG2	2.07	0.54
3:C:191:TRP:CE3	3:C:385:LEU:HB2	2.42	0.54
1:A:165:ARG:N	1:A:165:ARG:HD3	2.21	0.54
2:E:360:LEU:HD11	2:E:362:VAL:HG13	1.89	0.54
3:F:136:ARG:HH11	3:F:136:ARG:CB	2.11	0.54
1:J:119:ILE:O	1:J:119:ILE:HG22	2.06	0.54
2:B:182:VAL:O	2:B:186:LEU:HB2	2.08	0.54
3:C:125:GLN:HE21	3:C:126:GLN:HG3	1.71	0.54
1:D:120:ASN:O	1:D:124:GLN:HG2	2.07	0.54
2:H:390:HIS:CE1	2:H:428:HIS:HB2	2.42	0.54
3:L:191:TRP:CZ3	3:L:385:LEU:HB2	2.42	0.54
2:E:190:LYS:O	2:E:194:GLU:HB2	2.07	0.54
2:E:350:ARG:HG3	2:E:350:ARG:HH11	1.73	0.54
10:E:502:BMA:C1	6:N:101:NDG:H8C1	2.37	0.54
2:H:226:VAL:HG22	3:I:218:LEU:HG	1.90	0.54
1:J:165:ARG:O	1:J:166:LEU:HB2	2.08	0.54
2:B:365:TYR:CB	2:B:371:ASN:HD22	2.20	0.54
3:C:194:ILE:HB	3:C:382:MET:O	2.07	0.54
3:I:212:ARG:HA	3:I:230:ASN:HB2	1.90	0.54
1:J:169:GLU:OE1	1:J:169:GLU:HA	2.07	0.54
1:A:180:TYR:O	1:A:182:ALA:N	2.39	0.54
3:C:302:TYR:HA	3:C:336:ARG:HB2	1.89	0.54
1:D:115:LEU:HD22	2:E:178:ILE:HD11	1.89	0.54
2:E:200:MET:CE	3:F:119:PHE:HB3	2.37	0.54
1:G:103:GLU:C	1:G:105:LEU:H	2.10	0.54
1:G:160:ARG:HG2	2:H:213:LEU:HD22	1.90	0.54
1:G:162:LEU:HB2	2:H:210:GLN:NE2	2.22	0.54
1:G:181:ILE:O	1:G:184:LEU:HG	2.07	0.54
2:H:406:ASN:O	2:H:408:GLY:N	2.41	0.54
3:C:84:THR:HG22	3:C:88:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:389:ARG:O	3:C:390:ASP:HB3	2.07	0.54
2:E:329:GLN:HG2	2:E:475:ARG:O	2.08	0.54
2:E:389:ILE:O	2:E:425:ASN:ND2	2.41	0.54
1:G:165:ARG:O	1:G:166:LEU:HB2	2.08	0.54
1:J:133:ILE:HG12	2:K:193:LEU:HD21	1.90	0.54
2:K:365:TYR:HB2	2:K:371:ASN:ND2	2.23	0.54
1:A:181:ILE:O	1:A:181:ILE:CG1	2.55	0.54
2:B:348:SER:HB3	2:B:363:GLU:HB3	1.90	0.54
2:K:418:ASP:HA	2:K:453:ASP:HB3	1.89	0.54
1:D:162:LEU:H	2:E:210:GLN:NE2	2.06	0.54
2:E:370:GLY:HA3	2:E:459:ASN:HB3	1.89	0.54
2:H:220:VAL:CG2	3:I:140:ASP:HA	2.35	0.54
7:H:505:MAN:H3	6:H:506:NDG:H8C1	1.90	0.54
3:I:320:TYR:CD1	3:I:322:GLY:N	2.74	0.54
3:I:323:SER:HB3	3:I:326:GLU:HB3	1.90	0.54
9:I:501:NAG:H62	9:I:502:NAG:C1	2.37	0.54
1:J:103:GLU:C	1:J:105:LEU:H	2.10	0.54
2:K:476:PRO:O	2:K:477:LYS:HE3	2.08	0.54
3:L:323:SER:HB3	3:L:326:GLU:HB3	1.89	0.54
3:F:122:ARG:HG2	3:F:126:GLN:NE2	2.22	0.54
2:H:170:ARG:HA	2:H:173:GLU:OE2	2.08	0.54
2:K:177:ARG:NH2	2:K:181:THR:HG21	2.19	0.54
2:K:186:LEU:HD12	3:L:105:GLN:OE1	2.07	0.54
2:K:274:GLN:HE22	2:K:471:ALA:HA	1.73	0.54
1:A:168:LYS:CD	1:A:170:LYS:HE2	2.37	0.53
2:H:344:ALA:HB2	2:H:369:ALA:HB3	1.89	0.53
2:K:173:GLU:O	2:K:176:ILE:HB	2.07	0.53
3:L:194:ILE:HG23	3:L:233:ILE:CD1	2.36	0.53
1:A:182:ALA:C	1:A:184:LEU:H	2.12	0.53
2:B:418:ASP:HA	2:B:453:ASP:HB3	1.90	0.53
7:H:503:MAN:O1	7:P:101:MAN:C2	2.56	0.53
3:I:191:TRP:CZ3	3:I:385:LEU:HB2	2.42	0.53
1:A:133:ILE:O	1:A:137:VAL:HG23	2.09	0.53
3:C:197:ARG:CB	3:C:380:THR:HB	2.37	0.53
1:D:146:ASP:HB3	3:F:127:LEU:CD2	2.38	0.53
3:F:171:LYS:HB2	3:F:178:PRO:HB3	1.89	0.53
3:F:302:TYR:HA	3:F:336:ARG:HB2	1.89	0.53
1:G:147:ILE:CD1	2:H:207:ILE:HD11	2.38	0.53
1:J:162:LEU:HB2	2:K:210:GLN:NE2	2.23	0.53
2:K:365:TYR:HB3	2:K:371:ASN:HD22	1.73	0.53
3:L:248:LEU:N	3:L:248:LEU:HD22	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:308:MET:CG	3:C:335:ASN:HB2	2.39	0.53
3:F:125:GLN:HE21	3:F:126:GLN:HG3	1.74	0.53
3:F:323:SER:HB3	3:F:326:GLU:HB3	1.90	0.53
1:G:113:ILE:HD11	2:H:170:ARG:NH1	2.23	0.53
3:I:136:ARG:NH2	3:I:139:GLN:NE2	2.57	0.53
1:J:169:GLU:C	1:J:171:ASN:N	2.60	0.53
2:K:235:ILE:HD13	2:K:246:TYR:CD2	2.44	0.53
2:K:305:ILE:HG22	3:L:217:TYR:CE1	2.43	0.53
3:C:122:ARG:HG2	3:C:126:GLN:NE2	2.22	0.53
3:C:171:LYS:HB2	3:C:178:PRO:HB3	1.89	0.53
3:F:197:ARG:CB	3:F:380:THR:HB	2.35	0.53
3:F:212:ARG:HA	3:F:230:ASN:HB2	1.90	0.53
2:H:348:SER:HB3	2:H:363:GLU:HB3	1.89	0.53
2:H:443:THR:OG1	2:H:446:GLN:HG3	2.09	0.53
7:H:505:MAN:O1	6:H:506:NDG:C2	2.54	0.53
3:C:84:THR:O	3:C:88:ILE:HG13	2.09	0.53
1:D:133:ILE:O	1:D:137:VAL:HG23	2.09	0.53
3:F:84:THR:HG22	3:F:88:ILE:HD11	1.90	0.53
3:F:308:MET:CG	3:F:335:ASN:HB2	2.39	0.53
2:H:405:TRP:CZ2	2:H:412:LYS:HD2	2.42	0.53
1:A:192:VAL:HG12	1:A:193:VAL:H	1.73	0.53
2:B:428:HIS:CD2	2:B:431:ASN:HB2	2.43	0.53
3:C:244:LEU:HD22	3:C:263:PHE:CD1	2.44	0.53
2:H:365:TYR:CB	2:H:371:ASN:HD22	2.21	0.53
2:K:171:TYR:O	2:K:175:LYS:HB2	2.08	0.53
2:K:390:HIS:CE1	2:K:428:HIS:HB2	2.44	0.53
2:B:344:ALA:HB2	2:B:369:ALA:HB3	1.91	0.53
2:E:293:GLU:HG3	2:E:314:LEU:CA	2.37	0.53
2:H:420:GLY:O	2:H:424:TYR:HE2	1.92	0.53
3:I:130:ILE:HA	3:I:133:THR:CG2	2.36	0.53
2:K:200:MET:HB3	3:L:119:PHE:CE1	2.44	0.53
2:K:274:GLN:NE2	2:K:471:ALA:HA	2.24	0.53
2:K:301:ASN:ND2	2:K:305:ILE:HD11	2.23	0.53
3:L:130:ILE:HA	3:L:133:THR:CG2	2.37	0.53
1:A:125:GLN:OE1	3:C:106:ILE:HG21	2.09	0.53
1:D:181:ILE:O	1:D:181:ILE:CG1	2.56	0.53
2:E:301:ASN:ND2	2:E:305:ILE:HD11	2.23	0.53
10:E:502:BMA:H5	6:N:101:NDG:C8	2.30	0.53
3:F:191:TRP:CE3	3:F:385:LEU:HB2	2.43	0.53
2:H:178:ILE:HG21	3:I:98:ILE:HG21	1.89	0.53
2:H:233:GLU:O	2:H:237:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:130:GLN:HG3	1:J:178:ALA:O	2.09	0.53
2:K:348:SER:HB3	2:K:363:GLU:HB3	1.90	0.53
2:K:443:THR:OG1	2:K:446:GLN:HG3	2.08	0.53
3:L:244:LEU:HD22	3:L:263:PHE:CD1	2.44	0.53
2:E:186:LEU:HD21	3:F:106:ILE:HG13	1.90	0.53
10:E:502:BMA:O5	6:N:101:NDG:C8	2.48	0.53
1:G:130:GLN:HG3	1:G:178:ALA:O	2.09	0.53
3:C:172:PRO:HA	3:C:239:GLN:HE22	1.74	0.52
2:E:365:TYR:HB2	2:E:371:ASN:ND2	2.24	0.52
2:K:174:VAL:HG12	3:L:95:LEU:HD13	1.91	0.52
2:K:231:HIS:CD2	2:K:232:CYS:H	2.27	0.52
3:L:367:TRP:N	3:L:371:HIS:CE1	2.77	0.52
2:E:406:ASN:O	2:E:408:GLY:N	2.43	0.52
2:H:186:LEU:HD12	3:I:105:GLN:OE1	2.09	0.52
2:K:173:GLU:HA	2:K:176:ILE:CD1	2.39	0.52
3:L:197:ARG:CB	3:L:380:THR:HB	2.36	0.52
1:A:107:GLU:CG	1:J:97:LEU:HD21	2.38	0.52
1:D:119:ILE:CD1	2:E:178:ILE:HG12	2.39	0.52
9:E:501:NAG:H4	6:N:101:NDG:C1	2.38	0.52
1:G:173:GLN:C	1:G:175:GLU:H	2.12	0.52
3:I:335:ASN:CG	3:I:336:ARG:N	2.62	0.52
1:J:104:VAL:O	1:J:104:VAL:HG12	2.09	0.52
2:K:344:ALA:HB2	2:K:369:ALA:HB3	1.91	0.52
2:K:370:GLY:O	2:K:372:ALA:N	2.41	0.52
2:K:428:HIS:CD2	2:K:431:ASN:HB2	2.44	0.52
3:L:194:ILE:HB	3:L:382:MET:O	2.08	0.52
2:E:344:ALA:HB2	2:E:369:ALA:HB3	1.90	0.52
2:E:475:ARG:HG3	2:E:476:PRO:HD2	1.92	0.52
1:J:180:TYR:C	1:J:182:ALA:H	2.12	0.52
1:A:192:VAL:HG12	1:A:193:VAL:N	2.24	0.52
2:B:274:GLN:NE2	2:B:471:ALA:HA	2.24	0.52
3:C:323:SER:HB3	3:C:326:GLU:HB3	1.90	0.52
2:E:428:HIS:CD2	2:E:431:ASN:HB2	2.45	0.52
3:F:154:CYS:O	3:F:157:VAL:HB	2.09	0.52
6:H:506:NDG:O5	11:H:507:GAL:H3	2.09	0.52
2:K:164:GLN:CD	3:L:84:THR:HG23	2.30	0.52
3:L:154:CYS:HB2	3:L:192:THR:HG22	1.91	0.52
2:B:199:LYS:HG2	2:B:203:MET:HE2	1.91	0.52
2:B:352:GLU:O	2:B:358:TYR:HA	2.09	0.52
2:E:182:VAL:O	2:E:186:LEU:HB2	2.09	0.52
2:H:177:ARG:NH2	2:H:181:THR:HG21	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:391:LEU:HA	3:I:394:HIS:CD2	2.35	0.52
2:B:370:GLY:O	2:B:372:ALA:N	2.43	0.52
3:F:286:ASN:ND2	3:F:289:ASP:OD2	2.43	0.52
2:H:278:ASP:O	2:H:311:GLU:CD	2.48	0.52
7:H:503:MAN:C1	7:P:101:MAN:HO2	2.22	0.52
3:I:171:LYS:HB2	3:I:178:PRO:HB3	1.92	0.52
3:I:308:MET:CG	3:I:335:ASN:HB2	2.40	0.52
2:K:322:LEU:HD13	2:K:474:LEU:HD23	1.90	0.52
1:A:119:ILE:CD1	2:B:178:ILE:HG12	2.39	0.52
3:C:385:LEU:HD21	3:C:389:ARG:HG3	1.92	0.52
2:E:204:GLU:O	2:E:208:LYS:HG2	2.09	0.52
2:E:274:GLN:HB3	2:E:472:MET:HB2	1.91	0.52
1:J:173:GLN:C	1:J:175:GLU:H	2.12	0.52
2:K:263:MET:HE2	2:K:269:GLY:N	2.21	0.52
2:K:384:ASN:ND2	6:K:501:NDG:H2	2.25	0.52
2:B:276:ARG:HA	2:B:311:GLU:OE2	2.09	0.52
3:C:335:ASN:CG	3:C:336:ARG:N	2.63	0.52
3:F:125:GLN:HG2	3:F:126:GLN:N	2.24	0.52
1:G:104:VAL:O	1:G:104:VAL:HG12	2.10	0.52
3:L:212:ARG:HA	3:L:230:ASN:HB2	1.92	0.52
3:L:241:ALA:O	3:L:387:MET:HB2	2.09	0.52
2:B:384:ASN:ND2	4:M:2:HIS:NE2	2.58	0.52
2:B:426:ARG:NH2	4:M:6:NH2:N	2.58	0.52
2:H:167:ILE:CG2	3:I:88:ILE:HG23	2.38	0.52
3:L:209:VAL:HB	3:L:212:ARG:NH1	2.25	0.52
2:B:235:ILE:HD13	2:B:246:TYR:CD2	2.45	0.51
2:B:408:GLY:O	2:B:410:PRO:HD3	2.09	0.51
1:G:129:LEU:HD21	3:I:109:LEU:CB	2.40	0.51
1:G:169:GLU:OE1	1:G:169:GLU:HA	2.10	0.51
3:I:150:THR:CG2	3:I:151:GLY:H	2.08	0.51
3:L:88:ILE:O	3:L:88:ILE:HG22	2.10	0.51
3:L:335:ASN:C	3:L:337:CYS:N	2.63	0.51
2:E:274:GLN:NE2	2:E:471:ALA:HA	2.24	0.51
2:H:231:HIS:CD2	2:H:232:CYS:H	2.28	0.51
1:J:182:ALA:C	1:J:184:LEU:N	2.64	0.51
2:K:384:ASN:HD21	6:K:501:NDG:H2	1.72	0.51
3:L:194:ILE:HD12	3:L:233:ILE:CG1	2.26	0.51
1:A:107:GLU:HG3	1:J:97:LEU:CD2	2.40	0.51
3:C:212:ARG:HA	3:C:230:ASN:HB2	1.91	0.51
9:E:501:NAG:H61	6:N:101:NDG:O5	2.10	0.51
2:H:384:ASN:ND2	4:O:2:HIS:CE1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:194:ILE:HD12	3:I:233:ILE:CG1	2.25	0.51
1:A:111:ARG:NH1	1:J:96:GLU:HB2	2.22	0.51
2:E:370:GLY:O	2:E:372:ALA:N	2.42	0.51
2:E:418:ASP:HA	2:E:453:ASP:HB3	1.92	0.51
3:I:367:TRP:N	3:I:371:HIS:CE1	2.78	0.51
2:K:297:ILE:HA	2:K:312:TYR:CD1	2.45	0.51
2:B:274:GLN:HE22	2:B:471:ALA:HA	1.75	0.51
3:C:312:THR:HA	3:C:331:GLY:HA2	1.92	0.51
3:C:367:TRP:N	3:C:371:HIS:CE1	2.78	0.51
3:F:244:LEU:HD22	3:F:263:PHE:CD1	2.45	0.51
3:I:197:ARG:CB	3:I:380:THR:HB	2.36	0.51
3:I:244:LEU:HD22	3:I:263:PHE:CD1	2.46	0.51
1:J:162:LEU:O	1:J:163:GLU:CB	2.58	0.51
2:K:387:MET:SD	2:K:426:ARG:HG2	2.51	0.51
6:D:301:NDG:C2	7:E:503:MAN:O1	2.58	0.51
3:F:84:THR:O	3:F:88:ILE:HG13	2.10	0.51
3:F:312:THR:HA	3:F:331:GLY:HA2	1.93	0.51
1:A:107:GLU:HG3	1:J:97:LEU:CD1	2.40	0.51
1:A:181:ILE:O	1:A:181:ILE:HG13	2.10	0.51
2:B:476:PRO:O	2:B:477:LYS:HE3	2.09	0.51
2:H:171:TYR:O	2:H:174:VAL:HG12	2.10	0.51
1:J:115:LEU:HD21	3:L:95:LEU:C	2.31	0.51
1:G:181:ILE:HD12	2:H:185:SER:CB	2.40	0.51
3:I:312:THR:HA	3:I:331:GLY:HA2	1.92	0.51
2:B:177:ARG:HD3	2:B:181:THR:OG1	2.11	0.51
3:C:87:LYS:C	3:C:89:LEU:H	2.14	0.51
3:F:385:LEU:HD21	3:F:389:ARG:HG3	1.93	0.51
2:H:459:ASN:H	2:H:459:ASN:HD22	1.59	0.51
3:I:303:THR:CB	3:I:339:ALA:HB2	2.29	0.51
3:L:171:LYS:HB2	3:L:178:PRO:HB3	1.93	0.51
3:L:308:MET:CG	3:L:335:ASN:HB2	2.41	0.51
1:A:171:ASN:HD22	2:B:195:HIS:CG	2.29	0.51
2:B:354:GLU:HB2	2:B:358:TYR:CZ	2.46	0.51
2:B:414:CYS:O	2:B:417:GLU:O	2.29	0.51
3:C:286:ASN:ND2	3:C:289:ASP:OD2	2.44	0.51
1:D:124:GLN:NE2	1:D:187:GLU:OE1	2.44	0.51
2:E:278:ASP:O	2:E:311:GLU:CD	2.49	0.51
2:H:200:MET:HB3	3:I:119:PHE:CE1	2.46	0.51
3:I:387:MET:HA	3:I:387:MET:HE3	1.93	0.51
1:J:181:ILE:HD12	2:K:185:SER:CB	2.40	0.51
1:D:177:ALA:O	1:D:179:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:274:GLN:HE22	2:E:471:ALA:HA	1.76	0.50
1:G:188:ARG:HE	1:G:190:GLU:CG	2.23	0.50
2:H:190:LYS:HB2	3:I:109:LEU:HD21	1.94	0.50
3:L:303:THR:CB	3:L:339:ALA:HB2	2.28	0.50
1:D:168:LYS:CD	1:D:170:LYS:HE2	2.38	0.50
2:E:315:GLY:O	2:E:319:VAL:HG23	2.11	0.50
2:E:322:LEU:HD13	2:E:474:LEU:HD23	1.93	0.50
2:H:266:HIS:CE1	7:H:505:MAN:O3	2.64	0.50
2:H:179:GLU:HG3	2:H:180:SER:N	2.24	0.50
2:H:362:VAL:HG23	2:H:374:LEU:HD23	1.93	0.50
2:H:408:GLY:O	2:H:410:PRO:HD3	2.11	0.50
2:H:428:HIS:CD2	2:H:431:ASN:HB2	2.45	0.50
3:I:298:GLN:NE2	3:I:298:GLN:N	2.56	0.50
3:I:367:TRP:HB3	3:I:371:HIS:HE1	1.76	0.50
1:J:166:LEU:O	1:J:167:ASP:HB3	2.11	0.50
2:K:278:ASP:O	2:K:278:ASP:OD1	2.29	0.50
2:E:231:HIS:CD2	2:E:232:CYS:H	2.30	0.50
2:E:384:ASN:ND2	4:N:2:HIS:CD2	2.79	0.50
3:F:298:GLN:NE2	3:F:298:GLN:N	2.57	0.50
2:H:322:LEU:HD13	2:H:474:LEU:HD23	1.93	0.50
2:H:476:PRO:O	2:H:477:LYS:HE3	2.12	0.50
7:H:503:MAN:H2	7:P:101:MAN:H62	1.94	0.50
2:K:274:GLN:HB3	2:K:472:MET:HB2	1.92	0.50
1:A:171:ASN:HD22	2:B:195:HIS:CE1	2.30	0.50
3:C:363:ASP:O	3:C:364:GLY:O	2.28	0.50
1:D:183:ASN:O	1:D:184:LEU:C	2.49	0.50
6:D:301:NDG:H8C1	7:E:503:MAN:O1	2.11	0.50
3:F:335:ASN:CG	3:F:336:ARG:N	2.65	0.50
3:I:363:ASP:O	3:I:364:GLY:O	2.29	0.50
2:K:408:GLY:O	2:K:410:PRO:HD3	2.11	0.50
1:A:111:ARG:HH12	1:J:96:GLU:CB	2.21	0.50
2:E:414:CYS:O	2:E:418:ASP:HB2	2.12	0.50
3:F:88:ILE:O	3:F:92:VAL:HG23	2.11	0.50
1:G:115:LEU:HD21	3:I:95:LEU:C	2.31	0.50
3:I:88:ILE:O	3:I:88:ILE:HG22	2.12	0.50
3:I:194:ILE:HB	3:I:382:MET:O	2.12	0.50
3:I:370:TRP:O	3:I:371:HIS:HB3	2.12	0.50
1:J:115:LEU:HD11	3:L:96:GLU:HA	1.94	0.50
3:L:370:TRP:O	3:L:371:HIS:HB3	2.12	0.50
3:L:385:LEU:HD21	3:L:389:ARG:HG3	1.93	0.50
2:B:417:GLU:O	2:B:418:ASP:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:THR:CG2	3:C:151:GLY:H	2.02	0.50
3:F:125:GLN:NE2	3:F:126:GLN:HG3	2.27	0.50
2:H:261:CYS:HB3	2:H:263:MET:CE	2.41	0.50
2:K:165:LYS:O	2:K:169:ASN:N	2.45	0.50
3:L:87:LYS:O	3:L:91:GLU:HG3	2.12	0.50
1:A:112:ILE:HD13	2:B:171:TYR:HB2	1.93	0.50
3:C:88:ILE:O	3:C:92:VAL:HG23	2.12	0.50
3:C:298:GLN:NE2	3:C:298:GLN:N	2.58	0.50
3:C:367:TRP:HB3	3:C:371:HIS:HE1	1.77	0.50
2:E:199:LYS:HG2	2:E:203:MET:HE1	1.92	0.50
3:F:363:ASP:O	3:F:364:GLY:O	2.30	0.50
2:H:274:GLN:HB3	2:H:472:MET:HB2	1.93	0.50
2:K:197:ARG:O	2:K:201:GLN:HB2	2.12	0.50
2:B:435:ARG:O	2:B:454:GLY:HA2	2.12	0.50
3:C:209:VAL:HB	3:C:212:ARG:NH1	2.24	0.50
3:C:370:TRP:O	3:C:371:HIS:HB3	2.11	0.50
1:J:187:GLU:HG2	1:J:188:ARG:N	2.16	0.50
2:B:172:LYS:HE2	2:B:172:LYS:CA	2.31	0.49
2:E:408:GLY:O	2:E:410:PRO:HD3	2.12	0.49
3:F:273:ARG:NH1	3:F:309:LEU:HD11	2.27	0.49
1:G:115:LEU:HD11	3:I:96:GLU:HA	1.94	0.49
1:G:166:LEU:O	1:G:167:ASP:HB3	2.11	0.49
3:I:85:VAL:O	3:I:85:VAL:HG12	2.12	0.49
2:K:182:VAL:HG12	2:K:182:VAL:O	2.12	0.49
3:C:291:PHE:CD2	3:C:368:ALA:HB1	2.47	0.49
3:L:312:THR:HA	3:L:331:GLY:HA2	1.93	0.49
3:L:385:LEU:CD2	3:L:389:ARG:HG3	2.42	0.49
2:B:231:HIS:CD2	2:B:232:CYS:H	2.30	0.49
3:C:125:GLN:NE2	3:C:126:GLN:HG3	2.27	0.49
3:F:125:GLN:O	3:F:128:VAL:HG22	2.12	0.49
3:F:367:TRP:HB3	3:F:371:HIS:HE1	1.77	0.49
1:J:186:PHE:O	1:J:187:GLU:HB2	2.12	0.49
3:L:335:ASN:CG	3:L:336:ARG:N	2.65	0.49
2:H:293:GLU:HG3	2:H:314:LEU:CA	2.41	0.49
3:L:196:HIS:HA	3:L:380:THR:O	2.11	0.49
3:F:370:TRP:CG	3:F:370:TRP:O	2.65	0.49
1:G:112:ILE:HD11	3:I:92:VAL:CG2	2.42	0.49
2:H:199:LYS:HA	2:H:202:ARG:CZ	2.43	0.49
3:I:385:LEU:HD21	3:I:389:ARG:HG3	1.95	0.49
1:J:129:LEU:HD21	3:L:109:LEU:CB	2.41	0.49
3:L:85:VAL:O	3:L:85:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:130:ILE:CA	3:L:133:THR:HG23	2.40	0.49
3:L:286:ASN:ND2	3:L:289:ASP:OD2	2.46	0.49
3:L:291:PHE:CD2	3:L:368:ALA:HB1	2.47	0.49
2:B:409:ASP:OD1	2:B:411:THR:HB	2.13	0.49
2:B:443:THR:OG1	2:B:446:GLN:HG3	2.12	0.49
3:C:249:THR:HA	3:C:254:THR:O	2.13	0.49
3:F:367:TRP:N	3:F:371:HIS:CE1	2.80	0.49
2:H:182:VAL:HG12	2:H:182:VAL:O	2.12	0.49
2:H:435:ARG:O	2:H:454:GLY:HA2	2.12	0.49
1:J:115:LEU:CD1	3:L:96:GLU:HA	2.43	0.49
2:K:186:LEU:HA	2:K:189:MET:HB2	1.95	0.49
3:L:305:HIS:HE1	3:L:340:GLY:H	1.59	0.49
1:A:97:LEU:HB2	1:J:111:ARG:CZ	2.42	0.49
3:C:228:LEU:HG	3:C:232:LYS:HD2	1.95	0.49
1:D:112:ILE:HD13	2:E:171:TYR:HB2	1.94	0.49
1:D:128:LEU:C	1:D:128:LEU:HD13	2.33	0.49
1:D:181:ILE:O	1:D:181:ILE:HD12	2.12	0.49
2:H:370:GLY:O	2:H:372:ALA:N	2.45	0.49
3:C:372:ASP:C	3:C:374:TRP:H	2.16	0.49
2:E:362:VAL:HG23	2:E:374:LEU:HD23	1.95	0.49
9:E:501:NAG:O3	6:N:101:NDG:C1	2.60	0.49
1:J:186:PHE:HB3	2:K:177:ARG:NE	2.28	0.49
3:C:335:ASN:C	3:C:337:CYS:N	2.66	0.49
2:E:417:GLU:OE1	4:N:3:ARG:NH1	2.45	0.49
2:H:475:ARG:CG	2:H:476:PRO:HD2	2.43	0.49
2:K:293:GLU:HG2	2:K:294:PHE:H	1.77	0.49
2:K:428:HIS:CE1	4:P:1:GLY:N	2.81	0.49
2:K:435:ARG:O	2:K:454:GLY:HA2	2.13	0.49
2:B:274:GLN:HB3	2:B:472:MET:HB2	1.95	0.49
2:B:459:ASN:HD22	2:B:459:ASN:H	1.59	0.49
2:E:384:ASN:ND2	9:E:501:NAG:O1	2.46	0.49
3:F:372:ASP:C	3:F:374:TRP:H	2.16	0.49
2:H:164:GLN:OE1	3:I:84:THR:HA	2.13	0.49
2:H:178:ILE:O	2:H:183:ALA:HB2	2.13	0.49
2:H:182:VAL:CG1	3:I:102:HIS:NE2	2.76	0.49
1:J:172:LEU:O	1:J:175:GLU:HG2	2.13	0.49
2:K:194:GLU:CA	2:K:197:ARG:HH12	2.23	0.49
2:K:293:GLU:HG3	2:K:314:LEU:CA	2.39	0.49
2:K:328:GLN:O	2:K:349:PHE:N	2.42	0.49
3:L:298:GLN:NE2	3:L:298:GLN:N	2.56	0.49
2:B:413:HIS:CG	2:B:416:ARG:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:CYS:O	2:B:418:ASP:HB2	2.13	0.48
3:C:87:LYS:C	3:C:89:LEU:N	2.65	0.48
3:C:172:PRO:HA	3:C:239:GLN:NE2	2.28	0.48
1:D:171:ASN:HD22	2:E:195:HIS:CE1	2.31	0.48
3:F:370:TRP:O	3:F:371:HIS:HB3	2.13	0.48
2:H:458:MET:O	2:H:460:TRP:N	2.47	0.48
1:J:186:PHE:HB3	2:K:177:ARG:CZ	2.43	0.48
2:K:185:SER:O	2:K:187:ARG:N	2.46	0.48
2:K:371:ASN:OD1	2:K:371:ASN:O	2.31	0.48
2:K:475:ARG:CG	2:K:476:PRO:HD2	2.43	0.48
2:B:186:LEU:HD21	3:C:106:ILE:HG13	1.95	0.48
3:C:125:GLN:O	3:C:128:VAL:HG22	2.13	0.48
3:F:196:HIS:HA	3:F:380:THR:O	2.13	0.48
2:H:167:ILE:HD12	3:I:88:ILE:HG21	1.94	0.48
2:H:171:TYR:HA	2:H:174:VAL:CG1	2.42	0.48
3:I:293:PHE:CE2	3:I:303:THR:HG21	2.39	0.48
1:J:160:ARG:HB3	2:K:213:LEU:HD22	1.94	0.48
2:B:285:ARG:NH1	2:B:289:THR:HG21	2.28	0.48
3:C:89:LEU:O	3:C:92:VAL:N	2.47	0.48
1:D:180:TYR:C	1:D:182:ALA:N	2.66	0.48
2:E:297:ILE:HA	2:E:312:TYR:CD1	2.48	0.48
2:E:384:ASN:ND2	9:E:501:NAG:O5	2.46	0.48
2:E:425:ASN:C	2:E:427:CYS:N	2.66	0.48
3:I:172:PRO:HA	3:I:239:GLN:HE22	1.77	0.48
1:J:142:ARG:O	1:J:145:VAL:HG12	2.12	0.48
2:K:199:LYS:HA	2:K:202:ARG:CZ	2.42	0.48
2:K:409:ASP:OD1	2:K:411:THR:HB	2.14	0.48
3:L:367:TRP:HB3	3:L:371:HIS:HE1	1.78	0.48
1:A:139:GLN:NE2	3:C:120:VAL:HG11	2.27	0.48
2:B:405:TRP:CD2	2:B:412:LYS:HB3	2.48	0.48
3:C:182:PHE:CD1	3:C:182:PHE:C	2.87	0.48
3:C:243:ARG:HB2	3:C:387:MET:CE	2.43	0.48
3:F:87:LYS:C	3:F:89:LEU:H	2.17	0.48
3:F:241:ALA:O	3:F:387:MET:HB2	2.14	0.48
3:F:385:LEU:CD2	3:F:389:ARG:HG3	2.43	0.48
2:K:182:VAL:CG1	3:L:102:HIS:NE2	2.76	0.48
2:B:186:LEU:CD1	3:C:105:GLN:HB3	2.43	0.48
3:C:385:LEU:CD2	3:C:389:ARG:HG3	2.44	0.48
1:D:171:ASN:HD22	2:E:195:HIS:CG	2.31	0.48
1:D:181:ILE:O	1:D:181:ILE:HG13	2.13	0.48
9:E:501:NAG:HO3	6:N:101:NDG:C1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:ILE:HB	3:F:382:MET:O	2.13	0.48
2:H:186:LEU:HA	2:H:189:MET:HB2	1.96	0.48
2:H:231:HIS:HE2	2:H:475:ARG:HA	1.79	0.48
3:I:154:CYS:O	3:I:157:VAL:HB	2.13	0.48
3:C:241:ALA:O	3:C:387:MET:HB2	2.13	0.48
1:G:172:LEU:O	1:G:175:GLU:HG2	2.13	0.48
2:H:387:MET:SD	2:H:426:ARG:HG2	2.54	0.48
3:I:249:THR:HA	3:I:254:THR:O	2.14	0.48
1:J:122:GLN:O	1:J:126:LEU:HD13	2.14	0.48
9:C:501:NAG:O4	9:C:502:NAG:O5	2.30	0.48
2:E:292:ALA:O	2:E:293:GLU:HB3	2.13	0.48
2:H:179:GLU:O	2:H:183:ALA:HB3	2.13	0.48
3:I:370:TRP:O	3:I:370:TRP:CG	2.67	0.48
2:K:231:HIS:HE2	2:K:475:ARG:HA	1.78	0.48
1:A:177:ALA:O	1:A:179:SER:N	2.47	0.48
2:B:293:GLU:HG3	2:B:314:LEU:CA	2.40	0.48
2:B:458:MET:O	2:B:460:TRP:N	2.47	0.48
2:E:186:LEU:CD1	3:F:105:GLN:HB3	2.44	0.48
1:G:140:ILE:CD1	2:H:200:MET:SD	3.02	0.48
2:H:171:TYR:CA	2:H:174:VAL:HG12	2.43	0.48
3:I:136:ARG:NH2	3:I:139:GLN:HE21	2.12	0.48
3:I:151:GLY:HA2	3:I:156:GLN:HE21	1.78	0.48
3:I:209:VAL:HA	3:I:212:ARG:NH1	2.27	0.48
3:I:286:ASN:ND2	3:I:289:ASP:OD2	2.46	0.48
2:K:261:CYS:HB3	2:K:263:MET:CE	2.44	0.48
2:B:305:ILE:HG22	3:C:217:TYR:CE1	2.49	0.48
2:B:420:GLY:O	2:B:424:TYR:HE2	1.97	0.48
1:G:140:ILE:HD12	2:H:200:MET:SD	2.53	0.48
2:H:235:ILE:HD13	2:H:246:TYR:CD2	2.48	0.48
2:H:409:ASP:OD1	2:H:411:THR:HB	2.13	0.48
1:J:191:GLU:HG3	1:J:192:VAL:N	2.29	0.48
3:L:273:ARG:NH1	3:L:309:LEU:HD11	2.29	0.48
3:L:372:ASP:C	3:L:374:TRP:H	2.17	0.48
3:L:391:LEU:HG	3:L:394:HIS:CB	2.40	0.48
2:B:165:LYS:O	2:B:169:ASN:ND2	2.47	0.48
2:B:322:LEU:HD13	2:B:474:LEU:HD23	1.95	0.48
2:E:387:MET:SD	2:E:426:ARG:HG2	2.54	0.48
2:E:435:ARG:O	2:E:454:GLY:HA2	2.14	0.48
1:G:115:LEU:CD1	3:I:96:GLU:HA	2.43	0.48
3:I:209:VAL:HB	3:I:212:ARG:NH1	2.27	0.48
3:I:385:LEU:CD2	3:I:389:ARG:HG3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:179:GLU:O	2:K:183:ALA:HB3	2.13	0.48
2:K:365:TYR:CB	2:K:371:ASN:HD22	2.26	0.48
2:K:476:PRO:HG2	2:K:477:LYS:H	1.78	0.48
2:E:177:ARG:HD3	2:E:181:THR:OG1	2.14	0.47
2:E:293:GLU:HG2	2:E:294:PHE:H	1.78	0.47
2:E:365:TYR:CB	2:E:371:ASN:HD22	2.26	0.47
1:G:142:ARG:O	1:G:145:VAL:HG12	2.13	0.47
2:H:164:GLN:HG3	2:H:164:GLN:O	2.14	0.47
2:H:194:GLU:CA	2:H:197:ARG:HH12	2.22	0.47
2:K:178:ILE:O	2:K:183:ALA:HB2	2.13	0.47
3:L:234:HIS:NE2	3:L:267:PRO:HB3	2.28	0.47
1:A:111:ARG:HH22	1:J:96:GLU:CG	2.26	0.47
1:A:162:LEU:H	2:B:210:GLN:HE21	1.61	0.47
2:B:293:GLU:HG2	2:B:294:PHE:H	1.79	0.47
3:C:88:ILE:O	3:C:88:ILE:HG22	2.15	0.47
3:C:370:TRP:O	3:C:370:TRP:CG	2.67	0.47
3:F:387:MET:HA	3:F:387:MET:HE3	1.97	0.47
2:H:201:GLN:HA	2:H:201:GLN:NE2	2.29	0.47
3:I:273:ARG:NH1	3:I:309:LEU:HD11	2.29	0.47
2:B:263:MET:HE2	2:B:269:GLY:N	2.26	0.47
3:C:234:HIS:NE2	3:C:267:PRO:HB3	2.29	0.47
2:H:274:GLN:NE2	2:H:471:ALA:HA	2.29	0.47
1:J:168:LYS:O	1:J:171:ASN:ND2	2.47	0.47
2:B:389:ILE:O	2:B:425:ASN:ND2	2.47	0.47
3:C:195:GLN:HG3	3:C:227:TRP:CE3	2.49	0.47
2:E:414:CYS:O	2:E:417:GLU:O	2.33	0.47
3:F:228:LEU:HG	3:F:232:LYS:HD2	1.97	0.47
3:F:291:PHE:CD2	3:F:368:ALA:HB1	2.49	0.47
2:H:293:GLU:HG2	2:H:294:PHE:H	1.78	0.47
2:K:178:ILE:HD12	3:L:95:LEU:HD22	1.95	0.47
2:K:190:LYS:HB2	3:L:109:LEU:HD21	1.97	0.47
3:L:182:PHE:CD1	3:L:182:PHE:C	2.88	0.47
1:A:107:GLU:CG	1:J:97:LEU:CD2	2.92	0.47
2:E:409:ASP:OD1	2:E:411:THR:HB	2.14	0.47
3:F:209:VAL:HB	3:F:212:ARG:NH1	2.27	0.47
1:G:122:GLN:O	1:G:126:LEU:HD13	2.14	0.47
2:H:330:VAL:HG22	2:H:331:LEU:N	2.30	0.47
2:K:420:GLY:O	2:K:424:TYR:HE2	1.98	0.47
3:L:154:CYS:O	3:L:157:VAL:HB	2.14	0.47
3:L:370:TRP:O	3:L:370:TRP:CG	2.67	0.47
2:B:231:HIS:HE2	2:B:475:ARG:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:387:MET:HA	3:C:387:MET:HE3	1.95	0.47
1:D:162:LEU:H	2:E:210:GLN:HE21	1.62	0.47
3:F:87:LYS:C	3:F:89:LEU:N	2.68	0.47
1:G:172:LEU:HA	1:G:175:GLU:OE1	2.15	0.47
1:G:188:ARG:O	1:G:191:GLU:HG2	2.15	0.47
2:H:199:LYS:O	2:H:203:MET:HG3	2.14	0.47
2:H:425:ASN:C	2:H:427:CYS:N	2.64	0.47
3:L:230:ASN:HB3	3:L:272:TYR:CD2	2.49	0.47
1:A:189:PHE:C	1:A:191:GLU:N	2.67	0.47
2:B:362:VAL:HG23	2:B:374:LEU:HD23	1.96	0.47
1:D:130:GLN:NE2	1:D:182:ALA:HA	2.26	0.47
2:E:235:ILE:HD13	2:E:246:TYR:CD2	2.49	0.47
3:F:94:ILE:HD13	3:F:97:GLN:HE22	1.80	0.47
1:G:160:ARG:CG	2:H:213:LEU:HD22	2.45	0.47
2:H:185:SER:O	2:H:187:ARG:N	2.48	0.47
2:H:476:PRO:HG2	2:H:477:LYS:H	1.79	0.47
3:I:291:PHE:CD2	3:I:368:ALA:HB1	2.50	0.47
3:I:355:THR:HG22	3:I:356:ASP:OD2	2.15	0.47
3:I:372:ASP:C	3:I:374:TRP:H	2.17	0.47
2:K:276:ARG:HA	2:K:311:GLU:OE2	2.14	0.47
2:K:389:ILE:O	2:K:425:ASN:ND2	2.48	0.47
3:L:329:GLY:O	3:L:330:SER:HB3	2.15	0.47
1:A:101:TYR:HB2	1:J:104:VAL:HG11	1.97	0.47
1:D:180:TYR:C	1:D:182:ALA:H	2.18	0.47
3:F:106:ILE:HG22	3:F:107:GLN:NE2	2.29	0.47
1:J:158:CYS:O	2:K:218:CYS:HB3	2.15	0.47
2:K:406:ASN:N	2:K:407:PRO:HD3	2.29	0.47
3:L:332:TRP:HE3	3:L:343:ASN:ND2	2.13	0.47
1:D:132:ASN:HB3	3:F:113:TRP:CE2	2.50	0.47
2:E:330:VAL:HG22	2:E:331:LEU:N	2.30	0.47
3:F:121:THR:O	3:F:124:GLN:HB2	2.14	0.47
1:G:159:ALA:N	2:H:216:ALA:O	2.27	0.47
2:H:262:ASP:HB3	2:H:270:TRP:HB2	1.97	0.47
2:H:285:ARG:NH1	2:H:289:THR:HG21	2.30	0.47
2:H:414:CYS:O	2:H:418:ASP:HB2	2.14	0.47
3:I:305:HIS:HE1	3:I:340:GLY:H	1.61	0.47
3:L:228:LEU:HG	3:L:232:LYS:HD2	1.96	0.47
3:L:262:HIS:HD2	3:L:277:SER:OG	1.98	0.47
1:A:189:PHE:C	1:A:191:GLU:H	2.17	0.47
1:D:131:HIS:O	1:D:134:LYS:HB3	2.15	0.47
2:E:432:PRO:O	2:E:433:ASN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:243:ARG:HB2	3:I:387:MET:CE	2.45	0.47
3:I:335:ASN:C	3:I:337:CYS:N	2.66	0.47
2:B:297:ILE:HA	2:B:312:TYR:CD1	2.51	0.46
2:B:476:PRO:HG2	2:B:477:LYS:H	1.79	0.46
6:B:501:NDG:O4	6:M:101:NDG:C1	2.63	0.46
3:C:94:ILE:HD13	3:C:97:GLN:HE22	1.80	0.46
3:C:230:ASN:HB3	3:C:272:TYR:CD2	2.51	0.46
2:E:413:HIS:CG	2:E:416:ARG:HG3	2.50	0.46
3:F:293:PHE:CE2	3:F:303:THR:HG21	2.40	0.46
1:G:175:GLU:CG	1:G:176:LYS:H	2.28	0.46
2:H:178:ILE:HD12	3:I:95:LEU:HD22	1.97	0.46
2:H:266:HIS:CE1	7:H:505:MAN:HO3	2.33	0.46
3:I:196:HIS:HA	3:I:380:THR:O	2.15	0.46
3:I:392:SER:C	3:I:394:HIS:N	2.67	0.46
1:J:140:ILE:HD13	3:L:120:VAL:HG23	1.96	0.46
2:K:200:MET:HB3	3:L:119:PHE:CD1	2.50	0.46
2:K:278:ASP:O	2:K:311:GLU:CD	2.53	0.46
2:K:414:CYS:O	2:K:417:GLU:O	2.33	0.46
3:L:363:ASP:O	3:L:364:GLY:O	2.32	0.46
1:A:132:ASN:HB3	3:C:113:TRP:CE2	2.51	0.46
1:A:150:ALA:O	1:A:153:ALA:HB3	2.16	0.46
2:B:292:ALA:O	2:B:293:GLU:HB3	2.16	0.46
3:C:196:HIS:HD2	3:C:381:THR:HB	1.80	0.46
1:D:103:GLU:HA	1:D:106:ARG:NH1	2.26	0.46
3:F:88:ILE:O	3:F:88:ILE:HG22	2.16	0.46
3:F:182:PHE:CD1	3:F:182:PHE:C	2.87	0.46
1:G:168:LYS:O	1:G:171:ASN:ND2	2.48	0.46
2:H:166:GLU:HG3	2:H:167:ILE:N	2.30	0.46
1:A:182:ALA:C	1:A:184:LEU:N	2.68	0.46
3:C:262:HIS:HD2	3:C:277:SER:OG	1.99	0.46
2:E:420:GLY:O	2:E:424:TYR:HE2	1.98	0.46
2:H:170:ARG:CA	2:H:173:GLU:HG2	2.44	0.46
2:H:297:ILE:HA	2:H:312:TYR:CD1	2.50	0.46
1:A:160:ARG:HG2	1:A:160:ARG:NH1	2.28	0.46
3:C:276:TYR:OH	3:C:306:LEU:HB2	2.15	0.46
2:E:452:ASP:OD2	4:N:1:GLY:N	2.47	0.46
3:F:217:TYR:HB2	3:F:224:THR:OG1	2.15	0.46
3:F:355:THR:HG22	3:F:356:ASP:OD2	2.15	0.46
2:H:414:CYS:O	2:H:417:GLU:O	2.33	0.46
2:K:179:GLU:HG3	2:K:180:SER:N	2.25	0.46
3:L:276:TYR:OH	3:L:288:PHE:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:O	1:A:181:ILE:HD12	2.16	0.46
3:C:147:SER:HA	3:C:148:PRO:HD3	1.73	0.46
3:C:310:PHE:CE1	3:C:332:TRP:HA	2.51	0.46
2:E:390:HIS:HE1	2:E:428:HIS:CB	2.28	0.46
3:F:320:TYR:CD1	3:F:322:GLY:N	2.74	0.46
2:H:197:ARG:O	2:H:201:GLN:HB2	2.15	0.46
3:I:311:SER:OG	3:I:317:ASN:HB2	2.16	0.46
1:J:172:LEU:HA	1:J:175:GLU:OE1	2.16	0.46
2:K:417:GLU:O	2:K:418:ASP:CB	2.62	0.46
3:L:209:VAL:HA	3:L:212:ARG:NH1	2.28	0.46
2:B:432:PRO:O	2:B:433:ASN:CB	2.60	0.46
3:C:305:HIS:HE1	3:C:340:GLY:H	1.63	0.46
1:D:139:GLN:NE2	3:F:120:VAL:HG11	2.31	0.46
2:E:171:TYR:CE1	3:F:91:GLU:HB3	2.51	0.46
2:E:251:ASP:HB3	2:E:253:PHE:CD1	2.51	0.46
3:F:331:GLY:O	3:F:332:TRP:HB2	2.16	0.46
2:H:374:LEU:HA	2:H:389:ILE:HG23	1.97	0.46
3:I:241:ALA:O	3:I:387:MET:HB2	2.16	0.46
2:K:185:SER:C	2:K:187:ARG:N	2.69	0.46
2:K:459:ASN:H	2:K:459:ASN:HD22	1.62	0.46
3:L:189:ASN:ND2	3:L:389:ARG:HH21	2.13	0.46
2:B:374:LEU:HA	2:B:389:ILE:HG23	1.98	0.46
3:C:388:GLY:O	3:C:389:ARG:HG2	2.14	0.46
2:E:476:PRO:HG2	2:E:477:LYS:H	1.79	0.46
3:F:195:GLN:HG3	3:F:227:TRP:CE3	2.48	0.46
3:F:332:TRP:HE3	3:F:343:ASN:ND2	2.14	0.46
3:I:329:GLY:O	3:I:330:SER:HB3	2.15	0.46
2:K:201:GLN:HA	2:K:201:GLN:NE2	2.30	0.46
1:A:151:LEU:HD12	1:A:151:LEU:HA	1.76	0.46
1:A:170:LYS:HD2	1:A:170:LYS:C	2.35	0.46
1:A:186:PHE:HE2	2:B:177:ARG:HG3	1.81	0.46
2:B:425:ASN:C	2:B:427:CYS:N	2.68	0.46
1:D:182:ALA:O	1:D:183:ASN:O	2.34	0.46
3:F:209:VAL:HA	3:F:212:ARG:NH1	2.29	0.46
3:F:234:HIS:NE2	3:F:267:PRO:HB3	2.31	0.46
1:G:123:LEU:HD22	1:G:184:LEU:HA	1.97	0.46
2:H:413:HIS:CG	2:H:416:ARG:HG3	2.51	0.46
2:K:292:ALA:O	2:K:293:GLU:HB3	2.16	0.46
3:L:355:THR:HG22	3:L:356:ASP:OD2	2.15	0.46
2:B:205:GLU:HG3	2:B:206:ALA:H	1.81	0.46
3:C:154:CYS:O	3:C:157:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:ASN:ND2	3:C:389:ARG:HH21	2.14	0.46
3:C:311:SER:OG	3:C:317:ASN:HB2	2.16	0.46
2:E:165:LYS:HA	2:E:168:GLU:HB2	1.97	0.46
3:F:89:LEU:O	3:F:92:VAL:N	2.49	0.46
2:H:204:GLU:HG3	3:I:126:GLN:OE1	2.16	0.46
3:I:234:HIS:NE2	3:I:267:PRO:HB3	2.31	0.46
2:B:278:ASP:O	2:B:311:GLU:CD	2.54	0.46
3:F:305:HIS:HE1	3:F:340:GLY:H	1.62	0.46
3:F:311:SER:OG	3:F:317:ASN:HB2	2.16	0.46
1:G:128:LEU:C	1:G:130:GLN:N	2.69	0.46
3:I:172:PRO:HA	3:I:239:GLN:NE2	2.31	0.46
3:I:391:LEU:CA	3:I:394:HIS:HD2	2.22	0.46
3:C:275:PHE:C	3:C:275:PHE:CD1	2.90	0.45
1:D:170:LYS:HD2	1:D:170:LYS:C	2.37	0.45
1:D:186:PHE:CZ	1:D:188:ARG:NE	2.85	0.45
2:E:285:ARG:NH1	2:E:289:THR:HG21	2.30	0.45
3:F:329:GLY:O	3:F:330:SER:HB3	2.15	0.45
2:H:405:TRP:CD2	2:H:412:LYS:HB3	2.50	0.45
1:J:162:LEU:H	2:K:210:GLN:NE2	2.04	0.45
1:J:183:ASN:HB2	2:K:181:THR:HG23	1.98	0.45
2:K:262:ASP:HB3	2:K:270:TRP:HB2	1.99	0.45
2:K:452:ASP:OD2	4:P:1:GLY:N	2.43	0.45
1:A:191:GLU:HG3	1:A:192:VAL:N	2.31	0.45
2:H:274:GLN:HE22	2:H:471:ALA:HA	1.81	0.45
2:B:475:ARG:CG	2:B:476:PRO:HD2	2.46	0.45
2:E:231:HIS:HE2	2:E:475:ARG:HA	1.80	0.45
2:E:431:ASN:C	2:E:432:PRO:O	2.53	0.45
3:F:318:ASP:HB3	3:F:334:MET:HB2	1.99	0.45
3:I:262:HIS:HD2	3:I:277:SER:OG	1.99	0.45
2:K:360:LEU:HD11	2:K:362:VAL:CG1	2.46	0.45
2:B:171:TYR:CE1	3:C:91:GLU:HB3	2.51	0.45
1:D:188:ARG:HD3	1:D:188:ARG:HA	1.68	0.45
3:F:249:THR:HA	3:F:254:THR:O	2.16	0.45
3:I:130:ILE:CA	3:I:133:THR:HG23	2.40	0.45
3:L:390:ASP:C	3:L:392:SER:N	2.68	0.45
1:A:151:LEU:HD21	2:B:207:ILE:HD13	1.98	0.45
2:B:261:CYS:HB3	2:B:263:MET:CE	2.43	0.45
3:C:121:THR:O	3:C:124:GLN:HB2	2.17	0.45
1:D:98:GLU:CB	3:I:89:LEU:HD11	2.47	0.45
9:F:502:NAG:HO3	7:F:503:MAN:C1	2.06	0.45
1:G:188:ARG:NH2	1:G:190:GLU:OE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:360:LEU:HD12	2:H:361:TRP:H	1.82	0.45
3:I:189:ASN:ND2	3:I:389:ARG:HH21	2.15	0.45
2:K:285:ARG:NH1	2:K:289:THR:HG21	2.31	0.45
2:B:321:GLN:HE22	2:B:324:LYS:HE2	1.82	0.45
3:C:320:TYR:HD1	3:C:322:GLY:H	1.49	0.45
2:E:261:CYS:HB3	2:E:263:MET:CE	2.45	0.45
2:E:262:ASP:HB3	2:E:270:TRP:HB2	1.99	0.45
3:F:267:PRO:O	3:F:271:GLU:O	2.35	0.45
2:K:425:ASN:C	2:K:427:CYS:N	2.68	0.45
2:B:175:LYS:HG3	3:C:95:LEU:HD21	1.98	0.45
2:B:187:ARG:HD2	2:B:187:ARG:HA	1.61	0.45
2:B:330:VAL:HG22	2:B:331:LEU:N	2.31	0.45
3:C:209:VAL:HA	3:C:212:ARG:NH1	2.28	0.45
1:D:108:LEU:HD11	3:F:89:LEU:HD12	1.98	0.45
3:F:147:SER:HB3	3:F:168:TYR:CD2	2.52	0.45
3:F:308:MET:SD	3:F:335:ASN:HB2	2.57	0.45
2:H:406:ASN:N	2:H:407:PRO:HD3	2.31	0.45
3:I:87:LYS:O	3:I:91:GLU:HG3	2.16	0.45
3:I:267:PRO:O	3:I:271:GLU:O	2.34	0.45
3:L:151:GLY:HA2	3:L:156:GLN:HE21	1.82	0.45
2:B:328:GLN:O	2:B:349:PHE:N	2.46	0.45
3:C:125:GLN:HE21	3:C:126:GLN:CG	2.30	0.45
3:F:125:GLN:HE21	3:F:126:GLN:CG	2.30	0.45
2:H:195:HIS:O	2:H:198:ALA:HB3	2.17	0.45
2:H:328:GLN:O	2:H:349:PHE:N	2.44	0.45
1:J:162:LEU:HB3	1:J:163:GLU:H	1.58	0.45
2:K:179:GLU:HA	2:K:183:ALA:HB3	1.97	0.45
3:L:136:ARG:HH22	3:L:139:GLN:CG	2.29	0.45
1:A:98:GLU:OE1	1:A:98:GLU:C	2.55	0.45
2:E:226:VAL:HG22	3:F:218:LEU:HG	1.99	0.45
2:E:475:ARG:CG	2:E:476:PRO:HD2	2.47	0.45
3:F:388:GLY:O	3:F:389:ARG:HG2	2.16	0.45
2:H:197:ARG:CZ	2:H:197:ARG:HB3	2.47	0.45
2:H:213:LEU:C	2:H:215:SER:N	2.66	0.45
3:I:302:TYR:CA	3:I:336:ARG:HB2	2.47	0.45
2:K:208:LYS:O	2:K:212:GLU:HG2	2.16	0.45
3:L:249:THR:HA	3:L:254:THR:O	2.17	0.45
3:C:256:ARG:HG2	3:C:283:ASP:OD2	2.17	0.45
3:C:355:THR:HG22	3:C:356:ASP:OD2	2.16	0.45
3:C:390:ASP:OD2	3:C:391:LEU:HG	2.17	0.45
1:D:98:GLU:OE1	1:D:98:GLU:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:321:GLN:HE22	2:E:324:LYS:HE2	1.82	0.45
2:E:374:LEU:HA	2:E:389:ILE:HG23	1.99	0.45
1:G:181:ILE:HD12	2:H:185:SER:HA	1.99	0.45
2:H:200:MET:HB3	3:I:119:PHE:CD1	2.52	0.45
3:L:147:SER:HB3	3:L:168:TYR:CD2	2.52	0.45
3:L:172:PRO:HA	3:L:239:GLN:HE22	1.82	0.45
1:A:186:PHE:CZ	1:A:188:ARG:NH1	2.85	0.44
2:B:165:LYS:HA	2:B:168:GLU:HB2	1.98	0.44
2:B:167:ILE:CG2	3:C:88:ILE:HG21	2.48	0.44
3:C:308:MET:SD	3:C:335:ASN:HB2	2.57	0.44
2:E:187:ARG:C	2:E:189:MET:H	2.20	0.44
2:E:405:TRP:CD2	2:E:412:LYS:HB3	2.52	0.44
3:F:243:ARG:HB2	3:F:387:MET:CE	2.46	0.44
1:G:132:ASN:HB3	3:I:113:TRP:CE2	2.52	0.44
2:H:321:GLN:HE22	2:H:324:LYS:HE2	1.82	0.44
3:I:217:TYR:HB2	3:I:224:THR:OG1	2.17	0.44
3:I:388:GLY:O	3:I:389:ARG:HG2	2.17	0.44
2:K:350:ARG:O	2:K:361:TRP:HB2	2.17	0.44
1:D:108:LEU:HD21	3:F:89:LEU:CD1	2.48	0.44
2:E:301:ASN:CG	2:E:305:ILE:HG13	2.37	0.44
1:G:129:LEU:HD21	3:I:109:LEU:HB2	2.00	0.44
2:H:384:ASN:ND2	6:H:501:NDG:O5	2.49	0.44
3:I:228:LEU:HG	3:I:232:LYS:HD2	1.99	0.44
2:K:414:CYS:O	2:K:418:ASP:HB2	2.16	0.44
3:L:311:SER:OG	3:L:317:ASN:HB2	2.17	0.44
3:L:368:ALA:C	3:L:370:TRP:H	2.20	0.44
1:A:128:LEU:HD13	1:A:128:LEU:C	2.37	0.44
3:C:317:ASN:HD22	3:C:317:ASN:HA	1.60	0.44
2:E:365:TYR:HB3	2:E:371:ASN:ND2	2.32	0.44
2:H:383:ASP:O	2:H:387:MET:HG2	2.17	0.44
3:I:195:GLN:HG3	3:I:227:TRP:CE3	2.52	0.44
3:I:230:ASN:HB3	3:I:272:TYR:CD2	2.53	0.44
3:C:89:LEU:HD23	1:J:98:GLU:HA	2.00	0.44
3:C:273:ARG:NH1	3:C:309:LEU:HD11	2.31	0.44
1:D:188:ARG:NH2	2:E:173:GLU:OE1	2.51	0.44
2:E:172:LYS:HE2	2:E:172:LYS:CA	2.33	0.44
2:E:175:LYS:HG3	3:F:95:LEU:HD21	1.98	0.44
2:E:177:ARG:HH11	2:E:181:THR:HG21	1.82	0.44
2:E:278:ASP:O	2:E:278:ASP:OD1	2.35	0.44
1:G:177:ALA:O	1:G:181:ILE:HG23	2.17	0.44
2:H:179:GLU:HA	2:H:183:ALA:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:MET:O	2:H:193:LEU:HG	2.18	0.44
3:I:276:TYR:OH	3:I:288:PHE:HB3	2.18	0.44
1:J:122:GLN:HE22	3:L:103:ASP:HB2	1.80	0.44
1:J:128:LEU:C	1:J:130:GLN:N	2.69	0.44
1:J:173:GLN:C	1:J:175:GLU:N	2.71	0.44
2:K:330:VAL:HG22	2:K:331:LEU:N	2.32	0.44
2:K:334:MET:HA	2:K:469:GLN:O	2.16	0.44
2:K:413:HIS:CG	2:K:416:ARG:HG3	2.52	0.44
3:L:147:SER:HA	3:L:148:PRO:HD3	1.73	0.44
3:L:207:ASP:OD1	3:L:210:SER:HB2	2.18	0.44
2:B:187:ARG:C	2:B:189:MET:H	2.20	0.44
3:C:318:ASP:HB3	3:C:334:MET:HB2	2.00	0.44
1:D:192:VAL:O	1:D:193:VAL:C	2.56	0.44
3:F:309:LEU:O	3:F:333:TRP:HA	2.18	0.44
1:G:142:ARG:CZ	1:G:142:ARG:HB2	2.47	0.44
2:H:208:LYS:O	2:H:212:GLU:HG2	2.18	0.44
2:H:285:ARG:NH2	3:I:135:SER:O	2.50	0.44
2:H:359:ARG:HH21	2:H:394:GLN:NE2	2.07	0.44
3:I:151:GLY:HA2	3:I:156:GLN:NE2	2.32	0.44
3:L:275:PHE:CD1	3:L:275:PHE:C	2.90	0.44
3:L:302:TYR:CA	3:L:336:ARG:HB2	2.48	0.44
3:C:111:GLU:N	3:C:114:ARG:HH21	2.16	0.44
3:C:309:LEU:O	3:C:333:TRP:HA	2.18	0.44
3:F:196:HIS:HD2	3:F:381:THR:HB	1.81	0.44
3:I:87:LYS:C	3:I:89:LEU:H	2.21	0.44
2:K:374:LEU:HA	2:K:389:ILE:HG23	1.98	0.44
3:L:293:PHE:CE2	3:L:303:THR:HG21	2.38	0.44
3:C:173:LEU:H	3:C:239:GLN:NE2	2.15	0.44
3:C:182:PHE:CZ	3:C:222:LEU:HB2	2.52	0.44
1:D:114:HIS:C	1:D:116:GLN:N	2.70	0.44
3:F:86:GLN:O	3:F:86:GLN:HG2	2.18	0.44
3:F:111:GLU:N	3:F:114:ARG:HH21	2.16	0.44
1:G:175:GLU:CG	1:G:176:LYS:N	2.73	0.44
2:H:185:SER:C	2:H:187:ARG:N	2.70	0.44
3:I:147:SER:HB3	3:I:168:TYR:CD2	2.53	0.44
1:J:177:ALA:O	1:J:181:ILE:HG23	2.18	0.44
1:J:181:ILE:HD12	2:K:185:SER:HA	2.00	0.44
3:L:387:MET:HA	3:L:387:MET:HE3	2.00	0.44
7:L:501:MAN:O5	5:Q:2:NAG:O3	2.35	0.44
1:A:147:ILE:CG2	2:B:207:ILE:HD11	2.48	0.44
1:A:186:PHE:CD1	2:B:177:ARG:NH2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:196:HIS:HA	3:C:380:THR:O	2.16	0.44
3:C:332:TRP:HE3	3:C:343:ASN:ND2	2.16	0.44
3:C:368:ALA:C	3:C:370:TRP:H	2.21	0.44
2:E:231:HIS:CE1	2:E:476:PRO:HD3	2.53	0.44
3:F:264:LYS:O	3:F:265:LEU:HD23	2.17	0.44
3:F:276:TYR:OH	3:F:288:PHE:HB3	2.18	0.44
2:H:416:ARG:HG2	2:H:416:ARG:HH11	1.82	0.44
3:I:308:MET:SD	3:I:335:ASN:HB2	2.57	0.44
3:I:309:LEU:O	3:I:333:TRP:HA	2.18	0.44
1:J:120:ASN:OD1	1:J:187:GLU:CG	2.66	0.44
2:K:197:ARG:CZ	2:K:197:ARG:HB3	2.47	0.44
2:K:204:GLU:HG3	3:L:126:GLN:OE1	2.17	0.44
2:K:224:VAL:HA	2:K:225:PRO:HD3	1.85	0.44
2:B:231:HIS:CE1	2:B:476:PRO:HD3	2.53	0.44
2:B:390:HIS:O	2:B:393:MET:HG2	2.17	0.44
3:C:397:GLN:O	3:C:398:GLN:CB	2.64	0.44
3:F:265:LEU:HA	3:F:273:ARG:O	2.17	0.44
2:H:292:ALA:O	2:H:293:GLU:HB3	2.17	0.44
2:K:273:VAL:CG2	2:K:474:LEU:HD22	2.40	0.44
3:L:331:GLY:O	3:L:332:TRP:HB2	2.18	0.44
1:A:114:HIS:C	1:A:116:GLN:N	2.72	0.43
3:F:172:PRO:HA	3:F:239:GLN:HE22	1.83	0.43
2:H:251:ASP:HB3	2:H:253:PHE:CD1	2.53	0.43
2:H:317:LYS:HD3	2:H:358:TYR:OH	2.17	0.43
6:H:506:NDG:C2	11:H:507:GAL:O3	2.45	0.43
2:K:164:GLN:HG3	2:K:164:GLN:O	2.18	0.43
2:K:173:GLU:HA	2:K:176:ILE:HD12	2.00	0.43
2:K:405:TRP:CD2	2:K:412:LYS:HB3	2.52	0.43
3:L:136:ARG:HH22	3:L:139:GLN:HG2	1.83	0.43
1:A:104:VAL:HG22	1:J:100:ARG:CD	2.41	0.43
2:B:262:ASP:HB3	2:B:270:TRP:HB2	2.00	0.43
2:B:334:MET:HA	2:B:469:GLN:O	2.18	0.43
3:C:329:GLY:O	3:C:330:SER:HB3	2.18	0.43
3:I:182:PHE:CD1	3:I:182:PHE:C	2.91	0.43
3:I:196:HIS:HD2	3:I:381:THR:HB	1.83	0.43
2:K:194:GLU:HG2	2:K:197:ARG:HH12	1.83	0.43
2:K:431:ASN:C	2:K:432:PRO:O	2.53	0.43
3:L:135:SER:O	3:L:137:PRO:CD	2.62	0.43
3:L:197:ARG:HD2	3:L:197:ARG:HA	1.77	0.43
3:L:362:ASP:OD1	3:L:362:ASP:N	2.50	0.43
1:A:108:LEU:HD11	3:C:89:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:332:TRP:CD1	3:C:333:TRP:N	2.86	0.43
1:D:150:ALA:O	1:D:153:ALA:HB3	2.18	0.43
2:E:417:GLU:O	2:E:418:ASP:CB	2.57	0.43
3:F:335:ASN:C	3:F:337:CYS:N	2.66	0.43
2:H:263:MET:HE2	2:H:269:GLY:N	2.26	0.43
1:J:95:ASN:HA	1:J:98:GLU:HB3	1.99	0.43
2:K:189:MET:O	2:K:193:LEU:HG	2.17	0.43
2:K:362:VAL:HG23	2:K:374:LEU:HD23	2.00	0.43
2:K:456:VAL:CG1	2:K:457:TRP:N	2.80	0.43
3:L:196:HIS:HD2	3:L:381:THR:HB	1.82	0.43
1:A:131:HIS:O	1:A:134:LYS:HB3	2.18	0.43
2:B:199:LYS:HG2	2:B:203:MET:HE1	1.97	0.43
2:E:252:LEU:CD1	3:F:177:GLN:HG3	2.49	0.43
3:F:172:PRO:HA	3:F:239:GLN:NE2	2.34	0.43
3:F:185:ILE:HA	3:F:189:ASN:O	2.19	0.43
2:H:273:VAL:CG2	2:H:474:LEU:HD22	2.41	0.43
7:H:505:MAN:O1	6:H:506:NDG:H8C1	2.17	0.43
3:C:106:ILE:HG22	3:C:107:GLN:NE2	2.34	0.43
3:C:302:TYR:CA	3:C:336:ARG:HB2	2.48	0.43
2:E:390:HIS:HE1	2:E:428:HIS:HB2	1.81	0.43
2:E:456:VAL:CG1	2:E:457:TRP:N	2.81	0.43
3:F:276:TYR:OH	3:F:306:LEU:HB2	2.18	0.43
1:G:132:ASN:HB3	3:I:113:TRP:NE1	2.32	0.43
1:G:173:GLN:C	1:G:175:GLU:N	2.71	0.43
2:H:321:GLN:NE2	2:H:324:LYS:HE2	2.34	0.43
3:I:147:SER:HA	3:I:148:PRO:HD3	1.74	0.43
3:I:279:TYR:CD2	3:I:286:ASN:CB	3.01	0.43
2:K:174:VAL:HG12	2:K:174:VAL:O	2.19	0.43
3:F:197:ARG:HA	3:F:197:ARG:HD2	1.77	0.43
3:F:262:HIS:HD2	3:F:277:SER:OG	2.01	0.43
1:G:103:GLU:C	1:G:105:LEU:N	2.71	0.43
2:H:278:ASP:O	2:H:278:ASP:OD1	2.36	0.43
2:H:350:ARG:O	2:H:361:TRP:HB2	2.19	0.43
1:J:140:ILE:CD1	2:K:200:MET:SD	3.06	0.43
2:K:348:SER:O	2:K:362:VAL:HA	2.18	0.43
3:L:93:ARG:O	3:L:97:GLN:HB2	2.19	0.43
3:L:195:GLN:HG3	3:L:227:TRP:CE3	2.49	0.43
3:L:274:LEU:HD12	3:L:275:PHE:H	1.83	0.43
2:B:303:LYS:HB2	2:B:304:SER:H	1.65	0.43
2:E:172:LYS:O	2:E:176:ILE:HG13	2.19	0.43
1:G:183:ASN:HB2	2:H:181:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:GLU:HG2	2:H:197:ARG:HH12	1.82	0.43
2:H:301:ASN:CG	2:H:305:ILE:HG13	2.38	0.43
2:H:303:LYS:HA	2:H:303:LYS:HE3	2.01	0.43
3:I:332:TRP:HE3	3:I:343:ASN:ND2	2.17	0.43
2:K:458:MET:O	2:K:460:TRP:N	2.51	0.43
3:L:264:LYS:O	3:L:265:LEU:HD23	2.18	0.43
2:B:348:SER:O	2:B:362:VAL:HA	2.18	0.43
2:B:390:HIS:HE1	2:B:428:HIS:HB2	1.83	0.43
3:C:217:TYR:HB2	3:C:224:THR:OG1	2.19	0.43
2:E:167:ILE:CG2	3:F:88:ILE:HG21	2.48	0.43
2:H:371:ASN:ND2	2:H:374:LEU:CD1	2.80	0.43
2:H:389:ILE:O	2:H:425:ASN:ND2	2.51	0.43
3:I:275:PHE:CD1	3:I:275:PHE:C	2.92	0.43
2:K:165:LYS:O	2:K:168:GLU:N	2.52	0.43
2:K:317:LYS:HD3	2:K:358:TYR:OH	2.19	0.43
2:K:320:HIS:CD2	2:K:353:ASN:HA	2.54	0.43
2:K:384:ASN:ND2	6:K:501:NDG:C2	2.77	0.43
3:L:136:ARG:HD3	3:L:137:PRO:O	2.19	0.43
3:L:308:MET:SD	3:L:335:ASN:HB2	2.59	0.43
3:L:388:GLY:O	3:L:389:ARG:HG2	2.18	0.43
1:A:123:LEU:HB3	1:A:184:LEU:O	2.19	0.43
1:G:140:ILE:HD13	3:I:120:VAL:HG23	2.00	0.43
2:H:428:HIS:O	4:O:1:GLY:N	2.50	0.43
2:K:259:VAL:HG23	2:K:314:LEU:HD13	1.99	0.43
1:A:170:LYS:CD	1:A:174:LEU:HD11	2.49	0.43
2:B:317:LYS:HD3	2:B:358:TYR:OH	2.19	0.43
2:B:456:VAL:CG1	2:B:457:TRP:N	2.81	0.43
6:D:301:NDG:HA	7:E:503:MAN:HO1	1.63	0.43
2:E:172:LYS:HA	2:E:172:LYS:CE	2.35	0.43
2:E:187:ARG:HD2	2:E:187:ARG:HA	1.62	0.43
2:H:194:GLU:HB3	2:H:197:ARG:HH22	1.84	0.43
2:H:240:GLY:O	2:H:241:ARG:HD3	2.19	0.43
2:H:276:ARG:HA	2:H:311:GLU:OE2	2.19	0.43
1:A:162:LEU:HD23	2:B:213:LEU:HD11	2.00	0.42
2:B:251:ASP:HB3	2:B:253:PHE:CD1	2.53	0.42
3:C:274:LEU:HD12	3:C:275:PHE:H	1.83	0.42
3:C:279:TYR:CD2	3:C:286:ASN:CB	3.01	0.42
3:C:279:TYR:OH	3:C:282:GLY:O	2.35	0.42
1:D:110:ARG:O	1:D:110:ARG:HG3	2.19	0.42
1:D:170:LYS:CD	1:D:174:LEU:HD11	2.48	0.42
2:E:208:LYS:HE2	2:E:208:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:353:ASN:OD1	2:E:355:ALA:HB3	2.19	0.42
2:E:406:ASN:N	2:E:407:PRO:HD3	2.34	0.42
3:F:302:TYR:CA	3:F:336:ARG:HB2	2.47	0.42
1:J:103:GLU:C	1:J:105:LEU:N	2.71	0.42
1:J:175:GLU:CG	1:J:176:LYS:N	2.74	0.42
2:K:251:ASP:HB3	2:K:253:PHE:CD1	2.54	0.42
2:K:301:ASN:CG	2:K:305:ILE:HG13	2.40	0.42
2:K:360:LEU:HD12	2:K:361:TRP:H	1.84	0.42
2:K:416:ARG:HG2	2:K:416:ARG:HH11	1.84	0.42
3:L:217:TYR:HB2	3:L:224:THR:OG1	2.19	0.42
3:C:86:GLN:O	3:C:86:GLN:HG2	2.18	0.42
3:F:310:PHE:CE1	3:F:332:TRP:HA	2.55	0.42
2:H:231:HIS:CE1	2:H:476:PRO:HD3	2.54	0.42
2:H:352:GLU:HB3	2:H:356:GLN:HB2	2.01	0.42
3:I:368:ALA:C	3:I:370:TRP:H	2.22	0.42
1:J:188:ARG:O	1:J:191:GLU:HG2	2.18	0.42
1:A:108:LEU:HD12	2:B:167:ILE:HD13	2.01	0.42
2:E:167:ILE:HG22	3:F:88:ILE:HG21	2.01	0.42
2:E:303:LYS:HA	2:E:303:LYS:HE3	2.01	0.42
2:E:458:MET:O	2:E:460:TRP:N	2.52	0.42
3:F:189:ASN:ND2	3:F:389:ARG:HH21	2.16	0.42
3:F:230:ASN:HB3	3:F:272:TYR:CD2	2.54	0.42
3:F:298:GLN:H	3:F:298:GLN:HE21	1.66	0.42
2:H:334:MET:HA	2:H:469:GLN:O	2.19	0.42
2:H:350:ARG:HG3	2:H:350:ARG:NH1	2.32	0.42
3:I:185:ILE:HA	3:I:189:ASN:O	2.18	0.42
1:J:129:LEU:O	1:J:133:ILE:HG13	2.20	0.42
3:L:87:LYS:C	3:L:89:LEU:H	2.22	0.42
1:A:137:VAL:HG11	1:A:175:GLU:HG3	2.02	0.42
1:A:186:PHE:CE2	2:B:177:ARG:NE	2.88	0.42
2:B:177:ARG:HH11	2:B:181:THR:HG21	1.83	0.42
2:E:371:ASN:OD1	2:E:371:ASN:O	2.37	0.42
3:F:151:GLY:HA2	3:F:156:GLN:HE21	1.85	0.42
3:F:273:ARG:NH1	3:F:309:LEU:CD1	2.83	0.42
1:G:95:ASN:HA	1:G:98:GLU:HB3	2.00	0.42
2:H:224:VAL:HA	2:H:225:PRO:HD3	1.84	0.42
3:I:195:GLN:OE1	3:I:380:THR:HG22	2.20	0.42
1:J:140:ILE:HD12	2:K:200:MET:SD	2.60	0.42
2:K:199:LYS:O	2:K:203:MET:HG3	2.18	0.42
2:K:217:PRO:HB2	3:L:136:ARG:HH11	1.81	0.42
2:K:303:LYS:HE3	2:K:303:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:390:HIS:HE1	2:K:428:HIS:CB	2.32	0.42
3:L:316:ASP:OD2	3:L:322:GLY:O	2.37	0.42
2:B:166:GLU:HA	2:B:169:ASN:HD22	1.83	0.42
2:B:390:HIS:HE1	2:B:428:HIS:CB	2.32	0.42
2:E:231:HIS:CE1	2:E:475:ARG:HA	2.54	0.42
2:E:320:HIS:CD2	2:E:353:ASN:HA	2.55	0.42
3:F:197:ARG:NH1	3:F:365:ILE:HD11	2.35	0.42
1:G:136:GLN:HE22	3:I:116:ASN:HB2	1.85	0.42
2:H:265:SER:O	2:H:266:HIS:C	2.57	0.42
2:H:277:VAL:N	2:H:311:GLU:OE2	2.46	0.42
2:H:461:LYS:HG3	2:H:467:MET:HE1	2.02	0.42
7:H:505:MAN:O1	6:H:506:NDG:C7	2.59	0.42
3:I:93:ARG:O	3:I:97:GLN:HB2	2.19	0.42
3:I:173:LEU:H	3:I:239:GLN:NE2	2.16	0.42
3:I:256:ARG:HG2	3:I:283:ASP:OD2	2.18	0.42
3:I:318:ASP:HB3	3:I:334:MET:HB2	2.01	0.42
1:J:129:LEU:HD21	3:L:109:LEU:HB2	2.01	0.42
1:J:132:ASN:HB3	3:L:113:TRP:CE2	2.54	0.42
3:L:185:ILE:HA	3:L:189:ASN:O	2.20	0.42
1:A:96:GLU:CB	1:J:111:ARG:HH22	2.29	0.42
2:B:301:ASN:CG	2:B:305:ILE:HG13	2.39	0.42
2:B:303:LYS:HA	2:B:303:LYS:HE3	2.02	0.42
3:C:398:GLN:HE21	3:C:399:GLN:HG3	1.81	0.42
1:D:151:LEU:HA	1:D:151:LEU:HD12	1.75	0.42
2:E:208:LYS:HA	2:E:208:LYS:CE	2.37	0.42
2:E:265:SER:O	2:E:266:HIS:C	2.57	0.42
2:E:317:LYS:HD3	2:E:358:TYR:OH	2.19	0.42
3:F:274:LEU:HD12	3:F:275:PHE:H	1.85	0.42
1:G:120:ASN:OD1	1:G:187:GLU:HG2	2.20	0.42
3:I:197:ARG:NH1	3:I:365:ILE:HD11	2.35	0.42
3:I:310:PHE:CE1	3:I:332:TRP:HA	2.54	0.42
2:K:204:GLU:HA	3:L:123:LEU:HD11	2.01	0.42
2:K:303:LYS:HB2	2:K:304:SER:H	1.67	0.42
3:L:172:PRO:HA	3:L:239:GLN:NE2	2.34	0.42
3:L:279:TYR:CD2	3:L:286:ASN:CB	3.02	0.42
2:B:265:SER:O	2:B:266:HIS:C	2.57	0.42
2:B:320:HIS:CD2	2:B:353:ASN:HA	2.55	0.42
2:B:352:GLU:HB3	2:B:356:GLN:HB2	2.01	0.42
3:C:276:TYR:OH	3:C:288:PHE:HB3	2.20	0.42
1:D:151:LEU:HD21	2:E:207:ILE:HD13	2.02	0.42
2:E:165:LYS:O	2:E:169:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:199:LYS:HG2	2:E:203:MET:HE2	2.00	0.42
2:E:277:VAL:N	2:E:311:GLU:OE2	2.45	0.42
3:F:147:SER:HA	3:F:148:PRO:HD3	1.74	0.42
3:F:362:ASP:OD1	3:F:362:ASP:N	2.53	0.42
1:G:158:CYS:HA	2:H:217:PRO:HA	2.02	0.42
2:H:303:LYS:HE3	2:H:303:LYS:CA	2.50	0.42
2:H:371:ASN:OD1	2:H:371:ASN:O	2.37	0.42
3:I:92:VAL:O	3:I:96:GLU:CB	2.68	0.42
2:K:195:HIS:O	2:K:198:ALA:HB3	2.20	0.42
3:L:195:GLN:OE1	3:L:380:THR:HG22	2.20	0.42
3:L:243:ARG:HB2	3:L:387:MET:CE	2.50	0.42
3:L:332:TRP:CD1	3:L:333:TRP:N	2.88	0.42
1:A:100:ARG:NH2	1:J:107:GLU:OE2	2.53	0.42
3:C:185:ILE:HA	3:C:189:ASN:O	2.19	0.42
3:C:304:THR:HG23	3:C:304:THR:O	2.20	0.42
3:F:279:TYR:CD2	3:F:286:ASN:CB	3.01	0.42
1:G:160:ARG:HB3	2:H:213:LEU:HD22	2.00	0.42
2:H:353:ASN:OD1	2:H:355:ALA:HB3	2.20	0.42
3:I:362:ASP:OD1	3:I:362:ASP:N	2.52	0.42
9:I:501:NAG:HO4	9:I:502:NAG:C1	2.28	0.42
2:K:231:HIS:CE1	2:K:475:ARG:HA	2.54	0.42
3:L:105:GLN:O	3:L:109:LEU:HG	2.20	0.42
3:L:151:GLY:HA2	3:L:156:GLN:NE2	2.35	0.42
3:L:244:LEU:HD22	3:L:263:PHE:CE1	2.54	0.42
3:L:310:PHE:CE1	3:L:332:TRP:HA	2.54	0.42
1:A:151:LEU:HD11	2:B:207:ILE:HD13	2.02	0.42
1:A:169:GLU:O	1:A:172:LEU:N	2.47	0.42
2:B:168:GLU:O	2:B:172:LYS:HB2	2.20	0.42
2:B:350:ARG:HG3	2:B:350:ARG:NH1	2.34	0.42
2:B:359:ARG:HA	2:B:393:MET:O	2.19	0.42
2:B:384:ASN:OD1	6:B:501:NDG:C1	2.67	0.42
3:C:103:ASP:O	3:C:107:GLN:HG2	2.20	0.42
3:C:331:GLY:O	3:C:332:TRP:HB2	2.20	0.42
2:E:334:MET:HA	2:E:469:GLN:O	2.19	0.42
3:F:256:ARG:HG2	3:F:283:ASP:OD2	2.20	0.42
2:H:359:ARG:HA	2:H:393:MET:O	2.20	0.42
2:H:390:HIS:HE1	2:H:428:HIS:CB	2.33	0.42
1:J:97:LEU:N	1:J:97:LEU:HD23	2.35	0.42
3:L:304:THR:HG23	3:L:304:THR:O	2.18	0.42
2:B:441:ILE:C	2:B:441:ILE:HD12	2.40	0.42
3:C:244:LEU:HD22	3:C:263:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:HD23	1:D:108:LEU:HA	1.81	0.42
3:F:240:GLN:HB3	3:F:241:ALA:H	1.69	0.42
2:H:360:LEU:HD11	2:H:362:VAL:CG1	2.48	0.42
3:I:274:LEU:HD12	3:I:275:PHE:H	1.85	0.42
1:J:101:TYR:C	1:J:103:GLU:H	2.23	0.42
1:J:169:GLU:O	1:J:173:GLN:HG2	2.20	0.42
2:K:350:ARG:HG3	2:K:350:ARG:NH1	2.33	0.42
2:K:461:LYS:HG3	2:K:467:MET:HE1	2.02	0.42
3:L:89:LEU:C	3:L:89:LEU:HD13	2.40	0.42
3:L:276:TYR:OH	3:L:306:LEU:HB2	2.20	0.42
2:B:353:ASN:OD1	2:B:355:ALA:HB3	2.19	0.41
3:C:147:SER:HB3	3:C:168:TYR:CD2	2.55	0.41
1:D:95:ASN:O	1:D:96:GLU:C	2.59	0.41
1:D:158:CYS:HB3	2:E:214:CYS:HA	2.02	0.41
1:G:122:GLN:HE22	3:I:103:ASP:HB2	1.81	0.41
3:I:265:LEU:HA	3:I:273:ARG:O	2.20	0.41
3:L:197:ARG:NH1	3:L:365:ILE:HD11	2.35	0.41
3:L:267:PRO:O	3:L:271:GLU:O	2.38	0.41
2:B:371:ASN:O	2:B:371:ASN:OD1	2.37	0.41
3:C:293:PHE:CE2	3:C:303:THR:HG21	2.39	0.41
2:E:303:LYS:HB2	2:E:304:SER:H	1.65	0.41
1:G:101:TYR:C	1:G:103:GLU:H	2.22	0.41
2:H:201:GLN:HE21	2:H:201:GLN:CA	2.32	0.41
6:H:506:NDG:C4	11:H:507:GAL:H4	2.40	0.41
1:J:120:ASN:O	1:J:123:LEU:HB2	2.20	0.41
2:K:456:VAL:HG12	2:K:457:TRP:N	2.34	0.41
1:A:110:ARG:O	1:A:110:ARG:HG3	2.19	0.41
2:B:208:LYS:HE2	2:B:208:LYS:N	2.35	0.41
2:B:416:ARG:HG2	2:B:416:ARG:HH11	1.85	0.41
2:B:426:ARG:O	2:B:427:CYS:HB2	2.21	0.41
1:D:130:GLN:HE22	1:D:182:ALA:CA	2.29	0.41
1:D:184:LEU:HD23	1:D:184:LEU:H	1.86	0.41
2:E:321:GLN:NE2	2:E:324:LYS:HE2	2.36	0.41
2:E:343:TYR:O	2:E:369:ALA:CB	2.68	0.41
3:F:281:ASP:CG	3:F:282:GLY:H	2.23	0.41
3:F:385:LEU:CD2	3:F:386:PRO:HD2	2.41	0.41
2:H:231:HIS:CE1	2:H:475:ARG:HA	2.55	0.41
3:I:122:ARG:O	3:I:126:GLN:HG3	2.20	0.41
2:B:231:HIS:CE1	2:B:475:ARG:HA	2.55	0.41
3:C:368:ALA:O	3:C:370:TRP:N	2.54	0.41
1:G:150:ALA:O	1:G:153:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:TYR:C	1:G:182:ALA:N	2.72	0.41
2:H:431:ASN:C	2:H:432:PRO:O	2.56	0.41
3:I:304:THR:HG23	3:I:304:THR:O	2.20	0.41
3:I:316:ASP:OD2	3:I:322:GLY:O	2.39	0.41
3:I:389:ARG:O	3:I:390:ASP:CB	2.67	0.41
2:K:168:GLU:OE1	2:K:168:GLU:HA	2.20	0.41
2:K:178:ILE:HD13	3:L:98:ILE:CG2	2.50	0.41
2:B:406:ASN:N	2:B:407:PRO:HD3	2.35	0.41
2:B:431:ASN:C	2:B:432:PRO:O	2.55	0.41
3:C:221:THR:O	3:C:222:LEU:HB3	2.20	0.41
3:C:227:TRP:NE1	3:C:230:ASN:ND2	2.66	0.41
9:F:502:NAG:H3	7:F:503:MAN:C1	2.49	0.41
6:H:501:NDG:H3	6:O:101:NDG:C1	2.51	0.41
3:I:195:GLN:HG2	3:I:196:HIS:H	1.85	0.41
2:K:231:HIS:CE1	2:K:476:PRO:HD3	2.55	0.41
3:L:229:GLY:O	3:L:233:ILE:HG13	2.20	0.41
3:L:265:LEU:HA	3:L:273:ARG:O	2.21	0.41
3:C:207:ASP:OD1	3:C:210:SER:HB2	2.21	0.41
9:C:501:NAG:HO4	9:C:502:NAG:H62	1.84	0.41
2:E:416:ARG:HG2	2:E:416:ARG:HH11	1.86	0.41
3:F:207:ASP:OD1	3:F:210:SER:HB2	2.21	0.41
1:G:112:ILE:CD1	3:I:92:VAL:HG22	2.45	0.41
1:G:188:ARG:NE	1:G:190:GLU:HG2	2.33	0.41
3:I:105:GLN:O	3:I:109:LEU:HG	2.20	0.41
3:I:195:GLN:HG2	3:I:196:HIS:N	2.36	0.41
2:K:352:GLU:HB3	2:K:356:GLN:HB2	2.02	0.41
3:L:92:VAL:O	3:L:96:GLU:CB	2.68	0.41
3:L:318:ASP:HB3	3:L:334:MET:HB2	2.02	0.41
3:L:368:ALA:O	3:L:370:TRP:N	2.53	0.41
2:B:167:ILE:HG22	3:C:88:ILE:HG21	2.02	0.41
2:B:182:VAL:C	2:B:184:GLY:N	2.74	0.41
2:B:278:ASP:O	2:B:278:ASP:OD1	2.38	0.41
2:B:360:LEU:HD11	2:B:362:VAL:CG1	2.48	0.41
2:B:387:MET:HB2	2:B:426:ARG:HB3	2.02	0.41
7:B:502:MAN:C6	6:M:101:NDG:H8C1	2.51	0.41
1:G:183:ASN:C	1:G:185:LYS:N	2.72	0.41
2:H:390:HIS:HE1	2:H:428:HIS:HB2	1.84	0.41
2:H:425:ASN:O	2:H:426:ARG:C	2.57	0.41
3:L:309:LEU:O	3:L:333:TRP:HA	2.20	0.41
1:A:98:GLU:HB3	3:L:89:LEU:HD11	2.01	0.41
3:C:260:TYR:CZ	3:C:288:PHE:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ILE:HD11	3:F:92:VAL:HG21	2.03	0.41
1:D:162:LEU:HD23	2:E:213:LEU:HD11	2.02	0.41
2:E:425:ASN:O	2:E:426:ARG:C	2.59	0.41
2:E:456:VAL:HG12	2:E:457:TRP:N	2.36	0.41
3:F:275:PHE:CD1	3:F:275:PHE:C	2.92	0.41
1:G:101:TYR:C	1:G:103:GLU:N	2.74	0.41
2:H:348:SER:O	2:H:362:VAL:HA	2.20	0.41
2:H:384:ASN:HD22	4:O:2:HIS:CE1	2.39	0.41
1:J:112:ILE:HD11	3:L:92:VAL:CG2	2.45	0.41
1:J:112:ILE:CD1	3:L:92:VAL:HG22	2.47	0.41
3:L:122:ARG:O	3:L:126:GLN:HG3	2.20	0.41
1:A:143:VAL:HG22	3:C:124:GLN:HE22	1.84	0.41
2:B:405:TRP:CD2	4:M:3:ARG:HG3	2.55	0.41
2:B:405:TRP:CE2	4:M:3:ARG:HG3	2.56	0.41
3:C:362:ASP:OD1	3:C:362:ASP:N	2.53	0.41
1:D:185:LYS:O	1:D:186:PHE:C	2.59	0.41
1:D:189:PHE:O	1:D:192:VAL:HG23	2.21	0.41
6:D:301:NDG:C3	7:E:503:MAN:O1	2.67	0.41
2:E:165:LYS:HE2	2:E:165:LYS:HB3	1.91	0.41
2:E:259:VAL:HG23	2:E:314:LEU:HD13	2.03	0.41
2:E:350:ARG:O	2:E:361:TRP:HB2	2.20	0.41
2:E:390:HIS:CE1	2:E:428:HIS:CB	3.04	0.41
3:F:195:GLN:OE1	3:F:380:THR:HG22	2.20	0.41
3:F:368:ALA:C	3:F:370:TRP:H	2.23	0.41
2:H:432:PRO:O	2:H:433:ASN:CB	2.61	0.41
7:H:505:MAN:H2	6:H:506:NDG:H3	2.03	0.41
3:I:244:LEU:HD22	3:I:263:PHE:CE1	2.56	0.41
1:J:181:ILE:O	1:J:184:LEU:HG	2.21	0.41
1:J:186:PHE:HD1	2:K:177:ARG:HE	1.68	0.41
2:K:197:ARG:O	2:K:197:ARG:HG2	2.21	0.41
2:K:359:ARG:HH21	2:K:394:GLN:NE2	2.11	0.41
3:L:390:ASP:O	3:L:392:SER:N	2.47	0.41
1:A:97:LEU:O	1:A:97:LEU:HG	2.21	0.41
1:A:158:CYS:O	2:B:218:CYS:HB3	2.21	0.41
3:C:197:ARG:NH1	3:C:365:ILE:HD11	2.36	0.41
2:E:203:MET:O	2:E:207:ILE:HG12	2.21	0.41
2:H:458:MET:C	2:H:460:TRP:H	2.24	0.41
3:L:194:ILE:HA	3:L:194:ILE:HD13	1.85	0.41
3:L:273:ARG:NH1	3:L:309:LEU:CD1	2.84	0.41
3:L:298:GLN:H	3:L:298:GLN:HE21	1.65	0.41
1:A:95:ASN:O	1:A:96:GLU:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ARG:HA	3:C:137:PRO:HD2	1.83	0.40
2:E:166:GLU:HA	2:E:169:ASN:HD22	1.85	0.40
2:E:248:ILE:HD11	2:E:257:TYR:CE1	2.56	0.40
1:G:107:GLU:OE1	1:G:107:GLU:O	2.39	0.40
1:G:169:GLU:O	1:G:173:GLN:HG2	2.21	0.40
1:J:136:GLN:HE22	3:L:116:ASN:HB2	1.85	0.40
2:K:444:LYS:HA	2:K:464:TRP:CZ3	2.56	0.40
1:A:103:GLU:HA	1:A:106:ARG:NH1	2.26	0.40
1:A:111:ARG:NH2	1:J:96:GLU:CB	2.81	0.40
2:B:321:GLN:NE2	2:B:324:LYS:HE2	2.36	0.40
3:C:196:HIS:CE1	3:C:198:HIS:HB2	2.56	0.40
1:D:108:LEU:HD12	2:E:167:ILE:HD13	2.03	0.40
1:D:137:VAL:HG11	1:D:175:GLU:HG3	2.03	0.40
1:D:183:ASN:HB2	1:D:184:LEU:H	1.67	0.40
3:F:198:HIS:CE1	3:F:223:THR:HA	2.57	0.40
1:G:115:LEU:HD21	3:I:95:LEU:HB2	2.03	0.40
2:H:437:TYR:OH	2:H:447:ALA:HA	2.21	0.40
1:J:115:LEU:HD21	3:L:95:LEU:HB2	2.03	0.40
1:J:132:ASN:HB3	3:L:113:TRP:NE1	2.35	0.40
1:J:191:GLU:HG3	1:J:192:VAL:H	1.86	0.40
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.91	0.40
2:B:240:GLY:O	2:B:241:ARG:HD3	2.21	0.40
2:B:350:ARG:O	2:B:361:TRP:HB2	2.22	0.40
3:C:265:LEU:HA	3:C:273:ARG:O	2.21	0.40
3:C:267:PRO:O	3:C:271:GLU:O	2.40	0.40
2:E:348:SER:O	2:E:362:VAL:HA	2.21	0.40
3:F:103:ASP:O	3:F:107:GLN:HG2	2.21	0.40
3:F:216:GLY:HA3	3:F:226:PHE:HA	2.04	0.40
2:H:178:ILE:HD13	3:I:98:ILE:CG2	2.50	0.40
2:H:259:VAL:HG23	2:H:314:LEU:HD13	2.03	0.40
3:I:264:LYS:O	3:I:265:LEU:HD23	2.22	0.40
1:J:142:ARG:CZ	1:J:142:ARG:HB2	2.51	0.40
2:K:194:GLU:HB3	2:K:197:ARG:HH22	1.86	0.40
3:L:256:ARG:HG2	3:L:283:ASP:OD2	2.21	0.40
3:C:287:ALA:HB3	3:C:367:TRP:CE2	2.57	0.40
2:E:384:ASN:ND2	4:N:2:HIS:HE2	2.17	0.40
2:H:188:SER:HA	2:H:191:SER:OG	2.22	0.40
2:H:456:VAL:CG1	2:H:457:TRP:N	2.83	0.40
3:I:89:LEU:HD13	3:I:89:LEU:C	2.41	0.40
3:I:320:TYR:O	3:I:322:GLY:O	2.39	0.40
1:J:126:LEU:C	1:J:184:LEU:HD13	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:173:LEU:H	3:L:239:GLN:NE2	2.19	0.40
3:L:351:ASN:HD21	3:L:353:ARG:NE	2.20	0.40
1:A:121:MET:O	1:A:124:GLN:HB2	2.21	0.40
3:C:182:PHE:CE2	3:C:222:LEU:HB2	2.56	0.40
3:C:351:ASN:HD21	3:C:353:ARG:NE	2.20	0.40
1:D:121:MET:O	1:D:124:GLN:HB2	2.21	0.40
3:F:151:GLY:HA2	3:F:156:GLN:NE2	2.37	0.40
3:F:260:TYR:CZ	3:F:288:PHE:HB2	2.56	0.40
1:G:129:LEU:O	1:G:133:ILE:HG13	2.22	0.40
1:G:169:GLU:O	1:G:171:ASN:N	2.55	0.40
2:H:204:GLU:HG3	3:I:126:GLN:HE22	1.86	0.40
3:I:150:THR:CG2	3:I:151:GLY:N	2.74	0.40
3:I:260:TYR:CZ	3:I:288:PHE:HB2	2.56	0.40
3:I:352:TYR:CE1	3:I:374:TRP:HA	2.56	0.40
3:I:392:SER:O	3:I:394:HIS:N	2.53	0.40
2:K:303:LYS:HE3	2:K:303:LYS:CA	2.51	0.40
2:K:371:ASN:ND2	2:K:374:LEU:CD1	2.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/119 (82%)	74 (76%)	17 (18%)	6 (6%)	1	4
1	D	97/119 (82%)	75 (77%)	13 (13%)	9 (9%)	0	1
1	G	97/119 (82%)	75 (77%)	13 (13%)	9 (9%)	0	1
1	J	97/119 (82%)	74 (76%)	14 (14%)	9 (9%)	0	1
2	B	313/323 (97%)	265 (85%)	29 (9%)	19 (6%)	1	4
2	E	313/323 (97%)	268 (86%)	26 (8%)	19 (6%)	1	4
2	H	313/323 (97%)	260 (83%)	35 (11%)	18 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	313/323 (97%)	261 (83%)	32 (10%)	20 (6%)	1	3
3	C	315/323 (98%)	259 (82%)	38 (12%)	18 (6%)	1	5
3	F	315/323 (98%)	259 (82%)	39 (12%)	17 (5%)	2	5
3	I	311/323 (96%)	255 (82%)	41 (13%)	15 (5%)	2	7
3	L	311/323 (96%)	256 (82%)	40 (13%)	15 (5%)	2	7
4	M	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
4	N	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
4	O	3/5 (60%)	3 (100%)	0	0	100	100
4	P	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	2904/3080 (94%)	2389 (82%)	341 (12%)	174 (6%)	1	4

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
2	B	277	VAL
2	B	293	GLU
3	C	337	CYS
3	C	357	VAL
3	C	360	PRO
3	C	364	GLY
3	C	391	LEU
1	D	163	GLU
1	D	183	ASN
1	D	184	LEU
2	E	277	VAL
2	E	293	GLU
3	F	337	CYS
3	F	357	VAL
3	F	360	PRO
3	F	364	GLY
3	F	397	GLN
1	G	163	GLU
1	G	167	ASP
2	H	277	VAL
2	H	293	GLU
3	I	337	CYS
3	I	357	VAL
3	I	360	PRO

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Mol	Chain	Res	Type
3	I	364	GLY
1	J	162	LEU
1	J	163	GLU
1	J	167	ASP
2	K	277	VAL
2	K	293	GLU
2	K	407	PRO
3	L	337	CYS
3	L	357	VAL
3	L	360	PRO
3	L	364	GLY
1	A	178	ALA
1	A	186	PHE
1	A	188	ARG
2	B	176	ILE
2	B	266	HIS
2	B	371	ASN
2	B	407	PRO
2	B	427	CYS
2	B	459	ASN
2	B	476	PRO
3	C	173	LEU
3	C	199	ASP
3	C	330	SER
3	C	350	GLY
3	C	361	TYR
3	C	368	ALA
3	C	369	THR
3	C	394	HIS
3	C	397	GLN
1	D	178	ALA
1	D	186	PHE
1	D	192	VAL
2	E	176	ILE
2	E	266	HIS
2	E	371	ASN
2	E	407	PRO
2	E	427	CYS
2	E	476	PRO
3	F	173	LEU
3	F	199	ASP
3	F	350	GLY

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Mol	Chain	Res	Type
3	F	361	TYR
3	F	368	ALA
3	F	369	THR
1	G	162	LEU
1	G	166	LEU
1	G	168	LYS
2	H	186	LEU
2	H	266	HIS
2	H	371	ASN
2	H	407	PRO
2	H	427	CYS
2	H	459	ASN
2	H	476	PRO
3	I	173	LEU
3	I	199	ASP
3	I	330	SER
3	I	350	GLY
3	I	361	TYR
3	I	368	ALA
3	I	369	THR
1	J	166	LEU
1	J	168	LYS
2	K	166	GLU
2	K	186	LEU
2	K	266	HIS
2	K	371	ASN
2	K	419	ALA
2	K	427	CYS
2	K	476	PRO
3	L	173	LEU
3	L	199	ASP
3	L	350	GLY
3	L	361	TYR
3	L	368	ALA
3	L	369	THR
3	L	391	LEU
1	A	167	ASP
2	B	303	LYS
2	B	304	SER
2	B	351	PRO
2	B	419	ALA
3	C	281	ASP

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Mol	Chain	Res	Type
3	C	371	HIS
3	C	398	GLN
1	D	167	ASP
2	E	303	LYS
2	E	304	SER
2	E	419	ALA
2	E	459	ASN
3	F	281	ASP
3	F	330	SER
3	F	371	HIS
1	G	96	GLU
1	G	181	ILE
1	G	186	PHE
2	H	178	ILE
2	H	304	SER
2	H	419	ALA
3	I	281	ASP
3	I	371	HIS
1	J	96	GLU
1	J	181	ILE
1	J	187	GLU
2	K	303	LYS
2	K	304	SER
2	K	344	ALA
2	K	459	ASN
3	L	281	ASP
3	L	330	SER
3	L	371	HIS
2	B	188	SER
2	B	327	THR
2	B	344	ALA
3	C	359	PHE
2	E	188	SER
2	E	327	THR
2	E	351	PRO
2	H	303	LYS
2	H	327	THR
2	H	344	ALA
2	H	351	PRO
3	I	391	LEU
2	K	178	ILE
2	K	213	LEU

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Mol	Chain	Res	Type
2	K	327	THR
2	K	351	PRO
2	B	278	ASP
2	B	326	HIS
1	D	185	LYS
2	E	278	ASP
2	E	326	HIS
2	E	344	ALA
3	F	359	PHE
3	F	391	LEU
2	H	326	HIS
3	I	359	PHE
2	K	326	HIS
3	L	359	PHE
1	A	101	TYR
1	G	104	VAL
1	D	181	ILE
1	J	104	VAL
2	K	279	GLY
2	B	279	GLY
2	E	279	GLY
3	F	396	GLY
2	H	279	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	92/110 (84%)	83 (90%)	9 (10%)	8 24
1	D	92/110 (84%)	83 (90%)	9 (10%)	8 24
1	G	92/110 (84%)	88 (96%)	4 (4%)	29 62
1	J	92/110 (84%)	87 (95%)	5 (5%)	22 53
2	B	266/274 (97%)	249 (94%)	17 (6%)	17 45
2	E	266/274 (97%)	249 (94%)	17 (6%)	17 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	266/274 (97%)	248 (93%)	18 (7%)	16	42
2	K	266/274 (97%)	249 (94%)	17 (6%)	17	45
3	C	276/281 (98%)	258 (94%)	18 (6%)	17	44
3	F	276/281 (98%)	259 (94%)	17 (6%)	18	47
3	I	273/281 (97%)	253 (93%)	20 (7%)	14	38
3	L	273/281 (97%)	255 (93%)	18 (7%)	16	44
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	3 (100%)	0	100	100
4	O	3/3 (100%)	3 (100%)	0	100	100
4	P	3/3 (100%)	3 (100%)	0	100	100
All	All	2542/2672 (95%)	2373 (93%)	169 (7%)	16	44

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	110	ARG
1	A	128	LEU
1	A	142	ARG
1	A	151	LEU
1	A	165	ARG
1	A	169	GLU
1	A	175	GLU
1	A	188	ARG
2	B	172	LYS
2	B	186	LEU
2	B	205	GLU
2	B	224	VAL
2	B	251	ASP
2	B	253	PHE
2	B	274	GLN
2	B	285	ARG
2	B	303	LYS
2	B	322	LEU
2	B	326	HIS
2	B	350	ARG
2	B	352	GLU
2	B	400	ARG

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Mol	Chain	Res	Type
2	B	407	PRO
2	B	417	GLU
2	B	474	LEU
3	C	89	LEU
3	C	119	PHE
3	C	125	GLN
3	C	129	ASP
3	C	133	THR
3	C	136	ARG
3	C	192	THR
3	C	197	ARG
3	C	209	VAL
3	C	248	LEU
3	C	271	GLU
3	C	296	ASP
3	C	298	GLN
3	C	313	PRO
3	C	352	TYR
3	C	359	PHE
3	C	381	THR
3	C	383	LYS
1	D	98	GLU
1	D	110	ARG
1	D	128	LEU
1	D	142	ARG
1	D	151	LEU
1	D	165	ARG
1	D	169	GLU
1	D	175	GLU
1	D	184	LEU
2	E	172	LYS
2	E	186	LEU
2	E	205	GLU
2	E	224	VAL
2	E	251	ASP
2	E	253	PHE
2	E	274	GLN
2	E	285	ARG
2	E	303	LYS
2	E	322	LEU
2	E	326	HIS
2	E	350	ARG

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Mol	Chain	Res	Type
2	E	352	GLU
2	E	400	ARG
2	E	407	PRO
2	E	417	GLU
2	E	474	LEU
3	F	89	LEU
3	F	119	PHE
3	F	125	GLN
3	F	129	ASP
3	F	133	THR
3	F	136	ARG
3	F	192	THR
3	F	197	ARG
3	F	209	VAL
3	F	248	LEU
3	F	296	ASP
3	F	298	GLN
3	F	313	PRO
3	F	352	TYR
3	F	359	PHE
3	F	381	THR
3	F	383	LYS
1	G	107	GLU
1	G	166	LEU
1	G	169	GLU
1	G	171	ASN
2	H	166	GLU
2	H	177	ARG
2	H	205	GLU
2	H	209	THR
2	H	224	VAL
2	H	251	ASP
2	H	253	PHE
2	H	274	GLN
2	H	285	ARG
2	H	303	LYS
2	H	322	LEU
2	H	326	HIS
2	H	350	ARG
2	H	352	GLU
2	H	400	ARG
2	H	407	PRO

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Mol	Chain	Res	Type
2	H	417	GLU
2	H	474	LEU
3	I	83	LYS
3	I	98	ILE
3	I	119	PHE
3	I	125	GLN
3	I	127	LEU
3	I	133	THR
3	I	136	ARG
3	I	192	THR
3	I	197	ARG
3	I	209	VAL
3	I	248	LEU
3	I	296	ASP
3	I	298	GLN
3	I	313	PRO
3	I	352	TYR
3	I	359	PHE
3	I	381	THR
3	I	383	LYS
3	I	384	LEU
3	I	390	ASP
1	J	107	GLU
1	J	166	LEU
1	J	169	GLU
1	J	171	ASN
1	J	186	PHE
2	K	177	ARG
2	K	205	GLU
2	K	209	THR
2	K	224	VAL
2	K	251	ASP
2	K	253	PHE
2	K	274	GLN
2	K	285	ARG
2	K	303	LYS
2	K	322	LEU
2	K	326	HIS
2	K	350	ARG
2	K	352	GLU
2	K	400	ARG
2	K	407	PRO

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Mol	Chain	Res	Type
2	K	417	GLU
2	K	474	LEU
3	L	83	LYS
3	L	98	ILE
3	L	119	PHE
3	L	125	GLN
3	L	127	LEU
3	L	133	THR
3	L	136	ARG
3	L	192	THR
3	L	197	ARG
3	L	209	VAL
3	L	248	LEU
3	L	296	ASP
3	L	298	GLN
3	L	313	PRO
3	L	352	TYR
3	L	359	PHE
3	L	381	THR
3	L	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	130	GLN
1	A	132	ASN
2	B	169	ASN
2	B	210	GLN
2	B	231	HIS
2	B	238	ASN
2	B	274	GLN
2	B	288	ASN
2	B	320	HIS
2	B	356	GLN
2	B	371	ASN
2	B	379	GLN
2	B	394	GLN
2	B	459	ASN
2	B	469	GLN
3	C	97	GLN
3	C	107	GLN

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Mol	Chain	Res	Type
3	C	118	GLN
3	C	124	GLN
3	C	125	GLN
3	C	160	ASN
3	C	177	GLN
3	C	189	ASN
3	C	196	HIS
3	C	230	ASN
3	C	239	GLN
3	C	240	GLN
3	C	262	HIS
3	C	298	GLN
3	C	305	HIS
3	C	317	ASN
3	C	341	HIS
3	C	351	ASN
3	C	398	GLN
3	C	399	GLN
1	D	122	GLN
1	D	130	GLN
1	D	132	ASN
2	E	169	ASN
2	E	210	GLN
2	E	231	HIS
2	E	238	ASN
2	E	274	GLN
2	E	288	ASN
2	E	356	GLN
2	E	371	ASN
2	E	379	GLN
2	E	384	ASN
2	E	394	GLN
2	E	459	ASN
2	E	469	GLN
3	F	97	GLN
3	F	107	GLN
3	F	118	GLN
3	F	124	GLN
3	F	125	GLN
3	F	160	ASN
3	F	177	GLN
3	F	189	ASN

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Mol	Chain	Res	Type
3	F	196	HIS
3	F	230	ASN
3	F	239	GLN
3	F	240	GLN
3	F	262	HIS
3	F	298	GLN
3	F	305	HIS
3	F	317	ASN
3	F	341	HIS
3	F	351	ASN
3	F	398	GLN
1	G	124	GLN
1	G	130	GLN
1	G	132	ASN
1	G	136	GLN
1	G	171	ASN
2	H	169	ASN
2	H	201	GLN
2	H	210	GLN
2	H	231	HIS
2	H	238	ASN
2	H	274	GLN
2	H	288	ASN
2	H	320	HIS
2	H	356	GLN
2	H	371	ASN
2	H	379	GLN
2	H	384	ASN
2	H	394	GLN
2	H	459	ASN
2	H	469	GLN
3	I	107	GLN
3	I	125	GLN
3	I	139	GLN
3	I	160	ASN
3	I	189	ASN
3	I	196	HIS
3	I	230	ASN
3	I	239	GLN
3	I	240	GLN
3	I	262	HIS
3	I	298	GLN

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Mol	Chain	Res	Type
3	I	305	HIS
3	I	317	ASN
3	I	341	HIS
3	I	394	HIS
1	J	124	GLN
1	J	130	GLN
1	J	132	ASN
1	J	136	GLN
1	J	171	ASN
2	K	201	GLN
2	K	210	GLN
2	K	231	HIS
2	K	238	ASN
2	K	274	GLN
2	K	288	ASN
2	K	320	HIS
2	K	356	GLN
2	K	371	ASN
2	K	379	GLN
2	K	384	ASN
2	K	394	GLN
2	K	428	HIS
2	K	459	ASN
2	K	469	GLN
3	L	107	GLN
3	L	125	GLN
3	L	139	GLN
3	L	160	ASN
3	L	189	ASN
3	L	196	HIS
3	L	230	ASN
3	L	239	GLN
3	L	240	GLN
3	L	262	HIS
3	L	298	GLN
3	L	305	HIS
3	L	317	ASN
3	L	341	HIS
3	L	351	ASN
3	L	394	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Q	1	3,5	14,14,15	1.27	1 (7%)	17,19,21	1.32	3 (17%)
5	NAG	Q	2	5	14,14,15	1.31	2 (14%)	17,19,21	1.11	1 (5%)

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
5	NAG	Q	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	1	NAG	O7-C7	-4.10	1.14	1.23
5	Q	2	NAG	O7-C7	-3.71	1.14	1.23
5	Q	2	NAG	C2-N2	2.02	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	1	NAG	C3-C4-C5	2.43	114.58	110.24
5	Q	1	NAG	C6-C5-C4	-2.39	107.41	113.00
5	Q	1	NAG	C1-O5-C5	2.24	115.22	112.19
5	Q	2	NAG	C1-O5-C5	2.18	115.14	112.19

There are no chirality outliers.

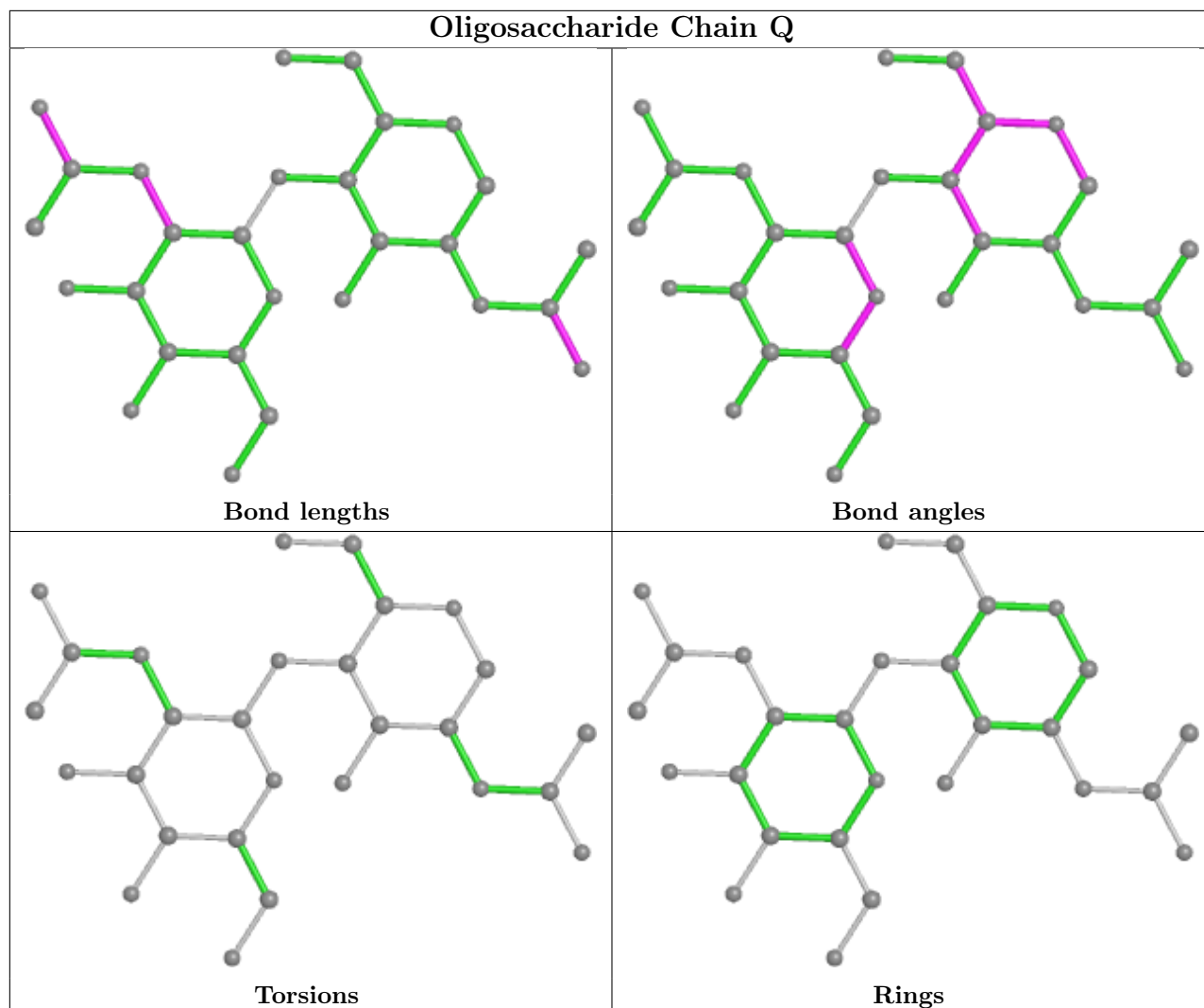
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	1	NAG	3	0
5	Q	2	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 8 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NDG	K	501	-	15,15,15	0.70	0	21,21,21	0.90	1 (4%)
6	NDG	O	101	-	15,15,15	0.59	0	21,21,21	0.59	0
6	NDG	M	101	-	15,15,15	0.50	0	21,21,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NDG	H	502	-	15,15,15	0.47	0	21,21,21	0.65	0
7	MAN	C	503	-	11,11,12	1.18	1 (9%)	15,15,17	2.52	4 (26%)
7	MAN	N	102	-	12,12,12	0.43	0	17,17,17	0.37	0
11	GAL	H	507	-	12,12,12	0.99	0	17,17,17	0.63	0
7	MAN	L	501	-	11,11,12	1.17	1 (9%)	15,15,17	2.52	4 (26%)
10	BMA	E	502	-	12,12,12	0.55	0	17,17,17	0.66	0
7	MAN	P	101	-	12,12,12	0.44	0	17,17,17	0.37	0
7	MAN	E	503	-	12,12,12	0.44	0	17,17,17	0.37	0
9	NAG	C	501	3	14,14,15	1.27	1 (7%)	17,19,21	1.33	3 (17%)
6	NDG	H	506	-	15,15,15	0.47	0	21,21,21	0.66	0
6	NDG	D	301	-	15,15,15	0.47	0	21,21,21	0.66	0
9	NAG	I	501	3	14,14,15	1.27	1 (7%)	17,19,21	1.33	3 (17%)
9	NAG	F	501	3	14,14,15	1.27	1 (7%)	17,19,21	1.33	3 (17%)
6	NDG	N	101	-	15,15,15	0.41	0	21,21,21	0.61	0
9	NAG	F	502	-	14,14,15	1.32	2 (14%)	17,19,21	1.11	1 (5%)
9	NAG	E	501	-	15,15,15	0.65	0	21,21,21	1.19	3 (14%)
7	MAN	H	505	-	12,12,12	0.44	0	17,17,17	0.37	0
7	MAN	B	502	-	12,12,12	0.46	0	17,17,17	0.45	0
7	MAN	J	301	-	11,11,12	1.17	1 (9%)	15,15,17	2.52	4 (26%)
10	BMA	H	504	-	12,12,12	0.54	0	17,17,17	0.38	0
6	NDG	H	501	-	15,15,15	0.48	0	21,21,21	0.76	0
7	MAN	F	503	-	11,11,12	1.18	1 (9%)	15,15,17	2.52	4 (26%)
9	NAG	I	502	-	14,14,15	1.30	1 (7%)	17,19,21	1.11	1 (5%)
7	MAN	H	503	-	12,12,12	0.44	0	17,17,17	0.37	0
9	NAG	C	502	-	14,14,15	1.31	1 (7%)	17,19,21	1.11	1 (5%)
6	NDG	B	501	-	15,15,15	0.38	0	21,21,21	0.60	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
6	NDG	K	501	-	-	6/6/26/26	0/1/1/1
6	NDG	O	101	-	-	4/6/26/26	0/1/1/1
6	NDG	M	101	-	-	5/6/26/26	0/1/1/1
6	NDG	H	502	-	-	6/6/26/26	0/1/1/1
7	MAN	C	503	-	-	0/2/19/22	0/1/1/1
7	MAN	N	102	-	-	1/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GAL	H	507	-	-	0/2/22/22	0/1/1/1
7	MAN	L	501	-	-	0/2/19/22	0/1/1/1
10	BMA	E	502	-	-	2/2/22/22	0/1/1/1
7	MAN	P	101	-	-	1/2/22/22	0/1/1/1
7	MAN	E	503	-	-	1/2/22/22	0/1/1/1
9	NAG	C	501	3	-	0/6/23/26	0/1/1/1
6	NDG	H	506	-	-	6/6/26/26	0/1/1/1
6	NDG	D	301	-	-	6/6/26/26	0/1/1/1
9	NAG	I	501	3	-	0/6/23/26	0/1/1/1
9	NAG	F	501	3	-	0/6/23/26	0/1/1/1
6	NDG	N	101	-	-	5/6/26/26	0/1/1/1
9	NAG	F	502	-	-	0/6/23/26	0/1/1/1
9	NAG	E	501	-	-	4/6/26/26	0/1/1/1
7	MAN	H	505	-	-	1/2/22/22	0/1/1/1
7	MAN	B	502	-	-	2/2/22/22	0/1/1/1
7	MAN	J	301	-	-	0/2/19/22	0/1/1/1
10	BMA	H	504	-	-	0/2/22/22	0/1/1/1
6	NDG	H	501	-	-	4/6/26/26	0/1/1/1
7	MAN	F	503	-	-	0/2/19/22	0/1/1/1
9	NAG	I	502	-	-	0/6/23/26	0/1/1/1
7	MAN	H	503	-	-	1/2/22/22	0/1/1/1
9	NAG	C	502	-	-	0/6/23/26	0/1/1/1
6	NDG	B	501	-	-	4/6/26/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	501	NAG	O7-C7	-4.13	1.13	1.23
9	C	501	NAG	O7-C7	-4.12	1.13	1.23
9	F	501	NAG	O7-C7	-4.12	1.13	1.23
9	F	502	NAG	O7-C7	-3.74	1.14	1.23
9	C	502	NAG	O7-C7	-3.72	1.14	1.23
9	I	502	NAG	O7-C7	-3.71	1.14	1.23
7	F	503	MAN	O5-C1	-3.38	1.38	1.43
7	C	503	MAN	O5-C1	-3.38	1.38	1.43
7	J	301	MAN	O5-C1	-3.35	1.38	1.43
7	L	501	MAN	O5-C1	-3.35	1.38	1.43
9	F	502	NAG	C2-N2	2.01	1.49	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	301	MAN	O5-C1-C2	6.42	120.67	110.77
7	C	503	MAN	O5-C1-C2	6.41	120.66	110.77
7	F	503	MAN	O5-C1-C2	6.38	120.62	110.77
7	L	501	MAN	O5-C1-C2	6.37	120.60	110.77
7	F	503	MAN	C1-O5-C5	5.84	120.10	112.19
7	L	501	MAN	C1-O5-C5	5.83	120.09	112.19
7	C	503	MAN	C1-O5-C5	5.82	120.08	112.19
7	J	301	MAN	C1-O5-C5	5.79	120.04	112.19
9	E	501	NAG	C3-C4-C5	2.59	114.86	110.24
9	E	501	NAG	C1-C2-C3	2.56	114.04	110.54
6	K	501	NDG	O5-C1-C2	2.50	112.03	109.52
9	I	501	NAG	C3-C4-C5	2.46	114.62	110.24
9	C	501	NAG	C3-C4-C5	2.45	114.62	110.24
9	F	501	NAG	C3-C4-C5	2.44	114.59	110.24
9	F	501	NAG	C6-C5-C4	-2.40	107.37	113.00
9	C	501	NAG	C6-C5-C4	-2.39	107.41	113.00
7	C	503	MAN	O3-C3-C2	-2.39	105.42	109.99
7	J	301	MAN	O3-C3-C2	-2.38	105.43	109.99
9	I	501	NAG	C6-C5-C4	-2.38	107.43	113.00
7	F	503	MAN	C1-C2-C3	2.38	112.59	109.67
7	L	501	MAN	C1-C2-C3	2.38	112.59	109.67
7	L	501	MAN	O3-C3-C2	-2.37	105.46	109.99
7	F	503	MAN	O3-C3-C2	-2.36	105.47	109.99
7	C	503	MAN	C1-C2-C3	2.31	112.51	109.67
7	J	301	MAN	C1-C2-C3	2.30	112.49	109.67
9	F	501	NAG	C1-O5-C5	2.26	115.25	112.19
9	I	501	NAG	C1-O5-C5	2.26	115.25	112.19
9	C	501	NAG	C1-O5-C5	2.25	115.25	112.19
9	I	502	NAG	C1-O5-C5	2.22	115.20	112.19
9	C	502	NAG	C1-O5-C5	2.21	115.19	112.19
9	F	502	NAG	C1-O5-C5	2.17	115.13	112.19
9	E	501	NAG	O5-C1-C2	2.15	111.68	109.52

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	NDG	C1-C2-N2-C7
6	B	501	NDG	C8-C7-N2-C2
6	B	501	NDG	O7-C7-N2-C2
6	D	301	NDG	C1-C2-N2-C7
6	D	301	NDG	C8-C7-N2-C2
6	D	301	NDG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	H	501	NDG	C8-C7-N2-C2
6	H	501	NDG	O7-C7-N2-C2
6	H	502	NDG	C1-C2-N2-C7
6	H	502	NDG	C8-C7-N2-C2
6	H	502	NDG	O7-C7-N2-C2
6	H	506	NDG	C1-C2-N2-C7
6	H	506	NDG	C8-C7-N2-C2
6	H	506	NDG	O7-C7-N2-C2
6	K	501	NDG	C1-C2-N2-C7
6	K	501	NDG	C8-C7-N2-C2
6	K	501	NDG	O7-C7-N2-C2
6	M	101	NDG	C8-C7-N2-C2
6	M	101	NDG	O7-C7-N2-C2
6	N	101	NDG	C8-C7-N2-C2
6	N	101	NDG	O7-C7-N2-C2
6	O	101	NDG	C8-C7-N2-C2
6	O	101	NDG	O7-C7-N2-C2
9	E	501	NAG	C1-C2-N2-C7
9	E	501	NAG	C8-C7-N2-C2
9	E	501	NAG	O7-C7-N2-C2
6	O	101	NDG	C4-C5-C6-O6
6	D	301	NDG	C4-C5-C6-O6
6	H	502	NDG	C4-C5-C6-O6
6	H	506	NDG	C4-C5-C6-O6
6	O	101	NDG	O5-C5-C6-O6
7	B	502	MAN	O5-C5-C6-O6
6	D	301	NDG	O5-C5-C6-O6
6	H	502	NDG	O5-C5-C6-O6
6	H	506	NDG	O5-C5-C6-O6
10	E	502	BMA	O5-C5-C6-O6
6	H	501	NDG	C4-C5-C6-O6
7	B	502	MAN	C4-C5-C6-O6
6	H	501	NDG	O5-C5-C6-O6
6	M	101	NDG	O5-C5-C6-O6
10	E	502	BMA	C4-C5-C6-O6
6	K	501	NDG	O5-C5-C6-O6
6	K	501	NDG	C4-C5-C6-O6
6	N	101	NDG	O5-C5-C6-O6
7	E	503	MAN	O5-C5-C6-O6
7	H	503	MAN	O5-C5-C6-O6
7	H	505	MAN	O5-C5-C6-O6
7	N	102	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	P	101	MAN	O5-C5-C6-O6
6	M	101	NDG	C4-C5-C6-O6
6	D	301	NDG	C3-C2-N2-C7
6	H	502	NDG	C3-C2-N2-C7
6	H	506	NDG	C3-C2-N2-C7
9	E	501	NAG	C4-C5-C6-O6
6	N	101	NDG	C3-C2-N2-C7
6	N	101	NDG	C1-C2-N2-C7
6	B	501	NDG	C3-C2-N2-C7
6	K	501	NDG	C3-C2-N2-C7
6	M	101	NDG	C1-C2-N2-C7

There are no ring outliers.

29 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	501	NDG	7	0
6	O	101	NDG	2	0
6	M	101	NDG	5	0
6	H	502	NDG	6	0
7	C	503	MAN	2	0
7	N	102	MAN	1	0
11	H	507	GAL	10	0
7	L	501	MAN	2	0
10	E	502	BMA	23	0
7	P	101	MAN	8	0
7	E	503	MAN	12	0
9	C	501	NAG	7	0
6	H	506	NDG	23	0
6	D	301	NDG	9	0
9	I	501	NAG	6	0
9	F	501	NAG	6	0
6	N	101	NDG	25	0
9	F	502	NAG	11	0
9	E	501	NAG	9	0
7	H	505	MAN	15	0
7	B	502	MAN	3	0
7	J	301	MAN	2	0
10	H	504	BMA	1	0
6	H	501	NDG	2	0
7	F	503	MAN	5	0
9	I	502	NAG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	503	MAN	15	0
9	C	502	NAG	9	0
6	B	501	NDG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.