



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:40 PM GMT

PDB ID : 1N86
Title : Crystal structure of human D-dimer from cross-linked fibrin complexed with GPR and GHRPLDK peptide ligands.
Authors : Yang, Z.; Pandi, L.; Doolittle, R.F.
Deposited on : 2002-11-19
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

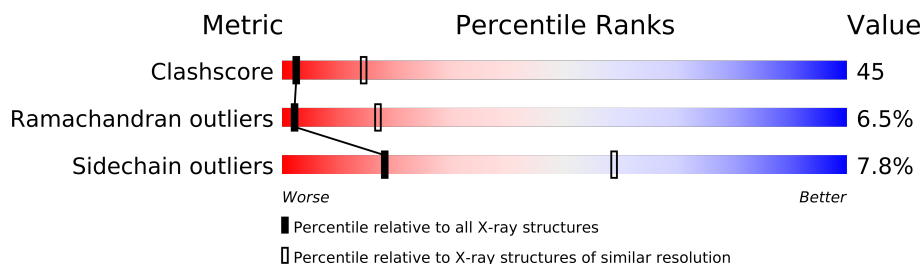
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	
1	D	87	
2	B	328	
2	E	328	
3	C	324	
3	F	324	
4	G	3	
4	H	3	
5	I	7	
5	J	7	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11054 atoms, of which 0 are hydrogen and 0 are deuterium.

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/alpha-E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			

- Molecule 2 is a protein called Fibrin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			
2	E	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			

- Molecule 3 is a protein called Fibrin gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	295	Total	C	N	O	S	0	0	0
			2364	1498	399	456	11			
3	F	295	Total	C	N	O	S	0	0	0
			2364	1498	399	456	11			

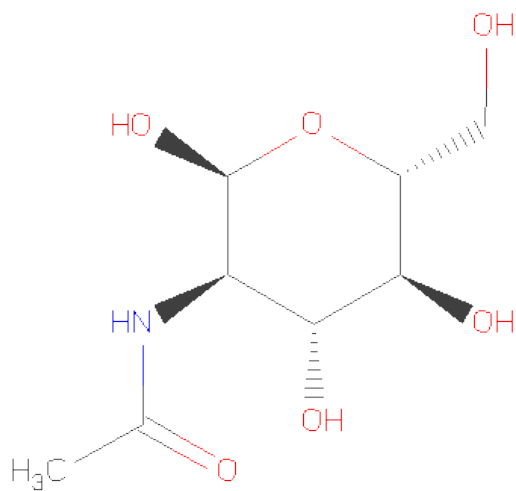
- Molecule 4 is a protein called fibrin alpha chain peptide ligand fragment Gly-Pro-Arg.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			23	13	6	4			
4	H	3	Total	C	N	O	0	0	0
			23	13	6	4			

- Molecule 5 is a protein called fibrin beta chain peptide ligand fragment Gly-His-Arg-Pro-Leu-Asp-Lys.

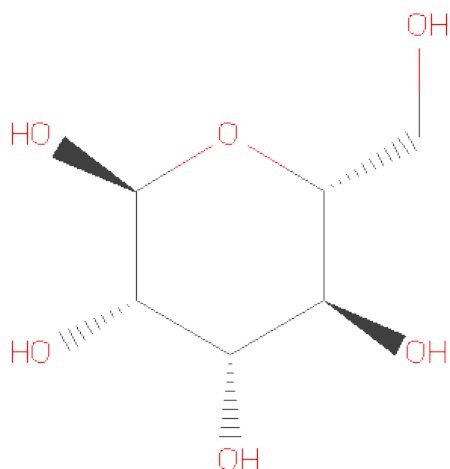
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			32	19	9	4			
5	J	4	Total	C	N	O	0	0	0
			32	19	9	4			

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	I	1	Total	C	N	O	0	0
			15	8	1	6		
6	E	1	Total	C	N	O	0	0
			15	8	1	6		
6	J	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

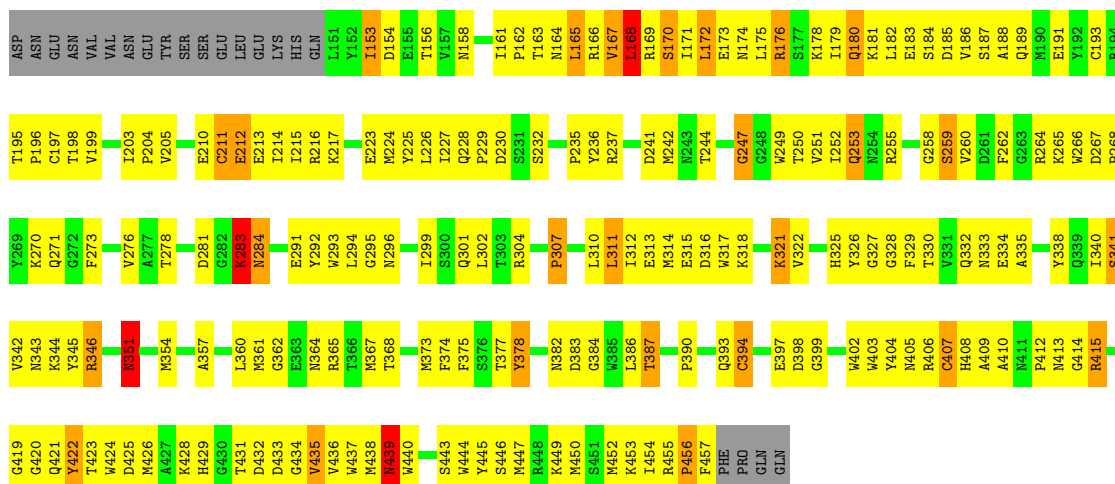


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			12	6	6		

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

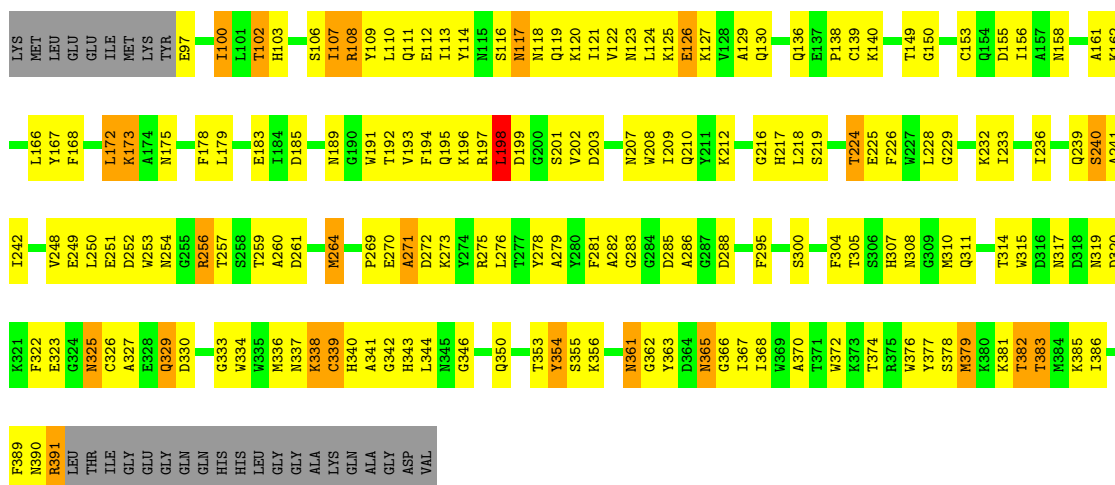
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		
8	F	1	Total	Ca	0	0
			1	1		
8	E	1	Total	Ca	0	0
			1	1		

Chain E:



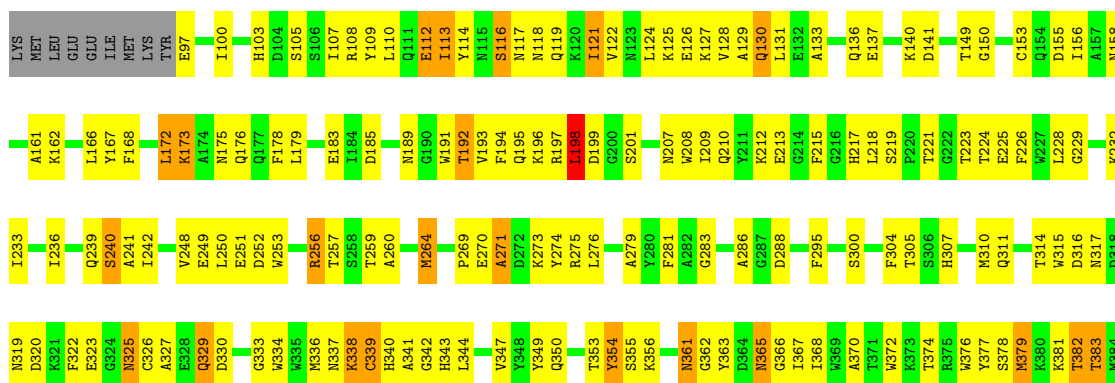
• Molecule 3: Fibrin gamma chain

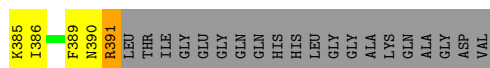
Chain C:



• Molecule 3: Fibrin gamma chain

Chain F:





- Molecule 4: fibrin alpha chain peptide ligand fragment Gly-Pro-Arg

Chain G:



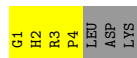
- Molecule 4: fibrin alpha chain peptide ligand fragment Gly-Pro-Arg

Chain H:



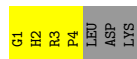
- Molecule 5: fibrin beta chain peptide ligand fragment Gly-His-Arg-Pro-Leu-Asp-Lys

Chain I:



- Molecule 5: fibrin beta chain peptide ligand fragment Gly-His-Arg-Pro-Leu-Asp-Lys

Chain J: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.33Å 130.09Å 298.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	84.0 (20.00-3.20)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11054	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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, NDG, MAN

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	0/609	0.69	0/811
1	D	0.38	0/609	0.64	0/811
2	B	0.38	0/2523	0.70	1/3409 (0.0%)
2	E	0.40	0/2523	0.69	1/3409 (0.0%)
3	C	0.43	0/2429	0.69	2/3285 (0.1%)
3	F	0.44	0/2429	0.69	1/3285 (0.0%)
4	G	0.71	0/23	0.74	0/28
4	H	0.61	0/23	0.76	0/28
5	I	0.55	0/33	0.56	0/43
5	J	0.47	0/33	0.54	0/43
All	All	0.41	0/11234	0.69	5/15152 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	338	LYS	N-CA-C	-5.44	96.30	111.00
3	F	338	LYS	N-CA-C	-5.27	96.78	111.00
2	E	346	ARG	N-CA-C	-5.26	96.79	111.00
2	B	346	ARG	N-CA-C	-5.14	97.13	111.00
3	C	102	THR	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	608	0	649	62	0
1	D	608	0	649	69	0
2	B	2462	0	2328	250	0
2	E	2462	0	2328	261	0
3	C	2364	0	2208	194	0
3	F	2364	0	2208	194	0
4	G	23	0	25	5	0
4	H	23	0	25	7	0
5	I	32	0	32	5	0
5	J	32	0	32	5	0
6	B	15	0	15	12	0
6	E	15	0	15	4	0
6	I	15	0	15	7	0
6	J	15	0	15	0	0
7	B	12	0	12	2	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
All	All	11054	0	10556	979	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 45.

All (979) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:365:ASN:HD22	3:F:365:ASN:H	1.03	1.02
3:C:326:CYS:HB3	3:C:336:MET:HE2	1.42	0.97
1:D:188:VAL:HG21	2:E:167:VAL:HG21	1.46	0.96
2:B:166:ARG:HH11	2:B:166:ARG:HB2	1.31	0.95
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.48	0.95
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.50	0.94
3:F:326:CYS:HB3	3:F:336:MET:HE2	1.45	0.94
3:F:307:HIS:HE1	3:F:341:ALA:H	1.17	0.93
3:C:365:ASN:H	3:C:365:ASN:HD22	1.04	0.93
2:B:351:ASN:HD21	2:B:354:MET:H	1.16	0.92
3:F:189:ASN:ND2	3:F:391:ARG:HE	1.66	0.92
3:C:307:HIS:HE1	3:C:341:ALA:H	1.15	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:189:ASN:ND2	3:C:391:ARG:HE	1.68	0.91
2:E:351:ASN:HD21	2:E:354:MET:H	1.19	0.91
3:F:172:LEU:H	3:F:239:GLN:HE21	1.13	0.90
1:A:119:ILE:HG12	1:A:123:LYS:HD3	1.53	0.90
2:B:351:ASN:ND2	2:B:354:MET:H	1.70	0.90
2:B:171:ILE:HD12	2:B:172:LEU:N	1.85	0.89
3:C:172:LEU:H	3:C:239:GLN:HE21	1.20	0.89
1:A:169:LEU:H	2:B:189:GLN:HE22	1.21	0.89
2:B:284:ASN:HD22	2:B:284:ASN:H	1.15	0.88
2:E:284:ASN:HD22	2:E:284:ASN:H	1.17	0.88
2:E:333:ASN:HD21	2:E:335:ALA:HB3	1.39	0.87
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.55	0.87
2:E:351:ASN:ND2	2:E:354:MET:H	1.72	0.87
2:E:283:LYS:HA	2:E:283:LYS:HE3	1.57	0.86
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.58	0.86
2:B:283:LYS:HA	2:B:283:LYS:HE3	1.56	0.86
1:D:132:HIS:HB3	3:F:107:ILE:HD11	1.58	0.86
2:B:373:MET:SD	2:B:405:ASN:HB2	2.15	0.85
2:E:166:ARG:HA	2:E:169:ARG:HD2	1.58	0.85
2:B:333:ASN:HD21	2:B:335:ALA:HB3	1.42	0.85
2:B:364:ASN:HD21	6:B:470:NDG:H6C1	1.40	0.84
1:D:131:GLN:O	1:D:135:LEU:HB2	1.76	0.84
2:E:373:MET:SD	2:E:405:ASN:HB2	2.17	0.84
2:E:310:LEU:HD12	2:E:311:LEU:H	1.41	0.84
3:F:105:SER:HA	3:F:108:ARG:HH12	1.41	0.84
2:E:361:MET:HB2	6:E:570:NDG:H8C3	1.60	0.84
3:C:167:TYR:O	3:C:179:LEU:HD12	1.78	0.83
3:C:304:PHE:HB3	3:C:338:LYS:HB3	1.61	0.82
3:F:365:ASN:N	3:F:365:ASN:HD22	1.78	0.82
2:E:311:LEU:HD11	2:E:313:GLU:HG3	1.59	0.82
3:F:149:THR:HG22	3:F:150:GLY:H	1.45	0.81
3:F:304:PHE:HB3	3:F:338:LYS:HB3	1.60	0.81
3:C:365:ASN:N	3:C:365:ASN:HD22	1.77	0.80
2:E:373:MET:CG	2:E:405:ASN:HB2	2.11	0.80
1:A:188:VAL:O	1:A:189:ILE:HD12	1.81	0.80
3:F:264:MET:HB2	3:F:279:ALA:HB2	1.62	0.80
2:B:310:LEU:HD12	2:B:311:LEU:H	1.45	0.80
2:E:357:ALA:HA	2:E:439:ASN:HD21	1.45	0.80
3:C:149:THR:HG22	3:C:150:GLY:H	1.47	0.80
3:C:307:HIS:CE1	3:C:341:ALA:H	2.00	0.79
2:B:364:ASN:ND2	6:B:470:NDG:H6C1	1.97	0.79
2:E:394:CYS:SG	2:E:407:CYS:N	2.55	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:394:CYS:SG	2:B:407:CYS:N	2.55	0.79
3:F:307:HIS:CE1	3:F:341:ALA:H	2.00	0.79
2:B:311:LEU:HD11	2:B:313:GLU:HG3	1.65	0.78
2:B:373:MET:CG	2:B:405:ASN:HB2	2.12	0.78
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.46	0.78
2:B:179:ILE:HD13	3:C:121:ILE:HG12	1.65	0.78
3:C:264:MET:HB2	3:C:279:ALA:HB2	1.65	0.78
2:B:351:ASN:C	2:B:351:ASN:HD22	1.87	0.77
3:F:340:HIS:O	4:H:1:GLY:HA2	1.85	0.77
2:E:351:ASN:C	2:E:351:ASN:HD22	1.87	0.77
3:F:167:TYR:O	3:F:179:LEU:HD12	1.84	0.77
2:E:439:ASN:N	2:E:439:ASN:HD22	1.81	0.77
2:B:456:PRO:O	2:B:457:PHE:HB3	1.85	0.77
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.66	0.76
2:B:161:ILE:HG22	2:B:165:LEU:HD11	1.65	0.76
3:C:197:ARG:HB2	3:C:382:THR:HB	1.67	0.76
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.67	0.76
2:B:367:MET:SD	2:B:406:ARG:HD3	2.26	0.75
2:E:310:LEU:HD12	2:E:311:LEU:N	2.01	0.75
2:B:439:ASN:N	2:B:439:ASN:HD22	1.81	0.75
3:F:197:ARG:HB2	3:F:382:THR:HB	1.66	0.75
2:E:398:ASP:HA	2:E:433:ASP:CB	2.17	0.75
2:B:310:LEU:HD12	2:B:311:LEU:N	2.02	0.75
2:B:241:ASP:OD1	2:B:244:THR:HB	1.87	0.75
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.66	0.74
2:E:456:PRO:O	2:E:457:PHE:HB3	1.84	0.74
2:B:364:ASN:CG	6:B:470:NDG:H1	2.08	0.74
2:E:188:ALA:O	2:E:191:GLU:HB3	1.87	0.74
3:F:105:SER:HA	3:F:108:ARG:NH1	2.03	0.74
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.69	0.73
2:E:412:PRO:HG3	2:E:450:MET:HE3	1.68	0.73
3:C:107:ILE:HG23	3:C:108:ARG:H	1.53	0.73
2:E:241:ASP:OD1	2:E:244:THR:HB	1.87	0.73
2:E:367:MET:SD	2:E:406:ARG:HD3	2.29	0.73
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.69	0.73
2:E:185:ASP:O	2:E:188:ALA:HB3	1.88	0.73
7:B:472:MAN:H5	6:I:471:NDG:O3	1.88	0.73
2:E:398:ASP:CA	2:E:433:ASP:HB3	2.19	0.73
2:B:398:ASP:HA	2:B:433:ASP:CB	2.18	0.72
1:D:152:VAL:HG13	1:D:153:ASP:N	2.04	0.72
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.54	0.72
2:E:255:ARG:HD3	2:E:262:PHE:CZ	2.24	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:B:470:NDG:H4	6:I:471:NDG:H1	1.72	0.72
2:B:398:ASP:CA	2:B:433:ASP:HB3	2.19	0.72
2:B:255:ARG:HD3	2:B:262:PHE:CZ	2.24	0.72
3:F:172:LEU:H	3:F:239:GLN:NE2	1.88	0.71
2:B:302:LEU:HD13	2:B:454:ILE:HD11	1.72	0.71
2:B:284:ASN:N	2:B:284:ASN:HD22	1.85	0.71
1:D:152:VAL:HG11	2:E:426:MET:O	1.90	0.71
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.72	0.71
6:B:470:NDG:C4	6:I:471:NDG:H1	2.21	0.71
3:C:366:GLY:O	3:C:368:ILE:HG23	1.90	0.71
3:C:113:ILE:O	3:C:116:SER:HB3	1.91	0.71
2:B:351:ASN:HD21	2:B:354:MET:N	1.87	0.71
3:F:304:PHE:HB3	3:F:338:LYS:CB	2.21	0.70
1:A:119:ILE:CG1	1:A:123:LYS:HD3	2.20	0.70
1:D:182:GLN:O	1:D:185:LEU:HB3	1.91	0.70
3:F:149:THR:HG22	3:F:150:GLY:N	2.06	0.70
2:E:168:LEU:HD22	2:E:168:LEU:H	1.56	0.70
3:C:242:ILE:H	3:C:242:ILE:HD12	1.57	0.70
3:F:366:GLY:O	3:F:368:ILE:HG23	1.91	0.70
1:A:188:VAL:C	1:A:189:ILE:HD12	2.12	0.69
2:B:266:TRP:HA	2:B:377:THR:HG21	1.73	0.69
2:E:415:ARG:H	2:E:434:GLY:HA2	1.56	0.69
2:E:264:ARG:NH1	3:F:136:GLN:HE21	1.89	0.69
1:A:169:LEU:H	2:B:189:GLN:NE2	1.91	0.69
2:E:310:LEU:HD22	2:E:329:PHE:CE2	2.27	0.69
3:C:295:PHE:HE2	3:C:305:THR:HG21	1.57	0.69
2:B:357:ALA:HA	2:B:439:ASN:ND2	2.08	0.69
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.74	0.69
2:B:228:GLN:HB2	2:B:235:PRO:HG3	1.74	0.69
2:E:435:VAL:O	2:E:446:SER:HA	1.93	0.69
1:D:136:LEU:O	1:D:140:VAL:HG12	1.92	0.69
2:E:168:LEU:H	2:E:168:LEU:CD2	2.05	0.69
3:F:113:ILE:HA	3:F:116:SER:HB3	1.74	0.69
3:F:295:PHE:CE2	3:F:305:THR:HG21	2.28	0.69
3:F:295:PHE:HE2	3:F:305:THR:HG21	1.57	0.69
2:E:325:HIS:HB2	2:E:346:ARG:HB2	1.75	0.69
2:E:357:ALA:HA	2:E:439:ASN:ND2	2.07	0.69
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.75	0.69
3:C:273:LYS:HE3	3:C:319:ASN:HD21	1.58	0.69
2:B:351:ASN:OD1	2:B:354:MET:HB2	1.93	0.68
3:C:232:LYS:O	3:C:236:ILE:HG13	1.92	0.68
2:B:179:ILE:CD1	3:C:121:ILE:HG12	2.23	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:191:GLU:OE2	2:B:194:ARG:HD2	1.92	0.68
3:F:340:HIS:CE1	4:H:1:GLY:N	2.61	0.68
2:E:284:ASN:ND2	2:E:284:ASN:H	1.90	0.68
2:E:228:GLN:HB2	2:E:235:PRO:HG3	1.75	0.68
2:E:266:TRP:HA	2:E:377:THR:HG21	1.73	0.68
3:C:107:ILE:HG23	3:C:108:ARG:N	2.08	0.68
2:B:295:GLY:O	2:B:299:ILE:HG13	1.92	0.68
3:F:153:CYS:SG	3:F:192:THR:HB	2.33	0.68
2:E:422:TYR:CE1	2:E:444:TRP:HA	2.29	0.68
3:C:295:PHE:CE2	3:C:305:THR:HG21	2.28	0.68
3:C:149:THR:HG22	3:C:150:GLY:N	2.08	0.68
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.74	0.68
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.75	0.68
1:A:129:LYS:HE3	1:A:129:LYS:HA	1.76	0.68
2:E:165:LEU:HD13	3:F:110:LEU:HD11	1.76	0.68
2:B:284:ASN:H	2:B:284:ASN:ND2	1.89	0.68
2:E:310:LEU:HD22	2:E:329:PHE:CD2	2.28	0.68
2:E:210:GLU:HA	2:E:227:ILE:HG21	1.76	0.68
2:E:311:LEU:HD12	2:E:312:ILE:N	2.09	0.67
2:E:284:ASN:N	2:E:284:ASN:HD22	1.88	0.67
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.29	0.67
2:B:210:GLU:HA	2:B:227:ILE:HG21	1.74	0.67
3:F:354:TYR:CE1	3:F:376:TRP:HA	2.29	0.67
2:E:343:ASN:HA	2:E:354:MET:SD	2.35	0.67
3:C:108:ARG:O	3:C:111:GLN:HB3	1.95	0.67
3:C:354:TYR:CE1	3:C:376:TRP:HA	2.30	0.67
1:D:178:TYR:O	1:D:182:GLN:HG2	1.95	0.67
1:A:136:LEU:HD13	1:A:136:LEU:C	2.15	0.67
2:B:311:LEU:HD12	2:B:312:ILE:N	2.10	0.67
2:B:161:ILE:HG22	2:B:165:LEU:CD1	2.25	0.66
2:B:415:ARG:H	2:B:434:GLY:HA2	1.60	0.66
3:C:219:SER:OG	3:C:224:THR:HG22	1.96	0.66
3:C:109:TYR:HA	3:C:112:GLU:CD	2.15	0.66
2:E:351:ASN:OD1	2:E:354:MET:HB2	1.95	0.66
1:D:127:ILE:O	1:D:130:VAL:HG12	1.96	0.66
3:F:264:MET:HB2	3:F:279:ALA:CB	2.24	0.66
3:F:242:ILE:HD12	3:F:242:ILE:H	1.58	0.66
2:B:325:HIS:HB2	2:B:346:ARG:HB2	1.76	0.66
2:E:351:ASN:HD21	2:E:354:MET:N	1.91	0.66
2:E:165:LEU:HD12	2:E:169:ARG:CZ	2.25	0.66
1:A:159:ARG:HG2	2:B:258:GLY:HA3	1.77	0.66
3:F:149:THR:HG23	3:F:168:PHE:O	1.96	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.77	0.66
3:C:192:THR:HG23	3:C:386:ILE:HG13	1.78	0.66
2:B:166:ARG:HB2	2:B:166:ARG:NH1	2.09	0.65
3:C:153:CYS:SG	3:C:192:THR:HB	2.36	0.65
2:B:313:GLU:OE1	2:B:453:LYS:HD2	1.97	0.65
3:C:117:ASN:O	3:C:121:ILE:HG13	1.94	0.65
3:C:103:HIS:O	3:C:107:ILE:HG22	1.96	0.65
2:E:360:LEU:O	2:E:365:ARG:HB2	1.96	0.65
3:F:117:ASN:C	3:F:119:GLN:H	2.00	0.64
3:F:117:ASN:O	3:F:119:GLN:N	2.30	0.64
3:F:219:SER:OG	3:F:224:THR:HG22	1.97	0.64
3:C:304:PHE:HB3	3:C:338:LYS:CB	2.25	0.64
1:A:144:LEU:HD21	2:B:175:LEU:HD21	1.78	0.64
3:F:228:LEU:O	3:F:232:LYS:HD2	1.98	0.64
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.79	0.64
3:F:109:TYR:O	3:F:112:GLU:HB2	1.98	0.64
3:F:192:THR:HG23	3:F:386:ILE:HG13	1.79	0.64
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.10	0.64
2:B:412:PRO:HG3	2:B:450:MET:HE3	1.79	0.64
2:E:295:GLY:O	2:E:299:ILE:HG13	1.98	0.64
2:B:310:LEU:HD22	2:B:329:PHE:CE2	2.33	0.64
3:C:172:LEU:H	3:C:239:GLN:NE2	1.93	0.64
2:B:343:ASN:HA	2:B:354:MET:SD	2.38	0.63
2:E:230:ASP:OD2	2:E:232:SER:HB2	1.97	0.63
3:C:365:ASN:ND2	3:C:365:ASN:H	1.87	0.63
3:C:149:THR:HG23	3:C:168:PHE:O	1.98	0.63
3:F:242:ILE:HD12	3:F:242:ILE:N	2.12	0.63
2:E:166:ARG:NH1	2:E:166:ARG:HB3	2.13	0.63
3:C:242:ILE:N	3:C:242:ILE:HD12	2.12	0.63
3:F:372:TRP:HZ3	3:F:379:MET:HE3	1.64	0.63
2:B:435:VAL:O	2:B:446:SER:HA	1.98	0.63
2:E:223:GLU:HG3	2:E:225:TYR:CE1	2.33	0.63
1:A:126:VAL:C	1:A:128:GLU:H	2.02	0.63
2:B:171:ILE:CD1	2:B:172:LEU:N	2.60	0.63
7:B:472:MAN:H3	6:I:471:NDG:HA	1.64	0.63
2:B:230:ASP:OD2	2:B:232:SER:HB2	1.99	0.63
2:E:402:TRP:HE3	2:E:413:ASN:ND2	1.96	0.63
2:B:360:LEU:O	2:B:365:ARG:HB2	1.99	0.63
3:C:337:ASN:C	3:C:339:CYS:H	2.00	0.62
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.46	0.62
2:B:176:ARG:HH11	2:B:176:ARG:HG2	1.63	0.62
3:C:228:LEU:O	3:C:232:LYS:HD2	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.64	0.62
2:B:310:LEU:HB2	2:B:329:PHE:CD2	2.35	0.62
1:D:186:GLU:HG2	1:D:189:ILE:HD12	1.80	0.62
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.42	0.62
1:A:169:LEU:N	2:B:189:GLN:HE22	1.96	0.62
3:F:250:LEU:HB3	3:F:379:MET:CE	2.29	0.62
2:B:428:LYS:HG2	2:B:429:HIS:CD2	2.34	0.62
2:B:161:ILE:CG2	2:B:165:LEU:HD11	2.29	0.62
3:F:232:LYS:O	3:F:236:ILE:HG13	2.00	0.62
2:B:210:GLU:OE1	2:B:212:GLU:HB3	2.00	0.62
3:F:389:PHE:C	3:F:391:ARG:H	2.03	0.62
3:C:156:ILE:HD13	3:C:167:TYR:HD2	1.65	0.62
2:E:161:ILE:C	2:E:163:THR:H	2.02	0.61
1:D:141:ARG:HD2	1:D:185:LEU:HD11	1.82	0.61
3:C:325:ASN:HD22	3:C:325:ASN:C	2.04	0.61
1:D:167:ARG:HG3	1:D:167:ARG:HH11	1.65	0.61
2:E:313:GLU:OE1	2:E:453:LYS:HD2	2.00	0.61
2:B:265:LYS:HE3	2:B:378:TYR:OH	2.01	0.61
3:F:337:ASN:C	3:F:339:CYS:H	2.03	0.61
1:A:186:GLU:C	1:A:188:VAL:H	2.03	0.61
2:E:224:MET:HE2	2:E:237:ARG:HD3	1.82	0.61
3:F:325:ASN:HD22	3:F:325:ASN:C	2.03	0.61
1:A:142:ALA:O	1:A:145:VAL:HB	1.99	0.61
3:C:172:LEU:N	3:C:239:GLN:HE21	1.97	0.61
3:F:365:ASN:ND2	3:F:365:ASN:H	1.86	0.61
3:C:108:ARG:O	3:C:112:GLU:HG3	2.01	0.61
2:B:158:ASN:O	2:B:159:SER:HB3	1.99	0.61
2:E:310:LEU:HB2	2:E:329:PHE:CD2	2.35	0.61
3:C:183:GLU:HB3	3:C:191:TRP:HB2	1.81	0.61
3:C:195:GLN:HE22	3:C:382:THR:HG21	1.66	0.60
2:E:412:PRO:HG3	2:E:450:MET:CE	2.31	0.60
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.83	0.60
2:E:265:LYS:HE3	2:E:378:TYR:OH	2.01	0.60
1:A:155:ASP:HA	1:A:171:ARG:NH1	2.16	0.60
2:B:333:ASN:ND2	2:B:335:ALA:HB3	2.13	0.60
3:C:264:MET:HB2	3:C:279:ALA:CB	2.30	0.60
2:B:402:TRP:HE3	2:B:413:ASN:ND2	1.99	0.60
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.84	0.60
2:E:439:ASN:HD22	2:E:439:ASN:H	1.49	0.60
2:E:264:ARG:NH1	3:F:136:GLN:NE2	2.50	0.60
1:D:132:HIS:HB3	3:F:107:ILE:CD1	2.29	0.60
6:B:470:NDG:H2	6:B:470:NDG:C6	2.31	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:310:LEU:HD22	2:B:329:PHE:CD2	2.37	0.60
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.84	0.60
2:E:181:LYS:O	2:E:184:SER:HB3	2.02	0.60
3:C:305:THR:HB	3:C:341:ALA:HB2	1.83	0.59
6:B:470:NDG:O4	6:I:471:NDG:H1	2.02	0.59
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.02	0.59
3:F:325:ASN:HD21	3:F:327:ALA:HB3	1.66	0.59
3:F:208:TRP:HA	3:F:314:THR:HG21	1.84	0.59
2:E:428:LYS:HG2	2:E:429:HIS:CD2	2.36	0.59
2:B:224:MET:CE	2:B:237:ARG:HD3	2.32	0.59
2:B:167:VAL:O	2:B:170:SER:HB3	2.02	0.59
2:E:333:ASN:HD21	2:E:335:ALA:CB	2.13	0.59
1:D:185:LEU:O	1:D:189:ILE:HG13	2.02	0.59
3:C:250:LEU:HB3	3:C:379:MET:CE	2.32	0.59
3:F:305:THR:HB	3:F:341:ALA:HB2	1.85	0.59
1:D:141:ARG:CD	1:D:185:LEU:HD11	2.33	0.59
3:C:372:TRP:HZ3	3:C:379:MET:HE3	1.67	0.59
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.18	0.59
3:C:103:HIS:HA	3:C:106:SER:HB3	1.85	0.59
1:D:160:SER:HA	2:E:258:GLY:O	2.03	0.59
2:B:412:PRO:HG3	2:B:450:MET:CE	2.33	0.59
2:E:224:MET:CE	2:E:237:ARG:HD3	2.33	0.59
3:C:389:PHE:C	3:C:391:ARG:H	2.06	0.59
3:C:207:ASN:ND2	3:C:210:GLN:HG3	2.18	0.59
3:F:249:GLU:HB3	3:F:383:THR:HG23	1.84	0.59
1:D:152:VAL:HG13	1:D:153:ASP:H	1.68	0.59
2:B:224:MET:HE2	2:B:237:ARG:HD3	1.85	0.58
3:C:153:CYS:HB2	3:C:192:THR:HB	1.85	0.58
1:D:144:LEU:HD23	2:E:175:LEU:HD11	1.85	0.58
3:F:326:CYS:CB	3:F:336:MET:HE2	2.28	0.58
1:D:130:VAL:O	1:D:134:GLN:HB2	2.03	0.58
2:B:439:ASN:ND2	2:B:439:ASN:N	2.51	0.58
3:F:113:ILE:HD13	3:F:114:TYR:N	2.19	0.58
1:D:152:VAL:CG1	1:D:153:ASP:N	2.67	0.58
2:B:223:GLU:HG3	2:B:225:TYR:CE1	2.38	0.58
3:F:113:ILE:HD13	3:F:114:TYR:H	1.68	0.58
2:E:402:TRP:CE3	2:E:413:ASN:ND2	2.70	0.58
3:F:153:CYS:HB2	3:F:192:THR:HB	1.86	0.58
3:C:252:ASP:OD2	3:C:256:ARG:HD3	2.04	0.58
2:E:163:THR:C	2:E:165:LEU:H	2.05	0.58
1:A:136:LEU:HD12	2:B:168:LEU:HD21	1.86	0.58
1:A:141:ARG:HB2	1:A:185:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:196:LYS:CD	3:F:383:THR:HB	2.34	0.57
1:D:126:VAL:O	1:D:129:LYS:HB2	2.04	0.57
5:J:2:HIS:C	5:J:3:ARG:HD3	2.25	0.57
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.04	0.57
2:E:432:ASP:CB	2:E:443:SER:HB3	2.35	0.57
2:E:165:LEU:HD12	2:E:169:ARG:NE	2.19	0.57
2:B:294:LEU:O	2:B:299:ILE:HD11	2.05	0.57
1:D:144:LEU:CD2	2:E:175:LEU:HD11	2.35	0.57
2:E:172:LEU:HB3	3:F:113:ILE:HD11	1.87	0.57
3:C:333:GLY:O	3:C:334:TRP:HB2	2.03	0.57
2:B:397:GLU:HB3	2:B:431:THR:HG21	1.86	0.57
2:B:432:ASP:CB	2:B:443:SER:HB3	2.35	0.57
3:F:333:GLY:O	3:F:334:TRP:HB2	2.04	0.57
1:A:145:VAL:HG12	1:A:146:ASP:N	2.20	0.57
3:F:121:ILE:O	3:F:124:LEU:N	2.38	0.57
1:D:123:LYS:HG2	1:D:123:LYS:O	2.05	0.57
3:F:340:HIS:CE1	4:H:1:GLY:H1	2.21	0.57
2:E:420:GLY:O	2:E:445:TYR:HA	2.04	0.57
3:C:156:ILE:HD13	3:C:167:TYR:CD2	2.39	0.57
2:E:439:ASN:N	2:E:439:ASN:ND2	2.51	0.57
2:B:402:TRP:CE3	2:B:413:ASN:ND2	2.72	0.57
2:B:151:LEU:O	2:B:152:TYR:HB3	2.04	0.57
3:F:108:ARG:O	3:F:112:GLU:HG3	2.04	0.57
3:C:196:LYS:CD	3:C:383:THR:HB	2.35	0.57
2:B:438:MET:O	2:B:440:TRP:N	2.38	0.57
3:F:124:LEU:CD2	3:F:128:VAL:HG23	2.34	0.57
1:D:148:LYS:NZ	2:E:425:ASP:OD2	2.38	0.57
3:C:208:TRP:HA	3:C:314:THR:HG21	1.86	0.57
3:C:326:CYS:CB	3:C:336:MET:HE2	2.25	0.56
2:E:165:LEU:CD1	3:F:110:LEU:HD11	2.34	0.56
3:F:172:LEU:N	3:F:239:GLN:HE21	1.92	0.56
3:F:156:ILE:HD13	3:F:167:TYR:HD2	1.70	0.56
2:E:161:ILE:HG22	3:F:103:HIS:NE2	2.21	0.56
2:E:162:PRO:O	2:E:166:ARG:HG3	2.06	0.56
2:E:171:ILE:HG22	2:E:172:LEU:N	2.19	0.56
3:C:322:PHE:HD1	3:C:338:LYS:HD2	1.70	0.56
2:E:171:ILE:O	2:E:174:ASN:N	2.37	0.56
2:B:439:ASN:H	2:B:439:ASN:HD22	1.51	0.56
3:C:339:CYS:HB2	4:G:1:GLY:O	2.05	0.56
3:F:248:VAL:HB	3:F:260:ALA:HB3	1.88	0.56
1:D:165:CYS:O	2:E:197:CYS:HB3	2.04	0.56
2:E:180:GLN:HA	2:E:180:GLN:HE21	1.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:102:THR:O	3:C:106:SER:N	2.38	0.56
1:A:152:VAL:HG21	2:B:426:MET:HG2	1.87	0.56
3:C:365:ASN:N	3:C:365:ASN:ND2	2.50	0.56
3:C:117:ASN:C	3:C:121:ILE:HG13	2.26	0.56
2:E:249:TRP:CZ3	2:E:455:ARG:HB2	2.41	0.56
1:D:185:LEU:CD1	1:D:186:GLU:HG3	2.36	0.56
1:D:150:LEU:HD11	1:D:154:ILE:HD11	1.86	0.56
2:E:170:SER:HA	2:E:173:GLU:CD	2.26	0.56
2:E:351:ASN:ND2	2:E:354:MET:HB2	2.21	0.56
2:B:255:ARG:NH1	2:B:413:ASN:HA	2.21	0.56
2:B:166:ARG:HH11	2:B:166:ARG:CB	2.13	0.55
2:B:162:PRO:HA	2:B:165:LEU:HD12	1.88	0.55
2:E:255:ARG:NH1	2:E:413:ASN:HA	2.21	0.55
2:E:402:TRP:HE3	2:E:413:ASN:HD22	1.54	0.55
2:B:351:ASN:HD21	2:B:354:MET:HB2	1.72	0.55
2:E:212:GLU:O	2:E:215:ILE:HG22	2.07	0.55
1:D:152:VAL:CG1	1:D:153:ASP:H	2.19	0.55
2:B:406:ARG:NE	5:I:3:ARG:O	2.40	0.55
6:E:570:NDG:O6	5:J:4:PRO:HB3	2.06	0.55
3:C:340:HIS:O	4:G:1:GLY:HA2	2.06	0.55
3:F:389:PHE:O	3:F:391:ARG:N	2.37	0.55
2:B:333:ASN:HD21	2:B:335:ALA:CB	2.15	0.55
3:F:156:ILE:HD13	3:F:167:TYR:CD2	2.41	0.55
2:B:410:ALA:HB1	2:B:437:TRP:CE3	2.42	0.55
2:E:351:ASN:C	2:E:351:ASN:ND2	2.56	0.55
4:H:2:PRO:O	4:H:3:ARG:NH1	2.40	0.55
3:F:251:GLU:OE1	3:F:381:LYS:HD2	2.07	0.55
1:D:147:MET:SD	2:E:179:ILE:HD11	2.47	0.55
3:C:253:TRP:CH2	3:C:350:GLN:HA	2.41	0.55
3:F:100:ILE:O	3:F:100:ILE:HG22	2.05	0.55
2:B:249:TRP:CZ3	2:B:455:ARG:HB2	2.41	0.55
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.07	0.55
2:E:294:LEU:O	2:E:299:ILE:HD11	2.06	0.55
2:E:255:ARG:HH11	2:E:255:ARG:HG3	1.72	0.55
2:E:438:MET:O	2:E:440:TRP:N	2.39	0.55
3:C:198:LEU:HD12	3:C:199:ASP:N	2.22	0.55
2:B:251:VAL:HB	2:B:292:TYR:OH	2.08	0.55
2:E:271:GLN:HA	2:E:271:GLN:HE21	1.72	0.55
2:B:351:ASN:C	2:B:351:ASN:ND2	2.56	0.54
3:C:251:GLU:OE1	3:C:381:LYS:HD2	2.08	0.54
3:F:253:TRP:CH2	3:F:350:GLN:HA	2.42	0.54
1:A:165:CYS:HA	2:B:196:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:SER:HA	2:B:258:GLY:O	2.07	0.54
2:E:410:ALA:HB1	2:E:437:TRP:CE3	2.42	0.54
3:C:127:LYS:O	3:C:130:GLN:HB2	2.06	0.54
6:B:470:NDG:H2	6:B:470:NDG:H6C1	1.88	0.54
3:F:109:TYR:HA	3:F:112:GLU:OE2	2.08	0.54
2:E:186:VAL:C	2:E:188:ALA:N	2.61	0.54
2:B:264:ARG:NH2	3:C:136:GLN:O	2.40	0.54
3:F:252:ASP:OD2	3:F:256:ARG:HD3	2.06	0.54
3:F:340:HIS:CE1	4:H:1:GLY:H2	2.26	0.54
2:B:255:ARG:HG3	2:B:255:ARG:HH11	1.73	0.54
3:F:172:LEU:HG	3:F:173:LYS:N	2.22	0.54
3:F:195:GLN:HE22	3:F:382:THR:HG21	1.72	0.54
1:A:144:LEU:CD2	2:B:175:LEU:HD11	2.38	0.54
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.08	0.54
2:E:186:VAL:C	2:E:188:ALA:H	2.10	0.54
2:B:197:CYS:O	3:C:139:CYS:HB3	2.08	0.54
3:C:250:LEU:HB3	3:C:379:MET:HE2	1.89	0.54
2:B:332:GLN:O	2:B:338:TYR:HA	2.08	0.54
1:D:183:LYS:C	1:D:185:LEU:N	2.60	0.54
1:D:127:ILE:C	1:D:129:LYS:H	2.09	0.54
2:B:424:TRP:C	2:B:426:MET:H	2.11	0.54
2:E:189:GLN:HA	2:E:189:GLN:NE2	2.22	0.54
3:F:117:ASN:C	3:F:119:GLN:N	2.61	0.54
2:B:325:HIS:O	2:B:345:TYR:HA	2.07	0.54
3:C:389:PHE:O	3:C:391:ARG:N	2.39	0.54
3:C:172:LEU:HG	3:C:173:LYS:HG3	1.89	0.54
2:E:424:TRP:C	2:E:426:MET:H	2.12	0.54
2:E:332:GLN:O	2:E:338:TYR:HA	2.08	0.54
2:E:255:ARG:HG3	2:E:255:ARG:NH1	2.23	0.54
2:E:340:ILE:HD12	2:E:403:TRP:CE3	2.43	0.54
5:I:2:HIS:O	5:I:3:ARG:HD3	2.08	0.53
2:B:364:ASN:HD21	6:B:470:NDG:C6	2.18	0.53
2:E:283:LYS:HD2	2:E:283:LYS:H	1.72	0.53
2:B:373:MET:HE2	2:B:404:TYR:O	2.08	0.53
3:F:264:MET:CB	3:F:279:ALA:HB2	2.36	0.53
2:B:255:ARG:HG3	2:B:255:ARG:NH1	2.23	0.53
2:E:204:PRO:HG3	3:F:217:HIS:CD2	2.43	0.53
2:E:168:LEU:N	2:E:168:LEU:HD22	2.23	0.53
2:B:420:GLY:O	2:B:445:TYR:HA	2.07	0.53
3:F:248:VAL:HG12	3:F:250:LEU:HD13	1.90	0.53
2:B:264:ARG:HD2	2:B:273:PHE:CE2	2.43	0.53
2:B:439:ASN:H	2:B:439:ASN:ND2	2.06	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:255:ARG:HD3	2:E:262:PHE:CE1	2.43	0.53
3:F:248:VAL:HG12	3:F:250:LEU:CD1	2.39	0.53
1:A:126:VAL:C	1:A:128:GLU:N	2.61	0.53
2:B:351:ASN:CG	2:B:354:MET:HB2	2.28	0.53
3:C:248:VAL:HG12	3:C:250:LEU:CD1	2.38	0.53
3:C:110:LEU:O	3:C:113:ILE:HB	2.09	0.53
3:C:363:TYR:HB3	4:G:3:ARG:NH2	2.23	0.53
3:C:107:ILE:C	3:C:107:ILE:HD13	2.29	0.53
3:C:209:ILE:O	3:C:212:LYS:HB3	2.09	0.53
3:F:207:ASN:ND2	3:F:210:GLN:HG3	2.23	0.53
1:D:183:LYS:C	1:D:185:LEU:H	2.12	0.53
2:E:439:ASN:H	2:E:439:ASN:ND2	2.06	0.53
2:E:228:GLN:OE1	3:F:176:GLN:HG3	2.09	0.53
2:E:199:VAL:O	3:F:141:ASP:HA	2.09	0.53
3:C:107:ILE:CG2	3:C:108:ARG:H	2.21	0.52
2:B:390:PRO:O	2:B:393:GLN:HG3	2.09	0.52
3:C:337:ASN:C	3:C:339:CYS:N	2.61	0.52
2:B:283:LYS:HE3	2:B:283:LYS:CA	2.33	0.52
2:E:325:HIS:O	2:E:345:TYR:HA	2.10	0.52
3:C:172:LEU:HG	3:C:173:LYS:N	2.23	0.52
3:F:250:LEU:HB3	3:F:379:MET:HE2	1.89	0.52
3:C:248:VAL:HG12	3:C:250:LEU:HD13	1.92	0.52
2:B:402:TRP:HE3	2:B:413:ASN:HD22	1.58	0.52
2:E:153:ILE:HG22	2:E:153:ILE:O	2.09	0.52
3:F:195:GLN:OE1	3:F:382:THR:CG2	2.57	0.52
2:B:271:GLN:HA	2:B:271:GLN:HE21	1.73	0.52
2:B:340:ILE:HD12	2:B:403:TRP:CE3	2.44	0.52
2:E:351:ASN:HD21	2:E:354:MET:HB2	1.75	0.52
2:E:390:PRO:O	2:E:393:GLN:HG3	2.10	0.52
2:B:386:LEU:O	2:B:387:THR:HG23	2.10	0.52
3:C:338:LYS:O	3:C:339:CYS:HB2	2.10	0.52
3:C:117:ASN:O	3:C:118:ASN:C	2.47	0.52
2:B:255:ARG:HD3	2:B:262:PHE:CE1	2.44	0.52
3:F:172:LEU:HG	3:F:173:LYS:HG3	1.91	0.51
3:F:153:CYS:CB	3:F:192:THR:HB	2.40	0.51
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.45	0.51
2:E:205:VAL:HG21	3:F:215:PHE:O	2.10	0.51
3:F:307:HIS:CE1	3:F:342:GLY:H	2.28	0.51
2:E:436:VAL:HG22	2:E:445:TYR:O	2.10	0.51
3:F:198:LEU:HD12	3:F:199:ASP:N	2.25	0.51
2:E:161:ILE:C	2:E:163:THR:N	2.64	0.51
1:D:147:MET:CE	2:E:179:ILE:HG12	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:212:GLU:HG3	2:B:213:GLU:N	2.25	0.51
3:F:325:ASN:ND2	3:F:325:ASN:C	2.64	0.51
3:F:325:ASN:O	3:F:329:GLN:HG3	2.11	0.51
2:E:421:GLN:HE21	2:E:421:GLN:HA	1.75	0.51
2:B:204:PRO:HG3	3:C:217:HIS:CD2	2.45	0.51
2:B:164:ASN:O	2:B:168:LEU:HB2	2.10	0.51
2:E:455:ARG:HG3	2:E:456:PRO:HD2	1.92	0.51
3:F:273:LYS:HG3	3:F:319:ASN:ND2	2.25	0.51
2:B:422:TYR:HE1	2:B:444:TRP:HA	1.74	0.51
3:C:153:CYS:CB	3:C:192:THR:HB	2.40	0.51
3:F:275:ARG:HA	3:F:311:GLN:HA	1.93	0.51
3:C:109:TYR:O	3:C:112:GLU:HB2	2.11	0.51
2:E:251:VAL:HB	2:E:292:TYR:OH	2.11	0.51
2:B:384:GLY:H	2:B:405:ASN:HA	1.76	0.51
2:E:264:ARG:HD2	2:E:273:PHE:CE2	2.46	0.51
3:F:337:ASN:C	3:F:339:CYS:N	2.64	0.51
2:E:186:VAL:O	2:E:188:ALA:N	2.44	0.51
1:D:148:LYS:HD3	2:E:425:ASP:O	2.11	0.51
1:D:177:ASP:O	1:D:180:ASP:HB2	2.11	0.51
3:C:195:GLN:OE1	3:C:382:THR:CG2	2.60	0.50
3:C:275:ARG:HA	3:C:311:GLN:HA	1.93	0.50
3:C:304:PHE:CD1	3:C:338:LYS:HB2	2.47	0.50
2:E:343:ASN:OD1	2:E:344:LYS:HG3	2.12	0.50
3:C:199:ASP:OD1	3:C:201:SER:N	2.44	0.50
2:B:406:ARG:O	2:B:407:CYS:HB2	2.10	0.50
2:E:307:PRO:O	2:E:456:PRO:O	2.29	0.50
3:F:197:ARG:CZ	3:F:367:ILE:HD11	2.41	0.50
3:C:248:VAL:HB	3:C:260:ALA:HB3	1.91	0.50
3:F:365:ASN:ND2	3:F:365:ASN:N	2.50	0.50
2:B:169:ARG:O	2:B:170:SER:C	2.50	0.50
2:E:406:ARG:O	2:E:407:CYS:HB2	2.11	0.50
3:F:128:VAL:O	3:F:131:LEU:HB3	2.12	0.50
1:A:148:LYS:NZ	2:B:425:ASP:OD2	2.44	0.50
3:F:304:PHE:CD1	3:F:338:LYS:HB2	2.47	0.50
1:A:188:VAL:HG12	1:A:188:VAL:O	2.12	0.50
2:E:262:PHE:CD2	2:E:413:ASN:HA	2.47	0.50
1:A:136:LEU:HD12	2:B:168:LEU:HD11	1.94	0.50
2:E:283:LYS:CA	2:E:283:LYS:HE3	2.34	0.50
1:A:165:CYS:O	2:B:197:CYS:HB3	2.12	0.50
3:C:97:GLU:HB3	3:C:100:ILE:HD11	1.93	0.50
3:F:199:ASP:OD1	3:F:201:SER:N	2.45	0.50
3:F:322:PHE:HD1	3:F:338:LYS:HD2	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:307:PRO:O	2:B:456:PRO:O	2.29	0.50
3:F:196:LYS:HD2	3:F:382:THR:O	2.12	0.50
3:C:194:PHE:HA	3:C:228:LEU:HB2	1.94	0.50
2:B:283:LYS:HD2	2:B:283:LYS:H	1.77	0.49
2:E:154:ASP:HB3	3:F:97:GLU:OE1	2.12	0.49
2:E:171:ILE:O	2:E:173:GLU:N	2.45	0.49
2:E:172:LEU:O	2:E:176:ARG:HB3	2.13	0.49
2:B:455:ARG:HG3	2:B:456:PRO:HD2	1.93	0.49
3:C:325:ASN:O	3:C:329:GLN:HG3	2.11	0.49
2:B:343:ASN:OD1	2:B:344:LYS:HG3	2.12	0.49
6:B:470:NDG:O3	6:I:471:NDG:H8C3	2.12	0.49
2:E:212:GLU:HG3	2:E:213:GLU:N	2.27	0.49
2:E:415:ARG:N	2:E:434:GLY:HA2	2.25	0.49
3:F:209:ILE:O	3:F:212:LYS:HB3	2.12	0.49
2:B:259:SER:OG	2:B:291:GLU:HG3	2.12	0.49
1:A:141:ARG:HB2	1:A:185:LEU:CD1	2.42	0.49
2:E:215:ILE:HB	2:E:242:MET:HE1	1.93	0.49
2:B:159:SER:OG	2:B:160:ASN:N	2.45	0.49
2:E:351:ASN:CG	2:E:354:MET:HB2	2.31	0.49
1:A:135:LEU:HD13	1:A:135:LEU:C	2.32	0.49
2:E:373:MET:HE2	2:E:404:TYR:O	2.12	0.49
3:C:325:ASN:ND2	3:C:325:ASN:C	2.65	0.49
2:E:384:GLY:H	2:E:405:ASN:HA	1.77	0.49
2:B:255:ARG:HH12	2:B:413:ASN:CA	2.26	0.49
1:D:171:ARG:HG3	1:D:171:ARG:HH11	1.78	0.49
1:D:136:LEU:HD13	3:F:110:LEU:HB3	1.95	0.49
2:B:177:SER:O	2:B:180:GLN:HG2	2.12	0.49
2:E:373:MET:HG3	2:E:405:ASN:CB	2.36	0.49
2:E:364:ASN:HD21	6:E:570:NDG:C6	2.26	0.49
3:C:251:GLU:HG3	3:C:257:THR:CG2	2.40	0.49
3:C:178:PHE:CD2	3:C:232:LYS:HD3	2.48	0.49
2:B:229:PRO:HG2	2:B:230:ASP:H	1.78	0.49
2:B:204:PRO:HA	3:C:216:GLY:O	2.12	0.49
1:A:162:ARG:HA	1:A:168:ALA:HB2	1.93	0.49
3:C:320:ASP:C	3:C:322:PHE:H	2.16	0.49
2:B:325:HIS:CB	2:B:346:ARG:HB2	2.43	0.49
3:C:307:HIS:CE1	3:C:342:GLY:H	2.31	0.49
1:D:122:LEU:HD12	1:D:122:LEU:C	2.34	0.49
3:C:196:LYS:HD2	3:C:382:THR:O	2.12	0.49
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.95	0.49
2:B:304:ARG:CB	2:B:304:ARG:HH11	2.26	0.49
1:A:133:ILE:CD1	3:C:107:ILE:HG13	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:251:GLU:HG3	3:F:257:THR:CG2	2.42	0.49
2:B:212:GLU:O	2:B:215:ILE:HG22	2.12	0.49
3:F:307:HIS:HE1	3:F:341:ALA:N	1.99	0.48
3:F:193:VAL:HG22	3:F:385:LYS:HB3	1.95	0.48
3:F:275:ARG:HA	3:F:310:MET:O	2.13	0.48
3:F:229:GLY:O	3:F:233:ILE:HG13	2.13	0.48
2:B:174:ASN:O	2:B:177:SER:HB2	2.13	0.48
3:F:194:PHE:HA	3:F:228:LEU:HB2	1.95	0.48
2:B:368:THR:HB	2:B:409:ALA:HB2	1.95	0.48
2:B:153:ILE:C	2:B:155:GLU:H	2.16	0.48
3:C:207:ASN:C	3:C:207:ASN:OD1	2.51	0.48
3:C:207:ASN:OD1	3:C:209:ILE:N	2.47	0.48
2:E:156:THR:C	2:E:158:ASN:H	2.17	0.48
3:F:288:ASP:OD1	3:F:288:ASP:C	2.52	0.48
2:E:255:ARG:NH1	2:E:413:ASN:CA	2.77	0.48
1:D:161:CYS:SG	1:D:165:CYS:SG	3.11	0.48
2:E:386:LEU:O	2:E:387:THR:HG23	2.13	0.48
1:D:127:ILE:C	1:D:129:LYS:N	2.66	0.48
3:C:273:LYS:HG3	3:C:319:ASN:ND2	2.28	0.48
1:A:124:ARG:N	1:A:124:ARG:HD2	2.29	0.48
3:F:389:PHE:C	3:F:391:ARG:N	2.67	0.48
3:F:239:GLN:O	3:F:241:ALA:N	2.46	0.48
2:B:407:CYS:HB2	5:I:1:GLY:O	2.13	0.48
3:C:114:TYR:O	3:C:117:ASN:HB2	2.13	0.48
2:B:262:PHE:CD2	2:B:413:ASN:HA	2.49	0.48
2:B:264:ARG:HD2	2:B:273:PHE:CZ	2.48	0.48
2:E:421:GLN:HA	2:E:421:GLN:NE2	2.27	0.48
2:E:325:HIS:CB	2:E:346:ARG:HB2	2.43	0.48
1:A:133:ILE:O	1:A:136:LEU:HB3	2.14	0.48
2:E:383:ASP:HA	2:E:404:TYR:O	2.12	0.48
2:B:255:ARG:NH1	2:B:413:ASN:CA	2.76	0.48
2:B:375:PHE:CE2	2:B:402:TRP:HA	2.48	0.48
3:C:372:TRP:HZ3	3:C:379:MET:CE	2.27	0.48
2:E:170:SER:HA	2:E:173:GLU:OE1	2.14	0.48
3:C:113:ILE:O	3:C:116:SER:N	2.47	0.48
1:D:156:ILE:O	1:D:157:LYS:C	2.49	0.48
1:D:171:ARG:HG3	1:D:171:ARG:NH1	2.29	0.48
2:E:217:LYS:HG2	3:F:213:GLU:HG3	1.96	0.48
2:E:171:ILE:C	2:E:173:GLU:N	2.67	0.48
1:A:136:LEU:C	1:A:136:LEU:CD1	2.82	0.48
2:B:384:GLY:N	2:B:406:ARG:H	2.12	0.48
6:B:470:NDG:C2	6:B:470:NDG:C6	2.92	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:375:PHE:CE2	2:E:402:TRP:HA	2.48	0.48
1:D:185:LEU:HD13	1:D:186:GLU:N	2.29	0.48
2:E:259:SER:OG	2:E:291:GLU:HG3	2.14	0.48
2:E:171:ILE:C	2:E:173:GLU:H	2.17	0.48
1:A:140:VAL:HG23	1:A:141:ARG:N	2.28	0.48
2:E:384:GLY:H	2:E:406:ARG:H	1.62	0.48
1:A:186:GLU:HA	1:A:189:ILE:HD13	1.96	0.48
2:E:255:ARG:HH12	2:E:413:ASN:CA	2.27	0.48
1:D:151:GLU:HG3	2:E:182:LEU:HD11	1.96	0.48
1:D:147:MET:HE1	2:E:179:ILE:HG12	1.96	0.48
2:E:198:THR:HG22	3:F:140:LYS:HB3	1.95	0.48
1:A:169:LEU:CD1	1:A:171:ARG:HB3	2.43	0.47
2:B:191:GLU:C	2:B:193:CYS:N	2.66	0.47
2:B:415:ARG:N	2:B:434:GLY:HA2	2.28	0.47
2:B:436:VAL:HG22	2:B:445:TYR:O	2.14	0.47
2:B:384:GLY:H	2:B:406:ARG:H	1.62	0.47
2:E:264:ARG:HD2	2:E:273:PHE:CZ	2.50	0.47
3:C:193:VAL:HG22	3:C:385:LYS:HB3	1.96	0.47
2:E:374:PHE:O	2:E:403:TRP:HA	2.14	0.47
2:E:167:VAL:O	2:E:169:ARG:N	2.47	0.47
2:E:165:LEU:HD12	2:E:169:ARG:NH2	2.30	0.47
3:C:240:SER:OG	3:C:242:ILE:HD11	2.14	0.47
2:E:368:THR:HB	2:E:409:ALA:HB2	1.95	0.47
2:B:438:MET:C	2:B:440:TRP:H	2.18	0.47
2:B:264:ARG:HH22	3:C:136:GLN:C	2.17	0.47
3:C:269:PRO:O	3:C:271:ALA:N	2.47	0.47
3:F:185:ASP:OD2	3:F:189:ASN:HB2	2.14	0.47
2:B:160:ASN:O	2:B:161:ILE:C	2.51	0.47
1:A:178:TYR:O	1:A:182:GLN:HG2	2.14	0.47
3:C:229:GLY:O	3:C:233:ILE:HG13	2.15	0.47
2:B:421:GLN:HE21	2:B:421:GLN:HA	1.80	0.47
2:E:167:VAL:O	2:E:170:SER:N	2.47	0.47
3:C:207:ASN:HD21	3:C:210:GLN:HG3	1.80	0.47
1:D:144:LEU:HD23	2:E:175:LEU:CD1	2.43	0.47
2:E:384:GLY:N	2:E:406:ARG:H	2.12	0.47
3:F:343:HIS:O	3:F:367:ILE:HA	2.15	0.47
2:E:182:LEU:C	2:E:184:SER:N	2.67	0.47
3:C:378:SER:O	3:C:379:MET:O	2.33	0.47
3:C:126:GLU:O	3:C:129:ALA:N	2.46	0.47
1:A:133:ILE:HG22	1:A:134:GLN:N	2.30	0.47
3:C:114:TYR:CE2	3:C:118:ASN:ND2	2.83	0.47
1:D:159:ARG:HG2	2:E:258:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:334:TRP:NE1	3:C:342:GLY:O	2.47	0.47
3:C:149:THR:CG2	3:C:150:GLY:H	2.24	0.47
2:E:438:MET:C	2:E:440:TRP:H	2.19	0.47
2:E:229:PRO:HG2	2:E:230:ASP:H	1.79	0.47
3:F:209:ILE:HG13	3:F:209:ILE:H	1.52	0.47
2:E:217:LYS:CG	3:F:213:GLU:HG3	2.45	0.47
3:F:338:LYS:O	3:F:339:CYS:HB2	2.14	0.47
3:F:295:PHE:CD2	4:H:2:PRO:HD3	2.50	0.47
3:C:107:ILE:CG2	3:C:108:ARG:N	2.76	0.47
3:C:156:ILE:HG21	3:C:167:TYR:CD2	2.50	0.47
2:E:189:GLN:HA	2:E:189:GLN:HE21	1.79	0.47
3:C:372:TRP:CZ3	3:C:379:MET:CE	2.98	0.47
2:B:171:ILE:HD12	2:B:172:LEU:CA	2.45	0.46
2:B:159:SER:O	2:B:163:THR:HG23	2.14	0.46
3:F:378:SER:O	3:F:379:MET:O	2.33	0.46
2:E:203:ILE:O	3:F:218:LEU:N	2.40	0.46
2:B:171:ILE:CG1	2:B:172:LEU:N	2.78	0.46
2:B:435:VAL:HG12	2:B:447:MET:HG2	1.95	0.46
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.50	0.46
3:C:372:TRP:CE3	3:C:379:MET:HE1	2.50	0.46
2:B:374:PHE:O	2:B:403:TRP:HA	2.15	0.46
1:D:185:LEU:HD13	1:D:186:GLU:HG3	1.97	0.46
2:B:203:ILE:O	3:C:218:LEU:N	2.38	0.46
2:B:321:LYS:O	2:B:322:VAL:HG13	2.16	0.46
3:F:330:ASP:OD2	3:F:340:HIS:NE2	2.48	0.46
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.97	0.46
3:C:122:VAL:O	3:C:123:ASN:C	2.54	0.46
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.75	0.46
3:F:196:LYS:HD3	3:F:383:THR:HB	1.96	0.46
3:F:314:THR:O	3:F:315:TRP:C	2.53	0.46
3:F:320:ASP:C	3:F:322:PHE:H	2.18	0.46
3:C:389:PHE:C	3:C:391:ARG:N	2.69	0.46
1:D:120:GLU:O	1:D:122:LEU:N	2.49	0.46
2:B:213:GLU:O	2:B:216:ARG:HB2	2.16	0.46
2:B:260:VAL:CG2	2:B:291:GLU:HB2	2.46	0.46
2:E:304:ARG:CB	2:E:304:ARG:HH11	2.28	0.46
2:B:211:CYS:SG	2:B:250:THR:HA	2.56	0.46
3:F:121:ILE:HG22	3:F:122:VAL:N	2.31	0.46
3:F:127:LYS:O	3:F:131:LEU:N	2.46	0.46
3:F:126:GLU:O	3:F:129:ALA:HB3	2.14	0.46
2:E:258:GLY:O	2:E:260:VAL:N	2.49	0.46
1:D:164:SER:HA	3:F:137:GLU:O	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:LEU:C	1:A:169:LEU:HD13	2.37	0.46
3:C:343:HIS:O	3:C:367:ILE:HA	2.16	0.46
2:B:265:LYS:O	2:B:268:PRO:HD2	2.16	0.46
2:E:435:VAL:HG12	2:E:447:MET:HG2	1.97	0.46
2:B:421:GLN:NE2	2:B:421:GLN:HA	2.31	0.46
2:B:405:ASN:C	2:B:407:CYS:N	2.68	0.45
3:C:149:THR:CG2	3:C:150:GLY:N	2.78	0.45
3:C:264:MET:CB	3:C:279:ALA:HB2	2.43	0.45
1:A:159:ARG:HB2	1:A:159:ARG:CZ	2.46	0.45
2:B:168:LEU:HD23	3:C:110:LEU:HD12	1.97	0.45
2:E:405:ASN:C	2:E:407:CYS:N	2.66	0.45
2:B:407:CYS:SG	5:I:3:ARG:CZ	3.04	0.45
5:I:2:HIS:CD2	5:I:4:PRO:HD3	2.51	0.45
2:E:422:TYR:HE1	2:E:444:TRP:HA	1.76	0.45
2:B:351:ASN:HD21	2:B:354:MET:CB	2.28	0.45
2:B:170:SER:OG	2:B:171:ILE:N	2.45	0.45
2:E:249:TRP:HE3	2:E:454:ILE:O	1.99	0.45
2:E:166:ARG:CZ	2:E:166:ARG:HB3	2.47	0.45
3:C:117:ASN:HB3	3:C:121:ILE:HD11	1.97	0.45
2:B:455:ARG:CG	2:B:456:PRO:HD2	2.46	0.45
2:E:455:ARG:CG	2:E:456:PRO:HD2	2.46	0.45
3:C:197:ARG:CZ	3:C:367:ILE:HD11	2.46	0.45
3:F:197:ARG:HG2	3:F:382:THR:CG2	2.46	0.45
3:F:242:ILE:CD1	3:F:242:ILE:H	2.29	0.45
3:F:178:PHE:CD2	3:F:232:LYS:HD3	2.52	0.45
2:E:182:LEU:O	2:E:183:GLU:C	2.53	0.45
5:J:2:HIS:O	5:J:3:ARG:HD3	2.17	0.45
3:C:288:ASP:C	3:C:288:ASP:OD1	2.54	0.45
3:C:197:ARG:HG2	3:C:382:THR:CG2	2.47	0.45
3:F:140:LYS:HA	3:F:140:LYS:HD2	1.79	0.45
2:E:253:GLN:NE2	2:E:452:MET:HG3	2.31	0.45
1:A:136:LEU:HD13	1:A:136:LEU:O	2.16	0.45
2:E:228:GLN:OE1	3:F:176:GLN:CG	2.63	0.45
3:F:250:LEU:HD23	3:F:379:MET:HE1	1.98	0.45
3:C:361:ASN:O	3:C:363:TYR:N	2.50	0.45
2:E:316:ASP:OD1	2:E:318:LYS:N	2.49	0.45
2:B:316:ASP:OD1	2:B:318:LYS:N	2.49	0.45
1:A:120:GLU:O	1:A:122:LEU:N	2.45	0.45
2:E:283:LYS:HD2	2:E:283:LYS:N	2.32	0.45
2:E:213:GLU:O	2:E:216:ARG:HB2	2.17	0.45
3:F:372:TRP:CZ3	3:F:379:MET:CE	2.99	0.45
3:F:361:ASN:O	3:F:363:TYR:N	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:239:GLN:O	3:C:241:ALA:N	2.50	0.45
2:B:188:ALA:O	2:B:191:GLU:HB3	2.17	0.45
2:B:215:ILE:HB	2:B:242:MET:HE1	1.98	0.45
3:C:259:THR:O	3:C:286:ALA:HB3	2.17	0.45
2:E:161:ILE:HA	2:E:164:ASN:HB2	1.99	0.45
2:B:214:ILE:HD11	2:B:227:ILE:HG22	1.98	0.45
3:C:281:PHE:CE2	3:C:283:GLY:HA2	2.52	0.45
2:E:321:LYS:O	2:E:322:VAL:HG13	2.16	0.45
2:E:178:LYS:HG2	2:E:178:LYS:O	2.17	0.45
3:C:225:GLU:O	3:C:226:PHE:HB3	2.17	0.45
3:F:269:PRO:O	3:F:271:ALA:N	2.50	0.45
2:E:407:CYS:HB2	5:J:1:GLY:O	2.16	0.45
6:B:470:NDG:H4	6:I:471:NDG:C1	2.45	0.45
2:B:412:PRO:C	2:B:414:GLY:N	2.71	0.45
2:E:193:CYS:C	2:E:195:THR:N	2.69	0.45
2:B:171:ILE:HA	2:B:174:ASN:HB3	1.97	0.44
2:E:215:ILE:HB	2:E:242:MET:CE	2.46	0.44
2:B:265:LYS:C	2:B:268:PRO:HD2	2.36	0.44
3:C:317:ASN:ND2	3:C:319:ASN:OD1	2.50	0.44
1:D:176:LYS:O	1:D:179:GLU:N	2.50	0.44
2:B:326:TYR:O	2:B:328:GLY:N	2.49	0.44
2:E:163:THR:C	2:E:165:LEU:N	2.71	0.44
3:C:185:ASP:OD2	3:C:189:ASN:HB2	2.17	0.44
3:C:156:ILE:HG22	3:C:161:ALA:HB3	1.98	0.44
3:F:149:THR:CG2	3:F:150:GLY:N	2.77	0.44
2:B:249:TRP:CE3	2:B:455:ARG:HB2	2.52	0.44
2:B:173:GLU:O	2:B:176:ARG:HB3	2.17	0.44
2:E:255:ARG:O	2:E:449:LYS:HA	2.17	0.44
2:B:255:ARG:O	2:B:449:LYS:HA	2.17	0.44
4:H:2:PRO:O	4:H:3:ARG:HG2	2.18	0.44
3:C:307:HIS:HE1	3:C:341:ALA:N	1.98	0.44
2:E:394:CYS:O	2:E:397:GLU:O	2.35	0.44
2:E:412:PRO:C	2:E:414:GLY:N	2.70	0.44
2:B:264:ARG:HH22	3:C:136:GLN:CA	2.30	0.44
1:D:135:LEU:O	1:D:136:LEU:C	2.55	0.44
1:A:130:VAL:O	1:A:133:ILE:HB	2.17	0.44
3:C:166:LEU:C	3:C:167:TYR:CD1	2.91	0.44
1:A:128:GLU:OE2	1:A:132:HIS:HD2	2.00	0.44
3:F:207:ASN:OD1	3:F:209:ILE:N	2.51	0.44
2:E:326:TYR:O	2:E:328:GLY:N	2.49	0.44
3:F:207:ASN:OD1	3:F:207:ASN:C	2.55	0.44
3:F:240:SER:OG	3:F:242:ILE:HD11	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:140:LYS:HD2	3:C:140:LYS:HA	1.82	0.44
3:C:121:ILE:O	3:C:121:ILE:HG22	2.18	0.44
2:B:302:LEU:CD1	2:B:454:ILE:HD11	2.45	0.44
3:C:126:GLU:O	3:C:127:LYS:C	2.56	0.44
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.77	0.44
3:F:259:THR:O	3:F:286:ALA:HB3	2.17	0.44
3:C:330:ASP:OD2	3:C:340:HIS:NE2	2.50	0.44
2:B:351:ASN:O	2:B:351:ASN:ND2	2.51	0.44
2:B:284:ASN:N	2:B:284:ASN:ND2	2.56	0.44
3:F:156:ILE:HG22	3:F:161:ALA:HB3	2.00	0.44
3:F:156:ILE:HG21	3:F:167:TYR:CD2	2.53	0.44
1:A:165:CYS:HB3	2:B:193:CYS:HA	1.99	0.44
2:E:342:VAL:O	2:E:343:ASN:HB3	2.18	0.43
3:C:249:GLU:O	3:C:383:THR:HG23	2.17	0.43
3:C:275:ARG:HA	3:C:310:MET:O	2.17	0.43
1:A:150:LEU:O	1:A:151:GLU:C	2.56	0.43
1:D:184:GLN:O	1:D:188:VAL:HG23	2.17	0.43
2:E:251:VAL:C	2:E:252:ILE:HD12	2.39	0.43
3:C:196:LYS:HD3	3:C:383:THR:HB	2.00	0.43
3:F:317:ASN:ND2	3:F:319:ASN:OD1	2.52	0.43
2:B:434:GLY:O	2:B:436:VAL:N	2.51	0.43
2:B:340:ILE:HD12	2:B:403:TRP:CD2	2.53	0.43
2:E:351:ASN:HD21	2:E:354:MET:CB	2.31	0.43
2:B:394:CYS:O	2:B:397:GLU:O	2.36	0.43
3:F:197:ARG:NH2	3:F:367:ILE:HD11	2.33	0.43
2:E:415:ARG:H	2:E:434:GLY:CA	2.26	0.43
1:D:151:GLU:HG3	2:E:182:LEU:CD1	2.49	0.43
2:B:259:SER:HG	2:B:291:GLU:HG3	1.83	0.43
2:B:360:LEU:HD12	2:B:368:THR:HG21	1.98	0.43
1:D:119:ILE:HG12	1:D:123:LYS:HD3	2.00	0.43
3:C:295:PHE:CD2	4:G:2:PRO:HD3	2.53	0.43
2:E:345:TYR:CG	2:E:351:ASN:HB2	2.54	0.43
1:D:186:GLU:HA	1:D:189:ILE:HB	2.00	0.43
2:E:182:LEU:O	2:E:184:SER:N	2.51	0.43
2:E:340:ILE:HD12	2:E:403:TRP:CD2	2.54	0.43
3:C:281:PHE:HB2	3:C:288:ASP:OD2	2.17	0.43
2:E:242:MET:HA	2:E:247:GLY:HA3	2.01	0.43
2:E:412:PRO:C	2:E:414:GLY:H	2.22	0.43
2:E:434:GLY:O	2:E:436:VAL:N	2.52	0.43
3:F:249:GLU:O	3:F:383:THR:HG23	2.19	0.43
3:C:339:CYS:O	3:C:340:HIS:HB3	2.19	0.43
2:E:167:VAL:O	2:E:168:LEU:C	2.56	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:342:VAL:O	2:B:343:ASN:HB3	2.18	0.43
1:D:129:LYS:HA	1:D:132:HIS:HB2	2.00	0.43
2:B:420:GLY:HA2	2:B:446:SER:O	2.18	0.43
2:E:211:CYS:SG	2:E:250:THR:HA	2.58	0.43
2:E:168:LEU:CB	3:F:110:LEU:HD13	2.49	0.43
2:B:171:ILE:O	2:B:174:ASN:N	2.52	0.43
2:E:284:ASN:N	2:E:284:ASN:ND2	2.58	0.43
2:E:214:ILE:HD11	2:E:227:ILE:HG22	2.00	0.43
2:B:212:GLU:O	2:B:213:GLU:C	2.56	0.43
1:D:157:LYS:O	1:D:158:ILE:C	2.56	0.43
3:C:209:ILE:HG13	3:C:209:ILE:H	1.52	0.43
3:C:198:LEU:C	3:C:198:LEU:HD12	2.40	0.43
3:C:322:PHE:CD1	3:C:338:LYS:HD2	2.50	0.43
2:E:314:MET:HA	2:E:449:LYS:O	2.19	0.43
3:F:128:VAL:O	3:F:131:LEU:N	2.52	0.43
2:E:405:ASN:O	2:E:406:ARG:C	2.56	0.42
3:F:124:LEU:O	3:F:125:LYS:C	2.55	0.42
2:E:340:ILE:HG12	2:E:341:SER:H	1.82	0.42
2:B:316:ASP:OD1	2:B:316:ASP:C	2.58	0.42
3:F:130:GLN:NE2	3:F:130:GLN:O	2.52	0.42
2:E:296:ASN:HA	2:E:296:ASN:HD22	1.67	0.42
3:F:199:ASP:OD1	3:F:201:SER:HB3	2.19	0.42
3:F:281:PHE:HB2	3:F:288:ASP:OD2	2.20	0.42
1:A:166:SER:OG	1:A:167:ARG:N	2.51	0.42
3:C:320:ASP:HB3	3:C:336:MET:HB2	2.01	0.42
1:A:119:ILE:O	1:A:119:ILE:HG23	2.18	0.42
3:C:117:ASN:O	3:C:120:LYS:N	2.52	0.42
3:F:273:LYS:HE3	3:F:319:ASN:ND2	2.29	0.42
3:F:354:TYR:HE1	3:F:376:TRP:HA	1.83	0.42
1:D:165:CYS:HA	2:E:196:PRO:HA	2.01	0.42
3:F:207:ASN:HD21	3:F:210:GLN:HG3	1.84	0.42
3:F:225:GLU:O	3:F:226:PHE:HB3	2.19	0.42
2:B:317:TRP:CZ2	2:B:419:GLY:N	2.86	0.42
2:B:383:ASP:HA	2:B:404:TYR:O	2.19	0.42
2:E:249:TRP:CE3	2:E:454:ILE:O	2.72	0.42
3:F:353:THR:HG22	3:F:354:TYR:N	2.35	0.42
2:B:340:ILE:HG12	2:B:341:SER:H	1.85	0.42
2:E:316:ASP:OD1	2:E:316:ASP:C	2.57	0.42
2:E:351:ASN:O	2:E:351:ASN:ND2	2.53	0.42
3:C:273:LYS:HE3	3:C:319:ASN:ND2	2.32	0.42
3:C:178:PHE:CE2	3:C:232:LYS:HB3	2.54	0.42
2:B:251:VAL:C	2:B:252:ILE:HD12	2.39	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:252:ILE:HG23	2:B:299:ILE:HD13	2.01	0.42
3:F:155:ASP:HA	3:F:158:ASN:HD22	1.84	0.42
3:F:300:SER:HB2	3:F:304:PHE:CD2	2.54	0.42
2:B:171:ILE:C	2:B:171:ILE:HD12	2.38	0.42
2:E:408:HIS:CE1	5:J:1:GLY:N	2.87	0.42
2:E:329:PHE:CD1	2:E:330:THR:N	2.88	0.42
3:C:156:ILE:HG21	3:C:167:TYR:CE2	2.55	0.42
2:E:255:ARG:N	2:E:450:MET:O	2.49	0.42
3:F:281:PHE:CE2	3:F:283:GLY:HA2	2.55	0.42
1:D:188:VAL:HG12	1:D:188:VAL:O	2.20	0.42
2:E:333:ASN:ND2	2:E:335:ALA:CB	2.78	0.42
2:B:333:ASN:ND2	2:B:335:ALA:CB	2.80	0.42
2:E:360:LEU:HD12	2:E:368:THR:HG21	2.00	0.42
2:B:409:ALA:O	2:B:438:MET:HB2	2.20	0.42
2:E:197:CYS:O	3:F:140:LYS:N	2.51	0.42
3:F:339:CYS:O	3:F:340:HIS:HB3	2.20	0.42
1:A:137:GLN:O	1:A:140:VAL:HG22	2.20	0.42
1:A:186:GLU:HA	1:A:186:GLU:OE1	2.19	0.42
2:E:409:ALA:O	2:E:438:MET:HB2	2.19	0.42
1:A:151:GLU:OE2	2:B:182:LEU:HD21	2.19	0.42
3:F:320:ASP:HB3	3:F:336:MET:HB2	2.02	0.42
2:E:249:TRP:CE3	2:E:455:ARG:HB2	2.54	0.42
2:B:215:ILE:HB	2:B:242:MET:CE	2.50	0.42
2:B:412:PRO:C	2:B:414:GLY:H	2.23	0.42
2:B:304:ARG:HB3	2:B:304:ARG:HH11	1.84	0.42
2:E:166:ARG:CB	2:E:166:ARG:NH1	2.83	0.42
1:D:122:LEU:O	1:D:126:VAL:HG13	2.19	0.42
3:F:149:THR:CG2	3:F:150:GLY:H	2.23	0.42
3:C:120:LYS:HA	3:C:123:ASN:ND2	2.35	0.42
1:D:152:VAL:O	1:D:155:ASP:HB3	2.20	0.42
2:E:212:GLU:O	2:E:213:GLU:C	2.57	0.41
3:C:372:TRP:CZ3	3:C:379:MET:HE1	2.55	0.41
3:C:314:THR:O	3:C:315:TRP:C	2.57	0.41
2:B:253:GLN:NE2	2:B:452:MET:HG3	2.35	0.41
3:F:166:LEU:C	3:F:167:TYR:CD1	2.93	0.41
2:E:252:ILE:HD13	2:E:454:ILE:HG23	2.02	0.41
1:D:149:ARG:O	1:D:152:VAL:HG12	2.19	0.41
2:E:270:LYS:HD2	2:E:334:GLU:OE2	2.20	0.41
2:E:415:ARG:O	2:E:434:GLY:HA2	2.19	0.41
3:C:353:THR:HG22	3:C:354:TYR:N	2.35	0.41
2:B:186:VAL:HG11	3:C:127:LYS:HG2	2.02	0.41
2:B:279:ASN:HA	2:B:286:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:355:SER:O	3:F:356:LYS:C	2.58	0.41
3:C:117:ASN:O	3:C:119:GLN:N	2.52	0.41
3:C:118:ASN:O	3:C:122:VAL:HG23	2.20	0.41
1:A:154:ILE:O	1:A:158:ILE:HG13	2.20	0.41
1:D:160:SER:O	2:E:259:SER:O	2.38	0.41
1:D:176:LYS:HD3	1:D:179:GLU:OE2	2.20	0.41
2:B:167:VAL:O	2:B:168:LEU:C	2.58	0.41
2:E:423:THR:HG23	2:E:426:MET:HE1	2.03	0.41
2:B:435:VAL:HG12	2:B:435:VAL:O	2.20	0.41
1:D:144:LEU:O	1:D:147:MET:N	2.51	0.41
2:B:421:GLN:HE21	2:B:421:GLN:CA	2.33	0.41
2:B:171:ILE:HG13	2:B:172:LEU:H	1.86	0.41
2:B:397:GLU:C	2:B:399:GLY:N	2.74	0.41
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.19	0.41
2:E:304:ARG:HH11	2:E:304:ARG:HB3	1.86	0.41
3:F:334:TRP:NE1	3:F:342:GLY:O	2.53	0.41
2:E:276:VAL:HA	2:E:292:TYR:CD1	2.56	0.41
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.19	0.41
3:C:242:ILE:H	3:C:242:ILE:CD1	2.29	0.41
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.56	0.41
3:F:100:ILE:HG23	3:F:103:HIS:HB2	2.03	0.41
3:F:113:ILE:CA	3:F:116:SER:HB3	2.48	0.41
3:F:372:TRP:HZ3	3:F:379:MET:CE	2.29	0.41
3:C:355:SER:O	3:C:356:LYS:C	2.58	0.41
1:A:153:ASP:O	1:A:157:LYS:HG2	2.20	0.41
2:E:345:TYR:CD2	2:E:351:ASN:HB2	2.56	0.41
1:D:130:VAL:HA	1:D:133:ILE:HG22	2.02	0.41
2:E:361:MET:HB2	6:E:570:NDG:C8	2.40	0.41
2:B:315:GLU:HB3	2:B:449:LYS:HB2	2.02	0.41
2:B:228:GLN:O	2:B:228:GLN:HG2	2.21	0.41
3:F:208:TRP:HB3	3:F:316:ASP:OD2	2.21	0.41
1:D:156:ILE:O	1:D:159:ARG:N	2.54	0.41
3:C:254:ASN:CB	3:C:256:ARG:HD2	2.51	0.41
3:C:363:TYR:CZ	4:G:3:ARG:HD3	2.56	0.41
1:A:175:LEU:O	1:A:178:TYR:HB2	2.21	0.41
1:A:175:LEU:O	1:A:176:LYS:C	2.59	0.41
3:C:272:ASP:CG	3:C:272:ASP:O	2.60	0.41
3:C:124:LEU:O	3:C:125:LYS:C	2.59	0.41
1:A:134:GLN:O	1:A:135:LEU:C	2.58	0.41
1:A:140:VAL:HG12	2:B:172:LEU:HD21	2.03	0.41
2:E:311:LEU:HD12	2:E:311:LEU:C	2.41	0.41
2:B:314:MET:HA	2:B:449:LYS:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:210:GLU:CD	2:B:212:GLU:HB3	2.41	0.41
3:F:242:ILE:CD1	3:F:242:ILE:N	2.83	0.41
3:F:274:TYR:O	3:F:275:ARG:C	2.58	0.41
2:E:317:TRP:CZ2	2:E:419:GLY:N	2.89	0.41
3:F:347:VAL:O	3:F:349:TYR:CD2	2.74	0.41
2:B:370:HIS:O	2:B:371:ASN:C	2.59	0.40
1:A:120:GLU:C	1:A:122:LEU:H	2.23	0.40
2:E:173:GLU:CG	2:E:174:ASN:N	2.84	0.40
3:F:100:ILE:HG23	3:F:103:HIS:CB	2.52	0.40
2:B:373:MET:SD	2:B:405:ASN:CB	3.01	0.40
2:E:188:ALA:O	2:E:191:GLU:N	2.55	0.40
2:E:315:GLU:HB3	2:E:449:LYS:HB2	2.02	0.40
1:D:144:LEU:CD2	2:E:175:LEU:HD21	2.51	0.40
2:B:424:TRP:CG	2:B:425:ASP:N	2.89	0.40
3:C:202:VAL:HG12	3:C:203:ASP:N	2.36	0.40
2:E:226:LEU:HD12	2:E:236:TYR:O	2.21	0.40
3:C:300:SER:HB2	3:C:304:PHE:CD2	2.57	0.40
3:F:113:ILE:O	3:F:117:ASN:N	2.50	0.40
2:B:342:VAL:HG23	2:B:354:MET:CG	2.52	0.40
1:A:140:VAL:CG2	1:A:141:ARG:N	2.85	0.40
2:E:241:ASP:O	2:E:247:GLY:HA2	2.21	0.40
2:B:161:ILE:O	2:B:162:PRO:C	2.60	0.40
2:B:267:ASP:O	2:B:270:LYS:HB3	2.21	0.40
2:E:420:GLY:HA2	2:E:446:SER:O	2.21	0.40
2:B:340:ILE:HB	2:B:403:TRP:CD1	2.56	0.40
3:C:202:VAL:HG23	3:C:225:GLU:HB2	2.04	0.40
3:F:221:THR:HB	3:F:223:THR:HG23	2.04	0.40
3:C:285:ASP:OD1	3:C:285:ASP:N	2.55	0.40
2:B:301:GLN:HE21	2:B:301:GLN:HB3	1.70	0.40
2:B:345:TYR:CG	2:B:351:ASN:HB2	2.56	0.40
2:B:167:VAL:HG12	2:B:168:LEU:N	2.36	0.40
2:B:249:TRP:HE3	2:B:454:ILE:O	2.04	0.40
2:B:255:ARG:HH11	2:B:255:ARG:CG	2.33	0.40
2:B:423:THR:HG23	2:B:426:MET:HE1	2.02	0.40
2:B:341:SER:HA	2:B:371:ASN:OD1	2.22	0.40
3:C:155:ASP:HA	3:C:158:ASN:HD22	1.86	0.40
3:C:261:ASP:HB2	3:C:282:ALA:HB3	2.03	0.40
1:A:169:LEU:HD22	1:A:170:ALA:N	2.37	0.40
2:B:311:LEU:HD12	2:B:311:LEU:C	2.42	0.40
3:F:124:LEU:O	3:F:124:LEU:HD23	2.21	0.40
3:C:199:ASP:OD1	3:C:201:SER:HB3	2.21	0.40
2:B:334:GLU:HB2	2:B:338:TYR:OH	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:130:GLN:O	3:F:133:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/87 (83%)	51 (71%)	18 (25%)	3 (4%)	4	31
1	D	72/87 (83%)	44 (61%)	23 (32%)	5 (7%)	2	14
2	B	305/328 (93%)	232 (76%)	50 (16%)	23 (8%)	2	12
2	E	305/328 (93%)	228 (75%)	54 (18%)	23 (8%)	2	12
3	C	293/324 (90%)	230 (78%)	46 (16%)	17 (6%)	3	21
3	F	293/324 (90%)	235 (80%)	42 (14%)	16 (6%)	3	23
4	G	1/3 (33%)	0	1 (100%)	0	100	100
4	H	1/3 (33%)	0	1 (100%)	0	100	100
5	I	2/7 (29%)	2 (100%)	0	0	100	100
5	J	2/7 (29%)	2 (100%)	0	0	100	100
All	All	1346/1498 (90%)	1024 (76%)	235 (18%)	87 (6%)	2	17

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	145	VAL
2	B	152	TYR
2	B	159	SER
2	B	160	ASN
2	B	259	SER
2	B	407	CYS
2	B	439	ASN
3	C	172	LEU

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Mol	Chain	Res	Type
3	C	240	SER
3	C	379	MET
1	D	121	VAL
2	E	259	SER
2	E	283	LYS
2	E	407	CYS
2	E	439	ASN
3	F	172	LEU
3	F	240	SER
3	F	379	MET
1	A	125	LYS
2	B	211	CYS
2	B	247	GLY
2	B	283	LYS
2	B	327	GLY
2	B	351	ASN
2	B	382	ASN
2	B	399	GLY
3	C	173	LYS
3	C	198	LEU
3	C	270	GLU
3	C	339	CYS
3	C	362	GLY
3	C	370	ALA
1	D	122	LEU
2	E	167	VAL
2	E	168	LEU
2	E	211	CYS
2	E	247	GLY
2	E	327	GLY
2	E	351	ASN
2	E	382	ASN
2	E	399	GLY
3	F	118	ASN
3	F	121	ILE
3	F	173	LYS
3	F	198	LEU
3	F	339	CYS
3	F	362	GLY
3	F	370	ALA
2	B	170	SER
2	B	394	CYS

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Mol	Chain	Res	Type
2	B	435	VAL
2	B	456	PRO
3	C	138	PRO
3	C	175	ASN
3	C	390	ASN
2	E	394	CYS
2	E	435	VAL
2	E	456	PRO
3	F	175	ASN
3	F	270	GLU
3	F	390	ASN
2	B	161	ILE
3	C	108	ARG
3	C	329	GLN
1	D	124	ARG
1	D	176	LYS
1	D	177	ASP
2	E	172	LEU
3	F	112	GLU
2	B	341	SER
2	B	345	TYR
3	C	117	ASN
3	C	271	ALA
2	E	153	ILE
2	E	212	GLU
3	F	329	GLN
2	B	212	GLU
2	E	170	SER
2	E	187	SER
2	E	341	SER
3	F	271	ALA
2	B	307	PRO
2	E	307	PRO
2	E	362	GLY
2	B	362	GLY
3	C	346	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	69/82 (84%)	62 (90%)	7 (10%)	11	41
1	D	69/82 (84%)	60 (87%)	9 (13%)	6	28
2	B	265/286 (93%)	247 (93%)	18 (7%)	22	65
2	E	265/286 (93%)	247 (93%)	18 (7%)	22	65
3	C	248/270 (92%)	229 (92%)	19 (8%)	18	59
3	F	248/270 (92%)	229 (92%)	19 (8%)	18	59
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
5	I	3/6 (50%)	3 (100%)	0	100	100
5	J	3/6 (50%)	3 (100%)	0	100	100
All	All	1174/1292 (91%)	1083 (92%)	91 (8%)	18	59

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	129	LYS
1	A	138	LYS
1	A	173	VAL
1	A	186	GLU
1	A	187	GLN
1	A	192	ASP
2	B	166	ARG
2	B	170	SER
2	B	178	LYS
2	B	190	MET
2	B	253	GLN
2	B	278	THR
2	B	281	ASP
2	B	283	LYS
2	B	284	ASN
2	B	301	GLN
2	B	311	LEU
2	B	321	LYS
2	B	351	ASN
2	B	378	TYR
2	B	387	THR
2	B	415	ARG
2	B	422	TYR

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Mol	Chain	Res	Type
2	B	439	ASN
3	C	100	ILE
3	C	107	ILE
3	C	126	GLU
3	C	162	LYS
3	C	198	LEU
3	C	224	THR
3	C	256	ARG
3	C	264	MET
3	C	276	LEU
3	C	323	GLU
3	C	325	ASN
3	C	354	TYR
3	C	361	ASN
3	C	365	ASN
3	C	374	THR
3	C	377	TYR
3	C	382	THR
3	C	383	THR
3	C	391	ARG
1	D	121	VAL
1	D	161	CYS
1	D	167	ARG
1	D	169	LEU
1	D	172	GLU
1	D	176	LYS
1	D	180	ASP
1	D	185	LEU
1	D	191	LYS
2	E	165	LEU
2	E	168	LEU
2	E	176	ARG
2	E	180	GLN
2	E	253	GLN
2	E	278	THR
2	E	281	ASP
2	E	283	LYS
2	E	284	ASN
2	E	301	GLN
2	E	311	LEU
2	E	321	LYS
2	E	351	ASN

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Mol	Chain	Res	Type
2	E	378	TYR
2	E	387	THR
2	E	415	ARG
2	E	422	TYR
2	E	439	ASN
3	F	113	ILE
3	F	116	SER
3	F	130	GLN
3	F	162	LYS
3	F	192	THR
3	F	198	LEU
3	F	256	ARG
3	F	264	MET
3	F	276	LEU
3	F	323	GLU
3	F	325	ASN
3	F	354	TYR
3	F	361	ASN
3	F	365	ASN
3	F	374	THR
3	F	377	TYR
3	F	382	THR
3	F	383	THR
3	F	391	ARG
4	H	2	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	187	GLN
2	B	158	ASN
2	B	189	GLN
2	B	243	ASN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	333	ASN
2	B	336	ASN

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Mol	Chain	Res	Type
2	B	339	GLN
2	B	351	ASN
2	B	364	ASN
2	B	405	ASN
2	B	408	HIS
2	B	421	GLN
2	B	429	HIS
2	B	439	ASN
3	C	115	ASN
3	C	117	ASN
3	C	123	ASN
3	C	144	GLN
3	C	177	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	365	ASN
1	D	134	GLN
1	D	184	GLN
1	D	187	GLN
2	E	158	ASN
2	E	180	GLN
2	E	189	GLN
2	E	243	ASN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	333	ASN
2	E	336	ASN
2	E	339	GLN
2	E	351	ASN
2	E	364	ASN
2	E	405	ASN
2	E	408	HIS
2	E	421	GLN

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Mol	Chain	Res	Type
2	E	429	HIS
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	118	ASN
3	F	130	GLN
3	F	136	GLN
3	F	144	GLN
3	F	177	GLN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	340	HIS
3	F	365	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	B	470	-	15,15,15	0.61	0	21,21,21	0.95	1 (4%)
7	MAN	B	472	-	12,12,12	0.47	0	17,17,17	0.38	0
6	NDG	E	570	-	15,15,15	0.41	0	21,21,21	0.48	0
6	NDG	I	471	-	15,15,15	0.46	0	21,21,21	0.49	0
6	NDG	J	571	-	15,15,15	0.57	0	21,21,21	0.50	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	B	470	-	-	0/6/26/26	0/1/1/1
7	MAN	B	472	-	-	0/2/22/22	0/1/1/1
6	NDG	E	570	-	-	0/6/26/26	0/1/1/1
6	NDG	I	471	-	-	0/6/26/26	0/1/1/1
6	NDG	J	571	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	470	NDG	C1-C2-C3	-2.44	107.11	110.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.