



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:11 AM GMT

PDB ID : 1FLC
Title : X-RAY STRUCTURE OF THE HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN OF INFLUENZA C VIRUS
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Deposited on : 1999-02-22
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>

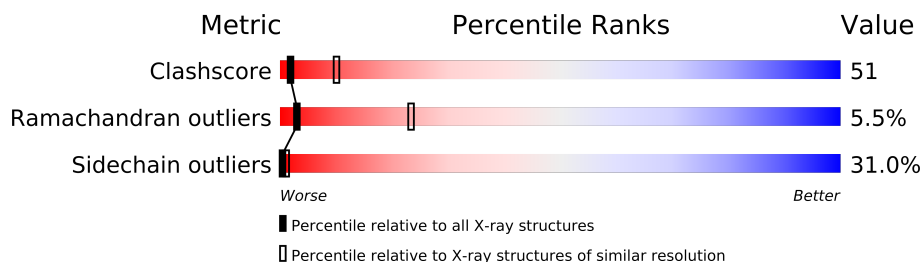
The following versions of software and data (see [references](#)) were used in the production of this report:

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	432	
1	C	432	
1	E	432	
2	B	175	
2	D	175	
2	F	175	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14285 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 HAEMAGGLUTININ-ESTERASE-FUSIONGLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3339	2113	565	636	25			
1	C	427	Total	C	N	O	S	0	0	0
			3338	2112	565	636	25			
1	E	427	Total	C	N	O	S	0	0	0
			3339	2113	565	636	25			

- Molecule 2 is a protein called HAEMAGGLUTININ-ESTERASE-FUSIONGLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1228	773	206	246	3			
2	D	162	Total	C	N	O	S	0	0	0
			1228	773	206	246	3			
2	F	162	Total	C	N	O	S	0	0	0
			1228	773	206	246	3			

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			39	22	2	15		
5	D	3	Total	C	N	O	0	0
			39	22	2	15		
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	3	Total	C	N	O	0	0
			39	22	2	15		

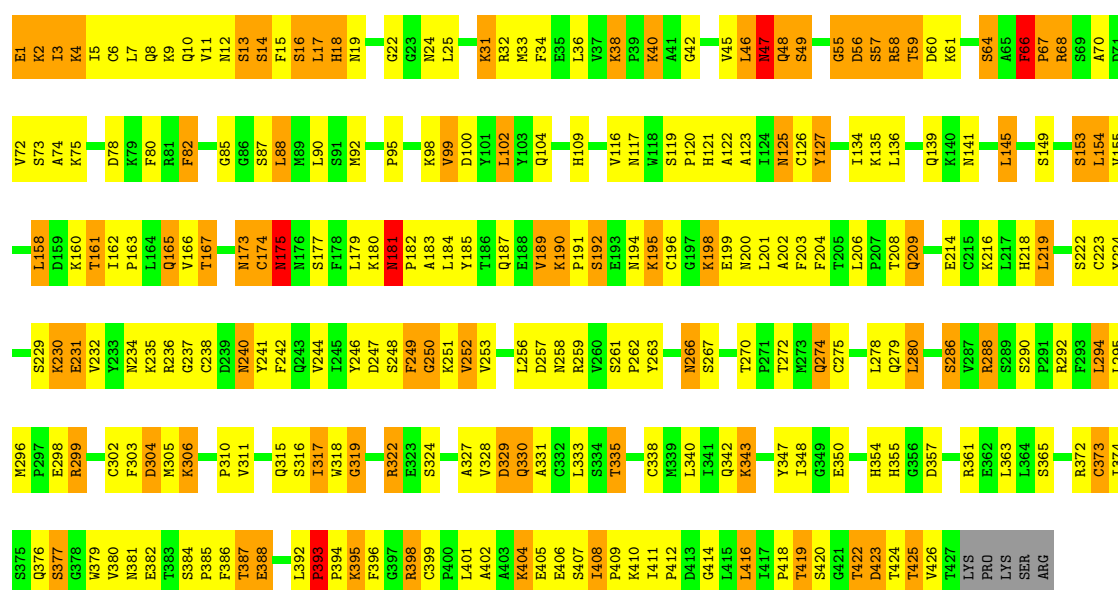
3 Residue-property plots

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: HAEMAGGLUTININ-ESTERASE-FUSIONGLYCOPROTEIN

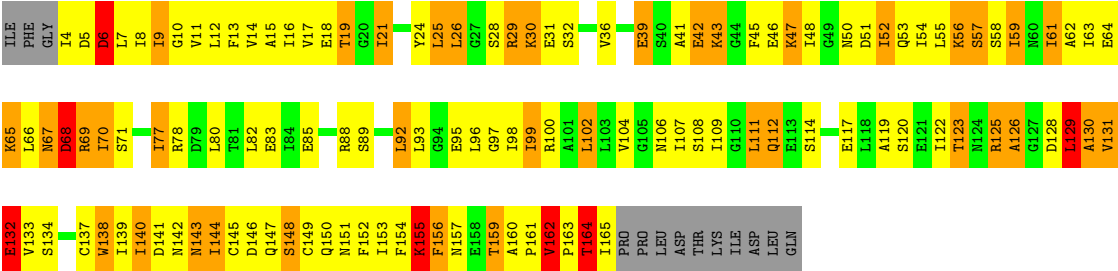
Chain A:





● Molecule 2: HAEMAGGLUTININ-ESTERASE-FUSIONGLYCOPROTEIN

Chain F:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.40Å 155.40Å 414.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	99.0 (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.54	Depositor
R, R_{free}	0.223 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14285	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: BMA, NAG, 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	0.68	0/3420	0.87	7/4622 (0.2%)
1	C	0.67	0/3418	0.87	6/4618 (0.1%)
1	E	0.68	0/3420	0.86	6/4622 (0.1%)
2	B	0.61	1/1241 (0.1%)	0.75	1/1678 (0.1%)
2	D	0.61	1/1241 (0.1%)	0.77	2/1678 (0.1%)
2	F	0.63	1/1241 (0.1%)	0.80	3/1678 (0.2%)
All	All	0.66	3/13981 (0.0%)	0.84	25/18896 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	39	GLU	CD-OE2	7.87	1.34	1.25
2	F	39	GLU	CD-OE2	7.71	1.34	1.25
2	B	39	GLU	CD-OE2	7.51	1.33	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	GLY	N-CA-C	6.17	128.54	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	175	ASN	C-N-CA	-6.11	106.43	121.70
1	A	304	ASP	N-CA-C	-6.03	94.71	111.00
1	E	304	ASP	N-CA-C	-5.91	95.04	111.00
1	C	304	ASP	N-CA-C	-5.87	95.15	111.00
1	A	175	ASN	C-N-CA	-5.71	107.42	121.70
2	B	69	ARG	N-CA-C	-5.70	95.61	111.00
1	A	55	GLY	N-CA-C	5.67	127.28	113.10
1	E	393	PRO	C-N-CD	5.64	140.24	128.40
1	A	319	GLY	N-CA-C	-5.63	99.02	113.10
1	C	175	ASN	C-N-CA	-5.63	107.63	121.70
1	E	55	GLY	N-CA-C	5.58	127.04	113.10
2	D	69	ARG	N-CA-C	-5.50	96.14	111.00
1	E	319	GLY	N-CA-C	-5.50	99.36	113.10
1	C	319	GLY	N-CA-C	-5.44	99.49	113.10
1	A	393	PRO	C-N-CD	5.43	139.80	128.40
2	F	162	VAL	N-CA-C	5.35	125.45	111.00
2	F	69	ARG	N-CA-C	-5.31	96.67	111.00
1	C	393	PRO	C-N-CD	5.30	139.52	128.40
1	C	66	PHE	N-CA-C	5.22	125.11	111.00
2	F	129	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	66	PHE	N-CA-C	5.17	124.95	111.00
1	A	181	ASN	C-N-CD	5.12	139.15	128.40
2	D	129	LEU	CA-CB-CG	5.10	127.03	115.30
1	E	66	PHE	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	PHE	Sidechain
1	C	249	PHE	Sidechain
1	E	249	PHE	Sidechain

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	3339	0	3251	331	0
1	C	3338	0	3245	349	0
1	E	3339	0	3250	336	0
2	B	1228	0	1232	198	0
2	D	1228	0	1232	234	0
2	F	1228	0	1232	188	0
3	A	39	0	34	1	0
3	C	39	0	34	3	0
3	E	39	0	34	6	0
4	A	117	0	102	0	0
4	C	78	0	68	0	0
4	E	117	0	102	4	0
5	B	39	0	34	11	0
5	D	39	0	34	5	0
5	F	39	0	34	8	0
6	C	39	0	34	0	0
All	All	14285	0	13952	1440	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 51.

All (1440) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:GLY:HA3	1:A:82:PHE:HB3	1.26	1.17
1:E:55:GLY:HA3	1:E:82:PHE:HB3	1.23	1.17
1:C:55:GLY:HA3	1:C:82:PHE:HB3	1.19	1.16
2:F:126:ALA:HB3	2:F:129:LEU:HG	1.25	1.15
2:B:126:ALA:HB3	2:B:129:LEU:HG	1.21	1.14
2:B:5:ASP:H	2:B:9:ILE:HG23	1.07	1.10
1:C:418:PRO:HD3	2:D:111:LEU:HD13	1.11	1.10
2:D:126:ALA:HB3	2:D:129:LEU:HG	1.28	1.10
1:A:249:PHE:HE2	1:C:252:VAL:HG11	1.07	1.10
1:A:257:ASP:HB2	1:E:249:PHE:CE1	1.88	1.09
2:D:30:LYS:HD2	2:D:32:SER:H	1.19	1.07
2:B:30:LYS:HD2	2:B:32:SER:H	1.21	1.05
1:A:249:PHE:CD2	1:C:252:VAL:HG21	1.91	1.05
1:E:418:PRO:HD3	2:F:111:LEU:HD13	1.31	1.04
5:B:1301:NDG:O3	5:B:1302:MAN:H5	1.57	1.03
2:B:129:LEU:O	2:B:131:VAL:HG12	1.56	1.03
1:A:2:LYS:HB3	2:B:31:GLU:HB2	1.37	1.03
1:E:377:SER:HB2	1:E:392:LEU:H	1.24	1.02
1:A:377:SER:HB2	1:A:392:LEU:H	1.20	1.02
2:F:129:LEU:O	2:F:131:VAL:HG12	1.58	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:30:LYS:HD2	2:F:32:SER:H	1.23	1.01
1:C:294:LEU:HD11	1:C:296:MET:HE3	1.42	1.01
1:C:55:GLY:CA	1:C:82:PHE:HB3	1.88	1.01
1:C:377:SER:HB2	1:C:392:LEU:H	1.21	1.01
1:C:10:GLN:NE2	2:D:25:LEU:HD21	1.75	1.01
1:E:166:VAL:HG21	1:E:185:TYR:HB3	1.42	1.01
1:E:55:GLY:CA	1:E:82:PHE:HB3	1.90	1.01
1:E:1:GLU:N	2:F:142:ASN:H	1.59	1.01
1:A:249:PHE:CE2	1:C:252:VAL:HG11	1.95	1.00
1:A:3:ILE:HA	2:B:30:LYS:HA	1.41	1.00
1:E:294:LEU:HD11	1:E:296:MET:HE3	1.38	1.00
1:C:249:PHE:HE2	1:E:252:VAL:HG11	1.27	1.00
1:A:55:GLY:CA	1:A:82:PHE:HB3	1.93	0.99
2:D:129:LEU:O	2:D:131:VAL:HG12	1.62	0.98
1:A:249:PHE:HD2	1:C:252:VAL:HG21	1.23	0.97
1:C:5:ILE:HG21	2:D:154:PHE:CD1	1.98	0.97
1:C:418:PRO:HD3	2:D:111:LEU:CD1	1.96	0.96
1:E:166:VAL:CG2	1:E:185:TYR:HB3	1.94	0.96
1:A:8:GLN:HE22	2:B:8:ILE:HA	1.28	0.95
1:A:216:LYS:HD3	1:A:305:MET:H	1.30	0.94
1:C:166:VAL:HG21	1:C:185:TYR:HB3	1.46	0.94
1:C:216:LYS:HD3	1:C:305:MET:H	1.32	0.94
1:C:3:ILE:HD11	2:D:140:ILE:HG22	1.48	0.93
1:E:1:GLU:H2	2:F:142:ASN:H	1.04	0.93
1:C:418:PRO:HG3	2:D:111:LEU:HB3	1.51	0.93
1:C:3:ILE:CD1	2:D:140:ILE:HG22	1.98	0.92
1:A:294:LEU:HD11	1:A:296:MET:HE3	1.51	0.92
1:A:257:ASP:HB2	1:E:249:PHE:CD1	2.05	0.92
1:C:166:VAL:CG2	1:C:185:TYR:HB3	2.00	0.92
1:A:166:VAL:HG21	1:A:185:TYR:HB3	1.49	0.92
1:C:10:GLN:HE21	2:D:25:LEU:HD21	1.34	0.91
1:A:8:GLN:HE22	2:B:8:ILE:CA	1.83	0.91
1:C:3:ILE:CG1	2:D:140:ILE:HG22	2.00	0.91
2:F:129:LEU:HA	2:F:140:ILE:HG12	1.53	0.91
1:E:216:LYS:HD3	1:E:305:MET:H	1.33	0.90
2:D:141:ASP:OD1	2:D:143:ASN:HB2	1.71	0.90
1:A:166:VAL:CG2	1:A:185:TYR:HB3	2.02	0.90
2:B:129:LEU:HA	2:B:140:ILE:HG12	1.54	0.89
1:C:9:LYS:HE2	2:D:112:GLN:HE22	1.36	0.89
1:E:8:GLN:HB3	2:F:25:LEU:HD12	1.55	0.88
2:B:4:ILE:HG22	2:B:9:ILE:HG21	1.55	0.88
1:C:31:LYS:NZ	1:C:411:ILE:HB	1.88	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:129:LEU:HA	2:D:140:ILE:HG12	1.56	0.88
1:E:184:LEU:HD12	1:E:185:TYR:H	1.38	0.88
2:D:160:ALA:N	2:D:161:PRO:HD3	1.89	0.88
1:A:31:LYS:NZ	1:A:411:ILE:HB	1.88	0.88
2:F:4:ILE:HG22	2:F:13:PHE:CD2	2.09	0.87
1:A:422:THR:HG21	2:F:51:ASP:HB3	1.55	0.87
1:C:426:VAL:CG2	2:D:4:ILE:HG23	2.04	0.87
1:A:184:LEU:HD12	1:A:185:TYR:H	1.40	0.87
1:E:31:LYS:NZ	1:E:411:ILE:HB	1.90	0.86
1:A:230:LYS:HD2	1:A:234:ASN:HD21	1.41	0.86
1:C:249:PHE:HD2	1:E:252:VAL:HG21	1.39	0.86
1:C:5:ILE:HG12	2:D:154:PHE:CE2	2.09	0.86
1:E:126:CYS:O	1:E:127:TYR:HB2	1.76	0.86
1:E:3:ILE:HD11	2:F:140:ILE:HG22	1.58	0.85
2:B:126:ALA:HB3	2:B:129:LEU:CG	2.03	0.85
1:A:80:PHE:HB3	1:A:82:PHE:CD2	2.11	0.85
1:A:231:GLU:CD	1:A:231:GLU:N	2.28	0.85
1:E:231:GLU:CD	1:E:231:GLU:N	2.30	0.85
1:C:249:PHE:CE2	1:E:252:VAL:HG11	2.12	0.84
1:C:426:VAL:HG21	2:D:4:ILE:HG23	1.59	0.84
2:B:5:ASP:HB2	2:B:9:ILE:HA	1.59	0.84
2:B:5:ASP:N	2:B:9:ILE:HG23	1.90	0.84
1:C:8:GLN:HB3	2:D:25:LEU:HD12	1.58	0.84
1:A:59:THR:HB	1:A:82:PHE:CD2	2.13	0.83
1:C:80:PHE:HB3	1:C:82:PHE:CD2	2.13	0.83
1:E:59:THR:HB	1:E:82:PHE:CD2	2.14	0.83
1:A:134:ILE:HD13	1:A:275:CYS:HB2	1.60	0.83
2:B:126:ALA:CB	2:B:129:LEU:HG	2.07	0.83
1:E:249:PHE:CG	1:E:250:GLY:N	2.43	0.83
2:F:126:ALA:HB3	2:F:129:LEU:CG	2.06	0.82
1:C:184:LEU:HD12	1:C:185:TYR:H	1.44	0.82
2:D:126:ALA:HB3	2:D:129:LEU:CG	2.09	0.82
1:E:4:LYS:O	2:F:28:SER:HA	1.79	0.82
1:E:80:PHE:HB3	1:E:82:PHE:CD2	2.14	0.82
2:F:126:ALA:CB	2:F:129:LEU:HG	2.09	0.82
1:C:249:PHE:CD2	1:E:252:VAL:HG21	2.15	0.82
1:E:181:ASN:HB3	1:E:182:PRO:HD3	1.60	0.82
1:C:249:PHE:CG	1:C:250:GLY:N	2.47	0.81
1:C:231:GLU:CD	1:C:231:GLU:N	2.34	0.81
1:A:249:PHE:CG	1:A:250:GLY:N	2.48	0.81
1:C:393:PRO:HB2	1:C:394:PRO:HD3	1.61	0.81
2:D:4:ILE:HG22	2:D:13:PHE:CB	2.10	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:181:ASN:HB3	1:C:182:PRO:HD3	1.62	0.80
1:C:25:LEU:HD11	2:D:107:ILE:CG2	2.11	0.80
2:B:68:ASP:C	2:B:70:ILE:H	1.83	0.80
1:A:126:CYS:O	1:A:127:TYR:HB2	1.80	0.80
2:F:65:LYS:HB2	2:F:65:LYS:HZ2	1.46	0.80
5:F:3301:NDG:O3	5:F:3302:MAN:H2	1.82	0.80
1:C:59:THR:HB	1:C:82:PHE:CD2	2.17	0.80
2:D:5:ASP:OD1	2:D:9:ILE:HA	1.80	0.80
1:A:181:ASN:HB3	1:A:182:PRO:HD3	1.62	0.80
1:A:288:ARG:NH1	1:A:288:ARG:HG3	1.97	0.79
1:C:230:LYS:HD2	1:C:234:ASN:HD21	1.45	0.79
1:C:3:ILE:HG13	2:D:140:ILE:O	1.82	0.79
1:C:420:SER:HB3	1:C:424:THR:OG1	1.83	0.79
1:C:38:LYS:H	1:C:38:LYS:HD3	1.48	0.79
1:C:25:LEU:HD11	2:D:107:ILE:HG21	1.62	0.79
1:E:134:ILE:HD13	1:E:275:CYS:HB2	1.65	0.79
1:A:19:ASN:ND2	5:F:3301:NDG:H8C2	1.97	0.79
1:E:1:GLU:HG2	1:E:2:LYS:N	1.98	0.79
2:D:4:ILE:HG22	2:D:9:ILE:HG21	1.63	0.78
1:E:230:LYS:HD2	1:E:234:ASN:HD21	1.48	0.78
1:E:405:GLU:O	1:E:408:ILE:HG23	1.84	0.78
1:E:28:THR:HG21	3:E:3501:NAG:H82	1.64	0.78
1:C:3:ILE:HG12	2:D:140:ILE:HG22	1.66	0.78
1:C:405:GLU:O	1:C:408:ILE:HG23	1.83	0.78
2:B:131:VAL:HG21	2:B:139:ILE:HB	1.64	0.78
1:C:3:ILE:HD11	2:D:140:ILE:CG2	2.13	0.78
1:E:45:VAL:C	1:E:46:LEU:HD23	2.04	0.78
2:F:68:ASP:C	2:F:70:ILE:H	1.85	0.78
2:B:125:ARG:O	2:B:129:LEU:HD21	1.82	0.78
1:A:45:VAL:C	1:A:46:LEU:HD23	2.03	0.78
1:E:240:ASN:ND2	1:E:263:TYR:OH	2.15	0.78
2:D:9:ILE:HD13	2:D:9:ILE:N	1.99	0.77
1:E:46:LEU:O	1:E:48:GLN:N	2.17	0.77
1:A:257:ASP:HB2	1:E:249:PHE:HE1	1.46	0.77
1:A:240:ASN:ND2	1:A:263:TYR:OH	2.18	0.77
2:B:126:ALA:N	2:B:129:LEU:HD11	2.00	0.77
1:A:288:ARG:HH11	1:A:288:ARG:HG3	1.49	0.77
2:D:146:ASP:OD2	2:D:148:SER:HB2	1.85	0.77
1:A:22:GLY:N	2:F:106:ASN:OD1	2.18	0.77
2:B:141:ASP:OD1	2:B:143:ASN:HB2	1.84	0.76
1:C:46:LEU:O	1:C:48:GLN:N	2.18	0.76
1:A:154:LEU:HD22	1:A:155:VAL:N	2.00	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:338:CYS:O	2:D:78:ARG:NH2	2.18	0.76
2:B:21:ILE:HD12	2:B:21:ILE:H	1.50	0.76
1:A:319:GLY:H	1:A:354:HIS:CD2	2.04	0.76
1:E:418:PRO:HD3	2:F:111:LEU:CD1	2.15	0.76
1:E:294:LEU:HD11	1:E:296:MET:CE	2.13	0.76
1:C:126:CYS:O	1:C:127:TYR:HB2	1.84	0.76
2:F:7:LEU:HD23	2:F:29:ARG:HH12	1.49	0.76
2:B:5:ASP:O	2:B:9:ILE:HD13	1.84	0.76
1:C:294:LEU:HD11	1:C:296:MET:CE	2.15	0.76
2:D:126:ALA:CB	2:D:129:LEU:HG	2.12	0.75
1:E:420:SER:HB3	1:E:424:THR:OG1	1.86	0.75
1:E:38:LYS:H	1:E:38:LYS:HD3	1.50	0.75
1:A:158:LEU:HD21	1:A:298:GLU:HA	1.67	0.75
2:B:131:VAL:HG11	2:B:139:ILE:C	2.07	0.75
1:C:134:ILE:HD13	1:C:275:CYS:HB2	1.68	0.75
1:A:393:PRO:HB2	1:A:394:PRO:HD3	1.67	0.75
2:B:162:VAL:HG22	2:B:162:VAL:O	1.87	0.75
2:B:129:LEU:O	2:B:131:VAL:N	2.19	0.74
1:E:158:LEU:HD21	1:E:298:GLU:HA	1.67	0.74
1:C:203:PHE:HD1	1:C:286:SER:HB3	1.51	0.74
2:F:129:LEU:O	2:F:131:VAL:N	2.21	0.74
1:E:154:LEU:HD22	1:E:155:VAL:N	2.03	0.74
1:C:5:ILE:O	2:D:138:TRP:CD1	2.40	0.74
1:C:3:ILE:O	2:D:139:ILE:HG23	1.86	0.74
1:C:45:VAL:C	1:C:46:LEU:HD23	2.07	0.74
1:E:379:TRP:HZ3	1:E:381:ASN:HB3	1.52	0.74
1:C:340:LEU:H	1:C:376:GLN:HE22	1.33	0.74
2:D:68:ASP:C	2:D:70:ILE:H	1.86	0.74
1:C:59:THR:O	1:C:82:PHE:CE2	2.41	0.74
2:B:125:ARG:C	2:B:129:LEU:HD21	2.08	0.74
2:B:131:VAL:CG2	2:B:139:ILE:H	2.01	0.74
2:B:138:TRP:N	2:B:138:TRP:CD1	2.56	0.74
2:B:4:ILE:HG22	2:B:9:ILE:CG2	2.18	0.74
1:C:163:PRO:HB2	1:C:165:GLN:OE1	1.88	0.74
2:B:65:LYS:HZ2	2:B:65:LYS:HB2	1.52	0.74
5:B:1301:NDG:H4	5:B:1302:MAN:H3	1.68	0.74
1:C:158:LEU:HD21	1:C:298:GLU:HA	1.70	0.74
1:A:163:PRO:HB2	1:A:165:GLN:OE1	1.87	0.73
2:F:55:LEU:HB3	2:F:107:ILE:HD12	1.70	0.73
2:D:65:LYS:HB2	2:D:65:LYS:NZ	2.03	0.73
1:C:388:GLU:CD	1:C:388:GLU:H	1.90	0.73
1:C:60:ASP:HA	1:C:82:PHE:CD1	2.22	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:66:PHE:HB3	1:E:67:PRO:HD3	1.70	0.73
1:C:240:ASN:ND2	1:C:263:TYR:OH	2.20	0.73
2:B:55:LEU:HB3	2:B:107:ILE:HD12	1.70	0.73
1:C:3:ILE:CD1	2:D:140:ILE:H	2.01	0.73
1:A:216:LYS:HD3	1:A:305:MET:N	2.02	0.73
2:F:141:ASP:OD1	2:F:143:ASN:HB2	1.87	0.73
1:E:392:LEU:HD22	1:E:393:PRO:HD2	1.68	0.73
1:A:46:LEU:O	1:A:48:GLN:N	2.22	0.73
2:B:62:ALA:O	2:B:66:LEU:HD13	1.89	0.73
1:E:31:LYS:HZ1	1:E:411:ILE:HB	1.52	0.73
1:C:319:GLY:H	1:C:354:HIS:CD2	2.06	0.73
1:C:379:TRP:HZ3	1:C:381:ASN:HB3	1.54	0.73
2:D:152:PHE:HD2	2:D:153:ILE:HD13	1.54	0.73
2:F:146:ASP:OD2	2:F:148:SER:HB2	1.88	0.72
2:F:9:ILE:HG22	2:F:10:GLY:H	1.53	0.72
1:A:420:SER:HB3	1:A:424:THR:OG1	1.88	0.72
2:D:112:GLN:HA	2:D:112:GLN:HE21	1.53	0.72
2:F:126:ALA:N	2:F:129:LEU:HD11	2.05	0.72
1:A:231:GLU:OE1	1:A:232:VAL:N	2.21	0.72
1:C:154:LEU:HD22	1:C:155:VAL:N	2.03	0.72
2:D:160:ALA:H	2:D:161:PRO:HD3	1.54	0.72
1:A:230:LYS:HD2	1:A:234:ASN:ND2	2.04	0.72
2:F:112:GLN:HE21	2:F:112:GLN:HA	1.53	0.72
1:A:249:PHE:HE2	1:C:252:VAL:CG1	1.94	0.72
1:E:60:ASP:HA	1:E:82:PHE:CD1	2.25	0.71
1:C:5:ILE:O	2:D:138:TRP:HD1	1.73	0.71
1:C:58:ARG:NH1	1:C:354:HIS:O	2.22	0.71
1:C:288:ARG:HG3	1:C:288:ARG:NH1	2.04	0.71
1:A:104:GLN:HB2	1:A:153:SER:HB2	1.71	0.71
1:E:216:LYS:HD3	1:E:305:MET:N	2.05	0.71
1:A:231:GLU:H	1:A:231:GLU:CD	1.91	0.71
1:E:388:GLU:CD	1:E:388:GLU:H	1.91	0.71
2:D:129:LEU:O	2:D:131:VAL:N	2.23	0.71
1:E:28:THR:HB	3:E:3501:NAG:H81	1.73	0.71
2:B:146:ASP:OD2	2:B:148:SER:HB2	1.91	0.71
1:C:318:TRP:HB3	1:C:322:ARG:HG3	1.72	0.71
1:A:66:PHE:HB3	1:A:67:PRO:HD3	1.73	0.71
1:E:393:PRO:HB2	1:E:394:PRO:HD3	1.71	0.71
1:A:392:LEU:HD22	1:A:393:PRO:HD2	1.70	0.71
1:C:315:GLN:NE2	1:C:343:LYS:H	1.89	0.71
1:E:373:CYS:HG	1:E:399:CYS:HG	1.36	0.71
1:E:288:ARG:NH1	1:E:288:ARG:HG3	2.04	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:405:GLU:O	1:A:408:ILE:HG23	1.91	0.71
1:E:1:GLU:O	2:F:141:ASP:HA	1.91	0.70
1:A:59:THR:O	1:A:82:PHE:CE2	2.44	0.70
1:C:249:PHE:CE1	1:E:257:ASP:HB2	2.26	0.70
1:E:426:VAL:HG11	2:F:4:ILE:HG21	1.72	0.70
1:E:288:ARG:HG3	1:E:288:ARG:HH11	1.56	0.70
5:D:2301:NDG:O3	5:D:2302:MAN:H2	1.91	0.70
2:D:131:VAL:CG2	2:D:139:ILE:H	2.05	0.70
1:A:2:LYS:O	2:B:31:GLU:N	2.23	0.70
1:C:319:GLY:HA2	1:C:347:TYR:HB3	1.74	0.70
2:F:65:LYS:HB2	2:F:65:LYS:NZ	2.04	0.70
1:E:319:GLY:H	1:E:354:HIS:CD2	2.09	0.70
2:B:140:ILE:HD12	2:B:141:ASP:H	1.56	0.70
2:F:131:VAL:CG2	2:F:139:ILE:H	2.05	0.70
2:D:131:VAL:HG21	2:D:139:ILE:HB	1.74	0.70
5:B:1301:NDG:O7	5:B:1301:NDG:C3	2.39	0.70
1:E:418:PRO:HG3	2:F:111:LEU:HB3	1.73	0.70
2:D:131:VAL:HG11	2:D:139:ILE:C	2.12	0.70
1:E:376:GLN:HB2	1:E:394:PRO:HD2	1.73	0.70
2:F:152:PHE:HD2	2:F:153:ILE:HD13	1.57	0.69
2:F:4:ILE:HB	2:F:9:ILE:CD1	2.22	0.69
1:C:288:ARG:HH11	1:C:288:ARG:HG3	1.57	0.69
2:D:21:ILE:HD12	2:D:21:ILE:H	1.57	0.69
2:F:131:VAL:HG11	2:F:139:ILE:C	2.12	0.69
2:B:140:ILE:CD1	2:B:141:ASP:H	2.06	0.69
1:A:8:GLN:NE2	2:B:8:ILE:HA	2.07	0.69
1:E:392:LEU:CD2	1:E:393:PRO:HD2	2.21	0.69
1:C:420:SER:H	1:C:424:THR:HG21	1.57	0.69
2:F:45:PHE:HA	2:F:48:ILE:HD12	1.74	0.69
1:A:38:LYS:HD3	1:A:38:LYS:H	1.56	0.69
2:B:112:GLN:HA	2:B:112:GLN:HE21	1.56	0.69
1:C:3:ILE:HD13	1:C:5:ILE:CD1	2.23	0.69
1:A:80:PHE:HB3	1:A:82:PHE:CE2	2.26	0.69
2:F:125:ARG:O	2:F:129:LEU:HD21	1.93	0.69
2:D:55:LEU:HB3	2:D:107:ILE:HD12	1.73	0.69
1:E:1:GLU:HA	2:F:141:ASP:HA	1.72	0.69
1:C:38:LYS:N	1:C:38:LYS:HD3	2.07	0.69
1:A:60:ASP:HA	1:A:82:PHE:CD1	2.28	0.69
1:C:216:LYS:HD3	1:C:305:MET:N	2.05	0.69
1:E:230:LYS:HD2	1:E:234:ASN:ND2	2.08	0.69
1:A:340:LEU:H	1:A:376:GLN:HE22	1.38	0.69
1:E:315:GLN:NE2	1:E:343:LYS:H	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:231:GLU:CD	1:E:231:GLU:H	1.96	0.69
2:F:62:ALA:O	2:F:66:LEU:HD13	1.94	0.68
1:A:9:LYS:O	2:B:15:ALA:N	2.25	0.68
1:E:25:LEU:HD11	2:F:107:ILE:HG21	1.75	0.68
1:E:340:LEU:H	1:E:376:GLN:HE22	1.40	0.68
1:C:426:VAL:HB	2:D:4:ILE:HD13	1.74	0.68
1:A:33:MET:HE2	2:B:100:ARG:HB2	1.73	0.68
1:A:379:TRP:HZ3	1:A:381:ASN:HB3	1.58	0.68
2:B:45:PHE:HA	2:B:48:ILE:HD12	1.76	0.68
1:C:60:ASP:HA	1:C:82:PHE:CE1	2.29	0.68
1:A:31:LYS:HB2	1:A:31:LYS:HZ3	1.58	0.68
1:C:230:LYS:HD2	1:C:234:ASN:ND2	2.08	0.68
1:A:319:GLY:HA2	1:A:347:TYR:HB3	1.75	0.68
2:B:65:LYS:NZ	2:B:65:LYS:HB2	2.08	0.68
1:E:9:LYS:HE2	2:F:112:GLN:HE22	1.57	0.68
1:C:1:GLU:OE1	1:C:2:LYS:HB2	1.94	0.68
1:E:247:ASP:O	1:E:249:PHE:O	2.10	0.68
1:E:1:GLU:N	2:F:142:ASN:N	2.39	0.68
1:A:315:GLN:NE2	1:A:343:LYS:H	1.90	0.68
1:A:58:ARG:NH1	1:A:354:HIS:O	2.26	0.68
1:A:425:THR:HB	2:B:16:ILE:HD11	1.73	0.68
1:E:25:LEU:HD11	2:F:107:ILE:CG2	2.24	0.68
2:B:129:LEU:CD2	2:B:153:ILE:HD12	2.24	0.68
1:C:392:LEU:HD22	1:C:393:PRO:HD2	1.75	0.68
1:C:249:PHE:CD1	1:C:250:GLY:N	2.59	0.68
1:A:376:GLN:HB2	1:A:394:PRO:HD2	1.76	0.68
1:A:294:LEU:HD11	1:A:296:MET:CE	2.24	0.68
1:E:59:THR:O	1:E:82:PHE:CE2	2.47	0.68
1:A:388:GLU:CD	1:A:388:GLU:H	1.97	0.67
2:D:125:ARG:O	2:D:129:LEU:HD21	1.95	0.67
1:A:252:VAL:HG11	1:E:249:PHE:HE2	1.59	0.67
1:E:163:PRO:HB2	1:E:165:GLN:OE1	1.93	0.67
1:A:426:VAL:HG11	2:B:4:ILE:HG12	1.77	0.67
1:A:119:SER:HB3	1:A:120:PRO:HD2	1.76	0.67
1:C:66:PHE:HB3	1:C:67:PRO:HD3	1.76	0.67
2:D:154:PHE:O	2:D:156:PHE:N	2.28	0.67
2:B:122:ILE:HB	2:B:138:TRP:CH2	2.30	0.67
1:C:3:ILE:HD11	2:D:140:ILE:CB	2.24	0.67
2:D:138:TRP:CD1	2:D:138:TRP:N	2.60	0.67
2:F:138:TRP:N	2:F:138:TRP:CD1	2.61	0.67
1:E:60:ASP:HA	1:E:82:PHE:CE1	2.30	0.67
2:B:152:PHE:HD2	2:B:153:ILE:HD13	1.60	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1:GLU:HA	2:F:141:ASP:CA	2.24	0.67
2:B:4:ILE:HG23	2:B:13:PHE:CD2	2.30	0.67
1:A:203:PHE:HD1	1:A:286:SER:HB3	1.60	0.67
1:E:231:GLU:OE1	1:E:232:VAL:N	2.25	0.67
1:E:1:GLU:CA	2:F:142:ASN:H	2.08	0.67
2:B:5:ASP:H	2:B:9:ILE:CG2	1.97	0.67
2:F:140:ILE:CD1	2:F:141:ASP:H	2.08	0.66
2:F:122:ILE:HB	2:F:138:TRP:CH2	2.30	0.66
1:A:249:PHE:CE2	1:C:252:VAL:CG1	2.75	0.66
1:A:420:SER:H	1:A:424:THR:HG21	1.59	0.66
1:E:294:LEU:C	1:E:294:LEU:HD22	2.15	0.66
2:F:125:ARG:C	2:F:129:LEU:HD21	2.15	0.66
1:A:392:LEU:CD2	1:A:393:PRO:HD2	2.26	0.66
1:A:66:PHE:O	1:A:67:PRO:C	2.34	0.66
2:D:45:PHE:HA	2:D:48:ILE:HD12	1.78	0.66
2:F:140:ILE:HD12	2:F:141:ASP:H	1.61	0.66
2:D:125:ARG:NH1	2:D:152:PHE:O	2.28	0.66
2:D:65:LYS:HB2	2:D:65:LYS:HZ2	1.58	0.66
1:E:58:ARG:NH2	1:E:317:ILE:O	2.29	0.66
2:F:131:VAL:HG21	2:F:139:ILE:HB	1.76	0.66
1:E:184:LEU:HD12	1:E:185:TYR:N	2.10	0.65
1:E:420:SER:H	1:E:424:THR:HG21	1.60	0.65
1:A:59:THR:HB	1:A:82:PHE:HD2	1.61	0.65
1:E:59:THR:HB	1:E:82:PHE:HD2	1.61	0.65
2:D:125:ARG:HB3	2:D:129:LEU:HD21	1.77	0.65
2:D:140:ILE:HD12	2:D:141:ASP:H	1.60	0.65
1:E:249:PHE:CD1	1:E:250:GLY:N	2.59	0.65
1:E:181:ASN:HB3	1:E:182:PRO:CD	2.26	0.65
2:D:62:ALA:O	2:D:66:LEU:HD13	1.96	0.65
2:D:126:ALA:N	2:D:129:LEU:HD11	2.11	0.65
2:D:140:ILE:CD1	2:D:141:ASP:H	2.08	0.65
1:A:257:ASP:CB	1:E:249:PHE:CE1	2.76	0.65
1:A:33:MET:CE	2:B:100:ARG:HB2	2.26	0.65
1:E:203:PHE:HD1	1:E:286:SER:HB3	1.62	0.65
2:D:122:ILE:HB	2:D:138:TRP:CH2	2.32	0.65
1:A:318:TRP:HB3	1:A:322:ARG:HG3	1.77	0.65
1:C:394:PRO:HG3	2:D:78:ARG:HG3	1.79	0.65
1:C:163:PRO:HG2	1:C:166:VAL:CG1	2.27	0.65
2:F:4:ILE:HB	2:F:9:ILE:HD13	1.79	0.65
1:E:319:GLY:HA2	1:E:347:TYR:HB3	1.77	0.65
2:D:9:ILE:HG21	2:D:13:PHE:HB2	1.79	0.65
1:E:1:GLU:CA	2:F:141:ASP:HA	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:GLU:N	1:A:1:GLU:OE1	2.27	0.65
2:D:30:LYS:HD2	2:D:32:SER:N	2.03	0.65
1:C:85:GLY:O	1:C:99:VAL:HG13	1.97	0.65
1:C:418:PRO:CG	2:D:111:LEU:HB3	2.27	0.65
1:E:10:GLN:HG3	2:F:15:ALA:HB3	1.79	0.65
1:E:1:GLU:H2	2:F:142:ASN:N	1.87	0.65
1:E:31:LYS:HB2	1:E:31:LYS:HZ3	1.61	0.65
2:F:21:ILE:H	2:F:21:ILE:HD12	1.62	0.65
1:C:66:PHE:O	1:C:67:PRO:C	2.31	0.64
2:B:116:TRP:HZ3	2:D:116:TRP:HH2	1.45	0.64
2:D:102:LEU:CD1	2:F:102:LEU:HD21	2.27	0.64
1:E:80:PHE:HB3	1:E:82:PHE:CE2	2.33	0.64
1:A:80:PHE:CB	1:A:82:PHE:CE2	2.80	0.64
2:D:125:ARG:C	2:D:129:LEU:HD21	2.18	0.64
2:D:152:PHE:CD2	2:D:153:ILE:HD13	2.33	0.64
2:D:30:LYS:CD	2:D:32:SER:H	2.04	0.64
1:E:126:CYS:HA	1:E:173:ASN:HD22	1.63	0.64
1:A:425:THR:CG2	2:B:16:ILE:HD11	2.28	0.64
1:A:126:CYS:HA	1:A:173:ASN:HD22	1.63	0.64
1:E:38:LYS:HD3	1:E:38:LYS:N	2.10	0.64
1:A:47:ASN:O	1:A:49:SER:N	2.30	0.64
1:C:416:LEU:HB2	2:D:52:ILE:HD13	1.79	0.64
1:C:416:LEU:HD22	2:D:56:LYS:HD2	1.78	0.64
2:F:125:ARG:HB3	2:F:129:LEU:HD21	1.80	0.64
1:A:424:THR:HG23	2:B:13:PHE:HA	1.80	0.64
2:F:129:LEU:CD2	2:F:153:ILE:HD12	2.28	0.64
1:C:47:ASN:O	1:C:49:SER:N	2.31	0.64
1:E:104:GLN:HB2	1:E:153:SER:HB2	1.78	0.64
1:C:31:LYS:HB2	1:C:31:LYS:HZ3	1.63	0.64
2:F:5:ASP:OD2	2:F:9:ILE:HA	1.97	0.64
1:C:5:ILE:HG12	2:D:154:PHE:CD2	2.32	0.63
2:D:4:ILE:HG22	2:D:13:PHE:CG	2.32	0.63
1:C:58:ARG:NH2	1:C:317:ILE:O	2.28	0.63
1:E:58:ARG:NH1	1:E:354:HIS:O	2.30	0.63
1:E:416:LEU:HD22	2:F:56:LYS:HD2	1.80	0.63
1:A:249:PHE:CD2	1:C:252:VAL:CG2	2.75	0.63
1:E:249:PHE:CD2	1:E:250:GLY:N	2.65	0.63
1:A:163:PRO:HG2	1:A:166:VAL:CG1	2.28	0.63
1:A:181:ASN:HB3	1:A:182:PRO:CD	2.27	0.63
2:B:116:TRP:CZ3	2:D:116:TRP:HH2	2.16	0.63
1:A:249:PHE:CD1	1:A:250:GLY:N	2.62	0.63
1:A:288:ARG:NH2	1:C:260:VAL:HG12	2.14	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:231:GLU:H	1:C:231:GLU:CD	2.01	0.63
1:A:34:PHE:HZ	2:B:66:LEU:HD23	1.63	0.63
1:A:162:ILE:HG23	1:A:163:PRO:HD2	1.81	0.63
1:C:376:GLN:HB2	1:C:394:PRO:HD2	1.80	0.63
2:F:17:VAL:O	2:F:19:THR:N	2.32	0.63
1:E:59:THR:HG21	1:E:80:PHE:CE2	2.34	0.63
1:E:294:LEU:HD21	1:E:296:MET:HE2	1.80	0.63
1:C:7:LEU:HD21	2:D:118:LEU:HD13	1.82	0.62
2:D:5:ASP:H	2:D:9:ILE:HD12	1.63	0.62
1:C:34:PHE:HE2	2:D:96:LEU:HD13	1.64	0.62
1:E:1:GLU:H1	2:F:142:ASN:CG	2.00	0.62
1:A:288:ARG:HH22	1:C:260:VAL:HG12	1.63	0.62
1:C:181:ASN:HB3	1:C:182:PRO:CD	2.28	0.62
1:E:66:PHE:O	1:E:67:PRO:C	2.32	0.62
5:B:1301:NDG:H3	5:B:1301:NDG:O7	1.99	0.62
1:E:66:PHE:HB3	1:E:67:PRO:CD	2.28	0.62
1:C:425:THR:HB	2:D:16:ILE:HD11	1.81	0.62
2:B:125:ARG:HB3	2:B:129:LEU:HD21	1.79	0.62
1:C:80:PHE:HB3	1:C:82:PHE:CE2	2.34	0.62
2:F:164:THR:HG23	2:F:165:ILE:H	1.64	0.62
2:B:17:VAL:O	2:B:17:VAL:HG23	2.00	0.62
1:E:3:ILE:HD11	2:F:140:ILE:H	1.63	0.62
1:A:3:ILE:HD13	1:A:5:ILE:CD1	2.29	0.62
1:A:319:GLY:H	1:A:354:HIS:HD2	1.47	0.62
1:A:190:LYS:HD3	1:A:191:PRO:HD2	1.80	0.62
1:C:80:PHE:CB	1:C:82:PHE:CE2	2.82	0.62
2:D:41:ALA:O	2:D:43:LYS:N	2.33	0.62
1:A:249:PHE:CE2	1:C:252:VAL:HG21	2.34	0.62
5:F:3300:NAG:O3	5:F:3301:NDG:N2	2.33	0.62
2:B:17:VAL:O	2:B:19:THR:N	2.32	0.62
1:C:104:GLN:HB2	1:C:153:SER:HB2	1.81	0.62
1:A:60:ASP:HA	1:A:82:PHE:CE1	2.35	0.61
1:E:80:PHE:CB	1:E:82:PHE:CE2	2.83	0.61
1:C:126:CYS:HA	1:C:173:ASN:HD22	1.63	0.61
1:C:414:GLY:H	2:D:56:LYS:HE3	1.65	0.61
2:F:152:PHE:CD2	2:F:153:ILE:HD13	2.35	0.61
2:B:4:ILE:CG2	2:B:9:ILE:HG21	2.29	0.61
1:A:184:LEU:HD12	1:A:185:TYR:N	2.12	0.61
1:C:31:LYS:HZ1	1:C:411:ILE:HB	1.60	0.61
2:F:17:VAL:HG23	2:F:17:VAL:O	2.00	0.61
2:B:125:ARG:NH1	2:B:152:PHE:O	2.34	0.61
1:E:163:PRO:HG2	1:E:166:VAL:CG1	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:68:ASP:C	2:B:70:ILE:N	2.52	0.61
1:E:46:LEU:N	1:E:46:LEU:HD23	2.16	0.61
1:C:59:THR:HB	1:C:82:PHE:HD2	1.63	0.61
1:A:426:VAL:HG21	2:B:4:ILE:HG21	1.81	0.61
1:A:249:PHE:CD2	1:A:250:GLY:N	2.69	0.61
1:C:392:LEU:CD2	1:C:393:PRO:HD2	2.30	0.61
1:C:203:PHE:CD1	1:C:286:SER:HB3	2.36	0.61
1:A:425:THR:CB	2:B:16:ILE:HD11	2.31	0.61
2:F:8:ILE:HG13	2:F:8:ILE:O	2.01	0.61
1:E:3:ILE:O	2:F:139:ILE:HG23	2.01	0.61
1:E:8:GLN:HB3	2:F:25:LEU:CD1	2.29	0.61
5:D:2301:NDG:H8C1	1:E:19:ASN:CB	2.30	0.61
1:E:3:ILE:HD13	1:E:5:ILE:CD1	2.31	0.61
1:E:294:LEU:HD22	1:E:295:LEU:N	2.15	0.61
1:E:190:LYS:HD3	1:E:191:PRO:HD2	1.82	0.61
1:A:31:LYS:HZ2	1:A:411:ILE:HB	1.66	0.60
1:E:318:TRP:HB3	1:E:322:ARG:HG3	1.82	0.60
1:A:357:ASP:O	1:A:361:ARG:HG3	2.01	0.60
1:E:1:GLU:CG	1:E:2:LYS:N	2.64	0.60
2:F:125:ARG:NH1	2:F:152:PHE:O	2.34	0.60
2:B:129:LEU:HD23	2:B:153:ILE:HD12	1.82	0.60
2:B:160:ALA:N	2:B:161:PRO:HD3	2.15	0.60
1:C:315:GLN:HE21	1:C:343:LYS:H	1.49	0.60
1:E:24:ASN:H	1:E:419:THR:HG22	1.67	0.60
2:B:123:THR:HG1	2:B:138:TRP:HZ3	1.48	0.60
1:C:3:ILE:HD11	2:D:140:ILE:H	1.64	0.60
1:A:31:LYS:HZ1	1:A:411:ILE:HB	1.61	0.60
2:D:4:ILE:HG22	2:D:13:PHE:HB2	1.82	0.60
1:E:92:MET:O	1:E:181:ASN:HB2	2.02	0.60
1:E:376:GLN:CB	1:E:394:PRO:HD2	2.32	0.60
1:A:241:TYR:O	1:A:258:ASN:HB2	2.01	0.60
1:A:5:ILE:HD12	1:A:5:ILE:N	2.16	0.60
5:F:3301:NDG:O7	5:F:3301:NDG:C3	2.49	0.60
2:B:131:VAL:HG11	2:B:139:ILE:O	2.01	0.60
2:B:102:LEU:CD1	2:D:102:LEU:HD21	2.31	0.60
2:D:142:ASN:HA	2:D:145:CYS:O	2.01	0.60
1:C:294:LEU:HD22	1:C:294:LEU:C	2.22	0.59
1:A:66:PHE:HB3	1:A:67:PRO:CD	2.31	0.59
1:A:261:SER:OG	1:A:262:PRO:HD2	2.03	0.59
1:E:59:THR:HG21	1:E:80:PHE:CD2	2.37	0.59
2:B:129:LEU:HD23	2:B:153:ILE:CD1	2.32	0.59
1:C:231:GLU:OE2	1:C:232:VAL:N	2.28	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:GLY:O	1:A:99:VAL:HG13	2.02	0.59
2:D:161:PRO:HG2	2:D:162:VAL:H	1.67	0.59
2:D:68:ASP:C	2:D:70:ILE:N	2.56	0.59
1:E:85:GLY:O	1:E:99:VAL:HG13	2.02	0.59
1:C:10:GLN:O	2:D:23:GLY:N	2.30	0.59
1:C:59:THR:HG21	1:C:80:PHE:CE2	2.38	0.59
1:C:241:TYR:O	1:C:258:ASN:HB2	2.02	0.59
2:D:17:VAL:O	2:D:17:VAL:HG23	2.02	0.59
5:B:1301:NDG:H8C2	1:C:19:ASN:CG	2.23	0.59
2:B:159:THR:O	2:B:160:ALA:HB3	2.02	0.59
1:A:331:ALA:O	1:A:335:THR:HG23	2.02	0.59
2:B:152:PHE:CD2	2:B:153:ILE:HD13	2.37	0.59
5:B:1301:NDG:C4	5:B:1302:MAN:H3	2.32	0.59
1:A:125:ASN:C	1:A:125:ASN:OD1	2.41	0.59
2:D:17:VAL:O	2:D:19:THR:N	2.35	0.59
1:A:416:LEU:O	2:B:24:TYR:OH	2.09	0.59
1:A:426:VAL:HG21	2:B:4:ILE:HG12	1.85	0.59
1:C:31:LYS:HZ2	1:C:411:ILE:HB	1.67	0.59
1:C:119:SER:HB3	1:C:120:PRO:HD2	1.84	0.59
1:C:249:PHE:CD2	1:C:250:GLY:N	2.71	0.58
5:F:3300:NAG:O3	5:F:3301:NDG:C7	2.51	0.58
1:C:18:HIS:CD2	1:C:412:PRO:HB3	2.37	0.58
1:C:5:ILE:HG21	2:D:154:PHE:CE1	2.38	0.58
2:F:154:PHE:O	2:F:156:PHE:N	2.36	0.58
1:C:3:ILE:HD12	2:D:140:ILE:H	1.68	0.58
1:C:46:LEU:HD23	1:C:46:LEU:N	2.18	0.58
1:A:315:GLN:HE21	1:A:343:LYS:H	1.49	0.58
1:C:319:GLY:H	1:C:354:HIS:HD2	1.51	0.58
2:D:29:ARG:HB2	2:D:36:VAL:HG13	1.84	0.58
2:D:9:ILE:H	2:D:9:ILE:HD13	1.68	0.58
1:C:66:PHE:HB3	1:C:67:PRO:CD	2.33	0.58
1:E:3:ILE:CD1	2:F:140:ILE:HG22	2.32	0.58
1:C:125:ASN:C	1:C:125:ASN:OD1	2.40	0.58
1:E:66:PHE:O	1:E:68:ARG:N	2.37	0.58
1:E:331:ALA:O	1:E:335:THR:HG23	2.03	0.58
1:C:184:LEU:HD12	1:C:185:TYR:N	2.17	0.58
1:E:125:ASN:C	1:E:125:ASN:OD1	2.42	0.58
1:C:87:SER:HB3	1:C:90:LEU:HD12	1.86	0.58
1:C:187:GLN:O	1:C:189:VAL:HG12	2.02	0.58
1:C:417:ILE:HA	2:D:24:TYR:OH	2.04	0.58
1:C:230:LYS:O	1:C:234:ASN:N	2.28	0.58
1:E:17:LEU:HD22	1:E:17:LEU:C	2.23	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:163:PRO:HG2	1:C:166:VAL:HG12	1.85	0.58
2:D:61:ILE:N	2:D:61:ILE:HD12	2.19	0.58
2:D:126:ALA:O	2:D:129:LEU:HD12	2.04	0.58
2:B:154:PHE:O	2:B:156:PHE:N	2.37	0.58
1:A:414:GLY:H	2:B:56:LYS:HE3	1.68	0.58
2:B:30:LYS:HD2	2:B:32:SER:N	2.05	0.57
1:A:10:GLN:HG3	2:B:15:ALA:HB3	1.84	0.57
1:A:187:GLN:O	1:A:189:VAL:HG12	2.04	0.57
2:B:131:VAL:O	2:B:132:GLU:C	2.42	0.57
1:A:163:PRO:HG2	1:A:166:VAL:HG12	1.86	0.57
2:B:126:ALA:O	2:B:129:LEU:HD12	2.04	0.57
1:E:315:GLN:HE21	1:E:343:LYS:H	1.50	0.57
2:F:29:ARG:HB2	2:F:36:VAL:HG13	1.85	0.57
1:E:311:VAL:O	1:E:338:CYS:HA	2.04	0.57
2:F:125:ARG:O	2:F:126:ALA:HB2	2.04	0.57
2:B:30:LYS:CD	2:B:32:SER:H	2.07	0.57
5:D:2301:NDG:H8C1	1:E:19:ASN:CG	2.25	0.57
2:B:131:VAL:HG21	2:B:139:ILE:CB	2.34	0.57
1:C:92:MET:O	1:C:181:ASN:HB2	2.04	0.57
2:F:131:VAL:HG11	2:F:139:ILE:O	2.05	0.57
1:A:244:VAL:CG2	1:E:249:PHE:CE1	2.88	0.57
2:F:162:VAL:HG13	2:F:164:THR:H	1.69	0.57
2:D:129:LEU:CD2	2:D:153:ILE:HD12	2.34	0.57
1:C:393:PRO:O	1:C:395:LYS:HG2	2.05	0.57
1:C:162:ILE:HG23	1:C:163:PRO:HD2	1.86	0.57
1:E:416:LEU:HB2	2:F:52:ILE:HD13	1.86	0.57
2:B:41:ALA:O	2:B:43:LYS:N	2.38	0.57
1:E:18:HIS:CD2	1:E:412:PRO:HB3	2.39	0.57
2:B:125:ARG:O	2:B:126:ALA:HB2	2.05	0.57
1:A:104:GLN:CB	1:A:153:SER:HB2	2.35	0.57
1:A:149:SER:OG	1:A:303:PHE:HB3	2.05	0.57
2:B:29:ARG:HB2	2:B:36:VAL:HG13	1.87	0.57
2:D:163:PRO:O	2:D:165:ILE:N	2.37	0.57
1:E:1:GLU:HA	2:F:142:ASN:N	2.20	0.56
2:B:141:ASP:HB3	2:B:144:ILE:HG12	1.87	0.56
2:D:161:PRO:O	2:D:162:VAL:HG13	2.05	0.56
2:F:7:LEU:N	2:F:7:LEU:HD22	2.19	0.56
2:D:21:ILE:CD1	2:D:21:ILE:H	2.15	0.56
2:F:41:ALA:O	2:F:43:LYS:N	2.38	0.56
2:F:131:VAL:HG21	2:F:139:ILE:H	1.71	0.56
2:D:102:LEU:HD13	2:F:102:LEU:HD21	1.86	0.56
1:C:331:ALA:O	1:C:335:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:59:THR:HG21	1:A:80:PHE:CD2	2.40	0.56
2:D:125:ARG:O	2:D:126:ALA:HB2	2.05	0.56
2:F:9:ILE:HG22	2:F:10:GLY:N	2.18	0.56
1:A:322:ARG:HD2	1:A:354:HIS:CE1	2.39	0.56
2:F:7:LEU:HD23	2:F:29:ARG:NH1	2.20	0.56
1:E:47:ASN:O	1:E:49:SER:N	2.38	0.56
1:A:18:HIS:CD2	1:A:412:PRO:HB3	2.41	0.56
1:E:379:TRP:CZ3	1:E:381:ASN:HB3	2.39	0.56
5:F:3300:NAG:O3	5:F:3301:NDG:C8	2.53	0.56
1:E:119:SER:HB3	1:E:120:PRO:HD2	1.87	0.56
1:C:66:PHE:O	1:C:68:ARG:N	2.38	0.56
1:C:66:PHE:CE1	1:C:70:ALA:HB2	2.41	0.56
2:F:97:GLY:O	2:F:100:ARG:HB3	2.04	0.56
1:A:59:THR:HG21	1:A:80:PHE:CE2	2.40	0.56
2:F:129:LEU:HD23	2:F:153:ILE:HD12	1.86	0.56
2:B:13:PHE:CD1	2:B:13:PHE:N	2.74	0.56
1:A:46:LEU:N	1:A:46:LEU:HD23	2.18	0.56
1:C:278:LEU:HD22	1:C:280:LEU:CD1	2.36	0.56
1:C:294:LEU:HD22	1:C:295:LEU:N	2.21	0.56
1:A:154:LEU:HD22	1:A:155:VAL:H	1.68	0.56
1:E:319:GLY:H	1:E:354:HIS:HD2	1.51	0.56
2:F:83:GLU:H	2:F:83:GLU:CD	2.08	0.56
2:F:129:LEU:HD23	2:F:153:ILE:CD1	2.36	0.56
1:C:393:PRO:HB2	1:C:394:PRO:CD	2.34	0.56
2:B:102:LEU:HD13	2:D:102:LEU:HD21	1.87	0.56
1:C:416:LEU:O	2:D:52:ILE:HD11	2.06	0.56
2:D:122:ILE:O	2:D:125:ARG:HB2	2.06	0.56
1:A:249:PHE:HD2	1:C:252:VAL:CG2	2.09	0.56
1:C:278:LEU:HD22	1:C:280:LEU:HD11	1.87	0.56
1:E:357:ASP:O	1:E:361:ARG:HG3	2.06	0.56
1:C:311:VAL:O	1:C:338:CYS:HA	2.05	0.55
1:C:17:LEU:C	1:C:17:LEU:HD22	2.25	0.55
1:E:187:GLN:O	1:E:189:VAL:HG12	2.06	0.55
2:D:30:LYS:HE3	2:D:32:SER:HB3	1.88	0.55
2:F:131:VAL:O	2:F:132:GLU:C	2.44	0.55
2:D:43:LYS:HB3	2:D:155:LYS:O	2.07	0.55
5:B:1301:NDG:HB	5:B:1302:MAN:H5	1.67	0.55
1:A:231:GLU:OE1	1:A:231:GLU:N	2.39	0.55
1:E:278:LEU:HD22	1:E:280:LEU:HD11	1.88	0.55
2:B:122:ILE:O	2:B:125:ARG:HB2	2.06	0.55
2:D:4:ILE:CG2	2:D:9:ILE:HG13	2.36	0.55
1:A:58:ARG:NH2	1:A:317:ILE:O	2.35	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:311:VAL:O	1:A:338:CYS:HA	2.06	0.55
2:F:123:THR:HG1	2:F:138:TRP:HZ3	1.52	0.55
1:E:422:THR:OG1	1:E:423:ASP:N	2.39	0.55
1:A:66:PHE:O	1:A:68:ARG:N	2.39	0.55
1:C:80:PHE:HB2	1:C:82:PHE:CE2	2.41	0.55
2:F:126:ALA:O	2:F:129:LEU:HD12	2.07	0.55
1:E:163:PRO:HG2	1:E:166:VAL:HG12	1.88	0.55
1:C:247:ASP:O	1:C:249:PHE:O	2.24	0.55
3:C:2500:NDG:H6C1	2:D:22:GLY:O	2.07	0.55
1:E:266:ASN:O	1:E:266:ASN:CG	2.44	0.55
1:A:190:LYS:CD	1:A:191:PRO:HD2	2.37	0.55
1:A:376:GLN:CB	1:A:394:PRO:HD2	2.37	0.55
1:E:162:ILE:HG23	1:E:163:PRO:HD2	1.89	0.55
1:A:203:PHE:CE2	1:C:262:PRO:HB3	2.42	0.55
2:B:47:LYS:NZ	1:C:423:ASP:OD2	2.35	0.55
1:A:92:MET:O	1:A:181:ASN:HB2	2.06	0.55
2:F:43:LYS:HB3	2:F:155:LYS:O	2.07	0.55
1:C:59:THR:HG21	1:C:80:PHE:CD2	2.42	0.54
1:A:244:VAL:HG21	1:E:249:PHE:CE1	2.42	0.54
1:C:424:THR:O	2:D:13:PHE:HB3	2.07	0.54
1:C:5:ILE:HG21	2:D:154:PHE:CG	2.40	0.54
1:E:294:LEU:CD1	1:E:296:MET:HE3	2.26	0.54
2:B:7:LEU:HD13	2:B:36:VAL:HG21	1.89	0.54
2:D:123:THR:HG1	2:D:138:TRP:HZ3	1.55	0.54
1:A:10:GLN:HG3	2:B:15:ALA:CB	2.36	0.54
1:A:17:LEU:HD22	1:A:17:LEU:C	2.28	0.54
1:A:1:GLU:O	1:A:3:ILE:HG13	2.08	0.54
2:D:148:SER:OG	2:D:160:ALA:HB3	2.08	0.54
1:A:249:PHE:CE1	1:C:244:VAL:CG2	2.90	0.54
1:A:333:LEU:HA	2:B:78:ARG:NH2	2.22	0.54
1:C:249:PHE:HE1	1:E:257:ASP:HB2	1.70	0.54
5:F:3301:NDG:H3	5:F:3301:NDG:O7	2.06	0.54
1:E:393:PRO:O	1:E:395:LYS:HG2	2.08	0.54
2:B:160:ALA:H	2:B:161:PRO:HD3	1.72	0.54
1:C:190:LYS:HD3	1:C:191:PRO:HD2	1.89	0.54
1:E:87:SER:HB3	1:E:90:LEU:HD12	1.90	0.54
2:F:164:THR:O	2:F:165:ILE:CB	2.56	0.54
1:C:24:ASN:H	1:C:419:THR:HG22	1.73	0.54
2:B:131:VAL:HG21	2:B:139:ILE:H	1.71	0.54
2:B:30:LYS:HE3	2:B:32:SER:HB3	1.90	0.54
5:B:1301:NDG:H4	5:B:1302:MAN:C3	2.30	0.54
1:C:422:THR:OG1	1:C:423:ASP:N	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1:GLU:CA	2:F:142:ASN:N	2.70	0.53
2:D:131:VAL:O	2:D:132:GLU:C	2.46	0.53
1:A:247:ASP:O	1:A:249:PHE:O	2.26	0.53
1:A:294:LEU:HD22	1:A:294:LEU:C	2.28	0.53
2:D:13:PHE:CD1	2:D:13:PHE:N	2.75	0.53
1:A:319:GLY:N	1:A:354:HIS:CD2	2.76	0.53
1:A:38:LYS:HD3	1:A:38:LYS:N	2.16	0.53
1:C:33:MET:HE2	2:D:100:ARG:HB2	1.90	0.53
1:A:319:GLY:N	1:A:354:HIS:HD2	2.07	0.53
2:B:148:SER:OG	2:B:160:ALA:HB3	2.08	0.53
1:E:116:VAL:HG13	1:E:117:ASN:N	2.23	0.53
2:D:119:ALA:HA	2:D:138:TRP:HH2	1.73	0.53
1:C:393:PRO:O	1:C:395:LYS:N	2.40	0.53
1:A:294:LEU:HD22	1:A:295:LEU:N	2.23	0.53
2:B:47:LYS:HZ1	1:C:423:ASP:CG	2.12	0.53
2:F:64:GLU:OE1	2:F:65:LYS:N	2.41	0.53
1:E:154:LEU:HD22	1:E:155:VAL:H	1.72	0.53
1:C:1:GLU:CA	2:D:142:ASN:OD1	2.57	0.53
1:C:5:ILE:N	1:C:5:ILE:HD12	2.23	0.53
2:D:131:VAL:HG21	2:D:139:ILE:H	1.72	0.53
2:D:64:GLU:OE1	2:D:65:LYS:N	2.41	0.53
1:E:241:TYR:O	1:E:242:PHE:HB3	2.08	0.53
1:E:241:TYR:O	1:E:258:ASN:HB2	2.09	0.53
1:E:20:GLY:HA3	2:F:104:VAL:HG12	1.89	0.53
1:A:3:ILE:HD13	1:A:5:ILE:HD13	1.90	0.53
2:F:7:LEU:H	2:F:7:LEU:HD22	1.74	0.53
1:C:154:LEU:HD22	1:C:155:VAL:H	1.71	0.53
1:A:266:ASN:CG	1:A:266:ASN:O	2.44	0.53
2:D:129:LEU:HD12	2:D:130:ALA:H	1.73	0.53
1:A:249:PHE:CZ	1:C:244:VAL:HG11	2.43	0.53
1:A:294:LEU:HD21	1:A:296:MET:HE2	1.91	0.53
1:E:5:ILE:HD12	1:E:5:ILE:N	2.23	0.53
2:D:129:LEU:HD23	2:D:153:ILE:CD1	2.39	0.53
1:A:393:PRO:O	1:A:395:LYS:HG2	2.08	0.53
1:A:68:ARG:CZ	1:A:68:ARG:HB3	2.39	0.53
2:F:61:ILE:N	2:F:61:ILE:HD12	2.24	0.53
2:B:129:LEU:HD12	2:B:130:ALA:H	1.71	0.53
1:A:203:PHE:CD1	1:A:286:SER:HB3	2.43	0.53
1:C:232:VAL:O	1:C:235:LYS:HB2	2.09	0.53
2:B:97:GLY:O	2:B:100:ARG:HB3	2.07	0.53
1:A:162:ILE:N	1:A:162:ILE:HD12	2.24	0.53
1:C:261:SER:OG	1:C:262:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:318:TRP:CB	1:C:322:ARG:HG3	2.37	0.53
1:C:288:ARG:CG	1:C:288:ARG:HH11	2.22	0.53
2:B:57:SER:O	2:B:61:ILE:HD13	2.09	0.53
1:C:4:LYS:HA	2:D:138:TRP:O	2.09	0.53
1:A:425:THR:HB	2:B:16:ILE:CD1	2.37	0.53
2:D:131:VAL:HG11	2:D:139:ILE:O	2.09	0.52
1:C:155:VAL:O	1:C:299:ARG:HG2	2.09	0.52
1:E:1:GLU:C	2:F:141:ASP:HA	2.28	0.52
2:D:125:ARG:O	2:D:126:ALA:CB	2.58	0.52
1:E:294:LEU:HD21	1:E:296:MET:CE	2.39	0.52
1:E:31:LYS:NZ	1:E:31:LYS:HB2	2.24	0.52
1:A:13:SER:C	1:A:15:PHE:H	2.11	0.52
1:A:278:LEU:HD22	1:A:280:LEU:HD11	1.91	0.52
1:A:288:ARG:HH11	1:A:288:ARG:CG	2.15	0.52
2:F:62:ALA:O	2:F:65:LYS:HB3	2.09	0.52
2:B:61:ILE:N	2:B:61:ILE:HD12	2.25	0.52
1:C:13:SER:C	1:C:15:PHE:H	2.12	0.52
1:C:357:ASP:O	1:C:361:ARG:HG3	2.09	0.52
1:E:13:SER:C	1:E:15:PHE:H	2.11	0.52
1:C:411:ILE:HG13	2:D:63:ILE:HD11	1.92	0.52
1:E:190:LYS:HD2	1:E:192:SER:OG	2.09	0.52
1:A:12:ASN:HB3	2:B:20:GLY:O	2.09	0.52
1:E:294:LEU:C	1:E:294:LEU:CD2	2.77	0.52
2:B:59:ILE:HG22	2:B:63:ILE:HD11	1.90	0.52
1:E:278:LEU:HD22	1:E:280:LEU:CD1	2.39	0.52
1:E:149:SER:OG	1:E:303:PHE:HB3	2.09	0.52
1:E:80:PHE:HB2	1:E:82:PHE:CE2	2.44	0.52
2:D:83:GLU:H	2:D:83:GLU:CD	2.13	0.52
2:D:141:ASP:HB3	2:D:144:ILE:HG12	1.91	0.52
1:C:424:THR:HG23	2:D:13:PHE:HA	1.90	0.52
1:E:66:PHE:CB	1:E:67:PRO:CD	2.87	0.52
2:F:163:PRO:C	2:F:164:THR:HG22	2.29	0.52
1:A:80:PHE:HB2	1:A:82:PHE:CE2	2.45	0.52
2:F:149:CYS:O	2:F:153:ILE:HG12	2.09	0.52
1:A:252:VAL:HG21	1:E:249:PHE:HD2	1.74	0.52
1:C:163:PRO:HG2	1:C:166:VAL:HG11	1.91	0.52
1:A:125:ASN:O	1:A:173:ASN:HB2	2.10	0.52
1:A:190:LYS:HD2	1:A:192:SER:OG	2.09	0.52
1:E:206:LEU:HB3	1:E:218:HIS:CD2	2.45	0.52
2:B:83:GLU:CD	2:B:83:GLU:H	2.14	0.52
1:E:256:LEU:HD12	1:E:257:ASP:N	2.24	0.51
2:F:159:THR:O	2:F:160:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:92:LEU:HA	2:D:95:GLU:HG3	1.92	0.51
2:F:13:PHE:N	2:F:13:PHE:CD1	2.77	0.51
1:E:317:ILE:HG22	1:E:324:SER:HB3	1.91	0.51
1:A:425:THR:HG22	2:B:16:ILE:HD11	1.93	0.51
1:E:230:LYS:O	1:E:234:ASN:N	2.30	0.51
1:E:232:VAL:O	1:E:235:LYS:HB2	2.10	0.51
1:C:149:SER:OG	1:C:303:PHE:HB3	2.10	0.51
2:B:8:ILE:O	2:B:8:ILE:HG13	2.10	0.51
1:A:8:GLN:NE2	2:B:9:ILE:H	2.08	0.51
1:C:294:LEU:HD21	1:C:296:MET:HE2	1.93	0.51
2:D:160:ALA:N	2:D:161:PRO:CD	2.68	0.51
1:A:181:ASN:O	1:A:183:ALA:N	2.44	0.51
1:C:414:GLY:N	2:D:56:LYS:HE3	2.26	0.51
1:A:256:LEU:HD12	1:A:257:ASP:N	2.26	0.51
1:E:68:ARG:CZ	1:E:68:ARG:HB3	2.40	0.51
1:E:190:LYS:CD	1:E:191:PRO:HD2	2.39	0.51
1:A:174:CYS:O	1:A:175:ASN:C	2.49	0.51
1:A:87:SER:HB3	1:A:90:LEU:HD12	1.92	0.51
2:F:142:ASN:HA	2:F:145:CYS:O	2.11	0.51
2:F:5:ASP:OD1	2:F:6:ASP:N	2.43	0.51
1:E:241:TYR:CG	1:E:242:PHE:N	2.79	0.51
1:A:116:VAL:HG13	1:A:117:ASN:N	2.26	0.51
1:A:422:THR:OG1	1:A:423:ASP:N	2.43	0.51
1:E:11:VAL:HG22	1:E:15:PHE:HB3	1.92	0.51
1:A:162:ILE:N	1:A:162:ILE:CD1	2.74	0.51
2:D:59:ILE:HG22	2:D:63:ILE:HD11	1.92	0.51
1:C:93:PHE:CD1	1:C:93:PHE:N	2.78	0.51
1:C:3:ILE:HD13	1:C:5:ILE:HD13	1.93	0.51
1:A:247:ASP:OD1	1:A:249:PHE:O	2.29	0.51
1:C:390:TYR:CE2	2:D:82:LEU:HG	2.45	0.51
1:E:141:ASN:HD22	1:E:279:GLN:HE21	1.58	0.51
2:F:119:ALA:HA	2:F:138:TRP:HH2	1.76	0.51
2:F:125:ARG:O	2:F:126:ALA:CB	2.59	0.51
2:B:125:ARG:O	2:B:126:ALA:CB	2.58	0.51
1:C:376:GLN:CB	1:C:394:PRO:HD2	2.41	0.51
1:A:163:PRO:HG2	1:A:166:VAL:HG11	1.93	0.51
1:C:66:PHE:CD2	1:C:67:PRO:HD3	2.46	0.51
1:A:266:ASN:ND2	1:A:266:ASN:O	2.44	0.51
1:E:3:ILE:CD1	2:F:140:ILE:H	2.25	0.50
1:A:8:GLN:NE2	2:B:9:ILE:N	2.58	0.50
2:D:159:THR:O	2:D:160:ALA:HB3	2.11	0.50
1:C:322:ARG:HD2	1:C:354:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:304:ASP:C	1:C:304:ASP:OD1	2.49	0.50
1:A:58:ARG:HD2	1:A:347:TYR:OH	2.11	0.50
1:A:158:LEU:HD21	1:A:298:GLU:CA	2.39	0.50
1:E:15:PHE:CD2	1:E:16:SER:N	2.80	0.50
1:A:206:LEU:HB3	1:A:218:HIS:CD2	2.46	0.50
5:B:1301:NDG:O3	5:B:1301:NDG:O7	2.27	0.50
1:E:393:PRO:O	1:E:395:LYS:N	2.44	0.50
1:E:125:ASN:O	1:E:173:ASN:HB2	2.11	0.50
1:A:241:TYR:CG	1:A:242:PHE:N	2.80	0.50
2:B:43:LYS:HB3	2:B:155:LYS:O	2.11	0.50
2:B:99:ILE:O	2:B:99:ILE:HG12	2.11	0.50
1:E:3:ILE:HD13	1:E:5:ILE:HD13	1.94	0.50
1:A:249:PHE:CE2	1:C:252:VAL:CB	2.95	0.50
2:B:21:ILE:N	2:B:21:ILE:HD12	2.23	0.50
1:E:66:PHE:CB	1:E:67:PRO:HD3	2.39	0.50
1:A:66:PHE:CB	1:A:67:PRO:CD	2.89	0.50
1:A:24:ASN:H	1:A:419:THR:HG22	1.77	0.50
1:A:135:LYS:O	1:A:139:GLN:HG2	2.12	0.50
2:F:122:ILE:O	2:F:125:ARG:HB2	2.11	0.50
1:A:393:PRO:O	1:A:395:LYS:N	2.44	0.50
2:D:4:ILE:HG21	2:D:9:ILE:HG13	1.93	0.50
1:C:398:ARG:NH1	2:D:70:ILE:O	2.44	0.50
1:C:222:SER:HB2	1:C:278:LEU:HD12	1.94	0.50
1:E:28:THR:CG2	3:E:3501:NAG:H82	2.37	0.50
1:A:45:VAL:O	1:A:46:LEU:HD23	2.12	0.50
2:D:62:ALA:O	2:D:65:LYS:HB3	2.12	0.50
1:A:11:VAL:HG22	1:A:15:PHE:HB3	1.94	0.50
2:F:59:ILE:HG22	2:F:63:ILE:HD11	1.94	0.50
1:E:10:GLN:HE21	2:F:25:LEU:HD21	1.76	0.50
2:B:43:LYS:HD3	2:B:156:PHE:HB2	1.94	0.50
1:A:1:GLU:C	1:A:3:ILE:H	2.14	0.50
1:A:3:ILE:HD12	1:A:3:ILE:C	2.32	0.50
2:D:129:LEU:HD23	2:D:153:ILE:HD12	1.93	0.50
1:C:6:CYS:HA	2:D:136:GLY:O	2.12	0.50
1:E:174:CYS:O	1:E:175:ASN:C	2.50	0.50
2:D:161:PRO:CG	2:D:162:VAL:H	2.22	0.50
1:C:11:VAL:HG22	1:C:15:PHE:HB3	1.94	0.50
1:C:55:GLY:C	1:C:82:PHE:HB3	2.32	0.49
1:E:3:ILE:HG13	2:F:140:ILE:O	2.10	0.49
2:B:162:VAL:CG2	2:B:162:VAL:O	2.60	0.49
1:C:398:ARG:NH1	1:C:398:ARG:HG2	2.27	0.49
1:C:317:ILE:HG22	1:C:324:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:319:GLY:N	1:C:354:HIS:CD2	2.78	0.49
1:C:266:ASN:CG	1:C:266:ASN:O	2.49	0.49
1:A:232:VAL:O	1:A:235:LYS:HB2	2.11	0.49
2:F:148:SER:HB3	2:F:160:ALA:O	2.11	0.49
2:D:43:LYS:HD3	2:D:156:PHE:HB2	1.93	0.49
1:C:38:LYS:NZ	1:C:38:LYS:O	2.44	0.49
1:C:377:SER:HB2	1:C:392:LEU:N	2.07	0.49
1:C:247:ASP:OD1	1:C:249:PHE:O	2.31	0.49
2:D:4:ILE:HA	2:D:13:PHE:CD2	2.47	0.49
3:C:2500:NDG:O7	2:D:21:ILE:HA	2.13	0.49
1:A:10:GLN:HA	2:B:15:ALA:HB3	1.95	0.49
1:A:418:PRO:HD3	2:B:111:LEU:HD13	1.94	0.49
2:B:163:PRO:C	2:B:165:ILE:H	2.15	0.49
1:E:121:HIS:C	1:E:123:ALA:N	2.66	0.49
1:E:231:GLU:N	1:E:231:GLU:OE1	2.45	0.49
2:F:148:SER:OG	2:F:160:ALA:HB3	2.11	0.49
1:A:189:VAL:HG23	1:A:196:CYS:HA	1.94	0.49
1:A:253:VAL:O	1:A:278:LEU:HD21	2.13	0.49
1:E:135:LYS:O	1:E:139:GLN:HG2	2.13	0.49
4:E:3650:NAG:H61	4:E:3651:NAG:C7	2.41	0.49
1:E:10:GLN:NE2	2:F:25:LEU:HD21	2.27	0.49
1:C:1:GLU:CA	2:D:142:ASN:N	2.75	0.49
1:C:34:PHE:CE2	2:D:96:LEU:HD13	2.46	0.49
1:A:55:GLY:C	1:A:82:PHE:HB3	2.33	0.49
2:B:119:ALA:HA	2:B:138:TRP:HH2	1.76	0.49
1:C:8:GLN:O	2:D:24:TYR:HA	2.13	0.49
1:E:162:ILE:N	1:E:162:ILE:HD12	2.27	0.49
1:A:266:ASN:ND2	1:A:266:ASN:C	2.66	0.49
2:D:5:ASP:OD2	2:D:9:ILE:HG23	2.12	0.49
2:B:161:PRO:C	2:B:162:VAL:HG12	2.33	0.49
2:B:39:GLU:OE1	2:B:155:LYS:HE3	2.13	0.49
1:A:333:LEU:HD11	1:A:340:LEU:HD23	1.93	0.49
1:A:377:SER:HB2	1:A:392:LEU:N	2.06	0.49
1:C:181:ASN:O	1:C:183:ALA:N	2.46	0.49
1:A:181:ASN:O	1:A:182:PRO:C	2.46	0.49
2:B:147:GLN:O	2:B:148:SER:C	2.51	0.49
1:E:155:VAL:O	1:E:299:ARG:HG2	2.12	0.49
2:D:57:SER:O	2:D:61:ILE:HD13	2.13	0.49
1:E:288:ARG:HH11	1:E:288:ARG:CG	2.24	0.49
1:A:426:VAL:HG11	2:B:4:ILE:CG1	2.42	0.49
1:A:252:VAL:HG11	1:E:249:PHE:CE2	2.44	0.49
1:E:393:PRO:HB2	1:E:394:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:4:ILE:CG1	2:F:5:ASP:N	2.74	0.49
1:C:319:GLY:N	1:C:354:HIS:HD2	2.10	0.49
2:F:43:LYS:HD3	2:F:156:PHE:HB2	1.95	0.49
1:E:189:VAL:HG23	1:E:196:CYS:HA	1.95	0.49
2:D:4:ILE:HA	2:D:13:PHE:CE2	2.48	0.48
1:C:231:GLU:HA	1:C:234:ASN:HB2	1.94	0.48
1:E:401:LEU:N	1:E:401:LEU:HD12	2.28	0.48
1:C:66:PHE:CB	1:C:67:PRO:CD	2.91	0.48
2:D:4:ILE:HB	2:D:9:ILE:CG1	2.43	0.48
2:D:4:ILE:HB	2:D:9:ILE:HG13	1.93	0.48
1:C:125:ASN:O	1:C:173:ASN:HB2	2.13	0.48
2:F:147:GLN:O	2:F:148:SER:C	2.52	0.48
1:E:247:ASP:OD1	1:E:249:PHE:O	2.31	0.48
2:F:30:LYS:CD	2:F:32:SER:H	2.10	0.48
1:A:66:PHE:CB	1:A:67:PRO:HD3	2.41	0.48
1:A:68:ARG:HA	1:A:350:GLU:OE2	2.14	0.48
1:C:385:PRO:HG2	1:C:386:PHE:CD2	2.49	0.48
1:C:20:GLY:HA3	2:D:104:VAL:HG12	1.93	0.48
1:A:5:ILE:CD1	1:A:5:ILE:N	2.76	0.48
1:A:257:ASP:CB	1:E:249:PHE:CD1	2.88	0.48
1:C:249:PHE:CD1	1:E:257:ASP:HB2	2.48	0.48
2:F:8:ILE:HG23	2:F:36:VAL:CG1	2.44	0.48
1:E:319:GLY:N	1:E:354:HIS:HD2	2.11	0.48
1:A:246:TYR:HA	1:A:251:LYS:O	2.13	0.48
1:E:329:ASP:HA	1:E:340:LEU:CD2	2.44	0.48
1:C:10:GLN:HG3	2:D:15:ALA:HB3	1.95	0.48
1:A:318:TRP:CB	1:A:322:ARG:HG3	2.44	0.48
1:C:85:GLY:O	1:C:99:VAL:CG1	2.61	0.48
2:F:92:LEU:HA	2:F:95:GLU:HG3	1.95	0.48
1:A:3:ILE:HD12	1:A:4:LYS:N	2.29	0.48
2:F:30:LYS:HE3	2:F:32:SER:HB3	1.95	0.48
2:D:4:ILE:HB	2:D:9:ILE:HD12	1.96	0.48
2:D:4:ILE:CG2	2:D:9:ILE:HG21	2.38	0.48
2:D:61:ILE:H	2:D:61:ILE:CD1	2.26	0.48
1:E:304:ASP:C	1:E:304:ASP:OD1	2.52	0.48
1:A:203:PHE:CD1	1:C:262:PRO:HD3	2.49	0.48
2:B:64:GLU:OE1	2:B:65:LYS:N	2.47	0.48
1:C:379:TRP:CZ3	1:C:381:ASN:HB3	2.42	0.48
2:F:21:ILE:H	2:F:21:ILE:CD1	2.20	0.48
1:A:278:LEU:HD22	1:A:280:LEU:CD1	2.43	0.48
1:C:135:LYS:O	1:C:139:GLN:HG2	2.12	0.48
2:D:154:PHE:O	2:D:155:LYS:C	2.52	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:ASN:HA	1:A:237:GLY:O	2.14	0.48
1:C:66:PHE:CB	1:C:67:PRO:HD3	2.44	0.48
1:A:304:ASP:C	1:A:304:ASP:OD1	2.52	0.48
1:E:121:HIS:O	1:E:123:ALA:N	2.46	0.48
1:C:174:CYS:O	1:C:175:ASN:C	2.52	0.48
1:C:374:ILE:HG13	1:C:374:ILE:O	2.14	0.47
1:E:331:ALA:O	1:E:335:THR:CG2	2.62	0.47
2:F:131:VAL:HG21	2:F:139:ILE:CB	2.44	0.47
2:B:125:ARG:HB3	2:B:129:LEU:CD2	2.45	0.47
1:A:66:PHE:CD2	1:A:67:PRO:HD3	2.49	0.47
1:A:385:PRO:HG2	1:A:386:PHE:CD2	2.48	0.47
1:A:202:ALA:HB3	1:A:296:MET:HE1	1.96	0.47
1:E:424:THR:HG23	2:F:13:PHE:HA	1.97	0.47
1:A:401:LEU:HD11	2:B:70:ILE:HD11	1.95	0.47
1:E:203:PHE:CD1	1:E:286:SER:HB3	2.45	0.47
2:B:164:THR:HG22	2:B:164:THR:O	2.14	0.47
1:A:244:VAL:HG22	1:E:249:PHE:CE1	2.49	0.47
1:C:68:ARG:CZ	1:C:68:ARG:HB3	2.45	0.47
2:B:43:LYS:O	2:B:46:GLU:HB2	2.14	0.47
1:E:33:MET:HE3	1:E:409:PRO:HB2	1.97	0.47
2:F:129:LEU:HD12	2:F:130:ALA:H	1.78	0.47
1:E:1:GLU:HA	2:F:141:ASP:CG	2.35	0.47
1:E:374:ILE:O	1:E:374:ILE:HG13	2.13	0.47
1:E:28:THR:HB	3:E:3501:NAG:C8	2.43	0.47
2:B:5:ASP:CB	2:B:9:ILE:HA	2.38	0.47
1:E:163:PRO:HG2	1:E:166:VAL:HG11	1.95	0.47
1:E:68:ARG:HA	1:E:350:GLU:OE2	2.15	0.47
1:A:66:PHE:CE1	1:A:70:ALA:HB2	2.49	0.47
1:A:47:ASN:C	1:A:49:SER:H	2.18	0.47
2:F:162:VAL:HA	2:F:163:PRO:HD3	1.47	0.47
2:F:54:ILE:O	2:F:57:SER:HB3	2.14	0.47
1:E:26:TYR:OH	1:E:425:THR:HG21	2.14	0.47
1:C:80:PHE:HB2	1:C:82:PHE:HE2	1.79	0.47
1:C:294:LEU:CD2	1:C:294:LEU:C	2.83	0.47
2:F:154:PHE:O	2:F:156:PHE:CD2	2.67	0.47
1:A:31:LYS:HB2	1:A:31:LYS:NZ	2.28	0.47
1:A:329:ASP:HA	1:A:340:LEU:CD2	2.45	0.47
1:E:127:TYR:N	1:E:173:ASN:ND2	2.62	0.47
2:D:67:ASN:OD1	2:D:67:ASN:N	2.48	0.47
1:C:121:HIS:O	1:C:123:ALA:N	2.48	0.47
1:E:55:GLY:C	1:E:82:PHE:HB3	2.33	0.47
1:C:5:ILE:CG1	2:D:154:PHE:CE2	2.91	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:ASP:HA	1:A:340:LEU:HD22	1.96	0.47
1:E:231:GLU:HA	1:E:234:ASN:HB2	1.97	0.47
1:A:34:PHE:HZ	2:B:66:LEU:CD2	2.28	0.47
1:A:304:ASP:OD1	1:A:306:LYS:HB2	2.14	0.47
2:B:6:ASP:HB2	2:B:7:LEU:H	1.43	0.47
1:C:100:ASP:OD1	1:C:100:ASP:C	2.53	0.47
1:A:1:GLU:HA	2:B:141:ASP:HA	1.98	0.46
1:A:1:GLU:O	1:A:3:ILE:N	2.41	0.46
1:C:10:GLN:HE22	2:D:25:LEU:HD21	1.74	0.46
1:C:160:LYS:HG3	1:C:162:ILE:CD1	2.45	0.46
1:A:19:ASN:CG	5:F:3301:NDG:H8C2	2.35	0.46
1:C:398:ARG:HH11	1:C:398:ARG:HG2	1.80	0.46
1:C:47:ASN:C	1:C:49:SER:H	2.18	0.46
2:D:77:ILE:HD12	2:D:77:ILE:H	1.80	0.46
1:C:387:THR:O	1:C:402:ALA:HA	2.15	0.46
1:A:377:SER:CB	1:A:392:LEU:H	2.09	0.46
2:B:21:ILE:CD1	2:B:21:ILE:H	2.12	0.46
1:C:127:TYR:N	1:C:173:ASN:ND2	2.63	0.46
2:F:164:THR:OG1	2:F:165:ILE:N	2.46	0.46
1:C:241:TYR:O	1:C:242:PHE:HB3	2.15	0.46
1:A:149:SER:HB3	1:A:304:ASP:O	2.15	0.46
1:A:25:LEU:HD23	1:A:418:PRO:HA	1.97	0.46
1:E:387:THR:HG22	1:E:400:PRO:HB2	1.96	0.46
2:B:131:VAL:HG22	2:B:139:ILE:H	1.78	0.46
1:A:374:ILE:O	1:A:374:ILE:HG13	2.14	0.46
1:A:354:HIS:C	1:A:355:HIS:ND1	2.69	0.46
1:E:38:LYS:NZ	1:E:38:LYS:O	2.47	0.46
1:C:398:ARG:HH11	1:C:398:ARG:CG	2.29	0.46
1:C:190:LYS:CD	1:C:191:PRO:HD2	2.46	0.46
1:A:222:SER:HB2	1:A:278:LEU:HD12	1.96	0.46
1:E:178:PHE:CD2	1:E:179:LEU:N	2.83	0.46
1:A:406:GLU:CD	1:A:406:GLU:H	2.19	0.46
2:B:93:LEU:HA	2:B:93:LEU:HD23	1.74	0.46
1:E:329:ASP:HA	1:E:340:LEU:HD22	1.97	0.46
1:A:331:ALA:O	1:A:335:THR:CG2	2.63	0.46
1:C:223:CYS:HA	1:C:274:GLN:O	2.16	0.46
2:D:41:ALA:C	2:D:43:LYS:H	2.19	0.46
1:C:156:ASN:HA	1:C:299:ARG:HG2	1.98	0.46
1:E:80:PHE:HB2	1:E:82:PHE:HE2	1.81	0.46
2:B:149:CYS:O	2:B:153:ILE:HG12	2.15	0.46
2:B:4:ILE:HG22	2:B:9:ILE:HD12	1.97	0.46
1:A:379:TRP:CZ3	1:A:381:ASN:HB3	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:102:LEU:HD11	2:D:102:LEU:HD21	1.98	0.46
2:F:163:PRO:O	2:F:164:THR:HG22	2.16	0.46
1:E:198:LYS:O	1:E:199:GLU:C	2.54	0.46
1:A:8:GLN:HE22	2:B:8:ILE:CB	2.28	0.46
1:E:401:LEU:HD11	2:F:70:ILE:HD11	1.97	0.46
1:A:15:PHE:CD2	1:A:16:SER:N	2.84	0.46
1:C:246:TYR:HA	1:C:251:LYS:O	2.16	0.46
1:A:249:PHE:CE1	1:C:244:VAL:HG22	2.51	0.46
1:E:247:ASP:OD1	1:E:247:ASP:C	2.54	0.46
1:A:230:LYS:O	1:A:234:ASN:N	2.33	0.46
2:F:68:ASP:C	2:F:70:ILE:N	2.56	0.46
1:A:42:GLY:HA2	1:A:363:LEU:HD22	1.98	0.46
1:A:141:ASN:HD22	1:A:279:GLN:HE21	1.64	0.46
1:C:163:PRO:HD3	1:C:202:ALA:HB2	1.96	0.46
2:D:61:ILE:N	2:D:61:ILE:CD1	2.79	0.46
1:E:66:PHE:CD2	1:E:67:PRO:HD3	2.50	0.46
2:B:142:ASN:HA	2:B:145:CYS:O	2.16	0.46
1:A:223:CYS:HA	1:A:274:GLN:O	2.15	0.46
2:D:107:ILE:O	2:D:108:SER:C	2.54	0.46
1:C:1:GLU:CA	2:D:142:ASN:H	2.28	0.46
2:B:154:PHE:O	2:B:155:LYS:C	2.54	0.46
1:E:398:ARG:HG2	1:E:398:ARG:NH1	2.30	0.46
2:B:92:LEU:HA	2:B:95:GLU:HG3	1.97	0.46
1:A:426:VAL:CG2	2:B:4:ILE:HG21	2.44	0.45
1:C:4:LYS:O	2:D:28:SER:HA	2.16	0.45
1:C:7:LEU:HA	1:C:7:LEU:HD13	1.73	0.45
2:D:149:CYS:O	2:D:153:ILE:N	2.36	0.45
1:A:393:PRO:HB2	1:A:394:PRO:CD	2.40	0.45
1:C:162:ILE:HD12	1:C:162:ILE:N	2.31	0.45
1:C:414:GLY:O	2:D:56:LYS:NZ	2.41	0.45
1:E:222:SER:HB2	1:E:278:LEU:HD12	1.98	0.45
1:A:198:LYS:O	1:A:199:GLU:C	2.54	0.45
1:E:7:LEU:HA	1:E:7:LEU:HD13	1.74	0.45
1:A:249:PHE:CE1	1:C:257:ASP:HB2	2.51	0.45
2:D:9:ILE:H	2:D:9:ILE:CD1	2.24	0.45
1:C:68:ARG:HA	1:C:350:GLU:OE2	2.16	0.45
1:E:88:LEU:HD23	1:E:88:LEU:N	2.31	0.45
2:F:77:ILE:H	2:F:77:ILE:HD12	1.81	0.45
1:C:5:ILE:HB	2:D:154:PHE:CZ	2.52	0.45
2:D:5:ASP:CG	2:D:9:ILE:HA	2.37	0.45
1:C:189:VAL:HG23	1:C:196:CYS:HA	1.98	0.45
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:158:LEU:CD2	1:A:158:LEU:N	2.79	0.45
1:C:315:GLN:HG3	1:C:317:ILE:HD13	1.99	0.45
1:C:3:ILE:HD11	2:D:140:ILE:N	2.29	0.45
2:D:4:ILE:HB	2:D:9:ILE:CD1	2.47	0.45
1:E:104:GLN:CB	1:E:153:SER:HB2	2.46	0.45
2:B:56:LYS:O	2:B:59:ILE:HG12	2.16	0.45
2:F:141:ASP:HB3	2:F:144:ILE:HG12	1.98	0.45
1:A:252:VAL:HG21	1:E:249:PHE:CD2	2.51	0.45
1:C:249:PHE:CE1	1:E:244:VAL:CG2	2.99	0.45
1:C:31:LYS:CE	1:C:411:ILE:HB	2.47	0.45
1:A:127:TYR:N	1:A:173:ASN:ND2	2.64	0.45
2:F:7:LEU:HB2	2:F:36:VAL:HG11	1.99	0.45
2:B:65:LYS:CB	2:B:65:LYS:NZ	2.76	0.45
1:C:68:ARG:H	1:C:68:ARG:HG2	1.48	0.45
1:E:1:GLU:CG	1:E:2:LYS:H	2.29	0.45
2:F:126:ALA:HB3	2:F:129:LEU:CD2	2.47	0.45
1:A:374:ILE:O	1:A:395:LYS:HA	2.17	0.45
2:B:154:PHE:O	2:B:156:PHE:CD2	2.70	0.45
1:E:246:TYR:HA	1:E:251:LYS:O	2.16	0.45
2:B:131:VAL:HG21	2:B:139:ILE:N	2.31	0.45
2:D:119:ALA:O	2:D:120:SER:C	2.54	0.45
1:C:329:ASP:HA	1:C:340:LEU:HD22	1.98	0.45
2:B:62:ALA:O	2:B:65:LYS:HB3	2.16	0.45
2:F:57:SER:O	2:F:61:ILE:HD13	2.17	0.45
1:C:88:LEU:HD23	1:C:88:LEU:N	2.30	0.45
1:E:281:LYS:O	1:E:285:TYR:OH	2.31	0.45
2:B:120:SER:OG	2:B:121:GLU:N	2.49	0.45
2:B:126:ALA:O	2:B:129:LEU:CD1	2.65	0.45
2:D:131:VAL:HG21	2:D:139:ILE:CB	2.43	0.45
1:C:256:LEU:HD12	1:C:257:ASP:N	2.31	0.45
1:A:296:MET:HE3	1:A:296:MET:HB2	1.84	0.45
2:F:4:ILE:HG22	2:F:13:PHE:CE2	2.51	0.45
1:C:38:LYS:O	1:C:38:LYS:CD	2.65	0.45
1:C:58:ARG:HD2	1:C:347:TYR:OH	2.16	0.45
1:A:38:LYS:HD3	1:A:38:LYS:O	2.17	0.45
1:A:38:LYS:HZ3	1:A:40:LYS:HD2	1.81	0.45
1:E:34:PHE:HE2	2:F:96:LEU:HD13	1.82	0.45
2:B:118:LEU:O	2:B:119:ALA:C	2.55	0.45
2:B:119:ALA:O	2:B:120:SER:C	2.54	0.45
1:C:424:THR:HG22	2:D:14:VAL:CG1	2.47	0.45
1:E:31:LYS:HZ2	1:E:411:ILE:HB	1.80	0.45
2:B:68:ASP:HB3	2:B:70:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:319:GLY:CA	1:A:354:HIS:HD2	2.30	0.45
1:E:66:PHE:CE1	1:E:70:ALA:HB2	2.52	0.45
1:C:75:LYS:O	1:C:78:ASP:HB2	2.17	0.45
1:E:31:LYS:NZ	1:E:31:LYS:CB	2.80	0.44
1:C:192:SER:C	1:C:194:ASN:H	2.20	0.44
1:E:121:HIS:C	1:E:123:ALA:H	2.21	0.44
1:E:425:THR:HB	2:F:16:ILE:HD11	1.99	0.44
2:B:50:ASN:O	2:B:53:GLN:HB2	2.18	0.44
2:F:42:GLU:HG2	2:F:42:GLU:H	1.58	0.44
2:F:149:CYS:HA	2:F:152:PHE:HB3	1.98	0.44
2:B:126:ALA:HB3	2:B:129:LEU:CD2	2.47	0.44
1:C:7:LEU:CD2	2:D:118:LEU:HD13	2.47	0.44
1:C:294:LEU:HD21	1:C:296:MET:CE	2.47	0.44
2:F:4:ILE:HD12	2:F:5:ASP:H	1.81	0.44
2:B:41:ALA:C	2:B:43:LYS:H	2.20	0.44
2:F:61:ILE:H	2:F:61:ILE:CD1	2.30	0.44
1:E:149:SER:HB3	1:E:304:ASP:O	2.17	0.44
1:C:74:ALA:O	1:C:75:LYS:C	2.54	0.44
1:E:93:PHE:CD1	1:E:93:PHE:N	2.85	0.44
1:E:224:TYR:CE1	1:E:274:GLN:HB3	2.52	0.44
2:B:141:ASP:HB3	2:B:144:ILE:CG1	2.47	0.44
2:B:4:ILE:HG23	2:B:13:PHE:CG	2.53	0.44
1:E:374:ILE:O	1:E:395:LYS:HA	2.16	0.44
1:E:426:VAL:HG22	1:E:427:THR:N	2.32	0.44
1:E:28:THR:CB	3:E:3501:NAG:C8	2.96	0.44
1:C:180:LYS:HD2	1:C:299:ARG:NH2	2.33	0.44
1:A:68:ARG:H	1:A:68:ARG:HG2	1.51	0.44
1:E:190:LYS:HA	1:E:190:LYS:HD3	1.74	0.44
2:D:149:CYS:HA	2:D:152:PHE:HB3	2.00	0.44
1:C:296:MET:CA	1:C:296:MET:HE2	2.46	0.44
1:E:234:ASN:HA	1:E:237:GLY:O	2.17	0.44
1:A:322:ARG:CD	1:A:354:HIS:CE1	3.00	0.44
1:C:161:THR:HG23	1:C:203:PHE:HB2	1.99	0.44
2:F:125:ARG:HB3	2:F:129:LEU:CD2	2.47	0.44
1:C:25:LEU:HD23	1:C:418:PRO:HA	1.99	0.44
1:E:181:ASN:O	1:E:183:ALA:N	2.51	0.44
1:C:234:ASN:HA	1:C:237:GLY:O	2.17	0.44
1:C:174:CYS:SG	1:C:178:PHE:HA	2.57	0.44
1:C:376:GLN:O	1:C:376:GLN:HG3	2.18	0.44
2:F:67:ASN:N	2:F:67:ASN:OD1	2.50	0.44
1:E:322:ARG:HD2	1:E:354:HIS:CE1	2.52	0.44
1:E:174:CYS:SG	1:E:178:PHE:HA	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:204:PHE:HE1	1:C:206:LEU:HD21	1.82	0.44
1:C:116:VAL:HG13	1:C:117:ASN:N	2.31	0.44
1:A:3:ILE:HD11	2:B:140:ILE:O	2.17	0.44
2:D:131:VAL:HG22	2:D:139:ILE:H	1.82	0.44
1:C:5:ILE:CG2	2:D:154:PHE:CE1	3.01	0.44
1:A:216:LYS:CD	1:A:305:MET:H	2.15	0.44
1:C:121:HIS:C	1:C:123:ALA:N	2.69	0.44
1:A:387:THR:O	1:A:402:ALA:HA	2.18	0.44
1:C:36:LEU:HA	1:C:36:LEU:HD23	1.70	0.44
2:F:111:LEU:HA	2:F:111:LEU:HD23	1.77	0.44
1:A:161:THR:HG23	1:A:203:PHE:HB2	2.00	0.44
1:E:28:THR:HG21	3:E:3501:NAG:C8	2.43	0.44
2:D:97:GLY:O	2:D:100:ARG:HB3	2.17	0.44
1:A:38:LYS:CD	1:A:38:LYS:O	2.66	0.44
5:D:2300:NAG:H83	1:E:20:GLY:C	2.38	0.44
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.70	0.44
1:E:42:GLY:HA2	1:E:363:LEU:HD22	1.99	0.44
2:D:141:ASP:HB3	2:D:144:ILE:CG1	2.48	0.44
1:A:38:LYS:HA	1:A:388:GLU:OE2	2.18	0.44
1:E:21:PHE:CD2	2:F:102:LEU:HD23	2.53	0.44
2:F:59:ILE:H	2:F:59:ILE:HG12	1.47	0.44
1:A:3:ILE:HD11	2:B:140:ILE:N	2.33	0.43
1:A:422:THR:C	1:A:424:THR:H	2.20	0.43
1:E:216:LYS:CD	1:E:305:MET:H	2.17	0.43
1:C:318:TRP:HA	1:C:318:TRP:CE3	2.53	0.43
1:E:318:TRP:CB	1:E:322:ARG:HG3	2.46	0.43
2:F:154:PHE:O	2:F:155:LYS:C	2.56	0.43
2:F:41:ALA:C	2:F:43:LYS:H	2.21	0.43
2:B:155:LYS:O	2:B:156:PHE:HB2	2.18	0.43
1:C:331:ALA:O	1:C:335:THR:CG2	2.66	0.43
1:C:219:LEU:C	1:C:219:LEU:CD2	2.86	0.43
2:F:119:ALA:O	2:F:120:SER:C	2.56	0.43
2:F:132:GLU:HG2	2:F:138:TRP:CE3	2.53	0.43
2:D:55:LEU:HD21	1:E:422:THR:HG22	1.99	0.43
1:E:230:LYS:O	1:E:233:TYR:N	2.51	0.43
1:C:38:LYS:HD3	1:C:38:LYS:O	2.18	0.43
1:C:408:ILE:HD12	1:C:409:PRO:HD2	1.99	0.43
1:C:141:ASN:HD22	1:C:279:GLN:HE21	1.65	0.43
1:E:261:SER:OG	1:E:262:PRO:HD2	2.18	0.43
1:E:5:ILE:HG23	2:F:26:LEU:HG	2.00	0.43
1:C:294:LEU:CD1	1:C:296:MET:HE3	2.31	0.43
2:D:9:ILE:HG21	2:D:13:PHE:CB	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:D:2301:NDG:C8	1:E:19:ASN:CG	2.86	0.43
1:A:13:SER:CB	2:B:18:GLU:O	2.67	0.43
2:B:102:LEU:HB3	1:C:21:PHE:CE1	2.53	0.43
1:C:104:GLN:CB	1:C:153:SER:HB2	2.46	0.43
1:A:266:ASN:HD22	1:A:266:ASN:N	2.14	0.43
1:C:52:ILE:HG12	1:C:53:GLY:N	2.32	0.43
2:F:132:GLU:CG	2:F:138:TRP:CE3	3.01	0.43
2:D:4:ILE:CB	2:D:9:ILE:HG13	2.48	0.43
2:D:4:ILE:HG22	2:D:13:PHE:HB3	1.99	0.43
2:D:42:GLU:H	2:D:42:GLU:HG2	1.59	0.43
2:D:111:LEU:HA	2:D:111:LEU:HD23	1.80	0.43
2:D:41:ALA:C	2:D:43:LYS:N	2.72	0.43
5:B:1301:NDG:O3	5:B:1302:MAN:C5	2.47	0.43
1:C:410:LYS:C	1:C:411:ILE:HD13	2.38	0.43
1:A:410:LYS:C	1:A:411:ILE:HD13	2.39	0.43
2:F:147:GLN:O	2:F:150:GLN:HB2	2.19	0.43
2:D:102:LEU:HD11	2:F:102:LEU:HD21	1.98	0.43
1:A:416:LEU:HB2	2:B:52:ILE:HD13	2.01	0.43
1:C:401:LEU:N	1:C:401:LEU:HD12	2.33	0.43
1:C:28:THR:HB	3:C:2501:NAG:C8	2.48	0.43
1:A:80:PHE:HB2	1:A:82:PHE:HE2	1.81	0.43
1:A:294:LEU:CD1	1:A:296:MET:HE3	2.37	0.43
2:D:59:ILE:HG12	2:D:59:ILE:H	1.52	0.43
2:F:147:GLN:O	2:F:150:GLN:N	2.51	0.43
1:E:266:ASN:ND2	1:E:266:ASN:C	2.70	0.43
1:A:404:LYS:HG2	1:A:404:LYS:H	1.32	0.43
1:C:426:VAL:HG23	2:D:4:ILE:HG23	1.93	0.43
1:C:230:LYS:O	1:C:233:TYR:N	2.52	0.43
1:C:44:SER:OG	1:C:45:VAL:N	2.51	0.43
1:C:158:LEU:HD21	1:C:298:GLU:CA	2.45	0.43
2:D:61:ILE:H	2:D:61:ILE:HD12	1.82	0.43
1:C:354:HIS:C	1:C:355:HIS:ND1	2.72	0.43
1:E:266:ASN:ND2	1:E:266:ASN:O	2.52	0.43
2:B:61:ILE:CD1	2:B:61:ILE:H	2.32	0.43
1:C:206:LEU:HB3	1:C:218:HIS:CD2	2.53	0.43
1:A:249:PHE:CE1	1:C:244:VAL:HG21	2.53	0.43
1:E:392:LEU:HA	1:E:393:PRO:HD2	1.56	0.43
1:C:377:SER:CB	1:C:392:LEU:H	2.10	0.43
1:C:190:LYS:HD2	1:C:192:SER:OG	2.18	0.43
1:E:387:THR:O	1:E:402:ALA:HA	2.19	0.43
1:A:88:LEU:N	1:A:88:LEU:HD23	2.34	0.43
2:B:77:ILE:H	2:B:77:ILE:HD12	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:366:GLY:C	1:E:368:ASP:H	2.21	0.43
2:B:131:VAL:CG1	2:B:139:ILE:H	2.31	0.43
2:D:107:ILE:HD13	2:D:107:ILE:HA	1.83	0.43
2:D:126:ALA:O	2:D:129:LEU:CD1	2.66	0.43
1:A:317:ILE:HG22	1:A:324:SER:HB3	1.99	0.43
1:E:38:LYS:CD	1:E:38:LYS:O	2.67	0.43
1:E:194:ASN:ND2	1:E:194:ASN:O	2.52	0.43
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.32	0.43
1:E:223:CYS:HA	1:E:274:GLN:O	2.18	0.43
1:C:27:ALA:HA	1:C:415:LEU:O	2.19	0.43
1:A:121:HIS:C	1:A:123:ALA:N	2.72	0.43
2:D:55:LEU:HD12	2:D:111:LEU:HG	2.01	0.43
2:D:39:GLU:OE1	2:D:155:LYS:HE3	2.19	0.43
1:A:294:LEU:CD2	1:A:294:LEU:C	2.87	0.43
2:D:147:GLN:O	2:D:150:GLN:HB2	2.19	0.43
1:E:253:VAL:O	1:E:278:LEU:HD21	2.19	0.43
1:E:241:TYR:CD2	1:E:242:PHE:N	2.87	0.43
1:E:404:LYS:HB2	1:E:406:GLU:HG2	2.00	0.43
2:B:115:LEU:HA	2:B:115:LEU:HD23	1.74	0.43
2:D:129:LEU:HD22	2:D:153:ILE:HG23	2.00	0.42
2:D:9:ILE:HG21	2:D:13:PHE:CG	2.53	0.42
1:A:231:GLU:HA	1:A:234:ASN:HB2	2.01	0.42
2:B:147:GLN:O	2:B:150:GLN:HB2	2.17	0.42
1:C:318:TRP:CG	1:C:322:ARG:HG3	2.54	0.42
1:E:338:CYS:O	2:F:78:ARG:NH2	2.52	0.42
1:A:135:LYS:HD3	1:A:327:ALA:HB3	2.00	0.42
1:C:42:GLY:HA2	1:C:363:LEU:HD22	2.00	0.42
1:A:209:GLN:HG2	1:A:214:GLU:HA	2.00	0.42
1:C:329:ASP:HA	1:C:340:LEU:CD2	2.49	0.42
2:D:67:ASN:O	2:D:68:ASP:O	2.37	0.42
2:F:141:ASP:O	2:F:144:ILE:HG12	2.19	0.42
1:A:423:ASP:CG	2:F:47:LYS:NZ	2.73	0.42
2:D:132:GLU:CG	2:D:138:TRP:CE3	3.02	0.42
1:E:162:ILE:N	1:E:162:ILE:CD1	2.82	0.42
1:C:249:PHE:CE1	1:E:244:VAL:HG21	2.54	0.42
1:E:156:ASN:HA	1:E:299:ARG:HG2	2.01	0.42
1:A:219:LEU:C	1:A:219:LEU:CD2	2.87	0.42
1:E:296:MET:HB2	1:E:296:MET:HE3	1.83	0.42
1:A:161:THR:C	1:A:162:ILE:HD12	2.40	0.42
1:E:319:GLY:N	1:E:354:HIS:CD2	2.81	0.42
1:E:85:GLY:O	1:E:99:VAL:CG1	2.68	0.42
1:E:398:ARG:CG	1:E:398:ARG:HH11	2.32	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:56:ASP:HB3	1:E:57:SER:H	1.29	0.42
1:E:36:LEU:HA	1:E:36:LEU:HD23	1.69	0.42
2:F:129:LEU:HD22	2:F:153:ILE:HG23	2.01	0.42
1:A:203:PHE:HE1	1:C:260:VAL:O	2.03	0.42
1:A:229:SER:C	1:A:231:GLU:OE1	2.58	0.42
2:F:68:ASP:HB3	2:F:70:ILE:HB	2.01	0.42
1:A:158:LEU:N	1:A:158:LEU:HD22	2.34	0.42
1:A:11:VAL:HG12	2:B:16:ILE:HA	2.01	0.42
1:E:398:ARG:HG2	1:E:398:ARG:HH11	1.85	0.42
1:C:198:LYS:O	1:C:199:GLU:C	2.58	0.42
1:A:373:CYS:HG	1:A:399:CYS:CB	2.32	0.42
2:D:93:LEU:HA	2:D:93:LEU:HD23	1.68	0.42
1:A:74:ALA:O	1:A:75:LYS:C	2.56	0.42
2:F:122:ILE:HB	2:F:138:TRP:HH2	1.83	0.42
1:E:392:LEU:HA	1:E:392:LEU:HD23	1.72	0.42
1:C:374:ILE:O	1:C:395:LYS:HA	2.19	0.42
1:C:422:THR:C	1:C:424:THR:H	2.23	0.42
1:E:158:LEU:CD2	1:E:298:GLU:HA	2.43	0.42
1:A:190:LYS:HE2	1:A:192:SER:OG	2.20	0.42
2:B:104:VAL:HG12	2:B:105:GLY:N	2.33	0.42
1:C:209:GLN:HG2	1:C:214:GLU:HA	2.01	0.42
2:D:126:ALA:HB3	2:D:129:LEU:CD2	2.50	0.42
1:A:401:LEU:HD12	1:A:401:LEU:N	2.33	0.42
1:A:315:GLN:HG3	1:A:317:ILE:HD13	2.01	0.42
2:B:41:ALA:HB1	2:B:155:LYS:HA	2.02	0.42
1:A:189:VAL:HG23	1:A:195:LYS:O	2.19	0.42
1:E:47:ASN:C	1:E:49:SER:H	2.22	0.42
1:C:190:LYS:HD3	1:C:190:LYS:HA	1.75	0.42
1:C:15:PHE:CD2	1:C:16:SER:N	2.87	0.42
1:C:149:SER:HB3	1:C:304:ASP:O	2.19	0.42
2:B:4:ILE:HG22	2:B:9:ILE:CG1	2.49	0.42
2:D:131:VAL:HG21	2:D:139:ILE:N	2.34	0.42
1:C:31:LYS:NZ	1:C:31:LYS:HB2	2.32	0.42
2:D:147:GLN:O	2:D:148:SER:C	2.57	0.42
1:C:38:LYS:H	1:C:38:LYS:CD	2.26	0.42
1:E:38:LYS:HD3	1:E:38:LYS:O	2.20	0.42
1:A:13:SER:HB2	2:B:18:GLU:O	2.20	0.42
2:D:45:PHE:O	2:D:47:LYS:N	2.53	0.42
1:A:85:GLY:O	1:A:99:VAL:CG1	2.67	0.42
1:E:266:ASN:N	1:E:266:ASN:HD22	2.18	0.42
2:D:30:LYS:CE	2:D:32:SER:HB3	2.49	0.42
1:E:31:LYS:CE	1:E:411:ILE:HB	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:67:ASN:O	2:F:68:ASP:O	2.38	0.42
1:E:158:LEU:HD21	1:E:298:GLU:CA	2.43	0.42
1:E:18:HIS:HD2	1:E:412:PRO:HD3	1.85	0.42
1:C:253:VAL:O	1:C:278:LEU:HD21	2.20	0.42
2:F:61:ILE:N	2:F:61:ILE:CD1	2.83	0.42
1:E:304:ASP:OD1	1:E:306:LYS:HB2	2.20	0.42
1:A:72:VAL:HG23	1:A:73:SER:O	2.19	0.42
2:F:99:ILE:O	2:F:99:ILE:HG12	2.20	0.42
1:C:417:ILE:HG12	2:D:24:TYR:CZ	2.55	0.42
1:E:294:LEU:CD2	1:E:295:LEU:N	2.80	0.42
1:A:166:VAL:HG22	1:A:167:THR:N	2.35	0.42
1:E:31:LYS:HZ2	1:E:31:LYS:C	2.24	0.42
1:C:181:ASN:O	1:C:182:PRO:C	2.55	0.42
1:A:192:SER:C	1:A:194:ASN:H	2.22	0.42
1:C:304:ASP:OD1	1:C:306:LYS:HB2	2.20	0.42
2:D:157:ASN:O	2:D:159:THR:HG23	2.20	0.41
1:E:181:ASN:O	1:E:182:PRO:C	2.55	0.41
1:C:319:GLY:CA	1:C:354:HIS:HD2	2.32	0.41
1:E:190:LYS:HA	1:E:191:PRO:HD2	1.82	0.41
1:C:241:TYR:CG	1:C:242:PHE:N	2.87	0.41
1:C:195:LYS:HA	1:C:195:LYS:HD2	1.41	0.41
1:E:366:GLY:C	1:E:368:ASP:N	2.73	0.41
1:A:5:ILE:HG22	1:A:6:CYS:N	2.34	0.41
2:B:149:CYS:O	2:B:153:ILE:N	2.41	0.41
2:D:132:GLU:HG2	2:D:138:TRP:CE3	2.55	0.41
2:D:149:CYS:O	2:D:153:ILE:HG12	2.21	0.41
1:A:10:GLN:HG2	2:B:17:VAL:HG22	2.02	0.41
1:A:33:MET:HE3	1:A:409:PRO:HB2	2.02	0.41
2:F:155:LYS:O	2:F:156:PHE:HB2	2.20	0.41
1:C:171:ALA:N	1:C:177:SER:O	2.49	0.41
1:C:281:LYS:O	1:C:285:TYR:OH	2.26	0.41
2:B:123:THR:OG1	2:B:138:TRP:HZ3	2.02	0.41
2:F:107:ILE:O	2:F:108:SER:C	2.59	0.41
2:D:51:ASP:O	2:D:55:LEU:HG	2.20	0.41
1:E:45:VAL:O	1:E:46:LEU:HD23	2.21	0.41
1:A:304:ASP:OD1	1:A:306:LYS:N	2.53	0.41
2:F:50:ASN:O	2:F:53:GLN:HB2	2.20	0.41
1:E:219:LEU:C	1:E:219:LEU:CD2	2.88	0.41
2:B:132:GLU:CG	2:B:138:TRP:CE3	3.04	0.41
1:E:160:LYS:HG3	1:E:162:ILE:CD1	2.50	0.41
2:D:68:ASP:HB3	2:D:70:ILE:HB	2.02	0.41
2:F:21:ILE:HD12	2:F:21:ILE:N	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:192:SER:C	1:E:194:ASN:H	2.24	0.41
1:A:18:HIS:ND1	1:A:18:HIS:N	2.68	0.41
1:A:75:LYS:O	1:A:78:ASP:HB2	2.20	0.41
1:A:95:PRO:HA	1:A:179:LEU:HD23	2.01	0.41
1:E:72:VAL:HG23	1:E:73:SER:O	2.20	0.41
2:B:80:LEU:HD12	2:B:80:LEU:HA	1.88	0.41
2:F:131:VAL:HG21	2:F:139:ILE:N	2.34	0.41
2:B:140:ILE:HD12	2:B:141:ASP:N	2.31	0.41
1:A:257:ASP:CG	1:A:259:ARG:HE	2.24	0.41
1:C:33:MET:HE3	1:C:409:PRO:HB2	2.02	0.41
2:F:157:ASN:O	2:F:159:THR:HG23	2.20	0.41
2:B:41:ALA:C	2:B:43:LYS:N	2.74	0.41
1:A:56:ASP:HB3	1:A:57:SER:H	1.26	0.41
2:F:126:ALA:O	2:F:129:LEU:CD1	2.68	0.41
1:E:377:SER:CB	1:E:392:LEU:H	2.11	0.41
2:D:61:ILE:HG22	2:D:62:ALA:N	2.35	0.41
2:D:65:LYS:CB	2:D:65:LYS:NZ	2.74	0.41
1:C:66:PHE:HE1	1:C:70:ALA:HB2	1.86	0.41
2:B:99:ILE:HD13	2:B:99:ILE:C	2.41	0.41
1:A:145:LEU:HA	1:A:145:LEU:HD12	1.88	0.41
1:E:201:LEU:C	1:E:201:LEU:CD2	2.89	0.41
1:E:330:GLN:NE2	4:E:3601:NAG:H83	2.35	0.41
1:E:40:LYS:N	1:E:379:TRP:O	2.51	0.41
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.85	0.41
1:E:404:LYS:HG2	1:E:404:LYS:H	1.34	0.41
2:B:125:ARG:C	2:B:129:LEU:HD11	2.40	0.41
2:F:55:LEU:HD12	2:F:111:LEU:HG	2.02	0.41
2:D:154:PHE:O	2:D:156:PHE:CD2	2.74	0.41
2:D:146:ASP:O	2:D:147:GLN:C	2.58	0.41
1:C:158:LEU:CD2	1:C:158:LEU:N	2.83	0.41
2:B:51:ASP:O	2:B:55:LEU:HG	2.20	0.41
1:C:34:PHE:HE2	2:D:96:LEU:CD1	2.29	0.41
2:B:39:GLU:HG2	2:B:40:SER:N	2.34	0.41
1:C:190:LYS:HE2	1:C:192:SER:OG	2.20	0.41
1:C:194:ASN:O	1:C:194:ASN:ND2	2.54	0.41
2:F:61:ILE:H	2:F:61:ILE:HD12	1.86	0.41
1:A:224:TYR:CE1	1:A:274:GLN:HB3	2.56	0.41
2:B:113:GLU:HB3	1:C:421:GLY:HA3	2.03	0.41
3:A:1500:NDG:H5	3:A:1501:NAG:C7	2.50	0.41
2:B:149:CYS:HA	2:B:152:PHE:HB3	2.02	0.41
2:D:119:ALA:HA	2:D:138:TRP:CH2	2.55	0.41
2:D:125:ARG:HB3	2:D:129:LEU:CD2	2.45	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:1301:NDG:C4	5:B:1302:MAN:C3	2.97	0.41
1:A:329:ASP:O	1:A:330:GLN:C	2.58	0.41
1:E:202:ALA:HB3	1:E:296:MET:HE1	2.03	0.41
1:A:31:LYS:CE	1:A:411:ILE:HB	2.49	0.41
1:A:411:ILE:HD13	1:A:411:ILE:N	2.36	0.41
1:C:231:GLU:N	1:C:231:GLU:OE2	2.52	0.41
2:B:67:ASN:O	2:B:68:ASP:O	2.38	0.41
1:E:44:SER:OG	1:E:45:VAL:N	2.54	0.41
1:A:102:LEU:HD21	1:A:104:GLN:NE2	2.35	0.41
1:E:354:HIS:C	1:E:355:HIS:ND1	2.73	0.41
1:C:102:LEU:HD21	1:C:104:GLN:NE2	2.35	0.41
2:B:59:ILE:HG12	2:B:59:ILE:H	1.49	0.41
1:E:18:HIS:ND1	1:E:18:HIS:N	2.68	0.41
1:C:191:PRO:O	1:C:194:ASN:N	2.50	0.41
1:C:190:LYS:HA	1:C:191:PRO:HD2	1.80	0.41
1:E:366:GLY:O	1:E:368:ASP:N	2.54	0.41
2:F:134:SER:OG	2:F:137:CYS:HB2	2.21	0.41
2:D:80:LEU:HA	2:D:80:LEU:HD12	1.93	0.41
2:B:5:ASP:CG	2:B:9:ILE:CG2	2.89	0.41
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.86	0.41
1:C:216:LYS:CD	1:C:305:MET:H	2.18	0.41
2:D:5:ASP:N	2:D:9:ILE:HD12	2.33	0.41
1:A:155:VAL:O	1:A:299:ARG:HG2	2.21	0.41
1:E:315:GLN:HG3	1:E:317:ILE:HD13	2.03	0.41
1:E:319:GLY:CA	1:E:354:HIS:HD2	2.33	0.41
2:D:21:ILE:HD12	2:D:21:ILE:N	2.29	0.41
2:F:51:ASP:O	2:F:55:LEU:HG	2.20	0.40
1:C:392:LEU:HD23	1:C:392:LEU:HA	1.81	0.40
1:E:38:LYS:CD	1:E:38:LYS:H	2.28	0.40
1:C:158:LEU:CD2	1:C:298:GLU:HA	2.47	0.40
1:A:11:VAL:N	2:B:15:ALA:O	2.38	0.40
2:F:41:ALA:C	2:F:43:LYS:N	2.75	0.40
4:E:3650:NAG:O4	4:E:3651:NAG:O7	2.39	0.40
1:E:406:GLU:H	1:E:406:GLU:CD	2.24	0.40
1:E:74:ALA:O	1:E:75:LYS:C	2.59	0.40
2:F:93:LEU:HD23	2:F:93:LEU:HA	1.70	0.40
1:A:100:ASP:OD1	1:A:100:ASP:C	2.60	0.40
1:E:27:ALA:HA	1:E:415:LEU:O	2.22	0.40
2:B:118:LEU:HA	2:B:118:LEU:HD23	1.94	0.40
2:B:119:ALA:O	2:B:122:ILE:N	2.55	0.40
1:E:25:LEU:HA	1:E:25:LEU:HD23	1.86	0.40
1:E:375:SER:HB2	1:E:395:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:39:GLU:OE1	2:F:155:LYS:HE3	2.22	0.40
1:E:189:VAL:HG23	1:E:195:LYS:O	2.22	0.40
1:A:310:PRO:HB3	1:A:396:PHE:CE1	2.56	0.40
1:E:391:LEU:HA	1:E:391:LEU:HD23	1.84	0.40
1:E:1:GLU:HA	2:F:141:ASP:C	2.41	0.40
2:B:132:GLU:HG2	2:B:138:TRP:CE3	2.56	0.40
1:A:31:LYS:CB	1:A:31:LYS:NZ	2.85	0.40
2:F:147:GLN:HG3	2:F:151:ASN:OD1	2.21	0.40
1:C:189:VAL:HG23	1:C:195:LYS:O	2.22	0.40
1:A:18:HIS:HD2	1:A:412:PRO:HD3	1.87	0.40
1:E:236:ARG:NH2	1:E:293:PHE:HZ	2.20	0.40
2:D:134:SER:OG	2:D:137:CYS:HB2	2.21	0.40
2:B:128:ASP:O	2:B:140:ILE:HD11	2.21	0.40
2:B:129:LEU:HD22	2:B:153:ILE:HG23	2.04	0.40
1:A:420:SER:HB2	2:B:12:LEU:O	2.21	0.40
2:D:118:LEU:HA	2:D:118:LEU:HD23	1.89	0.40
2:D:118:LEU:O	2:D:119:ALA:C	2.58	0.40
1:A:249:PHE:CE2	1:C:252:VAL:CG2	3.04	0.40
1:C:363:LEU:HA	1:C:363:LEU:HD23	1.71	0.40
4:E:3550:NAG:H61	4:E:3551:NAG:C7	2.52	0.40
2:B:26:LEU:HA	2:B:26:LEU:HD12	1.95	0.40
2:B:133:VAL:HB	2:B:134:SER:H	1.65	0.40
1:E:417:ILE:HA	2:F:24:TYR:OH	2.21	0.40
1:E:25:LEU:HD23	1:E:418:PRO:HA	2.03	0.40
2:D:123:THR:OG1	2:D:138:TRP:HZ3	2.04	0.40
2:D:41:ALA:HB1	2:D:155:LYS:HA	2.03	0.40
2:F:30:LYS:HD2	2:F:32:SER:N	2.08	0.40
1:E:158:LEU:CD2	1:E:158:LEU:N	2.84	0.40
1:E:58:ARG:HD2	1:E:347:TYR:OH	2.20	0.40
1:E:161:THR:HG23	1:E:203:PHE:HB2	2.02	0.40
1:A:195:LYS:HA	1:A:195:LYS:HD2	1.47	0.40
1:E:87:SER:O	1:E:88:LEU:C	2.59	0.40
1:E:242:PHE:CD1	1:E:242:PHE:C	2.94	0.40
2:D:11:VAL:HG13	2:D:11:VAL:O	2.20	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	425/432 (98%)	359 (84%)	49 (12%)	17 (4%)	5	32
1	C	425/432 (98%)	359 (84%)	50 (12%)	16 (4%)	5	34
1	E	425/432 (98%)	358 (84%)	51 (12%)	16 (4%)	5	34
2	B	160/175 (91%)	113 (71%)	32 (20%)	15 (9%)	1	7
2	D	160/175 (91%)	111 (69%)	32 (20%)	17 (11%)	1	5
2	F	160/175 (91%)	115 (72%)	29 (18%)	16 (10%)	1	6
All	All	1755/1821 (96%)	1415 (81%)	243 (14%)	97 (6%)	3	23

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	48	GLN
1	A	66	PHE
1	A	393	PRO
2	B	18	GLU
2	B	42	GLU
2	B	68	ASP
2	B	126	ALA
2	B	130	ALA
2	B	132	GLU
2	B	155	LYS
1	C	2	LYS
1	C	47	ASN
1	C	48	GLN
1	C	66	PHE
1	C	393	PRO
2	D	18	GLU
2	D	42	GLU
2	D	68	ASP
2	D	126	ALA
2	D	130	ALA

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Mol	Chain	Res	Type
2	D	132	GLU
2	D	155	LYS
2	D	161	PRO
2	D	163	PRO
2	D	164	THR
1	E	47	ASN
1	E	48	GLN
1	E	66	PHE
1	E	393	PRO
2	F	18	GLU
2	F	68	ASP
2	F	126	ALA
2	F	130	ALA
2	F	132	GLU
2	F	155	LYS
2	F	161	PRO
2	F	162	VAL
2	F	164	THR
1	A	64	SER
1	A	422	THR
2	B	67	ASN
2	B	133	VAL
2	B	156	PHE
1	C	64	SER
1	C	422	THR
2	D	67	ASN
2	D	133	VAL
1	E	64	SER
1	E	422	THR
2	F	42	GLU
2	F	67	ASN
2	F	133	VAL
2	F	156	PHE
1	A	2	LYS
1	A	177	SER
2	B	46	GLU
2	B	161	PRO
1	C	122	ALA
1	C	177	SER
1	C	407	SER
2	D	46	GLU
2	D	156	PHE

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Mol	Chain	Res	Type
1	E	122	ALA
1	E	177	SER
1	E	407	SER
2	F	46	GLU
1	A	14	SER
1	A	407	SER
2	B	162	VAL
1	C	14	SER
1	C	230	LYS
2	D	66	LEU
1	E	14	SER
1	E	230	LYS
1	A	4	LYS
1	A	122	ALA
1	A	181	ASN
2	B	164	THR
1	C	181	ASN
2	D	6	ASP
1	E	127	TYR
2	F	6	ASP
1	A	127	TYR
1	E	181	ASN
1	A	3	ILE
1	A	250	GLY
2	F	61	ILE
1	C	3	ILE
2	D	61	ILE
1	A	67	PRO
2	B	61	ILE
1	C	291	PRO
1	E	3	ILE
1	E	67	PRO
1	E	291	PRO
1	C	67	PRO

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/374 (99%)	269 (73%)	100 (27%)	1	2
1	C	368/374 (98%)	265 (72%)	103 (28%)	0	2
1	E	369/374 (99%)	265 (72%)	104 (28%)	0	2
2	B	134/147 (91%)	78 (58%)	56 (42%)	0	0
2	D	134/147 (91%)	82 (61%)	52 (39%)	0	0
2	F	134/147 (91%)	81 (60%)	53 (40%)	0	0
All	All	1508/1563 (96%)	1040 (69%)	468 (31%)	0	1

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	7	LEU
1	A	13	SER
1	A	14	SER
1	A	16	SER
1	A	17	LEU
1	A	18	HIS
1	A	31	LYS
1	A	32	ARG
1	A	38	LYS
1	A	40	LYS
1	A	46	LEU
1	A	47	ASN
1	A	49	SER
1	A	56	ASP
1	A	57	SER
1	A	58	ARG
1	A	59	THR
1	A	61	LYS
1	A	64	SER
1	A	68	ARG
1	A	82	PHE
1	A	88	LEU
1	A	98	LYS
1	A	99	VAL
1	A	102	LEU
1	A	109	HIS
1	A	125	ASN
1	A	136	LEU
1	A	145	LEU

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Mol	Chain	Res	Type
1	A	153	SER
1	A	154	LEU
1	A	158	LEU
1	A	160	LYS
1	A	161	THR
1	A	165	GLN
1	A	167	THR
1	A	173	ASN
1	A	174	CYS
1	A	175	ASN
1	A	180	LYS
1	A	189	VAL
1	A	190	LYS
1	A	192	SER
1	A	195	LYS
1	A	198	LYS
1	A	200	ASN
1	A	201	LEU
1	A	204	PHE
1	A	208	THR
1	A	209	GLN
1	A	219	LEU
1	A	230	LYS
1	A	231	GLU
1	A	236	ARG
1	A	238	CYS
1	A	240	ASN
1	A	248	SER
1	A	252	VAL
1	A	266	ASN
1	A	267	SER
1	A	270	THR
1	A	272	THR
1	A	274	GLN
1	A	280	LEU
1	A	286	SER
1	A	288	ARG
1	A	290	SER
1	A	292	ARG
1	A	294	LEU
1	A	299	ARG
1	A	302	CYS

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Mol	Chain	Res	Type
1	A	306	LYS
1	A	316	SER
1	A	317	ILE
1	A	322	ARG
1	A	328	VAL
1	A	329	ASP
1	A	330	GLN
1	A	335	THR
1	A	342	GLN
1	A	343	LYS
1	A	348	ILE
1	A	365	SER
1	A	372	ARG
1	A	373	CYS
1	A	377	SER
1	A	380	VAL
1	A	382	GLU
1	A	384	SER
1	A	387	THR
1	A	388	GLU
1	A	395	LYS
1	A	398	ARG
1	A	404	LYS
1	A	408	ILE
1	A	416	LEU
1	A	419	THR
1	A	423	ASP
1	A	425	THR
2	B	4	ILE
2	B	5	ASP
2	B	6	ASP
2	B	7	LEU
2	B	9	ILE
2	B	11	VAL
2	B	12	LEU
2	B	13	PHE
2	B	14	VAL
2	B	19	THR
2	B	21	ILE
2	B	25	LEU
2	B	26	LEU
2	B	29	ARG

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Mol	Chain	Res	Type
2	B	30	LYS
2	B	31	GLU
2	B	43	LYS
2	B	47	LYS
2	B	52	ILE
2	B	56	LYS
2	B	57	SER
2	B	58	SER
2	B	59	ILE
2	B	65	LYS
2	B	68	ASP
2	B	69	ARG
2	B	70	ILE
2	B	71	SER
2	B	77	ILE
2	B	80	LEU
2	B	82	LEU
2	B	88	ARG
2	B	89	SER
2	B	92	LEU
2	B	98	ILE
2	B	99	ILE
2	B	102	LEU
2	B	109	ILE
2	B	111	LEU
2	B	112	GLN
2	B	114	SER
2	B	117	GLU
2	B	123	THR
2	B	125	ARG
2	B	128	ASP
2	B	129	LEU
2	B	131	VAL
2	B	132	GLU
2	B	138	TRP
2	B	140	ILE
2	B	143	ASN
2	B	144	ILE
2	B	148	SER
2	B	155	LYS
2	B	159	THR
2	B	162	VAL

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Mol	Chain	Res	Type
1	C	7	LEU
1	C	13	SER
1	C	14	SER
1	C	16	SER
1	C	17	LEU
1	C	18	HIS
1	C	31	LYS
1	C	32	ARG
1	C	38	LYS
1	C	40	LYS
1	C	46	LEU
1	C	47	ASN
1	C	49	SER
1	C	56	ASP
1	C	57	SER
1	C	58	ARG
1	C	59	THR
1	C	61	LYS
1	C	63	ASN
1	C	64	SER
1	C	68	ARG
1	C	82	PHE
1	C	88	LEU
1	C	98	LYS
1	C	99	VAL
1	C	102	LEU
1	C	109	HIS
1	C	120	PRO
1	C	125	ASN
1	C	136	LEU
1	C	145	LEU
1	C	153	SER
1	C	154	LEU
1	C	158	LEU
1	C	160	LYS
1	C	161	THR
1	C	165	GLN
1	C	167	THR
1	C	170	THR
1	C	173	ASN
1	C	174	CYS
1	C	175	ASN

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Mol	Chain	Res	Type
1	C	180	LYS
1	C	189	VAL
1	C	190	LYS
1	C	192	SER
1	C	195	LYS
1	C	198	LYS
1	C	200	ASN
1	C	201	LEU
1	C	204	PHE
1	C	208	THR
1	C	209	GLN
1	C	219	LEU
1	C	230	LYS
1	C	231	GLU
1	C	236	ARG
1	C	238	CYS
1	C	240	ASN
1	C	248	SER
1	C	252	VAL
1	C	266	ASN
1	C	267	SER
1	C	270	THR
1	C	272	THR
1	C	274	GLN
1	C	280	LEU
1	C	286	SER
1	C	288	ARG
1	C	290	SER
1	C	292	ARG
1	C	294	LEU
1	C	299	ARG
1	C	302	CYS
1	C	306	LYS
1	C	316	SER
1	C	317	ILE
1	C	322	ARG
1	C	328	VAL
1	C	329	ASP
1	C	330	GLN
1	C	335	THR
1	C	342	GLN
1	C	343	LYS

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Mol	Chain	Res	Type
1	C	348	ILE
1	C	365	SER
1	C	372	ARG
1	C	373	CYS
1	C	377	SER
1	C	380	VAL
1	C	382	GLU
1	C	384	SER
1	C	387	THR
1	C	388	GLU
1	C	395	LYS
1	C	398	ARG
1	C	404	LYS
1	C	408	ILE
1	C	416	LEU
1	C	419	THR
1	C	423	ASP
1	C	425	THR
1	C	427	THR
2	D	7	LEU
2	D	9	ILE
2	D	11	VAL
2	D	12	LEU
2	D	14	VAL
2	D	19	THR
2	D	21	ILE
2	D	25	LEU
2	D	26	LEU
2	D	29	ARG
2	D	30	LYS
2	D	31	GLU
2	D	43	LYS
2	D	47	LYS
2	D	52	ILE
2	D	56	LYS
2	D	57	SER
2	D	58	SER
2	D	59	ILE
2	D	65	LYS
2	D	68	ASP
2	D	69	ARG
2	D	70	ILE

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Mol	Chain	Res	Type
2	D	71	SER
2	D	77	ILE
2	D	78	ARG
2	D	80	LEU
2	D	82	LEU
2	D	88	ARG
2	D	89	SER
2	D	92	LEU
2	D	98	ILE
2	D	99	ILE
2	D	102	LEU
2	D	109	ILE
2	D	111	LEU
2	D	112	GLN
2	D	114	SER
2	D	117	GLU
2	D	123	THR
2	D	125	ARG
2	D	128	ASP
2	D	129	LEU
2	D	131	VAL
2	D	132	GLU
2	D	138	TRP
2	D	140	ILE
2	D	143	ASN
2	D	144	ILE
2	D	148	SER
2	D	155	LYS
2	D	159	THR
1	E	7	LEU
1	E	13	SER
1	E	14	SER
1	E	16	SER
1	E	17	LEU
1	E	18	HIS
1	E	31	LYS
1	E	32	ARG
1	E	38	LYS
1	E	40	LYS
1	E	46	LEU
1	E	47	ASN
1	E	49	SER

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Mol	Chain	Res	Type
1	E	56	ASP
1	E	57	SER
1	E	58	ARG
1	E	59	THR
1	E	61	LYS
1	E	63	ASN
1	E	64	SER
1	E	68	ARG
1	E	82	PHE
1	E	88	LEU
1	E	98	LYS
1	E	99	VAL
1	E	100	ASP
1	E	102	LEU
1	E	109	HIS
1	E	120	PRO
1	E	125	ASN
1	E	136	LEU
1	E	145	LEU
1	E	153	SER
1	E	154	LEU
1	E	158	LEU
1	E	160	LYS
1	E	161	THR
1	E	165	GLN
1	E	167	THR
1	E	173	ASN
1	E	174	CYS
1	E	175	ASN
1	E	180	LYS
1	E	189	VAL
1	E	190	LYS
1	E	192	SER
1	E	195	LYS
1	E	198	LYS
1	E	200	ASN
1	E	201	LEU
1	E	204	PHE
1	E	208	THR
1	E	209	GLN
1	E	219	LEU
1	E	220	VAL

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Mol	Chain	Res	Type
1	E	230	LYS
1	E	231	GLU
1	E	236	ARG
1	E	238	CYS
1	E	240	ASN
1	E	248	SER
1	E	252	VAL
1	E	266	ASN
1	E	267	SER
1	E	270	THR
1	E	272	THR
1	E	274	GLN
1	E	280	LEU
1	E	286	SER
1	E	288	ARG
1	E	290	SER
1	E	292	ARG
1	E	294	LEU
1	E	299	ARG
1	E	302	CYS
1	E	306	LYS
1	E	316	SER
1	E	317	ILE
1	E	322	ARG
1	E	328	VAL
1	E	329	ASP
1	E	330	GLN
1	E	335	THR
1	E	342	GLN
1	E	343	LYS
1	E	348	ILE
1	E	365	SER
1	E	372	ARG
1	E	373	CYS
1	E	377	SER
1	E	380	VAL
1	E	382	GLU
1	E	384	SER
1	E	387	THR
1	E	388	GLU
1	E	395	LYS
1	E	398	ARG

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Mol	Chain	Res	Type
1	E	404	LYS
1	E	408	ILE
1	E	416	LEU
1	E	419	THR
1	E	423	ASP
1	E	425	THR
1	E	427	THR
2	F	6	ASP
2	F	9	ILE
2	F	11	VAL
2	F	12	LEU
2	F	14	VAL
2	F	19	THR
2	F	21	ILE
2	F	25	LEU
2	F	26	LEU
2	F	29	ARG
2	F	30	LYS
2	F	31	GLU
2	F	43	LYS
2	F	47	LYS
2	F	52	ILE
2	F	56	LYS
2	F	57	SER
2	F	58	SER
2	F	59	ILE
2	F	65	LYS
2	F	68	ASP
2	F	69	ARG
2	F	70	ILE
2	F	71	SER
2	F	77	ILE
2	F	80	LEU
2	F	82	LEU
2	F	85	GLU
2	F	88	ARG
2	F	89	SER
2	F	92	LEU
2	F	98	ILE
2	F	99	ILE
2	F	102	LEU
2	F	109	ILE

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Mol	Chain	Res	Type
2	F	111	LEU
2	F	112	GLN
2	F	114	SER
2	F	117	GLU
2	F	123	THR
2	F	125	ARG
2	F	128	ASP
2	F	129	LEU
2	F	131	VAL
2	F	132	GLU
2	F	138	TRP
2	F	140	ILE
2	F	143	ASN
2	F	144	ILE
2	F	148	SER
2	F	155	LYS
2	F	159	THR
2	F	164	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	18	HIS
1	A	63	ASN
1	A	104	GLN
1	A	141	ASN
1	A	209	GLN
1	A	234	ASN
1	A	240	ASN
1	A	266	ASN
1	A	315	GLN
1	A	330	GLN
1	A	342	GLN
1	A	354	HIS
1	A	376	GLN
2	B	112	GLN
2	B	143	ASN
2	B	150	GLN
2	B	157	ASN
1	C	8	GLN
1	C	10	GLN

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Mol	Chain	Res	Type
1	C	18	HIS
1	C	63	ASN
1	C	104	GLN
1	C	141	ASN
1	C	173	ASN
1	C	209	GLN
1	C	234	ASN
1	C	240	ASN
1	C	266	ASN
1	C	315	GLN
1	C	330	GLN
1	C	342	GLN
1	C	354	HIS
1	C	376	GLN
2	D	112	GLN
2	D	150	GLN
2	D	157	ASN
1	E	8	GLN
1	E	10	GLN
1	E	18	HIS
1	E	63	ASN
1	E	104	GLN
1	E	141	ASN
1	E	173	ASN
1	E	209	GLN
1	E	234	ASN
1	E	240	ASN
1	E	266	ASN
1	E	315	GLN
1	E	330	GLN
1	E	342	GLN
1	E	354	HIS
1	E	376	GLN
2	F	112	GLN
2	F	143	ASN
2	F	150	GLN
2	F	157	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 ⓘ

45 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NDG	A	1500	1,3	12,14,15	0.64	0	15,19,21	1.09	1 (6%)
3	NAG	A	1501	3	12,14,15	0.69	0	15,19,21	1.40	2 (13%)
3	BMA	A	1502	3	10,11,12	0.83	0	11,15,17	0.51	0
4	NAG	A	1550	1,4	12,14,15	0.71	0	15,19,21	1.36	2 (13%)
4	NAG	A	1551	4	12,14,15	0.59	0	15,19,21	0.70	0
4	BMA	A	1552	4	10,11,12	0.67	0	11,15,17	0.43	0
4	NAG	A	1600	1,4	12,14,15	0.49	0	15,19,21	0.99	2 (13%)
4	NAG	A	1601	4	12,14,15	0.64	0	15,19,21	1.04	2 (13%)
4	BMA	A	1602	4	10,11,12	0.93	1 (10%)	11,15,17	0.85	1 (9%)
4	NAG	A	1650	1,4	12,14,15	0.68	0	15,19,21	0.93	1 (6%)
4	NAG	A	1651	4	12,14,15	0.54	0	15,19,21	0.77	0
4	BMA	A	1652	4	10,11,12	0.57	0	11,15,17	0.36	0
5	NAG	B	1300	2,5	12,14,15	0.68	0	15,19,21	1.29	3 (20%)
5	NDG	B	1301	5	12,14,15	0.53	0	15,19,21	1.60	2 (13%)
5	MAN	B	1302	5	10,11,12	0.52	0	11,15,17	0.46	0
3	NDG	C	2500	1,3	12,14,15	0.54	0	15,19,21	1.22	2 (13%)
3	NAG	C	2501	3	12,14,15	0.62	0	15,19,21	0.81	1 (6%)
3	BMA	C	2502	3	10,11,12	0.61	0	11,15,17	0.45	0
4	NAG	C	2550	1,4	12,14,15	0.78	0	15,19,21	1.10	1 (6%)
4	NAG	C	2551	4	12,14,15	0.70	0	15,19,21	0.84	1 (6%)
4	BMA	C	2552	4	10,11,12	0.76	0	11,15,17	0.71	0
6	NAG	C	2600	1,6	12,14,15	0.84	0	15,19,21	0.93	1 (6%)
6	NDG	C	2601	6	12,14,15	0.76	0	15,19,21	0.96	0
6	BMA	C	2602	6	10,11,12	0.59	0	11,15,17	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	2650	1,4	12,14,15	0.81	0	15,19,21	1.24	2 (13%)
4	NAG	C	2651	4	12,14,15	0.65	0	15,19,21	0.95	1 (6%)
4	BMA	C	2652	4	10,11,12	0.50	0	11,15,17	0.90	1 (9%)
5	NAG	D	2300	2,5	12,14,15	0.81	0	15,19,21	1.15	2 (13%)
5	NDG	D	2301	5	12,14,15	0.66	0	15,19,21	1.21	2 (13%)
5	MAN	D	2302	5	10,11,12	0.59	0	11,15,17	0.36	0
3	NDG	E	3500	1,3	12,14,15	0.55	0	15,19,21	1.05	0
3	NAG	E	3501	3	12,14,15	0.59	0	15,19,21	1.08	1 (6%)
3	BMA	E	3502	3	10,11,12	0.65	0	11,15,17	0.29	0
4	NAG	E	3550	1,4	12,14,15	0.68	0	15,19,21	0.79	1 (6%)
4	NAG	E	3551	4	12,14,15	0.82	0	15,19,21	0.77	0
4	BMA	E	3552	4	10,11,12	0.69	0	11,15,17	0.66	0
4	NAG	E	3600	1,4	12,14,15	0.58	0	15,19,21	0.83	0
4	NAG	E	3601	4	12,14,15	0.73	0	15,19,21	1.19	2 (13%)
4	BMA	E	3602	4	10,11,12	0.73	0	11,15,17	0.62	0
4	NAG	E	3650	1,4	12,14,15	0.60	0	15,19,21	0.83	1 (6%)
4	NAG	E	3651	4	12,14,15	0.58	0	15,19,21	0.64	0
4	BMA	E	3652	4	10,11,12	0.68	0	11,15,17	0.51	0
5	NAG	F	3300	2,5	12,14,15	0.52	0	15,19,21	1.52	2 (13%)
5	NDG	F	3301	5	12,14,15	0.67	0	15,19,21	1.82	3 (20%)
5	MAN	F	3302	5	10,11,12	0.52	0	11,15,17	0.47	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
3	NDG	A	1500	1,3	-	0/6/23/26	1/1/1/1
3	NAG	A	1501	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1502	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1550	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1551	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1552	4	-	0/2/19/22	0/1/1/1
4	NAG	A	1600	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1601	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1602	4	-	0/2/19/22	0/1/1/1
4	NAG	A	1650	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1651	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1652	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1300	2,5	-	0/6/23/26	0/1/1/1
5	NDG	B	1301	5	-	1/6/23/26	0/1/1/1
5	MAN	B	1302	5	-	0/2/19/22	0/1/1/1
3	NDG	C	2500	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2501	3	-	0/6/23/26	0/1/1/1
3	BMA	C	2502	3	-	0/2/19/22	0/1/1/1
4	NAG	C	2550	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2551	4	-	0/6/23/26	0/1/1/1
4	BMA	C	2552	4	-	0/2/19/22	0/1/1/1
6	NAG	C	2600	1,6	-	0/6/23/26	0/1/1/1
6	NDG	C	2601	6	-	0/6/23/26	1/1/1/1
6	BMA	C	2602	6	-	0/2/19/22	0/1/1/1
4	NAG	C	2650	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2651	4	-	0/6/23/26	0/1/1/1
4	BMA	C	2652	4	-	0/2/19/22	0/1/1/1
5	NAG	D	2300	2,5	-	0/6/23/26	0/1/1/1
5	NDG	D	2301	5	-	0/6/23/26	1/1/1/1
5	MAN	D	2302	5	-	0/2/19/22	0/1/1/1
3	NDG	E	3500	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3501	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3502	3	-	0/2/19/22	0/1/1/1
4	NAG	E	3550	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	3551	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3552	4	-	0/2/19/22	0/1/1/1
4	NAG	E	3600	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	3601	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3602	4	-	0/2/19/22	0/1/1/1
4	NAG	E	3650	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	3651	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3652	4	-	0/2/19/22	0/1/1/1
5	NAG	F	3300	2,5	-	0/6/23/26	0/1/1/1
5	NDG	F	3301	5	-	0/6/23/26	0/1/1/1
5	MAN	F	3302	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1602	BMA	C4-C5	2.45	1.58	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3301	NDG	C3-C4-C5	-5.30	100.73	110.20
5	B	1301	NDG	C3-C4-C5	-4.44	102.27	110.20
4	A	1550	NAG	O5-C5-C6	-3.73	103.06	106.98
5	F	3300	NAG	C3-C4-C5	-3.53	103.90	110.20
3	A	1501	NAG	C4-C3-C2	-3.34	103.15	111.32
3	C	2500	NDG	C4-C3-C2	-3.12	103.67	111.32
4	C	2650	NAG	C2-N2-C7	-3.12	117.86	123.09
5	F	3301	NDG	C6-C5-C4	2.88	119.96	113.00
4	C	2651	NAG	C2-N2-C7	-2.87	118.27	123.09
4	C	2550	NAG	C2-N2-C7	-2.84	118.33	123.09
3	E	3501	NAG	C3-C2-N2	-2.81	107.49	111.76
3	A	1501	NAG	C2-N2-C7	-2.79	118.41	123.09
5	D	2300	NAG	C3-C4-C5	-2.74	105.31	110.20
5	F	3300	NAG	C6-C5-C4	2.66	119.42	113.00
5	B	1300	NAG	C3-C4-C5	-2.63	105.51	110.20
5	D	2300	NAG	C2-N2-C7	-2.58	118.75	123.09
4	C	2652	BMA	C4-C3-C2	-2.53	107.11	110.50
5	B	1301	NDG	C6-C5-C4	2.45	118.93	113.00
4	E	3601	NAG	C2-N2-C7	-2.43	119.02	123.09
3	A	1500	NDG	C2-N2-C7	-2.42	119.03	123.09
4	E	3550	NAG	C2-N2-C7	-2.42	119.03	123.09
4	E	3601	NAG	C3-C4-C5	2.38	114.45	110.20
3	C	2500	NDG	C2-N2-C7	-2.37	119.10	123.09
4	A	1601	NAG	C3-C4-C5	2.24	114.21	110.20
4	A	1600	NAG	C3-C2-N2	-2.16	108.47	111.76
3	C	2501	NAG	C2-N2-C7	-2.15	119.47	123.09
5	B	1300	NAG	C2-N2-C7	-2.14	119.50	123.09
4	C	2551	NAG	C2-N2-C7	-2.13	119.51	123.09
4	A	1650	NAG	C2-N2-C7	-2.13	119.52	123.09
4	E	3650	NAG	C2-N2-C7	-2.12	119.54	123.09
6	C	2600	NAG	C2-N2-C7	-2.09	119.58	123.09
4	A	1601	NAG	C2-N2-C7	-2.09	119.58	123.09
4	A	1600	NAG	C2-N2-C7	-2.08	119.60	123.09
5	F	3301	NDG	O4-C4-C5	2.07	114.75	109.28
4	A	1602	BMA	C3-C4-C5	2.06	113.89	110.20
4	C	2650	NAG	O5-C5-C4	2.05	113.26	110.65
5	D	2301	NDG	C3-C2-N2	-2.04	108.65	111.76
5	D	2301	NDG	C2-N2-C7	-2.04	119.66	123.09
4	A	1550	NAG	C2-N2-C7	-2.04	119.67	123.09
5	B	1300	NAG	O5-C5-C4	-2.04	108.07	110.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1301	NDG	C3-C2-N2-C7

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2301	NDG	C1-C2-C3-C4-C5-O
6	C	2601	NDG	C1-C2-C3-C4-C5-O
3	A	1500	NDG	C1-C2-C3-C4-C5-O

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.