Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1N73
Title	:	Fibrin D-Dimer, Lamprey complexed with the PEPTIDE LIGAND: GLY-HIS-ARG-PRO-AMIDE
Authors	:	Yang, Z.; Pandi, L.; Doolittle, R.F.
Deposited on	:	2002-11-12
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/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:

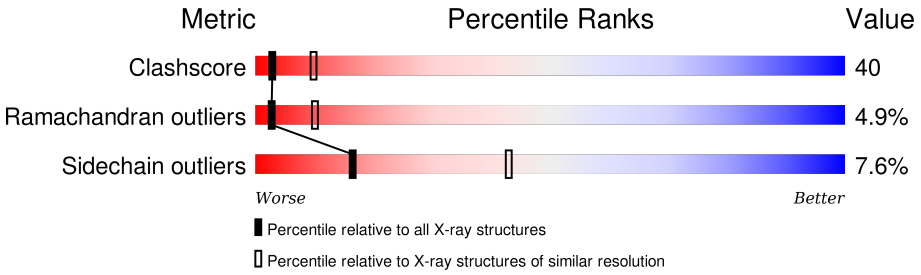
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	23% 39% 15% 24%
1	D	119	15% 49% 9% • 24%
2	B	323	42% 49% 6% • •
2	E	323	38% 52% 7% • •
3	C	330	47% 42% 8% • •
3	F	330	45% 46% 5% •
4	G	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	H	4	25% 75%
4	I	4	25% 50% 25%
4	J	4	25% 50% 25%

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
5	NAG	C	480	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12039 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 Fibrin alpha-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	S	0	0	0
			763	480	143	137	3			
1	D	90	Total	C	N	O	S	0	0	0
			758	477	142	136	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	THR	SEE REMARK 999	UNP P02674
D	153	ALA	THR	SEE REMARK 999	UNP P02674

- Molecule 2 is a protein called Fibrin beta chain.

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

- Molecule 3 is a protein called Fibrin gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	322	Total	C	N	O	S	0	0	0
			2630	1658	457	502	13			
3	F	322	Total	C	N	O	S	0	0	0
			2630	1658	457	502	13			

- Molecule 4 is a protein called peptide ligand: Gly-his-Arg-Pro-amide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			32	19	9	4			

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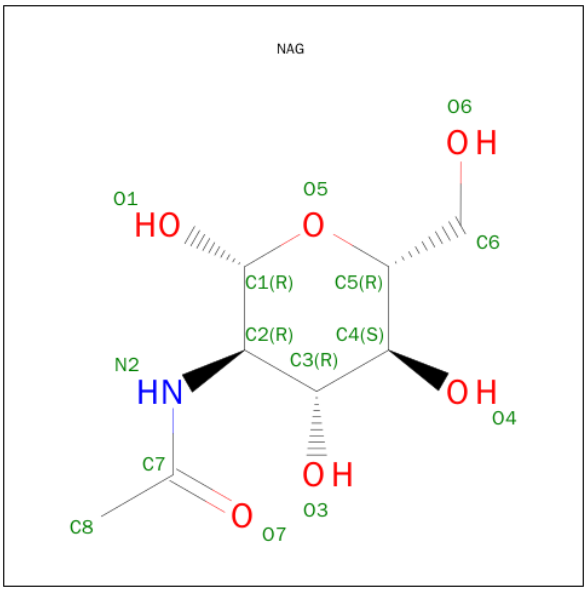
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	4	Total C N O 32 19 9 4	0	0	0
4	I	4	Total C N O 32 19 9 4	0	0	0
4	J	4	Total C N O 32 19 9 4	0	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0

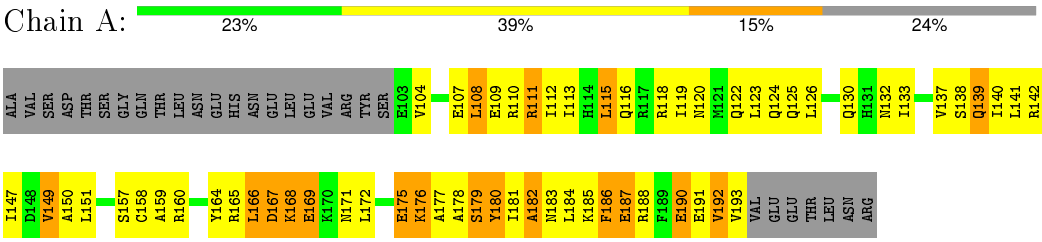
3 Residue-property plots (i)

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

Note EDS was not executed.

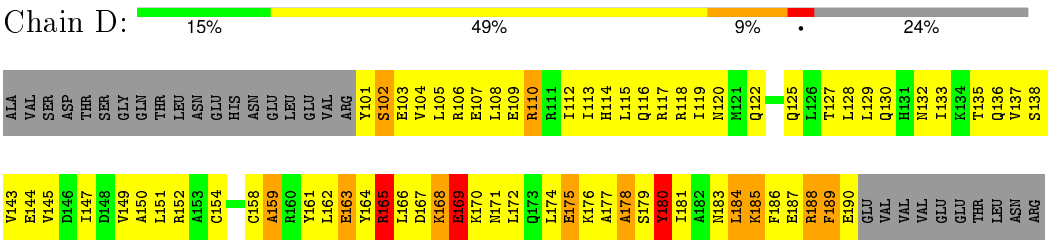
- Molecule 1: Fibrin alpha-1 chain

Chain A:



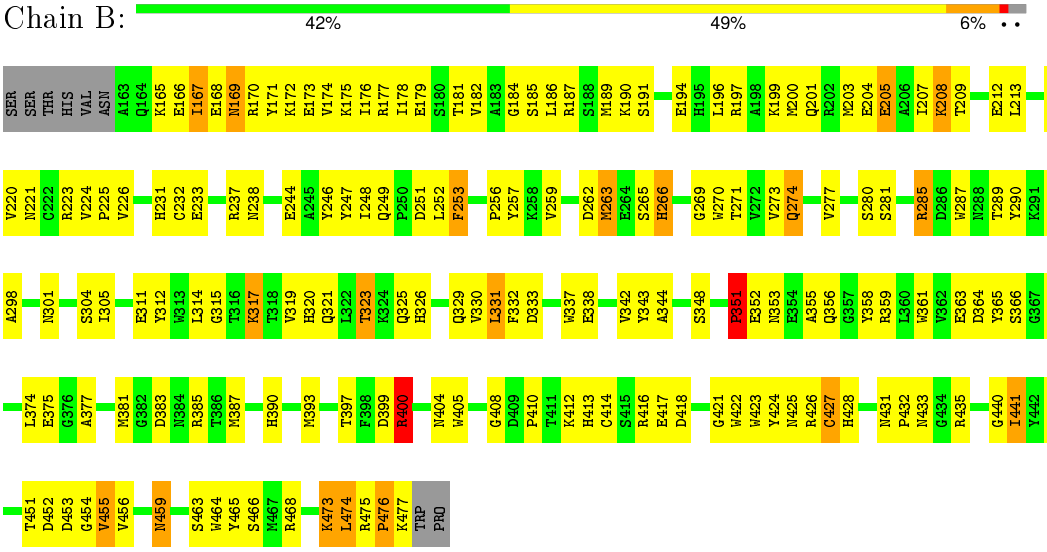
- Molecule 1: Fibrin alpha-1 chain

Chain D:



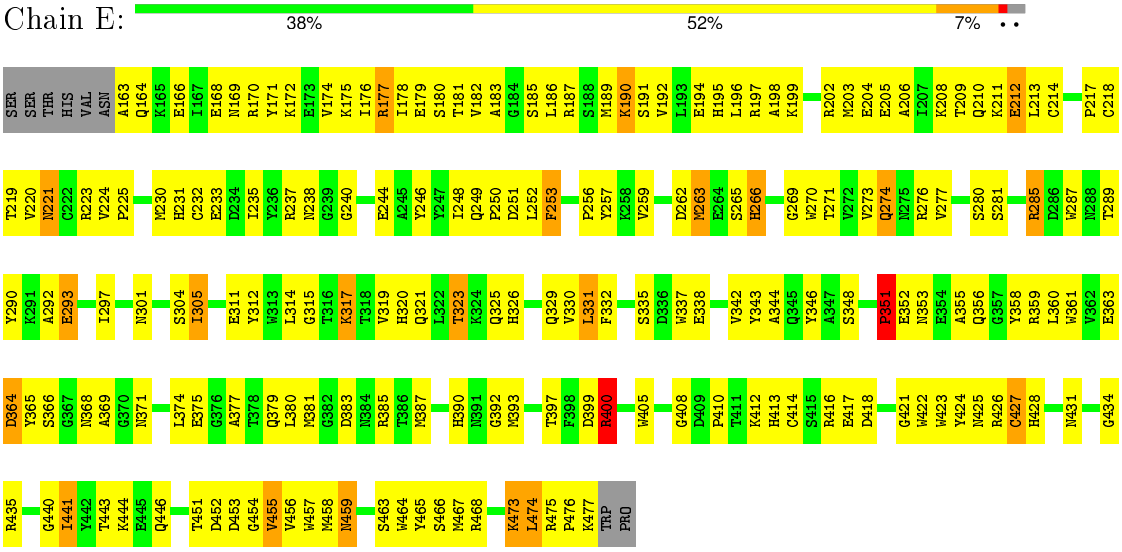
- Molecule 2: Fibrin beta chain

Chain B:



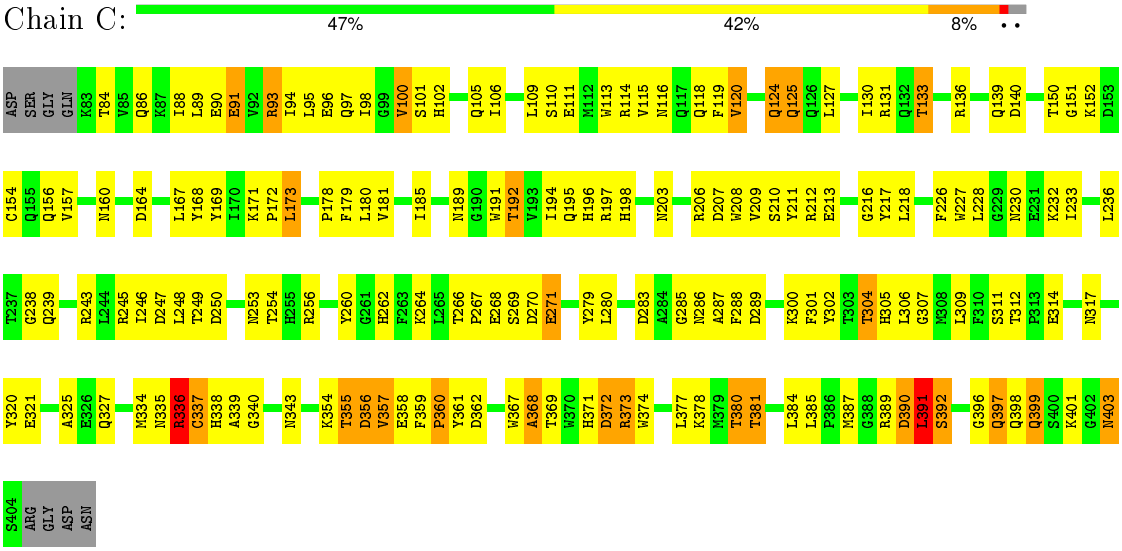
• Molecule 2: Fibrin beta chain

Chain E:



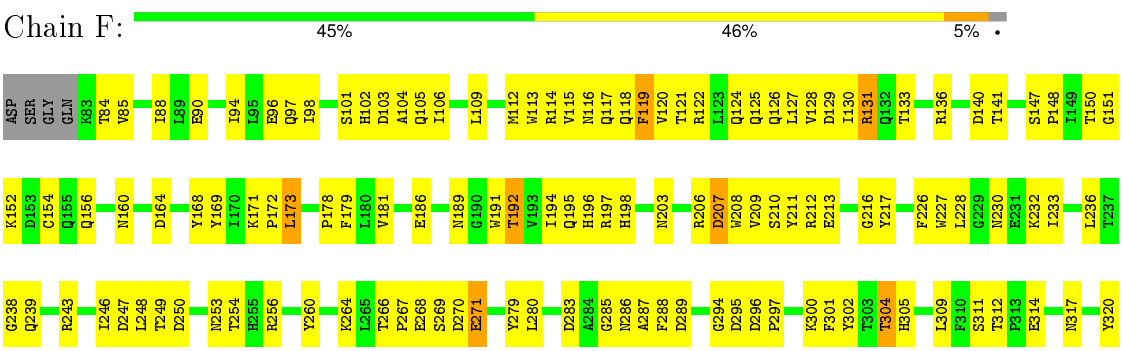
• Molecule 3: Fibrin gamma chain

Chain C:



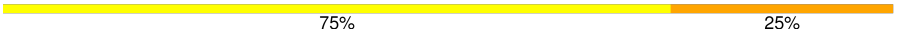
• Molecule 3: Fibrin gamma chain

Chain F:



- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide

Chain G:

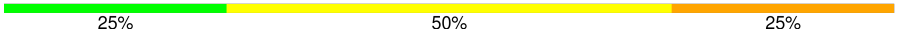


- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide

Chain H:

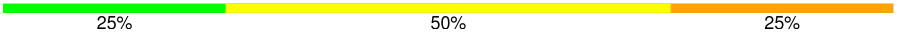
- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide

Chain I:



- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide

Chain J:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.73Å 99.30Å 120.73Å 99.58° 101.46° 92.36°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	81.7 (20.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.258 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12039	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.41	0/769	0.71	0/1030
1	D	0.36	0/765	0.63	0/1024
2	B	0.41	0/2602	0.65	0/3517
2	E	0.41	0/2602	0.65	0/3517
3	C	0.44	0/2701	0.69	1/3653 (0.0%)
3	F	0.43	0/2701	0.67	1/3653 (0.0%)
4	G	0.41	0/33	0.66	0/43
4	H	0.42	0/33	0.55	0/43
4	I	0.42	0/33	0.45	0/43
4	J	0.46	0/33	0.59	0/43
All	All	0.42	0/12272	0.67	2/16566 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	336	ARG	N-CA-C	-5.23	96.88	111.00
3	F	336	ARG	N-CA-C	-5.17	97.05	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	763	0	799	89	0
1	D	758	0	789	113	0
2	B	2535	0	2363	221	0
2	E	2535	0	2363	218	0
3	C	2630	0	2455	176	0
3	F	2630	0	2453	191	0
4	G	32	0	32	13	0
4	H	32	0	32	6	0
4	I	32	0	32	3	0
4	J	32	0	32	8	0
5	B	14	0	13	3	0
5	C	14	0	13	2	0
5	E	14	0	13	4	0
5	F	14	0	13	2	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	12039	0	11402	925	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 40.

All (925) 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)
3:C:203:ASN:HD21	5:C:480:NAG:C1	1.30	1.40
2:E:381:MET:HB2	5:E:480:NAG:C8	1.67	1.22
2:B:381:MET:HB2	5:B:480:NAG:C8	1.73	1.18
1:D:168:LYS:HD2	1:D:169:GLU:H	0.97	1.10
2:E:381:MET:HB2	5:E:480:NAG:H82	1.33	1.09
3:C:150:THR:HG22	3:C:151:GLY:H	1.20	1.05
2:E:371:ASN:HD21	2:E:374:LEU:HB2	1.26	1.01
3:C:247:ASP:HB2	3:C:381:THR:HG23	1.40	1.01
2:B:205:GLU:HA	2:B:208:LYS:HB2	1.39	1.00
2:B:381:MET:HB2	5:B:480:NAG:H82	1.43	0.99
3:F:150:THR:HG22	3:F:151:GLY:H	1.22	0.98
3:F:247:ASP:HB2	3:F:381:THR:HG23	1.40	0.98
3:C:245:ARG:HH22	3:C:391:LEU:HD11	1.27	0.96
3:C:189:ASN:ND2	3:C:389:ARG:HH21	1.62	0.96
2:B:371:ASN:HD21	2:B:374:LEU:HB2	1.31	0.94
1:D:168:LYS:CD	1:D:169:GLU:H	1.81	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:MET:SD	2:B:426:ARG:HG2	2.08	0.93
3:C:390:ASP:CG	3:C:391:LEU:H	1.68	0.93
1:D:108:LEU:HD11	3:F:88:ILE:HB	1.51	0.92
1:A:176:LYS:HE3	1:A:176:LYS:HA	1.52	0.92
1:D:168:LYS:HD2	1:D:169:GLU:N	1.82	0.92
3:C:336:ARG:HH11	4:G:2:HIS:CE1	1.88	0.91
3:F:302:TYR:HB3	3:F:336:ARG:HB3	1.52	0.90
1:D:101:TYR:HA	1:D:104:VAL:HG22	1.51	0.90
3:C:398:GLN:HG2	3:C:399:GLN:H	1.33	0.89
3:C:302:TYR:HB3	3:C:336:ARG:HB3	1.54	0.88
2:E:387:MET:SD	2:E:426:ARG:HG2	2.13	0.87
2:E:393:MET:SD	2:E:425:ASN:HB2	2.16	0.85
2:E:293:GLU:HB2	2:E:315:GLY:H	1.40	0.85
3:C:203:ASN:HD22	5:C:480:NAG:C1	1.83	0.85
1:D:115:LEU:HD21	3:F:96:GLU:HG2	1.58	0.85
2:E:197:ARG:NH1	2:E:197:ARG:HB3	1.91	0.85
1:A:112:ILE:HD12	2:B:167:ILE:HG22	1.58	0.85
2:B:393:MET:SD	2:B:425:ASN:HB2	2.17	0.84
1:D:188:ARG:NH1	1:D:188:ARG:HB3	1.92	0.84
1:A:109:GLU:HG2	2:B:167:ILE:HD12	1.59	0.83
3:C:305:HIS:HE1	3:C:339:ALA:H	1.26	0.83
3:C:357:VAL:HG12	3:C:358:GLU:H	1.45	0.82
2:B:263:MET:HE2	2:B:269:GLY:H	1.45	0.82
2:B:270:TRP:HB3	2:B:473:LYS:HB3	1.62	0.81
3:F:305:HIS:HE1	3:F:339:ALA:H	1.27	0.81
3:F:357:VAL:HG12	3:F:358:GLU:H	1.45	0.80
3:C:245:ARG:NH2	3:C:391:LEU:HD11	1.97	0.80
2:B:293:GLU:HB2	2:B:315:GLY:H	1.46	0.80
2:E:270:TRP:HB3	2:E:473:LYS:HB3	1.62	0.80
2:B:377:ALA:HA	2:B:459:ASN:HD21	1.47	0.80
2:E:263:MET:HE2	2:E:269:GLY:H	1.46	0.79
2:E:377:ALA:HA	2:E:459:ASN:HD21	1.46	0.79
3:C:86:GLN:HA	3:C:89:LEU:HG	1.64	0.79
3:C:305:HIS:CE1	3:C:339:ALA:H	2.00	0.79
1:A:186:PHE:CE2	2:B:177:ARG:HG3	2.18	0.79
1:D:139:GLN:O	1:D:143:VAL:HG23	1.83	0.79
2:B:292:ALA:O	2:B:293:GLU:HB3	1.83	0.78
2:E:381:MET:HB2	5:E:480:NAG:H81	1.61	0.78
1:A:120:ASN:HA	1:A:123:LEU:HD12	1.66	0.78
2:E:208:LYS:HE2	3:F:126:GLN:OE1	1.84	0.78
2:E:371:ASN:HD22	2:E:375:GLU:HG3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:PHE:HD2	2:E:177:ARG:HD2	1.49	0.78
3:F:305:HIS:CE1	3:F:339:ALA:H	2.02	0.77
1:A:118:ARG:NH1	3:C:96:GLU:HB3	2.00	0.77
1:A:120:ASN:HD21	1:A:188:ARG:H	1.31	0.77
3:C:397:GLN:HB3	3:F:397:GLN:O	1.84	0.77
3:F:150:THR:HG23	3:F:169:TYR:O	1.85	0.77
2:E:220:VAL:HG23	3:F:140:ASP:HA	1.66	0.77
2:B:381:MET:HB2	5:B:480:NAG:H81	1.62	0.77
1:A:118:ARG:HH12	3:C:96:GLU:HB3	1.49	0.77
1:D:176:LYS:O	1:D:180:TYR:HB2	1.84	0.77
3:F:209:VAL:HG12	3:F:212:ARG:HH12	1.49	0.76
2:E:292:ALA:O	2:E:293:GLU:HB3	1.84	0.75
3:C:300:LYS:O	3:C:304:THR:HG22	1.85	0.75
3:C:150:THR:HG22	3:C:151:GLY:N	2.01	0.75
2:B:371:ASN:HD22	2:B:375:GLU:HG3	1.50	0.75
1:D:108:LEU:O	1:D:112:ILE:HG12	1.87	0.75
2:E:435:ARG:N	2:E:454:GLY:HA2	2.03	0.74
2:B:177:ARG:O	2:B:182:VAL:HG23	1.87	0.74
2:B:344:ALA:HB2	2:B:369:ALA:HB3	1.70	0.74
2:E:344:ALA:HB2	2:E:369:ALA:HB3	1.69	0.74
1:A:133:ILE:O	1:A:137:VAL:HG23	1.86	0.74
2:E:171:TYR:HA	2:E:174:VAL:HG12	1.68	0.74
2:E:293:GLU:HB2	2:E:315:GLY:N	2.02	0.73
2:B:166:GLU:O	2:B:169:ASN:HB3	1.87	0.73
3:C:150:THR:HG23	3:C:169:TYR:O	1.88	0.73
3:C:268:GLU:HA	3:C:271:GLU:O	1.89	0.73
1:A:177:ALA:O	1:A:181:ILE:HG23	1.88	0.73
3:F:268:GLU:HA	3:F:271:GLU:O	1.88	0.73
2:B:285:ARG:NH1	2:B:289:THR:HG21	2.04	0.73
1:A:109:GLU:CG	2:B:167:ILE:HD12	2.18	0.73
2:B:170:ARG:HA	2:B:173:GLU:CD	2.10	0.72
3:C:390:ASP:CG	3:C:391:LEU:N	2.43	0.72
2:B:393:MET:HG3	2:B:425:ASN:HB2	1.72	0.72
1:A:192:VAL:HG12	1:A:193:VAL:H	1.53	0.72
3:C:111:GLU:O	3:C:115:VAL:HG23	1.89	0.72
2:B:168:GLU:O	2:B:172:LYS:HE2	1.89	0.72
2:E:285:ARG:NH1	2:E:289:THR:HG21	2.05	0.72
1:A:181:ILE:O	1:A:183:ASN:N	2.21	0.72
3:C:84:THR:O	3:C:88:ILE:HD13	1.90	0.72
2:B:293:GLU:HB2	2:B:315:GLY:N	2.06	0.71
2:E:393:MET:HG3	2:E:425:ASN:HB2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLN:HE22	1:A:182:ALA:HA	1.56	0.71
3:F:300:LYS:O	3:F:304:THR:HG22	1.91	0.71
2:E:405:TRP:CD2	2:E:412:LYS:HB3	2.25	0.71
3:F:354:LYS:HE2	3:F:374:TRP:CZ2	2.26	0.70
3:C:209:VAL:HG12	3:C:212:ARG:HH12	1.55	0.70
3:C:90:GLU:OE2	3:C:93:ARG:HD3	1.91	0.70
3:C:354:LYS:HE2	3:C:374:TRP:CZ2	2.27	0.70
3:F:150:THR:HG22	3:F:151:GLY:N	2.02	0.69
1:A:188:ARG:HH12	2:B:174:VAL:HG22	1.56	0.69
1:D:108:LEU:HD21	3:F:88:ILE:HG22	1.74	0.69
2:B:435:ARG:N	2:B:454:GLY:HA2	2.07	0.69
3:C:336:ARG:HG2	4:G:2:HIS:CE1	2.27	0.69
2:E:211:LYS:NZ	3:F:133:THR:HG21	2.07	0.69
2:E:393:MET:CG	2:E:425:ASN:HB2	2.23	0.69
2:B:185:SER:O	2:B:189:MET:HG3	1.93	0.69
2:E:177:ARG:HB2	2:E:177:ARG:NH1	2.08	0.69
2:B:443:THR:OG1	2:B:446:GLN:HG3	1.92	0.68
1:D:120:ASN:HD21	1:D:188:ARG:HG2	1.58	0.68
1:D:188:ARG:HH11	1:D:188:ARG:HB3	1.58	0.68
2:B:170:ARG:HA	2:B:173:GLU:OE1	1.93	0.68
3:F:399:GLN:C	3:F:401:LYS:H	1.97	0.68
2:E:443:THR:OG1	2:E:446:GLN:HG3	1.93	0.68
1:A:187:GLU:O	1:A:188:ARG:HD3	1.94	0.68
1:A:187:GLU:C	1:A:188:ARG:HD3	2.14	0.68
3:F:109:LEU:HD23	3:F:112:MET:CE	2.24	0.68
3:F:94:ILE:O	3:F:97:GLN:HG2	1.94	0.67
2:E:293:GLU:HG3	2:E:314:LEU:HA	1.76	0.67
1:D:132:ASN:HB3	3:F:113:TRP:CE2	2.30	0.67
2:B:393:MET:CG	2:B:425:ASN:HB2	2.25	0.67
1:D:113:ILE:O	1:D:117:ARG:HG3	1.94	0.67
1:D:119:ILE:HD11	2:E:178:ILE:HG12	1.76	0.67
2:E:270:TRP:CE2	2:E:331:LEU:HD23	2.30	0.67
2:B:238:ASN:CB	3:C:213:GLU:HG3	2.25	0.67
1:D:162:LEU:O	1:D:163:GLU:HB2	1.94	0.67
3:F:362:ASP:OD2	4:H:1:GLY:HA2	1.94	0.67
2:E:371:ASN:ND2	2:E:374:LEU:HB2	2.06	0.66
1:D:136:GLN:HG3	3:F:113:TRP:HE1	1.59	0.66
2:B:416:ARG:HH11	2:B:416:ARG:HG2	1.60	0.66
1:D:169:GLU:C	1:D:171:ASN:H	1.96	0.66
2:B:173:GLU:O	2:B:176:ILE:HG12	1.95	0.66
3:C:391:LEU:O	3:C:392:SER:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:295:ASP:HB2	4:H:2:HIS:NE2	2.10	0.66
3:F:203:ASN:HD22	5:F:480:NAG:C1	2.00	0.66
2:B:270:TRP:CE2	2:B:331:LEU:HD23	2.31	0.66
2:B:405:TRP:CD2	2:B:412:LYS:HB3	2.30	0.66
2:E:323:THR:OG1	2:E:351:PRO:HD2	1.96	0.66
3:C:194:ILE:HG23	3:C:233:ILE:HD11	1.78	0.65
2:B:293:GLU:HG3	2:B:314:LEU:HA	1.78	0.65
2:B:371:ASN:ND2	2:B:374:LEU:HB2	2.09	0.65
4:J:3:ARG:HD3	4:J:4:PRO:HD2	1.77	0.65
1:A:120:ASN:HD21	1:A:188:ARG:N	1.95	0.65
2:B:292:ALA:O	2:B:293:GLU:CB	2.45	0.65
2:E:231:HIS:HD2	2:E:233:GLU:H	1.44	0.65
2:E:377:ALA:HA	2:E:459:ASN:ND2	2.11	0.65
2:B:377:ALA:HA	2:B:459:ASN:ND2	2.12	0.65
3:F:373:ARG:HD2	3:F:374:TRP:CZ3	2.32	0.64
1:A:108:LEU:O	1:A:112:ILE:HG13	1.95	0.64
3:C:358:GLU:HA	3:C:358:GLU:OE1	1.96	0.64
3:C:194:ILE:HD12	3:C:233:ILE:HG12	1.80	0.64
2:E:231:HIS:CD2	2:E:233:GLU:H	2.15	0.64
2:B:175:LYS:O	2:B:179:GLU:HG3	1.97	0.64
3:C:270:ASP:O	3:C:271:GLU:HB2	1.98	0.64
2:B:238:ASN:HB3	3:C:213:GLU:HG3	1.80	0.64
1:A:137:VAL:O	1:A:141:LEU:HG	1.97	0.64
1:A:147:ILE:HG23	2:B:207:ILE:HD11	1.80	0.64
3:F:270:ASP:O	3:F:271:GLU:HB2	1.97	0.64
2:E:405:TRP:CE2	4:J:3:ARG:HG2	2.33	0.64
4:H:2:HIS:H	4:H:2:HIS:HD1	1.46	0.64
2:B:323:THR:OG1	2:B:351:PRO:HD2	1.95	0.64
1:D:172:LEU:HD12	1:D:175:GLU:OE1	1.98	0.63
2:B:231:HIS:HD2	2:B:233:GLU:H	1.44	0.63
2:B:231:HIS:CD2	2:B:233:GLU:H	2.16	0.63
3:F:358:GLU:HA	3:F:358:GLU:OE1	1.96	0.63
3:C:173:LEU:N	3:C:239:GLN:HE21	1.96	0.63
2:E:416:ARG:HH11	2:E:416:ARG:HG2	1.63	0.63
1:D:120:ASN:ND2	1:D:188:ARG:HG2	2.13	0.63
3:C:189:ASN:HD22	3:C:389:ARG:HH21	1.43	0.63
3:C:216:GLY:HA3	3:C:226:PHE:HA	1.81	0.63
3:F:335:ASN:C	3:F:337:CYS:H	2.01	0.62
2:E:177:ARG:HB2	2:E:177:ARG:HH11	1.64	0.62
3:C:373:ARG:HD2	3:C:374:TRP:CZ3	2.34	0.62
3:C:150:THR:CG2	3:C:151:GLY:H	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:GLU:HG3	2:B:172:LYS:HD3	1.81	0.62
2:E:287:TRP:HA	2:E:397:THR:HG21	1.82	0.62
1:A:109:GLU:HG2	2:B:167:ILE:HG23	1.79	0.62
1:D:115:LEU:CD2	3:F:96:GLU:HG2	2.29	0.62
2:E:197:ARG:HH11	2:E:197:ARG:HB3	1.60	0.62
2:E:280:SER:OG	2:E:311:GLU:HG3	2.00	0.62
3:F:216:GLY:HA3	3:F:226:PHE:HA	1.81	0.62
1:D:149:VAL:HA	1:D:152:ARG:NH1	2.14	0.62
3:F:248:LEU:HD12	3:F:377:LEU:HD13	1.80	0.62
1:D:144:GLU:HB2	2:E:203:MET:HE1	1.82	0.62
3:C:101:SER:O	3:C:105:GLN:HG3	2.00	0.62
2:E:348:SER:HB3	2:E:363:GLU:HB2	1.80	0.62
3:C:130:ILE:HA	3:C:133:THR:HG23	1.82	0.62
2:B:170:ARG:O	2:B:174:VAL:HG23	2.00	0.62
1:D:129:LEU:O	1:D:133:ILE:HG13	2.00	0.61
1:D:184:LEU:O	1:D:186:PHE:N	2.34	0.61
2:E:319:VAL:O	2:E:323:THR:HG23	2.01	0.61
1:D:127:THR:HG21	1:D:185:LYS:HE3	1.81	0.61
4:J:3:ARG:NH1	4:J:3:ARG:HB2	2.15	0.61
1:D:101:TYR:CZ	1:D:105:LEU:HD22	2.35	0.61
4:J:3:ARG:CD	4:J:4:PRO:HD2	2.30	0.61
1:A:167:ASP:OD1	1:A:168:LYS:HD2	2.00	0.61
2:B:348:SER:HB3	2:B:363:GLU:HB2	1.81	0.61
3:F:171:LYS:HB2	3:F:178:PRO:HB3	1.80	0.61
1:D:177:ALA:O	1:D:179:SER:N	2.32	0.61
3:C:136:ARG:HH22	3:C:139:GLN:HG2	1.66	0.61
3:C:248:LEU:HD12	3:C:377:LEU:HD13	1.83	0.61
1:D:101:TYR:HE1	3:F:85:VAL:HG11	1.64	0.61
1:A:113:ILE:HD11	2:B:170:ARG:NH1	2.14	0.61
2:E:405:TRP:CZ2	4:J:3:ARG:HG2	2.36	0.61
3:C:102:HIS:O	3:C:106:ILE:HG13	2.01	0.61
2:E:292:ALA:O	2:E:293:GLU:CB	2.48	0.61
3:F:194:ILE:HD12	3:F:233:ILE:HG12	1.83	0.61
3:F:359:PHE:N	3:F:360:PRO:HD3	2.16	0.61
3:C:320:TYR:HE1	3:C:327:GLN:NE2	1.99	0.60
3:C:116:ASN:O	3:C:120:VAL:HG23	2.00	0.60
2:B:231:HIS:CE1	2:B:476:PRO:HD3	2.36	0.60
2:E:171:TYR:HA	2:E:174:VAL:CG1	2.30	0.60
3:C:172:PRO:HA	3:C:239:GLN:NE2	2.16	0.60
3:F:102:HIS:O	3:F:106:ILE:HG13	2.02	0.60
1:D:172:LEU:O	1:D:176:LYS:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HB3	2:B:213:LEU:HB3	1.83	0.60
1:A:137:VAL:HG11	1:A:175:GLU:HG3	1.83	0.60
2:E:187:ARG:HA	2:E:187:ARG:NE	2.17	0.60
3:F:271:GLU:HG3	3:F:309:LEU:HD23	1.84	0.60
3:C:285:GLY:HA3	3:C:369:THR:HB	1.84	0.60
3:C:359:PHE:N	3:C:360:PRO:HD3	2.17	0.60
2:E:353:ASN:ND2	2:E:355:ALA:HB3	2.17	0.60
3:F:122:ARG:HB2	3:F:122:ARG:NH1	2.17	0.59
2:B:167:ILE:N	2:B:167:ILE:HD13	2.16	0.59
2:E:232:CYS:SG	2:E:271:THR:HA	2.42	0.59
3:F:196:HIS:CE1	3:F:198:HIS:HB2	2.37	0.59
3:C:335:ASN:C	3:C:337:CYS:H	2.04	0.59
2:B:287:TRP:HA	2:B:397:THR:HG21	1.84	0.59
3:F:302:TYR:CD1	3:F:336:ARG:HB2	2.36	0.59
2:E:476:PRO:HG2	2:E:477:LYS:H	1.68	0.59
3:C:302:TYR:CD1	3:C:336:ARG:HB2	2.37	0.59
3:F:194:ILE:HG23	3:F:233:ILE:HD11	1.83	0.59
3:C:189:ASN:HD21	3:C:389:ARG:HH21	1.45	0.59
3:F:127:LEU:O	3:F:130:ILE:HG22	2.03	0.59
3:C:271:GLU:HG3	3:C:309:LEU:HD23	1.85	0.59
2:B:252:LEU:HD22	2:B:252:LEU:H	1.68	0.59
3:F:285:GLY:HA3	3:F:369:THR:HB	1.84	0.59
1:D:114:HIS:O	1:D:117:ARG:HG3	2.03	0.59
2:B:252:LEU:HD22	2:B:252:LEU:N	2.18	0.58
2:B:263:MET:CE	2:B:269:GLY:H	2.16	0.58
1:A:139:GLN:OE1	3:C:120:VAL:HG11	2.03	0.58
2:B:476:PRO:HG2	2:B:477:LYS:H	1.66	0.58
2:B:224:VAL:HG13	3:C:218:LEU:HB2	1.85	0.58
2:E:381:MET:CB	5:E:480:NAG:H82	2.23	0.58
1:A:130:GLN:HE22	1:A:182:ALA:CA	2.16	0.58
2:B:351:PRO:HA	2:B:359:ARG:O	2.04	0.58
2:E:252:LEU:HD22	2:E:252:LEU:H	1.68	0.58
2:E:323:THR:HG21	2:E:351:PRO:HD3	1.86	0.58
2:E:231:HIS:CD2	2:E:232:CYS:N	2.72	0.58
2:B:319:VAL:O	2:B:323:THR:HG23	2.04	0.58
2:B:413:HIS:ND1	2:B:416:ARG:HG3	2.19	0.58
2:B:232:CYS:SG	2:B:271:THR:HA	2.44	0.58
3:F:125:GLN:O	3:F:128:VAL:HG22	2.04	0.58
2:E:351:PRO:HA	2:E:359:ARG:O	2.04	0.58
3:F:320:TYR:HE1	3:F:327:GLN:NE2	2.02	0.58
2:E:342:VAL:HB	2:E:368:ASN:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:THR:HG21	2:B:351:PRO:HD3	1.85	0.57
2:E:413:HIS:CG	2:E:416:ARG:HG3	2.39	0.57
1:A:159:ALA:HB2	2:B:216:ALA:HB3	1.85	0.57
1:D:175:GLU:O	1:D:179:SER:HB3	2.03	0.57
2:B:231:HIS:CD2	2:B:232:CYS:N	2.72	0.57
3:F:195:GLN:HE22	3:F:380:THR:HG21	1.69	0.57
2:E:194:GLU:HA	2:E:197:ARG:HH12	1.69	0.57
2:E:413:HIS:ND1	2:E:416:ARG:HG3	2.19	0.57
2:E:231:HIS:CE1	2:E:476:PRO:HD3	2.39	0.57
2:E:365:TYR:CG	2:E:366:SER:N	2.73	0.57
3:C:127:LEU:O	3:C:130:ILE:HG22	2.04	0.57
1:A:150:ALA:HB1	3:C:131:ARG:HG2	1.86	0.57
3:C:195:GLN:HE22	3:C:380:THR:HG21	1.70	0.57
3:F:208:TRP:HA	3:F:312:THR:HG21	1.86	0.57
3:C:208:TRP:HA	3:C:312:THR:HG21	1.86	0.57
1:D:109:GLU:O	1:D:113:ILE:HD13	2.04	0.57
2:E:387:MET:HB2	2:E:426:ARG:HB3	1.86	0.57
2:E:252:LEU:N	2:E:252:LEU:HD22	2.20	0.57
2:E:273:VAL:HG21	2:E:474:LEU:HD22	1.87	0.56
3:C:171:LYS:HB2	3:C:178:PRO:HB3	1.85	0.56
3:C:401:LYS:HG3	3:F:397:GLN:OE1	2.05	0.56
3:F:311:SER:OG	3:F:317:ASN:HB2	2.04	0.56
3:C:196:HIS:CE1	3:C:198:HIS:HB2	2.40	0.56
1:D:108:LEU:HD21	3:F:88:ILE:CG2	2.35	0.56
1:D:101:TYR:OH	1:D:105:LEU:HD22	2.06	0.56
2:E:199:LYS:HG2	2:E:203:MET:HE3	1.87	0.56
3:F:285:GLY:HA3	3:F:369:THR:CB	2.36	0.56
3:F:203:ASN:CG	5:F:480:NAG:C1	2.65	0.56
2:B:413:HIS:CG	2:B:416:ARG:HG3	2.41	0.56
2:E:329:GLN:HE21	2:E:477:LYS:HA	1.71	0.56
3:C:311:SER:OG	3:C:317:ASN:HB2	2.05	0.56
1:A:142:ARG:NH1	2:B:445:GLU:O	2.38	0.56
2:B:281:SER:HB2	2:B:311:GLU:HB2	1.88	0.56
2:B:387:MET:SD	2:B:426:ARG:CG	2.91	0.56
1:D:188:ARG:HH11	1:D:188:ARG:CB	2.18	0.56
2:B:262:ASP:OD2	2:B:473:LYS:NZ	2.39	0.56
2:B:330:VAL:HG22	2:B:331:LEU:N	2.21	0.56
1:D:109:GLU:O	1:D:112:ILE:HB	2.06	0.56
2:B:459:ASN:N	2:B:459:ASN:HD22	2.04	0.56
2:E:237:ARG:HG3	2:E:237:ARG:HH11	1.70	0.56
2:E:455:VAL:O	2:E:466:SER:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ASN:HA	2:B:172:LYS:CE	2.36	0.56
2:B:226:VAL:HG21	3:C:226:PHE:HB2	1.88	0.56
2:B:280:SER:OG	2:B:311:GLU:HG3	2.06	0.56
3:F:173:LEU:N	3:F:239:GLN:HE21	2.04	0.56
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.71	0.56
1:D:169:GLU:C	1:D:171:ASN:N	2.60	0.56
1:D:147:ILE:O	1:D:151:LEU:HD23	2.05	0.56
3:C:98:ILE:O	3:C:101:SER:HB3	2.07	0.56
2:E:441:ILE:H	2:E:441:ILE:HD12	1.69	0.55
2:B:371:ASN:O	2:B:375:GLU:HB2	2.06	0.55
1:D:113:ILE:HA	1:D:116:GLN:OE1	2.06	0.55
2:B:194:GLU:HB3	2:B:197:ARG:HH21	1.70	0.55
3:F:209:VAL:HA	3:F:212:ARG:NH1	2.22	0.55
2:E:387:MET:HB2	2:E:426:ARG:HG2	1.89	0.55
3:F:117:GLN:O	3:F:120:VAL:HG12	2.06	0.55
2:E:371:ASN:HD22	2:E:375:GLU:CG	2.18	0.55
3:C:302:TYR:HB3	3:C:336:ARG:CB	2.33	0.55
2:E:185:SER:O	2:E:189:MET:HG3	2.07	0.55
1:D:118:ARG:O	1:D:122:GLN:HG2	2.07	0.55
2:B:428:HIS:O	4:I:1:GLY:HA2	2.07	0.55
4:G:2:HIS:CG	4:G:4:PRO:HD3	2.42	0.55
2:B:454:GLY:O	2:B:456:VAL:HG23	2.07	0.55
2:B:273:VAL:HG21	2:B:474:LEU:HD22	1.87	0.55
1:D:167:ASP:OD1	1:D:168:LYS:HG3	2.07	0.55
1:A:143:VAL:O	1:A:147:ILE:HG13	2.06	0.55
2:B:169:ASN:HA	2:B:172:LYS:NZ	2.21	0.55
2:B:329:GLN:HE21	2:B:477:LYS:HA	1.72	0.55
2:E:293:GLU:CG	2:E:314:LEU:HA	2.36	0.55
3:F:124:GLN:O	3:F:127:LEU:HB3	2.06	0.55
2:E:435:ARG:HD3	2:E:453:ASP:CG	2.27	0.55
3:F:94:ILE:HD13	3:F:97:GLN:OE1	2.06	0.55
3:F:362:ASP:OD2	4:H:1:GLY:CA	2.55	0.55
2:E:353:ASN:HD21	2:E:355:ALA:HB3	1.72	0.55
2:E:182:VAL:O	2:E:186:LEU:HG	2.07	0.55
2:B:371:ASN:HD22	2:B:375:GLU:CG	2.19	0.55
2:B:263:MET:HE2	2:B:263:MET:HA	1.88	0.55
2:B:171:TYR:OH	3:C:91:GLU:OE2	2.24	0.55
1:D:136:GLN:HG3	3:F:113:TRP:NE1	2.21	0.55
1:D:170:LYS:O	1:D:174:LEU:HG	2.06	0.55
1:D:107:GLU:OE2	1:D:107:GLU:HA	2.07	0.55
3:C:94:ILE:O	3:C:97:GLN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:HG12	1:A:193:VAL:N	2.22	0.54
3:F:172:PRO:HA	3:F:239:GLN:NE2	2.21	0.54
3:F:179:PHE:CD2	3:F:232:LYS:HD3	2.42	0.54
2:B:251:ASP:OD2	2:B:253:PHE:HE1	1.91	0.54
2:E:168:GLU:O	2:E:172:LYS:N	2.38	0.54
2:B:365:TYR:CG	2:B:366:SER:N	2.75	0.54
2:B:387:MET:HB2	2:B:426:ARG:HB3	1.89	0.54
2:E:209:THR:O	2:E:212:GLU:HB3	2.07	0.54
1:D:186:PHE:CD2	2:E:177:ARG:HD2	2.36	0.54
1:A:147:ILE:O	1:A:151:LEU:HB2	2.07	0.54
2:B:194:GLU:O	2:B:197:ARG:HB3	2.08	0.54
2:E:251:ASP:HB3	2:E:253:PHE:CD1	2.43	0.54
2:E:425:ASN:C	2:E:427:CYS:N	2.57	0.54
1:D:178:ALA:HB2	2:E:192:VAL:HG21	1.89	0.54
2:B:251:ASP:HB3	2:B:253:PHE:CD1	2.42	0.54
2:B:317:LYS:HZ3	2:B:321:GLN:HG2	1.73	0.54
2:E:220:VAL:CG2	3:F:140:ASP:HA	2.37	0.54
1:D:158:CYS:O	2:E:218:CYS:HB3	2.08	0.54
2:E:195:HIS:O	2:E:198:ALA:HB3	2.07	0.54
4:G:3:ARG:O	4:G:4:PRO:C	2.45	0.54
1:A:119:ILE:CD1	2:B:174:VAL:HG13	2.38	0.54
1:A:120:ASN:ND2	1:A:188:ARG:H	2.02	0.54
2:B:167:ILE:H	2:B:167:ILE:HD13	1.73	0.54
2:E:204:GLU:HG3	3:F:126:GLN:HE22	1.73	0.54
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.71	0.54
3:C:173:LEU:N	3:C:239:GLN:NE2	2.56	0.54
1:A:190:GLU:HB3	2:B:170:ARG:NH1	2.23	0.53
3:F:373:ARG:HG3	3:F:374:TRP:CE3	2.44	0.53
2:B:387:MET:HB2	2:B:426:ARG:HG2	1.89	0.53
2:E:191:SER:HA	2:E:194:GLU:OE1	2.08	0.53
2:B:176:ILE:HG13	2:B:177:ARG:N	2.23	0.53
3:C:285:GLY:HA3	3:C:369:THR:CB	2.38	0.53
3:F:302:TYR:HB3	3:F:336:ARG:CB	2.32	0.53
1:A:123:LEU:HB3	1:A:184:LEU:O	2.08	0.53
1:A:181:ILE:C	1:A:183:ASN:H	2.11	0.53
1:A:169:GLU:OE1	1:A:169:GLU:C	2.46	0.53
3:C:209:VAL:HA	3:C:212:ARG:NH1	2.24	0.53
2:E:231:HIS:HD2	2:E:232:CYS:N	2.05	0.53
3:C:154:CYS:SG	3:C:192:THR:HB	2.49	0.53
1:D:130:GLN:NE2	1:D:179:SER:O	2.40	0.53
1:D:179:SER:O	1:D:181:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:HIS:HD2	2:B:232:CYS:N	2.05	0.53
2:E:168:GLU:C	2:E:170:ARG:H	2.11	0.53
1:A:145:VAL:O	1:A:149:VAL:HG23	2.09	0.53
2:B:205:GLU:HA	2:B:208:LYS:CB	2.27	0.53
2:E:274:GLN:HE21	2:E:274:GLN:C	2.12	0.53
2:E:414:CYS:SG	2:E:427:CYS:N	2.80	0.53
3:F:359:PHE:O	3:F:361:TYR:N	2.33	0.53
2:B:353:ASN:ND2	2:B:355:ALA:HB3	2.24	0.53
1:D:119:ILE:O	1:D:122:GLN:N	2.42	0.53
1:A:166:LEU:N	1:A:166:LEU:HD23	2.23	0.53
2:E:444:LYS:HB2	2:E:444:LYS:NZ	2.24	0.53
2:E:387:MET:HB2	2:E:426:ARG:CB	2.39	0.52
2:B:435:ARG:HD3	2:B:453:ASP:CG	2.28	0.52
2:E:281:SER:HB2	2:E:311:GLU:HB2	1.91	0.52
2:B:342:VAL:HB	2:B:368:ASN:OD1	2.08	0.52
2:E:371:ASN:O	2:E:375:GLU:HB2	2.10	0.52
2:B:441:ILE:H	2:B:441:ILE:HD12	1.74	0.52
2:E:197:ARG:CZ	2:E:197:ARG:HB3	2.40	0.52
2:B:263:MET:HE1	2:B:269:GLY:HA2	1.91	0.52
2:E:262:ASP:OD2	2:E:473:LYS:NZ	2.42	0.52
2:E:330:VAL:HG22	2:E:331:LEU:N	2.23	0.52
3:F:154:CYS:SG	3:F:192:THR:HB	2.49	0.52
2:E:194:GLU:HA	2:E:197:ARG:NH1	2.24	0.52
3:C:173:LEU:H	3:C:239:GLN:HE21	1.56	0.52
3:C:357:VAL:HG12	3:C:358:GLU:N	2.22	0.52
2:E:177:ARG:HE	2:E:181:THR:CB	2.21	0.52
3:C:194:ILE:HG23	3:C:233:ILE:CD1	2.40	0.52
1:D:101:TYR:C	1:D:103:GLU:H	2.13	0.52
3:F:246:ILE:HG22	3:F:248:LEU:CD2	2.40	0.52
2:B:365:TYR:HB2	2:B:371:ASN:OD1	2.10	0.52
2:B:293:GLU:CG	2:B:314:LEU:HA	2.39	0.52
2:E:251:ASP:OD2	2:E:253:PHE:HE1	1.93	0.52
2:B:301:ASN:HD21	2:B:305:ILE:HD11	1.74	0.52
3:C:336:ARG:NH1	4:G:2:HIS:CE1	2.69	0.51
3:F:90:GLU:O	3:F:94:ILE:HG12	2.09	0.51
2:E:202:ARG:O	2:E:205:GLU:HG2	2.09	0.51
1:D:119:ILE:HA	1:D:122:GLN:HG2	1.92	0.51
3:C:372:ASP:H	3:F:294:GLY:HA3	1.75	0.51
3:C:391:LEU:HD13	3:C:392:SER:N	2.26	0.51
3:F:368:ALA:HA	3:F:371:HIS:O	2.10	0.51
3:C:86:GLN:HA	3:C:89:LEU:CG	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:399:GLN:HG2	3:F:400:SER:N	2.26	0.51
1:D:119:ILE:HA	1:D:122:GLN:CG	2.40	0.51
2:B:416:ARG:NH1	2:B:416:ARG:HG2	2.24	0.51
3:C:191:TRP:CE3	3:C:385:LEU:HB2	2.45	0.51
2:E:211:LYS:HZ2	3:F:133:THR:HG21	1.74	0.51
3:C:373:ARG:HG3	3:C:374:TRP:CE3	2.45	0.51
2:B:425:ASN:C	2:B:427:CYS:N	2.59	0.51
3:C:320:TYR:CZ	4:G:3:ARG:HG2	2.46	0.51
3:F:194:ILE:HG23	3:F:233:ILE:CD1	2.41	0.51
2:B:184:GLY:HA2	2:B:187:ARG:NH2	2.26	0.51
1:A:172:LEU:O	1:A:176:LYS:HB2	2.11	0.51
2:E:211:LYS:HZ3	3:F:133:THR:HG21	1.75	0.51
3:C:246:ILE:HG22	3:C:248:LEU:CD2	2.41	0.51
2:B:301:ASN:CG	2:B:305:ILE:HG13	2.31	0.51
2:B:387:MET:O	2:B:425:ASN:O	2.28	0.51
3:F:335:ASN:C	3:F:337:CYS:N	2.64	0.51
3:C:209:VAL:HG23	3:C:210:SER:N	2.26	0.51
3:F:117:GLN:NE2	3:F:120:VAL:HG11	2.25	0.51
2:B:317:LYS:NZ	2:B:321:GLN:OE1	2.44	0.51
1:D:101:TYR:HA	1:D:104:VAL:CG2	2.31	0.51
2:E:459:ASN:HD22	2:E:459:ASN:N	2.07	0.51
4:J:3:ARG:HH11	4:J:3:ARG:HB2	1.74	0.51
2:B:414:CYS:SG	2:B:427:CYS:N	2.84	0.50
3:C:361:TYR:CE2	4:G:3:ARG:HD3	2.46	0.50
1:D:161:TYR:HD1	2:E:210:GLN:NE2	2.09	0.50
3:C:335:ASN:C	3:C:337:CYS:N	2.64	0.50
1:D:101:TYR:CE1	3:F:85:VAL:HG11	2.44	0.50
1:A:186:PHE:HE2	2:B:177:ARG:HG3	1.71	0.50
3:C:124:GLN:O	3:C:124:GLN:OE1	2.28	0.50
2:B:444:LYS:NZ	2:B:444:LYS:HB2	2.26	0.50
1:A:119:ILE:HD12	2:B:174:VAL:HG13	1.94	0.50
3:C:289:ASP:O	3:C:300:LYS:HE3	2.12	0.50
2:E:454:GLY:O	2:E:456:VAL:HG23	2.11	0.50
2:E:297:ILE:HA	2:E:312:TYR:CD1	2.46	0.50
2:E:225:PRO:HG3	3:F:217:TYR:HE1	1.76	0.50
2:E:343:TYR:CD1	2:E:343:TYR:C	2.85	0.50
1:A:113:ILE:HD11	2:B:170:ARG:HH12	1.75	0.50
3:C:173:LEU:H	3:C:239:GLN:NE2	2.10	0.50
2:E:223:ARG:HG3	2:E:304:SER:OG	2.12	0.50
3:C:368:ALA:HA	3:C:371:HIS:O	2.12	0.50
1:D:108:LEU:HD11	3:F:88:ILE:CB	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ILE:C	1:D:183:ASN:H	2.14	0.50
1:A:138:SER:OG	1:A:139:GLN:N	2.43	0.50
3:F:289:ASP:O	3:F:300:LYS:HE3	2.12	0.50
3:C:179:PHE:CD2	3:C:232:LYS:HD3	2.47	0.50
2:E:390:HIS:HE1	2:E:428:HIS:HB2	1.77	0.50
3:F:150:THR:CG2	3:F:151:GLY:H	2.04	0.50
2:B:170:ARG:O	2:B:173:GLU:HG2	2.11	0.50
1:D:137:VAL:O	1:D:141:LEU:HB2	2.11	0.50
1:A:140:ILE:HD12	2:B:196:LEU:HD22	1.93	0.50
1:D:108:LEU:O	1:D:108:LEU:HD23	2.11	0.49
1:D:177:ALA:C	1:D:179:SER:N	2.66	0.49
3:C:338:HIS:CE1	4:G:1:GLY:N	2.80	0.49
2:B:262:ASP:C	2:B:263:MET:HE3	2.33	0.49
3:F:209:VAL:HG23	3:F:210:SER:N	2.27	0.49
3:F:327:GLN:OE1	3:F:361:TYR:CD2	2.65	0.49
1:D:102:SER:O	1:D:106:ARG:HD2	2.12	0.49
1:D:158:CYS:HB3	2:E:214:CYS:HA	1.92	0.49
3:F:197:ARG:NH1	3:F:343:ASN:HA	2.28	0.49
3:F:337:CYS:SG	4:H:3:ARG:NH1	2.85	0.49
2:B:225:PRO:HG3	3:C:217:TYR:HE1	1.77	0.49
2:B:352:GLU:O	2:B:358:TYR:HA	2.13	0.49
2:E:375:GLU:O	2:E:385:ARG:NH1	2.45	0.49
2:B:387:MET:HB2	2:B:426:ARG:CB	2.42	0.49
2:E:190:LYS:HG3	2:E:194:GLU:OE1	2.13	0.49
1:D:136:GLN:HE22	3:F:116:ASN:HB3	1.78	0.49
3:F:320:TYR:HE1	3:F:327:GLN:HE22	1.61	0.49
2:B:244:GLU:HG3	2:B:246:TYR:CE1	2.48	0.49
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.61	0.49
3:C:181:VAL:HG12	3:C:228:LEU:HD11	1.94	0.49
3:F:197:ARG:H	3:F:380:THR:HG22	1.77	0.49
3:C:398:GLN:HG2	3:C:399:GLN:N	2.15	0.49
1:A:180:TYR:C	1:A:182:ALA:H	2.16	0.49
2:B:454:GLY:O	2:B:456:VAL:N	2.46	0.49
2:E:221:ASN:CG	3:F:141:THR:HG1	2.13	0.49
2:E:217:PRO:CB	3:F:136:ARG:NH1	2.76	0.49
1:D:113:ILE:O	1:D:116:GLN:HB2	2.13	0.49
2:E:263:MET:HE2	2:E:263:MET:HA	1.93	0.49
1:D:143:VAL:O	1:D:147:ILE:HG13	2.12	0.49
1:A:141:LEU:O	1:A:144:GLU:N	2.46	0.49
2:E:320:HIS:HD2	2:E:351:PRO:O	1.95	0.49
1:D:125:GLN:O	1:D:129:LEU:HD13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:197:ARG:HG2	3:F:380:THR:HG22	1.94	0.49
1:D:109:GLU:O	1:D:113:ILE:CD1	2.60	0.49
1:D:161:TYR:HD1	2:E:210:GLN:HE22	1.59	0.49
3:F:181:VAL:HG12	3:F:228:LEU:HD11	1.94	0.49
3:C:249:THR:HA	3:C:254:THR:O	2.13	0.49
1:A:183:ASN:OD1	2:B:181:THR:HG21	2.13	0.48
1:D:177:ALA:C	1:D:179:SER:H	2.17	0.48
2:E:263:MET:CE	2:E:269:GLY:H	2.21	0.48
1:A:138:SER:O	1:A:141:LEU:N	2.45	0.48
2:E:476:PRO:O	2:E:477:LYS:HG2	2.13	0.48
3:F:191:TRP:CE3	3:F:385:LEU:HB2	2.49	0.48
2:E:317:LYS:NZ	2:E:321:GLN:OE1	2.46	0.48
3:F:197:ARG:HG2	3:F:380:THR:CG2	2.44	0.48
3:C:320:TYR:HE1	3:C:327:GLN:HE22	1.61	0.48
1:A:169:GLU:C	1:A:171:ASN:N	2.67	0.48
2:B:297:ILE:HA	2:B:312:TYR:CD1	2.49	0.48
1:D:189:PHE:CD1	1:D:189:PHE:N	2.82	0.48
2:B:320:HIS:HD2	2:B:351:PRO:O	1.96	0.48
2:B:390:HIS:CE1	2:B:428:HIS:HB2	2.49	0.48
3:C:359:PHE:O	3:C:361:TYR:N	2.33	0.48
1:D:162:LEU:H	2:E:210:GLN:HE22	1.60	0.48
1:D:158:CYS:O	1:D:159:ALA:O	2.31	0.48
2:E:276:ARG:NH2	2:E:434:GLY:O	2.33	0.48
1:D:169:GLU:HA	1:D:169:GLU:OE1	2.12	0.48
2:B:331:LEU:HD12	2:B:332:PHE:N	2.29	0.48
1:A:169:GLU:C	1:A:171:ASN:H	2.16	0.48
1:A:139:GLN:O	1:A:143:VAL:HG23	2.13	0.48
1:D:132:ASN:HB3	3:F:113:TRP:NE1	2.28	0.48
2:E:189:MET:O	2:E:190:LYS:C	2.52	0.48
2:B:331:LEU:C	2:B:331:LEU:HD12	2.34	0.48
3:C:197:ARG:H	3:C:380:THR:HG22	1.78	0.48
2:B:249:GLN:HG3	2:B:256:PRO:HG3	1.94	0.48
1:A:158:CYS:O	2:B:218:CYS:HB3	2.13	0.48
3:F:151:GLY:HA2	3:F:156:GLN:HE21	1.78	0.48
1:D:150:ALA:HB2	3:F:131:ARG:HD2	1.95	0.48
2:E:454:GLY:O	2:E:456:VAL:N	2.47	0.48
3:C:111:GLU:OE1	3:C:114:ARG:NH1	2.45	0.48
3:F:154:CYS:SG	3:F:192:THR:HA	2.54	0.48
2:E:390:HIS:CE1	2:E:428:HIS:HB2	2.48	0.48
3:C:327:GLN:OE1	3:C:361:TYR:CD2	2.66	0.48
2:B:262:ASP:HB3	2:B:270:TRP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASN:O	1:A:175:GLU:HB3	2.14	0.48
2:E:416:ARG:NH1	2:E:416:ARG:HG2	2.26	0.48
2:E:352:GLU:O	2:E:358:TYR:HA	2.14	0.48
1:A:108:LEU:HG	2:B:167:ILE:HG21	1.96	0.47
2:E:331:LEU:HD12	2:E:332:PHE:N	2.29	0.47
2:E:393:MET:HE2	2:E:424:TYR:O	2.15	0.47
3:F:327:GLN:HG2	3:F:359:PHE:CD2	2.48	0.47
3:F:119:PHE:O	3:F:122:ARG:N	2.47	0.47
2:B:223:ARG:HG3	2:B:304:SER:OG	2.13	0.47
2:B:383:ASP:O	2:B:387:MET:HG2	2.14	0.47
2:E:441:ILE:N	2:E:441:ILE:HD12	2.28	0.47
2:B:196:LEU:O	2:B:200:MET:HG3	2.14	0.47
2:E:325:GLN:HG2	2:E:326:HIS:CD2	2.48	0.47
2:B:476:PRO:O	2:B:477:LYS:HG2	2.15	0.47
3:C:197:ARG:HG2	3:C:380:THR:CG2	2.45	0.47
2:B:455:VAL:O	2:B:466:SER:HA	2.14	0.47
2:E:365:TYR:HB2	2:E:371:ASN:OD1	2.14	0.47
1:A:126:LEU:HB3	1:A:184:LEU:HD13	1.96	0.47
2:E:270:TRP:HB3	2:E:473:LYS:CB	2.41	0.47
1:D:147:ILE:HG12	3:F:127:LEU:HD13	1.96	0.47
3:F:397:GLN:HG3	3:F:398:GLN:H	1.79	0.47
1:A:157:SER:HB2	3:C:136:ARG:O	2.14	0.47
2:B:390:HIS:HE1	2:B:428:HIS:HB2	1.79	0.47
3:F:189:ASN:OD1	3:F:391:LEU:HD23	2.14	0.47
1:A:183:ASN:C	1:A:185:LYS:N	2.67	0.47
3:C:355:THR:O	3:C:356:ASP:HB2	2.14	0.47
2:E:359:ARG:HD3	2:E:361:TRP:CZ2	2.48	0.47
2:E:252:LEU:CD2	2:E:252:LEU:H	2.28	0.47
2:E:428:HIS:CD2	2:E:431:ASN:HB2	2.49	0.47
3:C:167:LEU:HB3	3:C:180:LEU:HD11	1.96	0.47
3:C:125:GLN:HE21	3:C:125:GLN:C	2.17	0.47
2:E:365:TYR:CD2	2:E:371:ASN:HB2	2.49	0.47
3:F:302:TYR:C	3:F:335:ASN:ND2	2.68	0.47
1:A:119:ILE:HA	1:A:122:GLN:OE1	2.15	0.47
1:A:116:GLN:O	1:A:119:ILE:N	2.48	0.47
3:C:301:PHE:O	3:C:304:THR:HG23	2.14	0.47
2:B:475:ARG:HG3	2:B:476:PRO:HD2	1.97	0.47
2:E:203:MET:O	2:E:206:ALA:HB3	2.15	0.47
2:B:252:LEU:CD2	2:B:252:LEU:H	2.27	0.47
3:C:154:CYS:SG	3:C:192:THR:HA	2.55	0.47
3:F:114:ARG:O	3:F:118:GLN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:114:ARG:O	3:F:115:VAL:C	2.53	0.47
2:B:325:GLN:HG2	2:B:326:HIS:CD2	2.49	0.47
3:C:196:HIS:HD2	3:C:381:THR:HB	1.80	0.47
3:C:305:HIS:CE1	3:C:340:GLY:H	2.33	0.47
3:C:110:SER:O	3:C:114:ARG:HB2	2.15	0.47
2:E:405:TRP:CG	2:E:412:LYS:HB3	2.50	0.47
2:B:190:LYS:HB2	3:C:109:LEU:HD21	1.96	0.47
2:E:422:TRP:CG	2:E:423:TRP:N	2.82	0.47
3:C:337:CYS:HB2	4:G:1:GLY:O	2.15	0.47
2:B:165:LYS:HA	2:B:168:GLU:HB3	1.96	0.47
3:F:312:THR:HG1	3:F:314:GLU:CD	2.17	0.47
2:B:422:TRP:CG	2:B:423:TRP:N	2.83	0.47
3:C:279:TYR:CB	3:C:286:ASN:ND2	2.78	0.47
3:C:354:LYS:O	3:C:355:THR:C	2.52	0.47
2:E:353:ASN:OD1	2:E:356:GLN:HG2	2.15	0.47
2:B:224:VAL:HA	2:B:225:PRO:HD3	1.82	0.47
4:I:2:HIS:ND1	4:I:2:HIS:N	2.63	0.47
2:B:371:ASN:ND2	2:B:375:GLU:HG3	2.26	0.46
2:B:169:ASN:HA	2:B:172:LYS:HE2	1.96	0.46
1:D:136:GLN:HE22	3:F:116:ASN:CB	2.28	0.46
1:D:162:LEU:HD23	2:E:213:LEU:CD1	2.46	0.46
3:C:197:ARG:NH1	3:C:343:ASN:HA	2.30	0.46
3:C:197:ARG:HG2	3:C:380:THR:HG22	1.96	0.46
1:D:174:LEU:O	1:D:178:ALA:N	2.44	0.46
2:B:199:LYS:O	2:B:203:MET:HE2	2.14	0.46
2:B:375:GLU:O	2:B:385:ARG:NH1	2.47	0.46
3:F:354:LYS:O	3:F:355:THR:C	2.53	0.46
2:B:301:ASN:OD1	2:B:305:ILE:HG13	2.15	0.46
2:E:301:ASN:HD21	2:E:305:ILE:HD11	1.79	0.46
2:E:408:GLY:O	2:E:410:PRO:HD3	2.15	0.46
2:E:176:ILE:O	2:E:180:SER:HB3	2.15	0.46
2:E:262:ASP:C	2:E:263:MET:HE3	2.35	0.46
3:F:399:GLN:O	3:F:401:LYS:N	2.46	0.46
3:F:122:ARG:HH11	3:F:122:ARG:HB2	1.79	0.46
2:E:192:VAL:O	2:E:196:LEU:HG	2.15	0.46
3:F:243:ARG:NH1	3:F:387:MET:CE	2.77	0.46
2:E:164:GLN:C	2:E:166:GLU:H	2.19	0.46
2:B:274:GLN:C	2:B:274:GLN:HE21	2.18	0.46
2:B:209:THR:HA	2:B:212:GLU:OE1	2.15	0.46
3:C:391:LEU:O	3:C:392:SER:CB	2.62	0.46
1:D:113:ILE:HG22	1:D:117:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:425:ASN:O	2:E:426:ARG:C	2.52	0.46
1:D:118:ARG:HG3	1:D:118:ARG:HH11	1.79	0.46
3:F:246:ILE:HG22	3:F:248:LEU:HD21	1.97	0.46
2:B:343:TYR:CD1	2:B:343:TYR:C	2.88	0.46
1:A:119:ILE:HD11	2:B:178:ILE:HD11	1.98	0.46
3:C:152:LYS:HG3	3:C:156:GLN:NE2	2.30	0.46
2:B:181:THR:O	2:B:181:THR:HG22	2.15	0.46
1:A:167:ASP:OD1	1:A:168:LYS:N	2.48	0.46
2:E:387:MET:O	2:E:425:ASN:O	2.34	0.46
2:E:174:VAL:O	2:E:178:ILE:HG13	2.16	0.46
3:F:173:LEU:N	3:F:239:GLN:NE2	2.63	0.46
2:E:301:ASN:CG	2:E:305:ILE:HG13	2.36	0.46
3:F:207:ASP:OD1	3:F:207:ASP:N	2.47	0.46
3:F:164:ASP:O	3:F:168:TYR:OH	2.27	0.46
1:A:113:ILE:CD1	2:B:170:ARG:NH1	2.79	0.46
2:E:331:LEU:HD12	2:E:331:LEU:C	2.35	0.46
3:F:130:ILE:CG2	3:F:131:ARG:N	2.79	0.46
2:E:435:ARG:H	2:E:454:GLY:HA2	1.78	0.46
1:D:162:LEU:H	2:E:210:GLN:NE2	2.13	0.46
1:D:164:TYR:O	1:D:165:ARG:HB3	2.15	0.46
3:C:189:ASN:HD22	3:C:389:ARG:NH2	2.12	0.46
2:B:353:ASN:HD21	2:B:355:ALA:HB3	1.80	0.46
3:F:287:ALA:HB3	3:F:367:TRP:CZ2	2.51	0.46
3:C:287:ALA:HB3	3:C:367:TRP:CZ2	2.51	0.46
2:E:458:MET:SD	4:J:1:GLY:HA2	2.56	0.46
1:D:113:ILE:O	1:D:117:ARG:CG	2.63	0.46
3:F:285:GLY:HA3	3:F:369:THR:OG1	2.15	0.46
3:C:208:TRP:HE3	3:C:312:THR:HG23	1.81	0.46
2:E:290:TYR:CE2	2:E:421:GLY:HA3	2.51	0.46
2:E:244:GLU:HG3	2:E:246:TYR:CE1	2.51	0.46
3:C:253:ASN:HD21	3:C:378:LYS:NZ	2.13	0.46
2:B:330:VAL:HG22	2:B:331:LEU:H	1.81	0.45
3:F:399:GLN:C	3:F:401:LYS:N	2.66	0.45
2:E:475:ARG:HG3	2:E:476:PRO:HD2	1.97	0.45
2:E:197:ARG:CB	2:E:197:ARG:HH11	2.28	0.45
3:C:209:VAL:CG2	3:C:210:SER:N	2.79	0.45
2:B:435:ARG:O	2:B:454:GLY:HA2	2.17	0.45
1:D:141:LEU:O	1:D:144:GLU:HB3	2.15	0.45
3:C:266:THR:HB	3:C:267:PRO:HD2	1.98	0.45
2:E:360:LEU:O	2:E:392:GLY:N	2.39	0.45
2:B:408:GLY:O	2:B:410:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ASP:OD1	1:D:168:LYS:N	2.49	0.45
2:E:371:ASN:ND2	2:E:375:GLU:HG3	2.25	0.45
3:F:398:GLN:O	3:F:399:GLN:O	2.34	0.45
3:C:91:GLU:O	3:C:95:LEU:HG	2.15	0.45
3:C:246:ILE:HG22	3:C:248:LEU:HD21	1.99	0.45
3:C:243:ARG:NH1	3:C:387:MET:CE	2.78	0.45
2:B:365:TYR:CD2	2:B:371:ASN:HB2	2.52	0.45
1:A:120:ASN:ND2	1:A:187:GLU:HA	2.31	0.45
2:B:359:ARG:HD3	2:B:361:TRP:CZ2	2.52	0.45
2:B:441:ILE:N	2:B:441:ILE:HD12	2.31	0.45
2:B:220:VAL:O	2:B:220:VAL:HG23	2.17	0.45
2:E:194:GLU:CA	2:E:197:ARG:HH12	2.29	0.45
3:F:253:ASN:HD21	3:F:378:LYS:NZ	2.14	0.45
3:F:249:THR:HA	3:F:254:THR:O	2.16	0.45
3:F:160:ASN:N	3:F:160:ASN:HD22	2.12	0.45
3:F:130:ILE:HA	3:F:130:ILE:HD12	1.86	0.45
2:E:477:LYS:HA	2:E:477:LYS:HD3	1.82	0.45
2:B:393:MET:HE2	2:B:424:TYR:O	2.16	0.45
2:E:211:LYS:HG2	3:F:130:ILE:HD13	1.99	0.45
3:F:209:VAL:CG2	3:F:210:SER:N	2.80	0.45
1:D:165:ARG:N	1:D:165:ARG:CD	2.80	0.45
3:C:287:ALA:HB3	3:C:367:TRP:CH2	2.52	0.45
2:E:337:TRP:CD1	2:E:468:ARG:HB2	2.52	0.45
2:E:330:VAL:HG22	2:E:331:LEU:H	1.81	0.45
2:B:249:GLN:CG	2:B:256:PRO:HG3	2.47	0.45
3:F:296:ASP:OD1	3:F:297:PRO:HD2	2.17	0.45
3:C:302:TYR:HD1	3:C:336:ARG:HB2	1.81	0.45
1:A:184:LEU:HD21	2:B:185:SER:OG	2.17	0.45
2:B:263:MET:HE1	2:B:269:GLY:CA	2.47	0.45
3:F:117:GLN:C	3:F:120:VAL:HG12	2.37	0.45
3:F:206:ARG:HB2	3:F:211:TYR:CE2	2.52	0.45
2:E:452:ASP:HB2	2:E:463:SER:O	2.17	0.44
2:B:477:LYS:HD3	2:B:477:LYS:HA	1.84	0.44
2:B:265:SER:O	2:B:266:HIS:C	2.56	0.44
2:E:249:GLN:HG3	2:E:256:PRO:HG3	2.00	0.44
1:A:132:ASN:HD22	1:A:132:ASN:N	2.15	0.44
2:E:179:GLU:O	2:E:183:ALA:HB3	2.17	0.44
2:E:204:GLU:CG	3:F:126:GLN:HE22	2.30	0.44
1:A:130:GLN:NE2	1:A:182:ALA:HA	2.30	0.44
2:E:329:GLN:HG3	2:E:329:GLN:O	2.18	0.44
2:E:444:LYS:HA	2:E:464:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:353:ARG:HG2	3:F:353:ARG:HH11	1.83	0.44
3:F:266:THR:HB	3:F:267:PRO:HD2	1.98	0.44
3:C:327:GLN:HG2	3:C:359:PHE:CD2	2.53	0.44
3:F:355:THR:O	3:F:356:ASP:HB2	2.17	0.44
1:A:110:ARG:HG3	1:A:111:ARG:N	2.33	0.44
3:C:256:ARG:HD3	3:C:283:ASP:O	2.18	0.44
1:D:168:LYS:O	1:D:169:GLU:HB2	2.17	0.44
2:B:262:ASP:O	2:B:263:MET:HE3	2.17	0.44
2:E:174:VAL:HG13	2:E:175:LYS:N	2.33	0.44
2:B:199:LYS:C	2:B:203:MET:HE2	2.37	0.44
3:F:120:VAL:HG13	3:F:121:THR:N	2.33	0.44
3:F:385:LEU:HD23	3:F:391:LEU:HD11	2.00	0.44
2:E:263:MET:HE1	2:E:269:GLY:HA2	1.99	0.44
3:C:285:GLY:HA3	3:C:369:THR:OG1	2.17	0.44
3:C:160:ASN:HD22	3:C:160:ASN:N	2.14	0.44
2:B:297:ILE:HG22	2:B:298:ALA:N	2.33	0.44
3:C:306:LEU:HD12	3:C:307:GLY:N	2.32	0.44
2:E:383:ASP:O	2:E:387:MET:HG2	2.17	0.44
1:D:181:ILE:C	1:D:183:ASN:N	2.71	0.44
1:D:118:ARG:HG3	1:D:118:ARG:NH1	2.33	0.44
3:F:243:ARG:NH1	3:F:387:MET:HE1	2.33	0.44
2:B:290:TYR:CE2	2:B:421:GLY:HA3	2.53	0.44
2:E:440:GLY:O	2:E:465:TYR:HA	2.17	0.44
3:F:196:HIS:HD2	3:F:381:THR:HB	1.82	0.43
3:C:302:TYR:C	3:C:335:ASN:ND2	2.72	0.43
3:F:302:TYR:HD1	3:F:336:ARG:HB2	1.81	0.43
1:A:115:LEU:HD13	2:B:174:VAL:HG11	1.99	0.43
3:F:397:GLN:HG3	3:F:398:GLN:N	2.33	0.43
2:E:441:ILE:H	2:E:441:ILE:CD1	2.25	0.43
3:C:243:ARG:NH1	3:C:387:MET:HE1	2.34	0.43
3:C:271:GLU:CG	3:C:309:LEU:HD23	2.48	0.43
3:F:356:ASP:HB3	3:F:357:VAL:H	1.64	0.43
3:C:195:GLN:OE1	3:C:380:THR:HG23	2.18	0.43
2:B:353:ASN:OD1	2:B:356:GLN:HG2	2.18	0.43
3:C:260:TYR:CZ	3:C:288:PHE:HB2	2.53	0.43
2:B:425:ASN:O	2:B:426:ARG:C	2.55	0.43
3:F:336:ARG:O	3:F:337:CYS:HB2	2.18	0.43
1:D:115:LEU:CG	3:F:96:GLU:HG2	2.49	0.43
2:B:428:HIS:CD2	2:B:431:ASN:HB2	2.52	0.43
3:C:396:GLY:O	3:C:398:GLN:N	2.52	0.43
2:E:387:MET:SD	2:E:426:ARG:CG	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ARG:O	1:D:109:GLU:HB2	2.19	0.43
3:C:397:GLN:O	3:F:283:ASP:HB2	2.18	0.43
2:E:399:ASP:O	2:E:400:ARG:HB2	2.17	0.43
2:B:337:TRP:CD1	2:B:468:ARG:HB2	2.53	0.43
2:B:201:GLN:O	2:B:204:GLU:HB3	2.18	0.43
2:E:265:SER:O	2:E:266:HIS:C	2.57	0.43
2:E:417:GLU:HB3	2:E:451:THR:HG21	2.01	0.43
1:D:101:TYR:CA	1:D:104:VAL:HG22	2.36	0.43
2:B:170:ARG:C	2:B:173:GLU:HG2	2.39	0.43
3:F:152:LYS:HG3	3:F:156:GLN:NE2	2.33	0.43
3:F:208:TRP:HE3	3:F:312:THR:HG23	1.84	0.43
2:B:190:LYS:O	2:B:194:GLU:HG3	2.19	0.43
2:E:301:ASN:OD1	2:E:305:ILE:HG13	2.18	0.43
3:F:305:HIS:CE1	3:F:340:GLY:H	2.37	0.43
3:F:128:VAL:HG23	3:F:129:ASP:N	2.34	0.43
2:B:285:ARG:HB3	2:B:285:ARG:HH11	1.82	0.43
2:E:325:GLN:O	2:E:326:HIS:ND1	2.52	0.43
3:C:362:ASP:N	3:C:362:ASP:OD1	2.51	0.43
3:C:336:ARG:HG2	4:G:2:HIS:HE1	1.80	0.43
1:A:177:ALA:O	1:A:179:SER:N	2.44	0.43
2:E:435:ARG:O	2:E:454:GLY:HA2	2.19	0.43
4:J:3:ARG:HH11	4:J:3:ARG:CB	2.32	0.43
2:B:329:GLN:HG2	2:B:475:ARG:O	2.18	0.43
3:F:173:LEU:H	3:F:239:GLN:HE21	1.65	0.43
3:F:173:LEU:H	3:F:239:GLN:NE2	2.17	0.43
1:A:191:GLU:HA	1:A:191:GLU:OE1	2.17	0.43
2:B:167:ILE:CD1	2:B:167:ILE:H	2.25	0.42
2:B:174:VAL:O	2:B:178:ILE:HG13	2.19	0.42
2:B:172:LYS:HB2	2:B:172:LYS:HE3	1.87	0.42
3:C:90:GLU:O	3:C:94:ILE:HG12	2.19	0.42
1:D:178:ALA:CB	2:E:192:VAL:HG21	2.49	0.42
3:F:115:VAL:O	3:F:118:GLN:HB3	2.19	0.42
3:F:287:ALA:HB3	3:F:367:TRP:CH2	2.54	0.42
3:F:271:GLU:CG	3:F:309:LEU:HD23	2.48	0.42
2:B:444:LYS:HA	2:B:464:TRP:CZ3	2.53	0.42
1:A:183:ASN:O	1:A:183:ASN:OD1	2.36	0.42
3:F:357:VAL:HG12	3:F:358:GLU:N	2.22	0.42
2:E:262:ASP:HB3	2:E:270:TRP:HB2	2.01	0.42
2:B:405:TRP:CG	2:B:412:LYS:HB3	2.54	0.42
2:E:413:HIS:HB3	2:E:416:ARG:HB2	2.01	0.42
2:B:186:LEU:HD21	3:C:106:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:356:GLN:HE21	2:E:356:GLN:HA	1.83	0.42
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.66	0.42
3:C:164:ASP:O	3:C:168:TYR:OH	2.23	0.42
2:B:270:TRP:CZ2	2:B:331:LEU:HD23	2.54	0.42
3:F:256:ARG:HD3	3:F:283:ASP:O	2.19	0.42
3:C:113:TRP:CE3	3:C:114:ARG:N	2.88	0.42
3:C:270:ASP:O	3:C:271:GLU:CB	2.65	0.42
1:D:162:LEU:HD23	2:E:213:LEU:HD12	2.00	0.42
3:F:362:ASP:OD2	4:H:1:GLY:N	2.51	0.42
2:E:163:ALA:O	2:E:166:GLU:HB3	2.20	0.42
3:C:185:ILE:HA	3:C:189:ASN:O	2.19	0.42
1:D:115:LEU:HD21	3:F:96:GLU:HA	2.02	0.42
1:D:119:ILE:HD11	2:E:178:ILE:CG1	2.48	0.42
3:C:398:GLN:HE21	3:C:399:GLN:CD	2.23	0.42
1:A:112:ILE:O	1:A:116:GLN:HG3	2.19	0.42
1:A:183:ASN:O	1:A:186:PHE:HB2	2.19	0.42
3:F:373:ARG:HD2	3:F:374:TRP:CH2	2.54	0.42
3:F:109:LEU:HD23	3:F:112:MET:HE3	1.99	0.42
1:D:162:LEU:O	1:D:163:GLU:CB	2.63	0.42
3:F:173:LEU:HB2	3:F:239:GLN:HG2	2.01	0.42
2:E:235:ILE:HG22	2:E:240:GLY:HA3	2.02	0.42
2:E:457:TRP:HB3	2:E:467:MET:CE	2.50	0.42
1:A:186:PHE:CE2	1:A:188:ARG:NE	2.88	0.42
3:F:250:ASP:C	3:F:250:ASP:OD1	2.58	0.42
3:C:151:GLY:HA2	3:C:156:GLN:HE21	1.84	0.42
3:F:270:ASP:O	3:F:271:GLU:CB	2.65	0.42
3:C:100:VAL:HG12	3:C:101:SER:N	2.35	0.42
3:C:312:THR:HG1	3:C:314:GLU:CD	2.19	0.42
3:C:243:ARG:HH11	3:C:387:MET:HE3	1.85	0.42
2:E:335:SER:HB3	2:E:468:ARG:HH21	1.84	0.42
2:E:457:TRP:HB3	2:E:467:MET:HE3	2.02	0.42
3:F:279:TYR:CB	3:F:286:ASN:ND2	2.83	0.42
1:D:135:THR:O	1:D:138:SER:HB3	2.20	0.42
3:F:236:LEU:C	3:F:238:GLY:H	2.22	0.42
2:E:230:MET:HB2	2:E:250:PRO:HA	2.02	0.42
3:C:320:TYR:OH	4:G:3:ARG:HG2	2.20	0.42
3:C:320:TYR:CD2	3:C:321:GLU:N	2.88	0.42
3:F:301:PHE:O	3:F:304:THR:HG23	2.20	0.42
2:B:440:GLY:O	2:B:465:TYR:HA	2.19	0.42
3:F:88:ILE:HG22	3:F:88:ILE:O	2.20	0.42
2:B:270:TRP:HB3	2:B:473:LYS:CB	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:HE21	1:A:125:GLN:HA	1.85	0.42
4:G:3:ARG:N	4:G:4:PRO:HD3	2.34	0.41
1:A:107:GLU:O	1:A:109:GLU:N	2.53	0.41
2:E:219:THR:HB	3:F:141:THR:HG23	2.02	0.41
2:E:248:ILE:HD11	2:E:257:TYR:CE1	2.54	0.41
3:C:206:ARG:HB2	3:C:211:TYR:CE2	2.55	0.41
3:F:125:GLN:HG2	3:F:126:GLN:N	2.35	0.41
2:B:248:ILE:HD11	2:B:257:TYR:CE1	2.55	0.41
1:D:110:ARG:C	1:D:112:ILE:N	2.74	0.41
3:F:84:THR:O	3:F:88:ILE:HG13	2.21	0.41
3:C:373:ARG:HD2	3:C:374:TRP:CH2	2.55	0.41
1:D:144:GLU:CB	2:E:203:MET:HE1	2.49	0.41
2:B:220:VAL:HG23	3:C:140:ASP:HA	2.01	0.41
3:F:372:ASP:O	3:F:374:TRP:N	2.53	0.41
2:E:418:ASP:HA	2:E:453:ASP:HB3	2.01	0.41
2:E:287:TRP:CA	2:E:397:THR:HG21	2.50	0.41
1:D:145:VAL:O	1:D:149:VAL:HG23	2.21	0.41
1:D:152:ARG:C	1:D:154:CYS:N	2.73	0.41
2:E:224:VAL:HA	2:E:225:PRO:HD3	1.83	0.41
3:F:249:THR:HB	3:F:379:MET:HB3	2.01	0.41
2:B:452:ASP:HB2	2:B:463:SER:O	2.20	0.41
3:C:113:TRP:HA	3:C:116:ASN:HB2	2.03	0.41
2:E:285:ARG:HH11	2:E:285:ARG:HB3	1.85	0.41
3:F:243:ARG:HH11	3:F:387:MET:HE3	1.84	0.41
3:F:147:SER:HA	3:F:148:PRO:HD3	1.83	0.41
2:E:346:TYR:HA	2:E:364:ASP:O	2.20	0.41
3:F:94:ILE:O	3:F:98:ILE:HG13	2.21	0.41
2:B:405:TRP:CZ3	4:I:3:ARG:NH1	2.88	0.41
3:C:154:CYS:HA	3:C:157:VAL:HB	2.02	0.41
2:B:249:GLN:CD	2:B:256:PRO:HG3	2.41	0.41
2:B:331:LEU:HD11	2:B:333:ASP:OD1	2.20	0.41
2:E:270:TRP:CZ2	2:E:331:LEU:HD23	2.55	0.41
1:D:119:ILE:HD13	1:D:119:ILE:HA	1.86	0.41
1:A:167:ASP:CG	1:A:168:LYS:HD2	2.41	0.41
3:C:236:LEU:C	3:C:238:GLY:H	2.24	0.41
3:F:389:ARG:HB3	3:F:390:ASP:H	1.66	0.41
2:B:399:ASP:O	2:B:400:ARG:HB2	2.19	0.41
1:A:104:VAL:O	1:A:107:GLU:HB3	2.20	0.41
2:B:168:GLU:C	2:B:172:LYS:HE2	2.41	0.41
2:E:353:ASN:ND2	2:E:355:ALA:CB	2.83	0.41
3:F:160:ASN:ND2	3:F:160:ASN:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:ASP:OD1	3:C:250:ASP:C	2.57	0.41
4:G:3:ARG:N	4:G:4:PRO:CD	2.84	0.41
1:D:101:TYR:C	1:D:103:GLU:N	2.74	0.41
2:B:172:LYS:HG3	2:B:172:LYS:H	1.67	0.41
2:B:238:ASN:CG	3:C:213:GLU:HG3	2.41	0.41
2:E:329:GLN:HG2	2:E:475:ARG:O	2.21	0.41
2:B:224:VAL:HG21	2:B:247:TYR:CE1	2.56	0.41
2:E:259:VAL:HA	2:E:297:ILE:HG12	2.03	0.41
3:F:186:GLU:O	3:F:189:ASN:HB2	2.21	0.41
1:D:101:TYR:CE1	1:D:105:LEU:HB2	2.56	0.41
2:E:387:MET:HB2	2:E:426:ARG:CG	2.51	0.41
1:A:108:LEU:HD13	3:C:89:LEU:CD2	2.51	0.41
3:C:88:ILE:O	3:C:91:GLU:HB2	2.21	0.41
2:B:259:VAL:HA	2:B:297:ILE:HG12	2.03	0.41
3:F:350:GLY:O	3:F:375:TYR:HA	2.21	0.41
3:F:260:TYR:CZ	3:F:288:PHE:HB2	2.56	0.41
1:A:107:GLU:C	1:A:109:GLU:N	2.74	0.40
1:A:147:ILE:CG2	2:B:207:ILE:HD11	2.49	0.40
2:B:311:GLU:O	2:B:312:TYR:HB3	2.21	0.40
3:C:262:HIS:CE1	3:C:387:MET:HG2	2.56	0.40
3:F:101:SER:O	3:F:104:ALA:N	2.54	0.40
2:B:417:GLU:HB3	2:B:451:THR:HG21	2.01	0.40
3:F:196:HIS:HA	3:F:380:THR:O	2.21	0.40
3:C:336:ARG:O	3:C:337:CYS:HB2	2.21	0.40
3:F:396:GLY:HA2	3:F:401:LYS:HD3	2.02	0.40
2:B:169:ASN:CA	2:B:172:LYS:HE2	2.51	0.40
2:E:199:LYS:HG2	2:E:203:MET:CE	2.50	0.40
2:B:356:GLN:HE21	2:B:356:GLN:HA	1.86	0.40
2:B:432:PRO:O	2:B:433:ASN:HB2	2.20	0.40
2:B:413:HIS:HB3	2:B:416:ARG:HB2	2.02	0.40
3:C:136:ARG:NH2	3:C:139:GLN:HG2	2.33	0.40
3:C:325:ALA:N	3:C:334:MET:HE2	2.36	0.40
3:F:386:PRO:C	3:F:388:GLY:H	2.24	0.40
2:B:418:ASP:HA	2:B:453:ASP:HB3	2.02	0.40
1:A:150:ALA:CB	3:C:131:ARG:HG2	2.51	0.40
3:C:312:THR:OG1	3:C:314:GLU:OE1	2.24	0.40
2:E:238:ASN:CB	3:F:213:GLU:HG3	2.51	0.40
1:D:110:ARG:C	1:D:112:ILE:H	2.24	0.40
1:D:176:LYS:O	1:D:180:TYR:CB	2.64	0.40
1:A:147:ILE:O	1:A:151:LEU:CB	2.70	0.40
2:B:329:GLN:O	2:B:329:GLN:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:LEU:N	2:B:252:LEU:CD2	2.85	0.40
3:F:120:VAL:CG1	3:F:121:THR:N	2.85	0.40
1:A:111:ARG:CG	1:A:111:ARG:HH11	2.35	0.40
2:E:274:GLN:NE2	2:E:274:GLN:C	2.74	0.40
1:D:189:PHE:O	1:D:190:GLU:HB2	2.22	0.40
3:F:101:SER:O	3:F:105:GLN:HG3	2.22	0.40
2:E:379:GLN:O	2:E:380:LEU:HD23	2.21	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	89/119 (75%)	62 (70%)	16 (18%)	11 (12%)	0 1
1	D	88/119 (74%)	58 (66%)	20 (23%)	10 (11%)	0 1
2	B	313/323 (97%)	261 (83%)	41 (13%)	11 (4%)	4 18
2	E	313/323 (97%)	259 (83%)	43 (14%)	11 (4%)	4 18
3	C	320/330 (97%)	268 (84%)	36 (11%)	16 (5%)	3 9
3	F	320/330 (97%)	264 (82%)	44 (14%)	12 (4%)	4 16
4	G	2/4 (50%)	1 (50%)	1 (50%)	0	100 100
4	H	2/4 (50%)	1 (50%)	1 (50%)	0	100 100
4	I	2/4 (50%)	2 (100%)	0	0	100 100
4	J	2/4 (50%)	2 (100%)	0	0	100 100
All	All	1451/1560 (93%)	1178 (81%)	202 (14%)	71 (5%)	3 10

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	SER
1	A	182	ALA
1	A	186	PHE
2	B	455	VAL
3	C	337	CYS
3	C	356	ASP
3	C	373	ARG
3	C	390	ASP
3	C	392	SER
3	C	399	GLN
1	D	159	ALA
1	D	163	GLU
1	D	185	LYS
2	E	455	VAL
3	F	337	CYS
3	F	356	ASP
3	F	373	ARG
3	F	399	GLN
1	A	149	VAL
1	A	167	ASP
1	A	178	ALA
1	A	190	GLU
2	B	266	HIS
2	B	364	ASP
2	B	400	ARG
2	B	427	CYS
3	C	355	THR
1	D	178	ALA
1	D	180	TYR
1	D	184	LEU
2	E	266	HIS
2	E	364	ASP
2	E	400	ARG
2	E	427	CYS
3	F	355	THR
3	F	395	GLY
1	A	139	GLN
1	A	192	VAL
2	B	169	ASN
2	B	293	GLU
2	B	351	PRO
2	B	459	ASN
3	C	173	LEU

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Mol	Chain	Res	Type
3	C	271	GLU
3	C	360	PRO
3	C	368	ALA
1	D	166	LEU
2	E	293	GLU
2	E	351	PRO
2	E	459	ASN
3	F	173	LEU
3	F	271	GLU
3	F	360	PRO
3	F	368	ALA
1	A	108	LEU
3	C	357	VAL
3	C	391	LEU
3	C	403	ASN
2	E	169	ASN
2	E	190	LYS
3	F	357	VAL
1	A	166	LEU
3	C	397	GLN
1	D	102	SER
1	D	165	ARG
1	D	169	GLU
2	B	277	VAL
2	E	277	VAL
3	F	393	GLY
3	C	120	VAL
2	B	476	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	84/110 (76%)	73 (87%)	11 (13%)	5 15
1	D	83/110 (76%)	73 (88%)	10 (12%)	6 18
2	B	266/274 (97%)	247 (93%)	19 (7%)	18 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	266/274 (97%)	249 (94%)	17 (6%)	22 53
3	C	280/286 (98%)	259 (92%)	21 (8%)	17 44
3	F	280/286 (98%)	265 (95%)	15 (5%)	27 62
4	G	3/3 (100%)	2 (67%)	1 (33%)	0 1
4	H	3/3 (100%)	3 (100%)	0	100 100
4	I	3/3 (100%)	2 (67%)	1 (33%)	0 1
4	J	3/3 (100%)	2 (67%)	1 (33%)	0 1
All	All	1271/1352 (94%)	1175 (92%)	96 (8%)	16 43

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	115	LEU
1	A	124	GLN
1	A	164	TYR
1	A	165	ARG
1	A	168	LYS
1	A	169	GLU
1	A	175	GLU
1	A	176	LYS
1	A	180	TYR
1	A	187	GLU
2	B	167	ILE
2	B	191	SER
2	B	205	GLU
2	B	208	LYS
2	B	221	ASN
2	B	253	PHE
2	B	263	MET
2	B	274	GLN
2	B	285	ARG
2	B	317	LYS
2	B	323	THR
2	B	331	LEU
2	B	338	GLU
2	B	351	PRO
2	B	400	ARG
2	B	404	ASN
2	B	441	ILE

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Mol	Chain	Res	Type
2	B	473	LYS
2	B	474	LEU
3	C	91	GLU
3	C	93	ARG
3	C	100	VAL
3	C	118	GLN
3	C	119	PHE
3	C	124	GLN
3	C	125	GLN
3	C	133	THR
3	C	192	THR
3	C	207	ASP
3	C	264	LYS
3	C	269	SER
3	C	280	LEU
3	C	304	THR
3	C	336	ARG
3	C	372	ASP
3	C	380	THR
3	C	381	THR
3	C	384	LEU
3	C	391	LEU
3	C	403	ASN
1	D	110	ARG
1	D	128	LEU
1	D	165	ARG
1	D	168	LYS
1	D	169	GLU
1	D	175	GLU
1	D	180	TYR
1	D	187	GLU
1	D	188	ARG
1	D	189	PHE
2	E	177	ARG
2	E	212	GLU
2	E	221	ASN
2	E	253	PHE
2	E	263	MET
2	E	274	GLN
2	E	285	ARG
2	E	305	ILE
2	E	317	LYS

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Mol	Chain	Res	Type
2	E	323	THR
2	E	331	LEU
2	E	338	GLU
2	E	351	PRO
2	E	400	ARG
2	E	441	ILE
2	E	473	LYS
2	E	474	LEU
3	F	103	ASP
3	F	119	PHE
3	F	131	ARG
3	F	192	THR
3	F	207	ASP
3	F	264	LYS
3	F	269	SER
3	F	280	LEU
3	F	304	THR
3	F	336	ARG
3	F	372	ASP
3	F	380	THR
3	F	381	THR
3	F	384	LEU
3	F	394	HIS
4	G	3	ARG
4	I	2	HIS
4	J	3	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	120	ASN
1	A	125	GLN
1	A	130	GLN
1	A	132	ASN
1	A	173	GLN
2	B	201	GLN
2	B	210	GLN
2	B	231	HIS
2	B	238	ASN
2	B	266	HIS
2	B	274	GLN

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Mol	Chain	Res	Type
2	B	288	ASN
2	B	320	HIS
2	B	325	GLN
2	B	329	GLN
2	B	356	GLN
2	B	371	ASN
2	B	428	HIS
2	B	459	ASN
2	B	469	GLN
3	C	102	HIS
3	C	118	GLN
3	C	125	GLN
3	C	156	GLN
3	C	160	ASN
3	C	189	ASN
3	C	196	HIS
3	C	230	ASN
3	C	239	GLN
3	C	253	ASN
3	C	262	HIS
3	C	305	HIS
3	C	317	ASN
3	C	398	GLN
3	C	403	ASN
1	D	124	GLN
1	D	132	ASN
1	D	136	GLN
2	E	164	GLN
2	E	210	GLN
2	E	231	HIS
2	E	238	ASN
2	E	266	HIS
2	E	274	GLN
2	E	288	ASN
2	E	320	HIS
2	E	329	GLN
2	E	356	GLN
2	E	371	ASN
2	E	428	HIS
2	E	459	ASN
2	E	469	GLN
3	F	105	GLN

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Mol	Chain	Res	Type
3	F	116	ASN
3	F	132	GLN
3	F	156	GLN
3	F	160	ASN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	253	ASN
3	F	262	HIS
3	F	305	HIS
3	F	317	ASN
3	F	335	ASN
4	G	2	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	NAG	B	480	2	14,14,15	0.74	0	15,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	C	480	3	14,14,15	0.47	0	15,19,21	1.01	1 (6%)
5	NAG	E	480	2	14,14,15	0.73	0	15,19,21	0.65	0
5	NAG	F	480	3	14,14,15	0.55	0	15,19,21	0.72	1 (6%)

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	B	480	2	-	0/6/23/26	0/1/1/1
5	NAG	C	480	3	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	480	2	-	0/6/23/26	0/1/1/1
5	NAG	F	480	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	480	NAG	C2-N2-C7	-2.87	119.35	123.04
5	F	480	NAG	C2-N2-C7	-2.00	120.47	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	480	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	480	NAG	3	0
5	C	480	NAG	2	0
5	E	480	NAG	4	0
5	F	480	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.