



wwPDB EM Map/Model Validation Report ⓘ

Apr 26, 2016 – 04:25 PM EDT

PDB ID : 5IRE
EMDB ID: : EMD-8116
Title : The cryo-EM structure of Zika Virus
Authors : Sirohi, D.; Chen, Z.; Sun, L.; Klose, T.; Pierson, T.; Rossmann, M.; Kuhn, R.
Deposited on : 2016-03-13
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

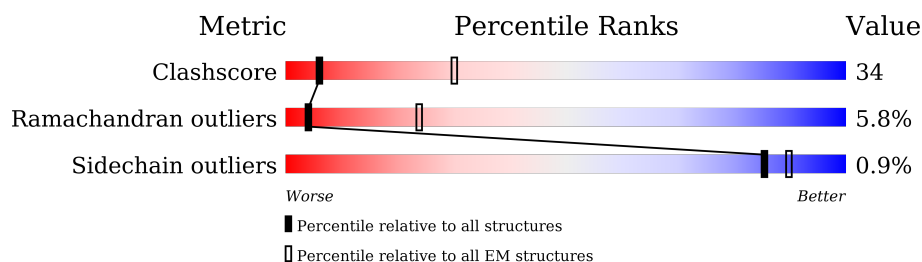
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	504	66% 28% . .
1	C	504	62% 32% 6% .
1	E	504	67% 27% 5% .
2	B	75	80% 19% .
2	D	75	73% 24% .
2	F	75	73% 23% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	600	-	-	X	-
3	NAG	E	600	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11024 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

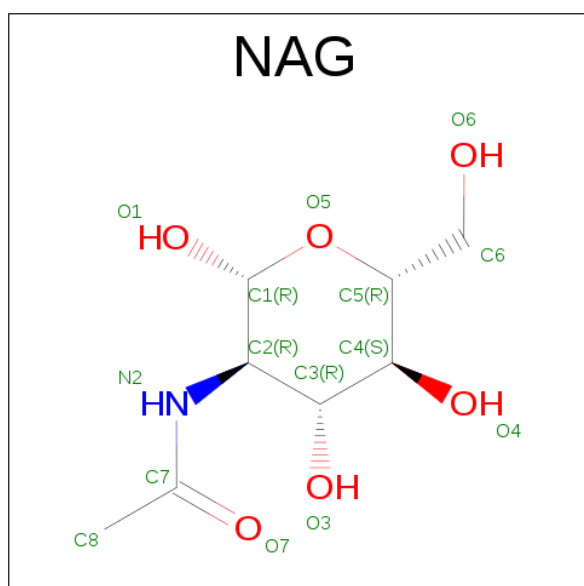
- Molecule 1 is a protein called E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	501	Total	C	N	O	S	0	0
			3167	1993	576	582	16		
1	C	501	Total	C	N	O	S	0	0
			3225	2035	589	586	15		
1	E	501	Total	C	N	O	S	0	0
			3186	2003	581	585	17		

- Molecule 2 is a protein called M protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	75	Total	C	N	O	0	0
			456	285	85	86		
2	D	75	Total	C	N	O	0	0
			456	285	85	86		
2	F	75	Total	C	N	O	0	0
			450	282	82	86		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

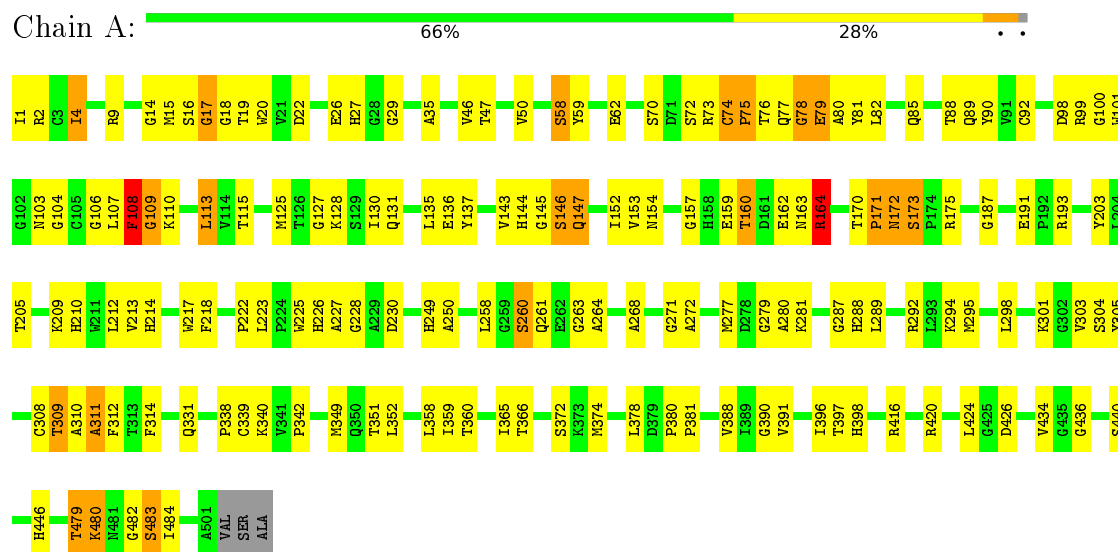


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 28	C 16	N 2	O 10	0
3	A	1	Total 28	C 16	N 2	O 10	0
3	C	1	Total 28	C 16	N 2	O 10	0
3	C	1	Total 28	C 16	N 2	O 10	0
3	E	1	Total 28	C 16	N 2	O 10	0
3	E	1	Total 28	C 16	N 2	O 10	0

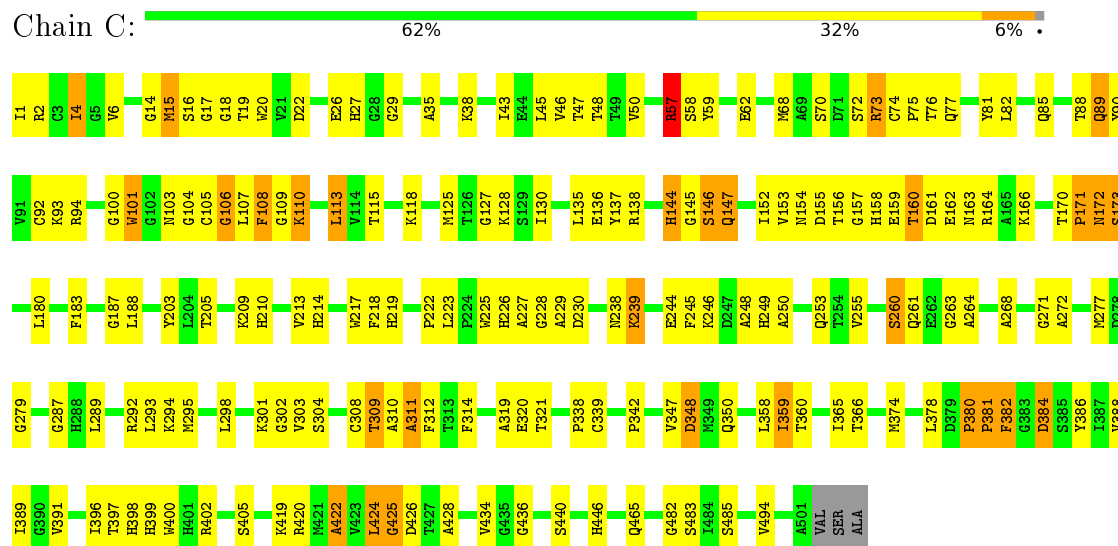
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

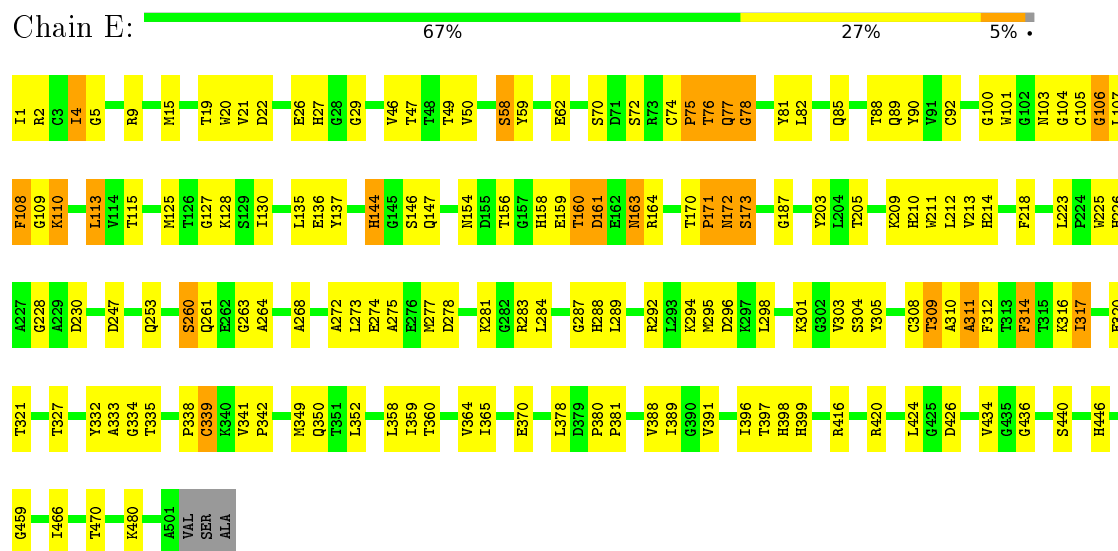
- Molecule 1: E protein



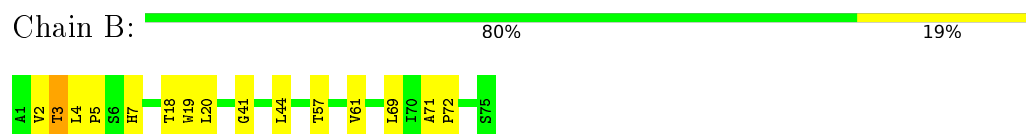
- Molecule 1: E protein



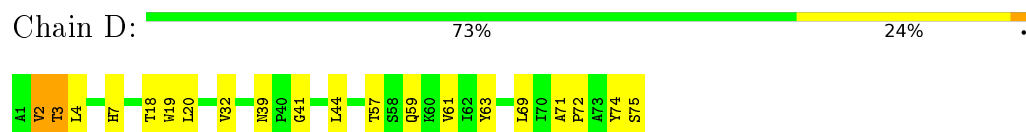
- Molecule 1: E protein



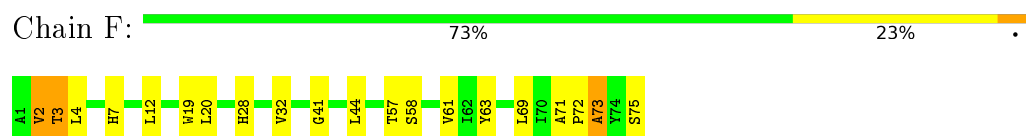
- Molecule 2: M protein



- Molecule 2: M protein



- Molecule 2: M protein



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	11842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	14000	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.56	2/3228 (0.1%)	0.64	3/4439 (0.1%)
1	C	0.60	2/3289 (0.1%)	0.62	3/4514 (0.1%)
1	E	0.53	0/3247	0.60	1/4460 (0.0%)
2	B	0.41	0/466	0.48	0/650
2	D	0.47	0/466	0.54	1/650 (0.2%)
2	F	0.42	0/460	0.48	0/643
All	All	0.55	4/11156 (0.0%)	0.60	8/15356 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	ARG	NE-CZ	-7.87	1.22	1.33
1	C	73	ARG	CZ-NH1	-7.82	1.22	1.33
1	A	164	ARG	CZ-NH1	-7.61	1.23	1.33
1	A	164	ARG	NE-CZ	-7.48	1.23	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	CYS	C-N-CD	-13.49	90.92	120.60
1	C	73	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	113	LEU	CA-CB-CG	5.36	127.64	115.30
1	C	113	LEU	CA-CB-CG	5.35	127.61	115.30
1	E	113	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	164	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	C	380	PRO	C-N-CD	5.09	139.08	128.40
2	D	71	ALA	C-N-CD	5.06	139.03	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ILE	Peptide
1	C	359	ILE	Peptide
1	E	359	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3167	0	2593	176	0
1	C	3225	0	2708	307	0
1	E	3186	0	2621	223	0
2	B	456	0	329	16	0
2	D	456	0	329	24	0
2	F	450	0	318	24	0
3	A	28	0	25	1	0
3	C	28	0	25	9	0
3	E	28	0	24	1	0
All	All	11024	0	8972	677	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (677) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ARG:HD3	1:C:166:LYS:CE	1.23	1.61
1:C:382:PHE:CE2	1:C:405:SER:HA	1.41	1.56
1:A:222:PRO:HG3	2:B:3:THR:CB	1.38	1.53
1:C:27:HIS:CE1	1:C:45:LEU:HD21	1.44	1.52
1:C:465:GLN:HE21	1:C:494:VAL:CG1	1.26	1.49
1:A:100:GLY:HA2	1:A:108:PHE:CB	1.43	1.47
1:C:101:TRP:CH2	1:E:327:THR:OG1	1.67	1.46
1:A:222:PRO:CG	2:B:3:THR:CB	1.91	1.45
1:E:1:ILE:HG12	1:E:147:GLN:NE2	1.21	1.44
1:E:308:CYS:CA	1:E:339:CYS:SG	2.05	1.44
1:C:138:ARG:HD3	1:C:166:LYS:NZ	1.28	1.43
1:C:320:GLU:O	1:E:108:PHE:CE1	1.67	1.42
1:C:465:GLN:NE2	1:C:494:VAL:HG13	1.36	1.39
1:C:27:HIS:CE1	1:C:45:LEU:CD2	2.04	1.39
1:A:175:ARG:HH22	1:E:349:MET:CE	1.35	1.38
1:C:27:HIS:ND1	1:C:287:GLY:CA	1.85	1.37
1:A:100:GLY:CA	1:A:108:PHE:HB3	1.53	1.37
1:C:138:ARG:NH1	1:C:166:LYS:HE2	1.36	1.35
1:C:138:ARG:CG	1:C:166:LYS:HE3	1.58	1.33
1:E:74:CYS:HB2	1:E:77:GLN:NE2	1.44	1.33
1:C:138:ARG:CD	1:C:166:LYS:CE	2.04	1.32
1:C:183:PHE:CE1	1:C:301:LYS:CB	2.12	1.32
1:C:183:PHE:HE1	1:C:301:LYS:CB	1.40	1.31
1:C:27:HIS:CE1	1:C:287:GLY:HA2	1.64	1.31
1:E:308:CYS:N	1:E:339:CYS:SG	2.04	1.31
1:C:68:MET:CE	1:C:255:VAL:HB	1.65	1.26
1:C:154:ASN:HD21	3:C:600:NAG:C7	1.47	1.26
1:E:109:GLY:O	1:E:110:LYS:HG3	1.08	1.25
1:A:175:ARG:NH2	1:E:349:MET:CE	1.95	1.25
1:C:138:ARG:HH11	1:C:166:LYS:CE	1.48	1.24
1:C:27:HIS:ND1	1:C:45:LEU:HD23	1.52	1.24
1:C:138:ARG:CD	1:C:166:LYS:HE3	1.64	1.24
1:C:109:GLY:O	1:C:110:LYS:HG3	1.09	1.23
1:C:27:HIS:HD1	1:C:287:GLY:CA	1.45	1.23
1:A:100:GLY:CA	1:A:108:PHE:CB	2.11	1.22
1:A:159:GLU:O	1:A:160:THR:HG23	1.40	1.21
1:A:175:ARG:NH2	1:E:349:MET:SD	2.15	1.20
1:A:74:CYS:HB3	1:A:75:PRO:CD	1.72	1.19
1:E:308:CYS:HB2	1:E:339:CYS:SG	1.83	1.18
1:E:210:HIS:HB2	1:E:275:ALA:O	1.44	1.18
1:E:308:CYS:CB	1:E:339:CYS:SG	2.32	1.18
1:A:100:GLY:HA2	1:A:108:PHE:CA	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:PHE:CZ	1:C:405:SER:HA	1.82	1.15
1:E:308:CYS:HA	1:E:339:CYS:SG	1.82	1.15
1:A:222:PRO:HG2	2:B:3:THR:CB	1.72	1.14
1:C:320:GLU:C	1:E:108:PHE:CE1	2.20	1.14
1:C:27:HIS:ND1	1:C:287:GLY:HA2	1.54	1.14
1:C:382:PHE:CE2	1:C:405:SER:CA	2.29	1.14
1:E:159:GLU:O	1:E:160:THR:HG23	1.49	1.13
1:C:27:HIS:NE2	1:C:48:THR:HG23	1.64	1.12
1:C:320:GLU:C	1:E:108:PHE:HE1	1.50	1.12
1:E:74:CYS:O	1:E:77:GLN:CG	1.97	1.12
1:C:90:TYR:OH	1:C:118:LYS:HE2	1.49	1.11
1:C:159:GLU:O	1:C:160:THR:HG23	1.48	1.11
1:E:109:GLY:O	1:E:110:LYS:CG	1.96	1.11
1:C:109:GLY:O	1:C:110:LYS:CG	1.97	1.10
1:A:74:CYS:HB3	1:A:75:PRO:HD2	1.14	1.10
2:D:69:LEU:O	2:D:72:PRO:HD2	1.50	1.10
1:E:15:MET:CB	1:E:21:VAL:HG23	1.82	1.09
1:E:74:CYS:CB	1:E:77:GLN:NE2	2.16	1.08
1:C:68:MET:HE1	1:C:255:VAL:HB	1.24	1.08
1:E:1:ILE:CG1	1:E:147:GLN:NE2	2.16	1.08
1:C:27:HIS:NE2	1:C:48:THR:CG2	2.19	1.06
1:C:108:PHE:CE1	1:E:321:THR:CB	2.39	1.06
1:C:465:GLN:HE21	1:C:494:VAL:HG11	1.20	1.05
1:C:154:ASN:ND2	3:C:600:NAG:C7	2.20	1.05
1:E:335:THR:CB	1:E:370:GLU:HA	1.86	1.05
1:E:74:CYS:C	1:E:77:GLN:HE21	1.59	1.05
1:E:15:MET:CB	1:E:21:VAL:CG2	2.34	1.04
1:E:74:CYS:HB3	1:E:75:PRO:HD2	1.36	1.04
1:E:312:PHE:HD2	1:E:389:ILE:HG22	1.18	1.04
1:E:74:CYS:CA	1:E:77:GLN:HE21	1.71	1.03
1:C:277:MET:CE	1:C:279:GLY:O	2.06	1.03
1:A:107:LEU:O	1:A:109:GLY:N	1.90	1.02
1:A:74:CYS:CB	1:A:75:PRO:HD2	1.78	1.02
1:C:420:ARG:O	1:C:424:LEU:HB2	1.58	1.02
1:C:138:ARG:CD	1:C:166:LYS:NZ	2.18	1.01
1:C:27:HIS:HD1	1:C:287:GLY:HA3	0.88	1.01
1:A:175:ARG:HH22	1:E:349:MET:HE2	0.85	1.00
1:A:146:SER:O	1:A:374:MET:HA	1.61	1.00
1:C:68:MET:HE1	1:C:255:VAL:CB	1.90	1.00
1:C:146:SER:O	1:C:374:MET:HA	1.61	0.99
1:C:465:GLN:NE2	1:C:494:VAL:CG1	2.05	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:C	1:A:109:GLY:H	1.66	0.98
1:A:74:CYS:O	1:A:75:PRO:O	1.80	0.98
1:C:108:PHE:HE1	1:E:321:THR:CB	1.75	0.97
1:C:90:TYR:CE1	1:C:118:LYS:CG	2.47	0.97
1:E:74:CYS:HB2	1:E:77:GLN:HE22	1.00	0.97
1:C:108:PHE:HE1	1:E:321:THR:CA	1.77	0.97
1:C:101:TRP:HH2	1:E:327:THR:OG1	1.38	0.97
1:E:309:THR:HG22	1:E:310:ALA:H	1.26	0.96
1:C:90:TYR:CE1	1:C:118:LYS:HG3	2.00	0.96
1:C:465:GLN:HE21	1:C:494:VAL:HG13	0.91	0.96
1:E:1:ILE:HG12	1:E:147:GLN:HE22	1.31	0.96
1:C:108:PHE:CE1	1:E:321:THR:CA	2.48	0.95
1:C:309:THR:HG22	1:C:310:ALA:H	1.30	0.95
1:C:90:TYR:OH	1:C:118:LYS:CE	2.14	0.95
1:C:154:ASN:ND2	3:C:600:NAG:C8	2.30	0.94
1:A:100:GLY:HA2	1:A:108:PHE:HA	1.47	0.94
1:C:163:ASN:O	1:C:180:LEU:HD22	1.66	0.93
1:A:100:GLY:HA2	1:A:108:PHE:HB3	1.08	0.93
1:A:309:THR:HG22	1:A:310:ALA:H	1.29	0.93
1:E:312:PHE:O	1:E:396:ILE:HG12	1.68	0.93
1:E:247:ASP:CB	1:E:253:GLN:HA	1.99	0.93
1:C:138:ARG:HD3	1:C:166:LYS:HZ1	1.31	0.93
1:C:154:ASN:HD21	3:C:600:NAG:C8	1.81	0.92
1:C:277:MET:HE3	1:C:279:GLY:O	1.67	0.91
2:D:74:TYR:O	2:F:28:HIS:CB	2.17	0.91
1:C:68:MET:CE	1:C:255:VAL:CB	2.47	0.91
1:E:74:CYS:O	1:E:77:GLN:HG2	1.68	0.91
1:A:16:SER:O	1:A:18:GLY:N	2.03	0.91
1:C:101:TRP:CZ3	1:E:327:THR:OG1	2.23	0.91
1:E:19:THR:CB	1:E:295:MET:H	1.83	0.90
1:C:138:ARG:HD3	1:C:166:LYS:HE2	1.53	0.90
1:E:312:PHE:CE2	1:E:341:VAL:HG13	2.07	0.90
1:C:320:GLU:O	1:E:108:PHE:CD1	2.25	0.90
1:E:49:THR:HG22	1:E:283:ARG:HG2	1.53	0.90
1:E:160:THR:O	1:E:161:ASP:O	1.90	0.90
1:E:74:CYS:O	1:E:75:PRO:O	1.88	0.89
1:C:27:HIS:ND1	1:C:45:LEU:CD2	2.22	0.89
1:C:138:ARG:HG3	1:C:166:LYS:HE3	1.52	0.88
1:E:19:THR:CB	1:E:295:MET:N	2.37	0.88
1:C:90:TYR:CE1	1:C:118:LYS:HG2	2.09	0.87
1:C:171:PRO:O	1:C:173:SER:N	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:THR:N	1:E:108:PHE:HE1	1.70	0.87
1:A:159:GLU:O	1:A:160:THR:CG2	2.22	0.87
1:A:175:ARG:NH2	1:E:349:MET:HE2	1.70	0.87
1:C:89:GLN:H	1:C:239:LYS:NZ	1.71	0.87
1:C:108:PHE:CD1	1:E:321:THR:HA	2.10	0.87
1:C:73:ARG:HG3	1:C:77:GLN:HG3	1.56	0.87
1:E:210:HIS:CB	1:E:275:ALA:O	2.22	0.87
1:A:171:PRO:O	1:A:173:SER:N	2.07	0.86
1:C:75:PRO:O	1:C:76:THR:OG1	1.93	0.86
1:E:1:ILE:CG1	1:E:147:GLN:HE21	1.81	0.85
1:E:312:PHE:CD2	1:E:389:ILE:HG22	2.09	0.85
1:E:171:PRO:O	1:E:173:SER:N	2.07	0.85
1:C:238:ASN:O	1:C:239:LYS:HB2	1.75	0.85
1:A:99:ARG:O	1:A:108:PHE:HA	1.77	0.84
1:C:154:ASN:ND2	3:C:600:NAG:O7	2.07	0.84
1:E:74:CYS:CB	1:E:77:GLN:HE21	1.85	0.84
1:E:316:LYS:O	1:E:317:ILE:O	1.95	0.84
1:C:347:VAL:O	1:C:348:ASP:CB	2.26	0.84
1:A:100:GLY:HA3	1:A:108:PHE:CB	2.05	0.84
1:E:77:GLN:O	1:E:78:GLY:O	1.95	0.83
1:C:27:HIS:HE1	1:C:45:LEU:HD21	1.40	0.83
1:E:74:CYS:O	1:E:77:GLN:HG3	1.76	0.83
1:C:101:TRP:CH2	1:E:327:THR:CB	2.62	0.82
2:D:69:LEU:O	2:D:72:PRO:CD	2.28	0.82
1:C:424:LEU:O	1:C:425:GLY:O	1.98	0.82
1:A:1:ILE:HG12	1:A:147:GLN:HE21	1.45	0.81
1:C:46:VAL:HG12	1:C:47:THR:HG23	1.62	0.81
1:A:46:VAL:HG12	1:A:47:THR:HG23	1.62	0.81
1:C:89:GLN:H	1:C:239:LYS:HZ1	1.25	0.81
1:A:193:ARG:HH21	1:E:398:HIS:CE1	1.99	0.81
1:E:273:LEU:CD2	2:F:12:LEU:CB	2.58	0.81
1:C:27:HIS:ND1	1:C:287:GLY:HA3	1.65	0.81
1:C:1:ILE:HG12	1:C:147:GLN:HE21	1.45	0.80
1:E:46:VAL:HG12	1:E:47:THR:HG23	1.62	0.80
1:C:321:THR:CA	1:E:108:PHE:HE1	1.95	0.80
1:A:74:CYS:HB3	1:A:75:PRO:HD3	1.64	0.80
1:C:321:THR:HA	1:E:108:PHE:CE1	2.17	0.80
1:E:19:THR:O	1:E:294:LYS:HA	1.82	0.80
1:A:100:GLY:CA	1:A:108:PHE:HB2	2.09	0.79
1:C:321:THR:CA	1:E:108:PHE:CE1	2.66	0.79
1:C:382:PHE:CZ	1:C:405:SER:CA	2.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:ILE:HG12	1:E:147:GLN:HE21	0.98	0.79
1:C:17:GLY:O	1:C:19:THR:N	2.16	0.79
1:C:321:THR:HA	1:E:108:PHE:CD1	2.17	0.79
1:E:273:LEU:HD21	2:F:12:LEU:CB	2.12	0.78
1:C:90:TYR:HE1	1:C:118:LYS:HG3	1.44	0.78
1:C:93:LYS:CB	1:C:245:PHE:CE2	2.66	0.78
1:C:245:PHE:HD2	1:C:253:GLN:HE21	1.29	0.78
1:C:27:HIS:H	1:C:287:GLY:HA3	1.47	0.78
1:E:27:HIS:H	1:E:287:GLY:HA3	1.47	0.78
1:E:74:CYS:CA	1:E:77:GLN:NE2	2.45	0.78
1:C:101:TRP:O	1:C:104:GLY:N	2.16	0.77
1:C:108:PHE:CE1	1:E:321:THR:HA	2.18	0.77
1:E:312:PHE:HD2	1:E:389:ILE:CG2	1.96	0.77
1:A:143:VAL:HB	1:A:163:ASN:CB	2.15	0.77
1:A:27:HIS:H	1:A:287:GLY:HA3	1.47	0.77
1:C:138:ARG:HH11	1:C:166:LYS:HE2	0.66	0.76
2:D:19:TRP:CD1	2:D:20:LEU:HG	2.20	0.76
2:B:19:TRP:CD1	2:B:20:LEU:HG	2.20	0.76
2:F:19:TRP:CD1	2:F:20:LEU:HG	2.20	0.76
1:C:101:TRP:CZ3	1:E:327:THR:CB	2.67	0.76
1:A:78:GLY:O	1:A:79:GLU:O	2.04	0.76
1:A:74:CYS:CB	1:A:75:PRO:CD	2.43	0.75
1:C:109:GLY:C	1:C:110:LYS:HG3	2.04	0.75
1:C:138:ARG:CZ	1:C:166:LYS:HE2	2.14	0.75
1:A:78:GLY:O	1:A:79:GLU:C	2.23	0.75
1:E:309:THR:HG22	1:E:310:ALA:N	2.01	0.74
1:E:312:PHE:HE2	1:E:341:VAL:HG13	1.52	0.74
1:C:75:PRO:HG2	1:C:107:LEU:O	1.86	0.74
1:E:109:GLY:C	1:E:110:LYS:HG3	2.04	0.74
1:E:210:HIS:CE1	1:E:277:MET:SD	2.79	0.74
1:C:90:TYR:CZ	1:C:118:LYS:HG2	2.23	0.74
1:C:426:ASP:H	1:C:446:HIS:CD2	2.06	0.74
1:C:465:GLN:CD	1:C:494:VAL:HG13	2.07	0.74
1:E:426:ASP:H	1:E:446:HIS:CD2	2.07	0.73
1:C:163:ASN:C	1:C:180:LEU:HD22	2.09	0.73
1:E:74:CYS:HB3	1:E:75:PRO:CD	2.16	0.73
1:A:107:LEU:C	1:A:109:GLY:N	2.38	0.73
1:E:159:GLU:O	1:E:160:THR:CG2	2.33	0.73
2:D:75:SER:C	2:F:69:LEU:HD11	2.09	0.73
1:C:309:THR:HG22	1:C:310:ALA:N	2.04	0.72
1:A:136:GLU:HA	1:A:170:THR:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TYR:CE2	1:C:230:ASP:HB2	2.24	0.72
1:C:43:ILE:CD1	1:C:293:LEU:HD11	2.19	0.72
1:A:309:THR:HG22	1:A:310:ALA:N	2.04	0.72
1:C:136:GLU:HA	1:C:170:THR:HG22	1.71	0.72
1:A:479:THR:O	1:A:480:LYS:CB	2.35	0.72
1:A:426:ASP:H	1:A:446:HIS:CD2	2.07	0.72
1:E:15:MET:CB	1:E:21:VAL:HG22	2.18	0.71
1:A:62:GLU:HA	1:A:260:SER:HA	1.73	0.71
1:E:75:PRO:O	1:E:77:GLN:HG2	1.89	0.71
1:C:159:GLU:O	1:C:160:THR:CG2	2.34	0.71
1:C:62:GLU:HA	1:C:260:SER:HA	1.73	0.71
1:C:277:MET:HE2	1:C:279:GLY:O	1.89	0.71
1:E:136:GLU:HA	1:E:170:THR:HG22	1.71	0.70
1:E:19:THR:CB	1:E:295:MET:CA	2.70	0.70
1:C:382:PHE:CG	1:C:405:SER:HB3	2.26	0.70
1:E:161:ASP:HB2	1:E:164:ARG:HH21	1.54	0.70
1:E:74:CYS:O	1:E:77:GLN:NE2	2.23	0.70
1:C:14:GLY:O	1:C:16:SER:N	2.24	0.70
2:D:2:VAL:O	2:D:4:LEU:N	2.25	0.70
1:E:74:CYS:C	1:E:77:GLN:NE2	2.42	0.70
2:F:2:VAL:O	2:F:4:LEU:N	2.24	0.70
1:E:305:TYR:CD1	1:E:338:PRO:O	2.45	0.70
1:C:138:ARG:HG2	1:C:166:LYS:HE3	1.69	0.70
1:C:314:PHE:HE2	1:C:398:HIS:HB2	1.57	0.70
1:C:27:HIS:ND1	1:C:287:GLY:N	2.39	0.70
1:A:314:PHE:HE2	1:A:398:HIS:HB2	1.56	0.69
1:A:100:GLY:HA3	1:A:108:PHE:HB2	1.72	0.69
1:A:77:GLN:O	1:A:79:GLU:N	2.25	0.69
1:A:175:ARG:NH2	1:E:349:MET:HE1	2.03	0.69
1:C:384:ASP:CB	1:C:399:HIS:HE1	2.05	0.69
1:E:100:GLY:N	1:E:103:ASN:OD1	2.26	0.69
1:E:312:PHE:CE1	1:E:332:TYR:CB	2.76	0.69
1:E:62:GLU:HA	1:E:260:SER:HA	1.73	0.69
1:C:100:GLY:N	1:C:103:ASN:OD1	2.26	0.68
1:C:108:PHE:HE1	1:E:321:THR:N	1.91	0.68
1:C:93:LYS:CB	1:C:245:PHE:CZ	2.76	0.68
1:C:382:PHE:HA	1:C:402:ARG:CB	2.23	0.68
1:E:275:ALA:CB	1:E:284:LEU:HD23	2.24	0.68
2:F:71:ALA:HB3	2:F:72:PRO:HD3	1.75	0.68
1:A:100:GLY:N	1:A:103:ASN:OD1	2.26	0.68
1:E:75:PRO:HG2	1:E:107:LEU:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASP:HB2	1:C:81:TYR:CE2	2.27	0.67
1:A:100:GLY:HA3	1:A:108:PHE:HB3	1.62	0.67
1:C:384:ASP:CB	1:C:399:HIS:CE1	2.77	0.67
2:F:3:THR:O	2:F:4:LEU:C	2.33	0.67
1:A:100:GLY:C	1:A:108:PHE:HB3	2.15	0.67
1:C:163:ASN:O	1:C:180:LEU:CD2	2.41	0.67
1:A:19:THR:CB	1:A:295:MET:H	2.08	0.67
1:A:80:ALA:HA	1:C:229:ALA:HB3	1.77	0.67
1:A:88:THR:O	1:A:90:TYR:N	2.28	0.67
1:E:88:THR:O	1:E:90:TYR:N	2.28	0.66
1:A:230:ASP:HB2	1:C:81:TYR:CZ	2.31	0.66
1:A:81:TYR:HB2	1:A:85:GLN:OE1	1.96	0.66
1:E:81:TYR:HB2	1:E:85:GLN:OE1	1.96	0.66
1:C:88:THR:O	1:C:90:TYR:N	2.28	0.66
1:E:210:HIS:NE2	1:E:277:MET:SD	2.69	0.66
1:C:138:ARG:HD3	1:C:166:LYS:HZ2	1.56	0.66
1:C:154:ASN:ND2	3:C:600:NAG:H81	2.11	0.66
1:E:272:ALA:HB2	2:F:7:HIS:CD2	2.31	0.66
1:A:154:ASN:CG	3:A:600:NAG:C1	2.64	0.65
1:C:81:TYR:HB2	1:C:85:GLN:OE1	1.96	0.65
1:C:43:ILE:HD12	1:C:293:LEU:HD11	1.77	0.65
1:C:272:ALA:HB2	2:D:7:HIS:CD2	2.32	0.65
1:E:161:ASP:OD2	1:E:164:ARG:NH2	2.30	0.65
2:D:3:THR:O	2:D:4:LEU:C	2.33	0.65
1:E:349:MET:HE3	1:E:352:LEU:HD21	1.79	0.65
1:A:170:THR:HB	1:A:171:PRO:HD2	1.78	0.65
1:A:76:THR:O	1:A:77:GLN:HG2	1.95	0.65
1:C:57:ARG:NH1	1:C:219:HIS:O	2.29	0.65
1:C:146:SER:CB	1:C:374:MET:CB	2.75	0.65
1:C:27:HIS:CE1	1:C:287:GLY:CA	2.47	0.65
1:C:238:ASN:O	1:C:239:LYS:CB	2.42	0.65
1:C:245:PHE:HD2	1:C:253:GLN:NE2	1.95	0.65
1:E:273:LEU:HD22	1:E:273:LEU:H	1.62	0.65
1:A:72:SER:OG	1:A:113:LEU:HD23	1.98	0.64
1:E:135:LEU:O	1:E:171:PRO:HD3	1.97	0.64
1:C:101:TRP:CD1	1:C:106:GLY:HA2	2.32	0.64
1:E:436:GLY:O	1:E:440:SER:N	2.29	0.64
1:E:72:SER:OG	1:E:113:LEU:HD23	1.98	0.64
1:C:108:PHE:CE1	1:E:320:GLU:O	2.49	0.64
1:C:68:MET:CE	1:C:255:VAL:CG2	2.76	0.64
1:A:146:SER:CB	1:A:374:MET:CB	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:SER:OG	1:C:113:LEU:HD23	1.98	0.64
1:C:58:SER:OG	1:C:226:HIS:HB3	1.98	0.64
1:C:135:LEU:O	1:C:171:PRO:HD3	1.98	0.64
1:C:170:THR:HB	1:C:171:PRO:HD2	1.79	0.64
1:A:135:LEU:O	1:A:171:PRO:HD3	1.97	0.63
1:C:108:PHE:CE1	1:E:320:GLU:C	2.72	0.63
1:A:163:ASN:O	1:A:164:ARG:HG3	1.98	0.63
2:D:39:ASN:HD22	1:E:459:GLY:HA2	1.63	0.63
2:D:75:SER:O	2:F:69:LEU:HD11	1.97	0.63
1:C:183:PHE:CD1	1:C:301:LYS:CB	2.78	0.63
1:E:312:PHE:CD2	1:E:389:ILE:CG2	2.77	0.63
1:E:275:ALA:HB1	1:E:284:LEU:HD23	1.81	0.63
1:E:76:THR:C	1:E:77:GLN:HG2	2.18	0.63
1:E:58:SER:OG	1:E:226:HIS:HB3	1.98	0.63
1:E:170:THR:HB	1:E:171:PRO:HD2	1.79	0.63
1:C:88:THR:C	1:C:90:TYR:H	2.02	0.63
1:E:88:THR:C	1:E:90:TYR:H	2.02	0.63
1:A:436:GLY:O	1:A:440:SER:N	2.29	0.62
1:C:188:LEU:HG	1:C:293:LEU:HD23	1.81	0.62
1:C:436:GLY:O	1:C:440:SER:N	2.29	0.62
1:A:58:SER:OG	1:A:226:HIS:HB3	1.98	0.62
1:C:108:PHE:HD1	1:E:321:THR:HA	1.62	0.62
1:A:14:GLY:O	1:A:35:ALA:CB	2.48	0.62
1:A:88:THR:C	1:A:90:TYR:H	2.02	0.62
1:C:152:ILE:HG22	1:C:153:VAL:HG23	1.81	0.62
1:C:245:PHE:CD2	1:C:253:GLN:NE2	2.68	0.62
1:C:43:ILE:CD1	1:C:293:LEU:CD1	2.77	0.62
1:A:193:ARG:HH21	1:E:398:HIS:HE1	1.43	0.62
1:C:359:ILE:O	1:C:359:ILE:HG13	1.99	0.61
1:C:382:PHE:CD2	1:C:405:SER:CA	2.82	0.61
1:A:152:ILE:HG22	1:A:153:VAL:HG23	1.81	0.61
3:C:600:NAG:C6	3:C:601:NAG:H82	2.31	0.61
1:A:172:ASN:O	1:A:173:SER:HB3	2.00	0.61
1:A:308:CYS:O	1:A:309:THR:O	2.19	0.61
1:C:172:ASN:O	1:C:173:SER:HB3	2.00	0.61
1:E:172:ASN:O	1:E:173:SER:HB3	2.00	0.60
1:A:482:GLY:O	1:A:484:ILE:N	2.35	0.60
1:C:89:GLN:N	1:C:239:LYS:NZ	2.45	0.60
1:C:382:PHE:HE2	1:C:405:SER:HA	1.49	0.60
1:C:85:GLN:HE22	1:C:94:ARG:HE	1.50	0.60
1:E:74:CYS:O	1:E:75:PRO:C	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:PHE:HE1	1:E:332:TYR:CB	2.13	0.60
1:A:81:TYR:CZ	1:C:230:ASP:HB2	2.36	0.60
1:C:27:HIS:HD1	1:C:45:LEU:HD23	1.56	0.59
1:E:311:ALA:HB3	1:E:334:GLY:H	1.67	0.59
1:C:27:HIS:CG	1:C:287:GLY:N	2.70	0.59
1:C:205:THR:HG22	1:C:210:HIS:ND1	2.18	0.59
1:C:248:ALA:O	1:C:250:ALA:N	2.36	0.59
1:C:308:CYS:O	1:C:309:THR:O	2.20	0.59
1:C:59:TYR:CE1	1:C:225:TRP:HB3	2.38	0.59
1:A:59:TYR:CE1	1:A:225:TRP:HB3	2.38	0.58
1:C:101:TRP:CZ3	1:E:327:THR:HB	2.39	0.58
1:C:465:GLN:HG3	1:C:494:VAL:CG1	2.34	0.58
1:C:319:ALA:HB3	1:E:108:PHE:CE2	2.38	0.58
1:A:70:SER:HA	1:A:82:LEU:HD11	1.86	0.58
1:C:382:PHE:CZ	1:C:405:SER:CB	2.87	0.58
1:E:59:TYR:CE1	1:E:225:TRP:HB3	2.38	0.58
1:A:217:TRP:CD1	2:B:7:HIS:HA	2.39	0.58
1:C:382:PHE:CE1	1:C:405:SER:HB2	2.37	0.58
1:A:205:THR:HG22	1:A:210:HIS:ND1	2.18	0.58
1:C:68:MET:HE1	1:C:255:VAL:CG2	2.32	0.58
1:E:335:THR:CB	1:E:370:GLU:CA	2.74	0.58
1:E:288:HIS:CD2	1:E:424:LEU:HD22	2.39	0.57
1:C:68:MET:HE2	1:C:255:VAL:HB	1.77	0.57
1:E:309:THR:CG2	1:E:310:ALA:H	2.09	0.57
1:E:205:THR:HG22	1:E:210:HIS:ND1	2.18	0.57
1:E:70:SER:HA	1:E:82:LEU:HD11	1.86	0.57
1:C:68:MET:HE2	1:C:255:VAL:CG2	2.35	0.57
1:E:311:ALA:HB1	1:E:333:ALA:HB3	1.87	0.57
1:E:101:TRP:O	1:E:104:GLY:N	2.37	0.57
1:A:482:GLY:O	1:A:483:SER:C	2.41	0.56
1:A:309:THR:CG2	1:A:310:ALA:H	2.12	0.56
1:C:348:ASP:O	1:C:386:TYR:CD2	2.58	0.56
2:D:39:ASN:ND2	1:E:459:GLY:HA2	2.20	0.56
1:A:288:HIS:CD2	1:A:424:LEU:HD22	2.39	0.56
1:C:27:HIS:CG	1:C:45:LEU:HD23	2.38	0.56
1:A:172:ASN:HD21	1:E:314:PHE:HB2	1.70	0.56
1:C:27:HIS:NE2	1:C:48:THR:HG21	2.17	0.56
1:C:70:SER:HA	1:C:82:LEU:HD11	1.86	0.56
1:E:19:THR:CB	1:E:296:ASP:N	2.68	0.56
1:C:108:PHE:CD1	1:E:321:THR:CB	2.88	0.56
1:E:1:ILE:HG21	1:E:147:GLN:HE22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:CB	1:A:295:MET:CB	2.84	0.56
1:E:358:LEU:HD12	1:E:378:LEU:HB3	1.88	0.56
1:C:50:VAL:HG11	1:C:130:ILE:HG12	1.88	0.56
1:E:261:GLN:O	1:E:264:ALA:N	2.28	0.56
1:E:310:ALA:O	1:E:311:ALA:HB2	2.06	0.56
2:F:72:PRO:O	2:F:73:ALA:HB2	2.06	0.56
1:C:108:PHE:CE1	1:E:321:THR:N	2.72	0.55
1:C:19:THR:CB	1:C:295:MET:H	2.19	0.55
1:E:27:HIS:N	1:E:287:GLY:HA3	2.20	0.55
1:A:310:ALA:O	1:A:311:ALA:HB2	2.05	0.55
1:C:89:GLN:N	1:C:239:LYS:HZ1	2.02	0.55
1:C:27:HIS:CE1	1:C:48:THR:CG2	2.89	0.55
1:C:382:PHE:CE2	1:C:405:SER:CB	2.90	0.55
1:C:382:PHE:CD2	1:C:405:SER:HB3	2.42	0.55
1:A:101:TRP:N	1:A:108:PHE:HB3	2.22	0.55
2:D:75:SER:HB3	2:F:32:VAL:HG23	1.88	0.55
1:A:101:TRP:O	1:A:104:GLY:N	2.37	0.55
1:A:214:HIS:H	2:B:7:HIS:HE1	1.55	0.55
1:E:19:THR:CB	1:E:295:MET:CB	2.84	0.55
1:A:50:VAL:HG11	1:A:130:ILE:HG12	1.88	0.55
1:C:358:LEU:HD12	1:C:378:LEU:HB3	1.88	0.55
1:A:261:GLN:O	1:A:264:ALA:N	2.28	0.55
1:E:19:THR:CB	1:E:295:MET:C	2.75	0.55
1:A:358:LEU:HD12	1:A:378:LEU:HB3	1.88	0.54
1:C:138:ARG:CD	1:C:166:LYS:HZ1	2.00	0.54
1:C:244:GLU:OE2	2:F:20:LEU:HA	2.05	0.54
1:C:424:LEU:C	1:C:425:GLY:O	2.45	0.54
1:C:321:THR:HA	1:E:108:PHE:HD1	1.71	0.54
1:E:74:CYS:O	1:E:77:GLN:CD	2.45	0.54
1:C:161:ASP:HB3	1:C:164:ARG:HH21	1.72	0.54
1:C:310:ALA:O	1:C:311:ALA:HB2	2.06	0.54
1:A:272:ALA:HB2	2:B:7:HIS:CD2	2.42	0.54
1:C:15:MET:CB	1:C:35:ALA:HB1	2.38	0.54
1:E:50:VAL:HG11	1:E:130:ILE:HG12	1.88	0.54
1:A:74:CYS:C	1:A:75:PRO:O	2.46	0.54
1:E:333:ALA:O	1:E:370:GLU:O	2.26	0.53
3:C:600:NAG:H62	3:C:601:NAG:H82	1.89	0.53
1:C:380:PRO:HB2	1:C:381:PRO:CD	2.38	0.53
1:C:43:ILE:HD12	1:C:293:LEU:CD1	2.39	0.53
1:C:90:TYR:CZ	1:C:118:LYS:CG	2.89	0.53
1:A:27:HIS:N	1:A:287:GLY:HA3	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:HB3	1:A:115:THR:HG22	1.91	0.53
1:C:217:TRP:CD1	2:D:7:HIS:HA	2.43	0.53
1:E:273:LEU:HD22	1:E:273:LEU:N	2.22	0.53
1:C:101:TRP:HH2	1:E:327:THR:CB	2.14	0.53
1:C:70:SER:HB3	1:C:115:THR:HG22	1.90	0.53
1:C:27:HIS:N	1:C:287:GLY:HA3	2.20	0.53
1:C:73:ARG:HB3	1:C:77:GLN:HB2	1.91	0.53
1:C:108:PHE:CD1	1:E:321:THR:CA	2.81	0.53
1:A:19:THR:CB	1:A:295:MET:N	2.72	0.52
1:C:382:PHE:CE1	1:C:405:SER:CB	2.92	0.52
1:C:75:PRO:C	1:C:76:THR:HG1	2.02	0.52
1:C:261:GLN:HA	1:E:263:GLY:HA3	1.92	0.52
1:C:261:GLN:O	1:C:264:ALA:N	2.29	0.52
1:A:14:GLY:O	1:A:35:ALA:HB2	2.10	0.52
1:C:154:ASN:HD22	3:C:600:NAG:C8	2.22	0.52
1:E:301:LYS:O	1:E:305:TYR:HE2	1.93	0.52
1:E:161:ASP:CB	1:E:164:ARG:HH21	2.23	0.52
1:C:309:THR:CG2	1:C:310:ALA:H	2.12	0.51
1:C:90:TYR:OH	1:C:118:LYS:HE3	2.04	0.51
1:C:146:SER:O	1:C:147:GLN:O	2.29	0.51
1:E:70:SER:HB3	1:E:115:THR:HG22	1.91	0.51
1:C:319:ALA:CB	1:E:108:PHE:CE2	2.93	0.51
1:A:172:ASN:OD1	1:E:398:HIS:HD2	1.94	0.51
1:A:279:GLY:O	1:A:281:LYS:N	2.44	0.51
1:C:264:ALA:O	1:C:268:ALA:N	2.42	0.51
1:C:382:PHE:CD1	1:C:405:SER:HB3	2.46	0.51
1:A:135:LEU:O	1:A:171:PRO:CD	2.58	0.51
1:E:85:GLN:HG2	1:E:92:CYS:SG	2.51	0.51
1:A:59:TYR:N	1:A:125:MET:O	2.41	0.51
1:A:78:GLY:HA3	1:C:227:ALA:O	2.10	0.51
1:E:59:TYR:N	1:E:125:MET:O	2.41	0.51
1:A:159:GLU:O	1:A:160:THR:CB	2.59	0.50
1:C:135:LEU:O	1:C:171:PRO:CD	2.59	0.50
1:A:301:LYS:O	1:A:305:TYR:HE2	1.93	0.50
1:C:101:TRP:HZ3	1:E:327:THR:HB	1.77	0.50
1:C:384:ASP:CA	1:C:399:HIS:HE1	2.23	0.50
1:A:85:GLN:HG2	1:A:92:CYS:SG	2.51	0.50
1:C:85:GLN:HG2	1:C:92:CYS:SG	2.51	0.50
1:A:277:MET:CE	1:A:279:GLY:O	2.59	0.50
1:E:77:GLN:C	1:E:78:GLY:O	2.48	0.50
1:A:146:SER:O	1:A:374:MET:CA	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ALA:O	1:A:268:ALA:N	2.43	0.50
1:C:20:TRP:CG	1:C:20:TRP:O	2.65	0.50
1:C:465:GLN:CG	1:C:494:VAL:HG13	2.42	0.49
1:C:59:TYR:N	1:C:125:MET:O	2.41	0.49
2:F:41:GLY:O	2:F:44:LEU:N	2.45	0.49
1:A:137:TYR:CZ	1:A:289:LEU:HD21	2.47	0.49
2:B:71:ALA:N	2:B:72:PRO:HD2	2.26	0.49
1:C:1:ILE:HG12	1:C:147:GLN:NE2	2.23	0.49
1:E:264:ALA:O	1:E:268:ALA:N	2.43	0.49
1:C:263:GLY:HA3	1:E:261:GLN:HA	1.93	0.49
1:C:137:TYR:CZ	1:C:289:LEU:HD21	2.47	0.49
2:D:41:GLY:O	2:D:44:LEU:N	2.45	0.49
1:C:68:MET:HE2	1:C:255:VAL:CB	2.38	0.49
1:E:163:ASN:O	1:E:164:ARG:C	2.51	0.49
1:E:135:LEU:O	1:E:171:PRO:CD	2.59	0.49
2:B:41:GLY:O	2:B:44:LEU:N	2.45	0.49
2:D:32:VAL:HG22	2:D:72:PRO:HG3	1.95	0.49
1:A:271:GLY:HA2	2:B:18:THR:HB	1.95	0.49
1:A:482:GLY:C	1:A:484:ILE:N	2.66	0.49
1:A:170:THR:O	1:A:171:PRO:C	2.51	0.49
1:E:170:THR:O	1:E:171:PRO:C	2.51	0.49
2:D:32:VAL:HG22	2:D:72:PRO:CG	2.42	0.48
1:A:303:VAL:O	1:A:304:SER:OG	2.27	0.48
1:E:128:LYS:N	1:E:203:TYR:O	2.45	0.48
1:A:20:TRP:CG	1:A:20:TRP:O	2.65	0.48
1:C:170:THR:O	1:C:171:PRO:C	2.51	0.48
1:C:27:HIS:CG	1:C:287:GLY:CA	2.86	0.48
1:A:17:GLY:O	1:A:20:TRP:CB	2.62	0.48
1:E:1:ILE:CG2	1:E:147:GLN:HE22	2.26	0.48
1:A:128:LYS:N	1:A:203:TYR:O	2.45	0.48
1:A:143:VAL:CB	1:A:163:ASN:CB	2.91	0.48
1:E:75:PRO:HG3	1:E:107:LEU:O	2.13	0.48
1:E:137:TYR:CZ	1:E:289:LEU:HD21	2.47	0.48
1:E:316:LYS:C	1:E:317:ILE:O	2.50	0.48
1:A:163:ASN:O	1:A:164:ARG:CG	2.62	0.47
1:A:74:CYS:O	1:A:75:PRO:C	2.47	0.47
1:A:80:ALA:HA	1:C:229:ALA:CB	2.43	0.47
1:C:348:ASP:O	1:C:386:TYR:HD2	1.96	0.47
1:E:308:CYS:O	1:E:309:THR:O	2.32	0.47
1:C:88:THR:C	1:C:90:TYR:N	2.67	0.47
1:C:226:HIS:CD2	1:C:228:GLY:H	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:THR:C	1:E:90:TYR:N	2.67	0.47
1:C:303:VAL:O	1:C:304:SER:OG	2.27	0.47
1:E:211:TRP:HA	1:E:274:GLU:HA	1.96	0.47
1:E:226:HIS:CD2	1:E:228:GLY:H	2.33	0.47
1:C:1:ILE:HG21	1:C:147:GLN:NE2	2.30	0.47
1:A:1:ILE:HG12	1:A:147:GLN:NE2	2.22	0.47
1:C:128:LYS:N	1:C:203:TYR:O	2.45	0.47
1:C:214:HIS:H	2:D:7:HIS:HE1	1.62	0.47
1:E:146:SER:CB	1:E:364:VAL:O	2.63	0.47
2:F:71:ALA:HB3	2:F:72:PRO:CD	2.42	0.47
1:A:226:HIS:NE2	1:A:230:ASP:O	2.43	0.46
1:A:88:THR:C	1:A:90:TYR:N	2.67	0.46
1:E:275:ALA:HB2	1:E:284:LEU:CD2	2.45	0.46
1:C:382:PHE:CD2	1:C:405:SER:CB	2.98	0.46
1:E:212:LEU:N	1:E:273:LEU:O	2.49	0.46
2:D:75:SER:HB2	2:F:32:VAL:CG2	2.45	0.46
1:C:157:GLY:C	1:C:159:GLU:H	2.17	0.46
1:C:213:VAL:HG11	1:C:218:PHE:HB2	1.97	0.46
1:E:213:VAL:HG11	1:E:218:PHE:HB2	1.98	0.46
1:E:426:ASP:H	1:E:446:HIS:HD2	1.60	0.46
1:C:19:THR:CB	1:C:295:MET:N	2.79	0.46
1:C:380:PRO:HG2	1:C:400:TRP:CZ3	2.50	0.46
1:A:213:VAL:HG11	1:A:218:PHE:HB2	1.97	0.46
1:A:226:HIS:CD2	1:A:228:GLY:H	2.33	0.46
1:A:1:ILE:HG21	1:A:147:GLN:NE2	2.30	0.46
1:A:214:HIS:H	2:B:7:HIS:CE1	2.34	0.46
1:C:419:LYS:O	1:C:422:ALA:HB3	2.16	0.46
1:E:187:GLY:O	1:E:294:LYS:N	2.43	0.46
1:C:68:MET:HE3	1:C:255:VAL:HB	1.83	0.46
1:C:222:PRO:HG3	2:D:3:THR:CB	2.46	0.45
1:C:426:ASP:H	1:C:446:HIS:HD2	1.60	0.45
1:C:465:GLN:NE2	1:C:494:VAL:HG11	2.03	0.45
1:C:74:CYS:HB3	1:C:75:PRO:HD2	1.98	0.45
1:E:226:HIS:NE2	1:E:230:ASP:O	2.43	0.45
1:A:187:GLY:O	1:A:294:LYS:N	2.43	0.45
1:C:22:ASP:HA	1:C:292:ARG:HA	1.99	0.45
1:C:319:ALA:HB3	1:E:108:PHE:CZ	2.52	0.45
1:E:144:HIS:HB3	1:E:360:THR:HG23	1.98	0.45
1:C:188:LEU:HG	1:C:293:LEU:CD2	2.45	0.45
1:C:27:HIS:H	1:C:287:GLY:CA	2.24	0.45
1:E:275:ALA:CB	1:E:284:LEU:CD2	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:CYS:CB	1:E:77:GLN:HE22	1.91	0.45
1:A:365:ILE:O	1:A:365:ILE:HG13	2.17	0.45
1:A:222:PRO:CD	2:B:4:LEU:H	2.30	0.45
1:E:365:ILE:HG13	1:E:365:ILE:O	2.17	0.45
1:A:22:ASP:HA	1:A:292:ARG:HA	1.99	0.45
1:A:308:CYS:N	1:A:339:CYS:SG	2.90	0.45
3:E:600:NAG:C7	3:E:600:NAG:O3	2.65	0.45
1:A:222:PRO:HD2	2:B:4:LEU:H	1.81	0.45
1:C:144:HIS:HB3	1:C:360:THR:HG23	1.98	0.45
1:A:261:GLN:O	1:A:263:GLY:N	2.50	0.45
1:A:416:ARG:NH2	1:A:420:ARG:HH21	2.15	0.45
1:C:72:SER:HG	1:C:113:LEU:HD23	1.81	0.45
1:C:365:ILE:HG13	1:C:365:ILE:O	2.17	0.45
1:A:426:ASP:H	1:A:446:HIS:HD2	1.60	0.44
1:C:147:GLN:OE1	1:C:162:GLU:CB	2.65	0.44
1:C:187:GLY:O	1:C:294:LYS:N	2.43	0.44
2:D:75:SER:CB	2:F:32:VAL:CG2	2.95	0.44
1:E:349:MET:HE3	1:E:349:MET:HA	1.99	0.44
1:C:138:ARG:CD	1:C:166:LYS:HZ2	2.22	0.44
1:C:261:GLN:O	1:C:263:GLY:N	2.51	0.44
1:C:382:PHE:CD1	1:C:405:SER:CB	3.00	0.44
1:E:261:GLN:O	1:E:263:GLY:N	2.50	0.44
1:A:131:GLN:HE21	1:C:76:THR:HG21	1.82	0.44
1:A:388:VAL:HG13	1:A:397:THR:HG22	2.00	0.44
1:C:246:LYS:HE2	1:E:274:GLU:OE2	2.18	0.44
1:C:308:CYS:N	1:C:339:CYS:SG	2.90	0.44
2:D:63:TYR:CE1	2:F:63:TYR:CE1	3.05	0.44
1:E:342:PRO:HG3	1:E:391:VAL:HG13	2.00	0.44
1:C:127:GLY:HA3	1:C:218:PHE:CZ	2.53	0.44
1:C:319:ALA:CB	1:E:108:PHE:CZ	3.01	0.44
1:C:424:LEU:HB3	1:C:428:ALA:HB2	2.00	0.44
1:C:101:TRP:HZ3	1:E:327:THR:CB	2.23	0.44
1:E:416:ARG:NH2	1:E:420:ARG:HH21	2.15	0.44
1:A:144:HIS:HB3	1:A:360:THR:HG23	1.98	0.44
1:C:342:PRO:HG3	1:C:391:VAL:HG13	2.00	0.44
1:E:214:HIS:H	2:F:7:HIS:HE1	1.65	0.44
1:C:2:ARG:HG3	1:C:2:ARG:O	2.18	0.43
1:C:388:VAL:HG13	1:C:397:THR:HG22	2.00	0.43
1:E:127:GLY:HA3	1:E:218:PHE:CZ	2.53	0.43
1:C:245:PHE:CD2	1:C:245:PHE:O	2.71	0.43
1:C:246:LYS:CE	1:E:274:GLU:OE2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:GLY:HA2	2:D:18:THR:HB	1.99	0.43
1:E:22:ASP:HA	1:E:292:ARG:HA	1.99	0.43
1:A:127:GLY:HA3	1:A:218:PHE:CZ	2.53	0.43
1:A:88:THR:HG23	1:C:88:THR:HG23	2.00	0.43
1:C:424:LEU:O	1:C:425:GLY:C	2.56	0.43
1:E:20:TRP:O	1:E:20:TRP:CG	2.71	0.43
1:E:273:LEU:CD2	1:E:273:LEU:H	2.30	0.43
1:A:81:TYR:HD2	1:C:227:ALA:HB3	1.82	0.43
1:C:27:HIS:CE1	1:C:48:THR:HG21	2.53	0.43
1:A:277:MET:HE3	1:A:279:GLY:O	2.18	0.43
1:A:227:ALA:HB3	1:C:81:TYR:HD2	1.84	0.43
1:C:424:LEU:HA	1:C:424:LEU:HD23	1.78	0.43
1:E:275:ALA:HB2	1:E:284:LEU:HD23	1.99	0.43
1:A:2:ARG:O	1:A:2:ARG:HG3	2.18	0.43
1:C:146:SER:O	1:C:374:MET:CA	2.49	0.43
1:E:466:ILE:O	1:E:470:THR:N	2.37	0.43
1:A:59:TYR:HB2	1:A:125:MET:HG2	2.01	0.42
1:A:349:MET:C	1:A:351:THR:N	2.73	0.42
1:C:26:GLU:O	1:C:29:GLY:N	2.52	0.42
1:C:338:PRO:HB3	1:C:366:THR:HA	2.01	0.42
1:A:191:GLU:HB3	1:E:399:HIS:CD2	2.53	0.42
1:A:227:ALA:HB3	1:C:81:TYR:CD2	2.54	0.42
1:A:27:HIS:H	1:A:287:GLY:CA	2.25	0.42
1:C:73:ARG:O	1:C:74:CYS:HB2	2.19	0.42
1:C:73:ARG:HA	1:C:73:ARG:HD2	1.81	0.42
1:E:72:SER:HG	1:E:113:LEU:HD23	1.83	0.42
2:F:57:THR:O	2:F:61:VAL:HG23	2.20	0.42
2:F:73:ALA:C	2:F:75:SER:H	2.23	0.42
1:A:73:ARG:O	1:A:74:CYS:HB2	2.19	0.42
1:E:77:GLN:O	1:E:78:GLY:C	2.51	0.42
1:C:93:LYS:CB	1:C:245:PHE:CD2	3.03	0.42
1:E:2:ARG:O	1:E:2:ARG:HG3	2.19	0.42
1:A:146:SER:O	1:A:147:GLN:O	2.38	0.42
1:A:171:PRO:C	1:A:173:SER:N	2.73	0.42
1:E:105:CYS:O	1:E:106:GLY:O	2.37	0.42
1:A:209:LYS:O	1:A:210:HIS:CG	2.72	0.42
1:E:210:HIS:O	1:E:274:GLU:HG3	2.20	0.42
1:A:100:GLY:CA	1:A:108:PHE:HA	2.34	0.42
1:A:338:PRO:HB3	1:A:366:THR:HA	2.01	0.42
2:B:57:THR:O	2:B:61:VAL:HG23	2.20	0.42
1:C:155:ASP:O	1:C:157:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LYS:O	1:C:210:HIS:CG	2.72	0.42
1:E:59:TYR:HB2	1:E:125:MET:HG2	2.02	0.42
1:E:388:VAL:HG13	1:E:397:THR:HG22	2.00	0.42
2:F:58:SER:O	2:F:61:VAL:N	2.52	0.42
1:A:157:GLY:HA3	1:A:164:ARG:NH2	2.35	0.42
1:C:246:LYS:HE3	2:F:19:TRP:CZ3	2.55	0.42
1:C:298:LEU:HA	1:C:298:LEU:HD23	1.83	0.42
1:E:380:PRO:HB2	1:E:381:PRO:HD2	2.02	0.42
1:A:17:GLY:O	1:A:20:TRP:N	2.48	0.41
1:A:26:GLU:O	1:A:29:GLY:N	2.52	0.41
1:C:381:PRO:O	1:C:402:ARG:CB	2.68	0.41
1:C:89:GLN:N	1:C:239:LYS:HZ3	2.14	0.41
2:D:57:THR:O	2:D:61:VAL:HG23	2.20	0.41
1:C:100:GLY:HA3	1:E:5:GLY:HA3	2.02	0.41
1:C:245:PHE:CG	1:C:245:PHE:O	2.72	0.41
1:C:483:SER:C	1:C:485:SER:N	2.73	0.41
1:C:59:TYR:HB2	1:C:125:MET:HG2	2.02	0.41
1:C:382:PHE:CZ	1:C:405:SER:HB2	2.56	0.41
1:E:288:HIS:NE2	1:E:424:LEU:HD22	2.35	0.41
1:A:19:THR:CB	1:A:295:MET:CA	2.99	0.41
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.83	0.41
2:D:59:GLN:O	2:F:63:TYR:OH	2.37	0.41
1:E:209:LYS:O	1:E:210:HIS:CG	2.73	0.41
1:E:26:GLU:O	1:E:29:GLY:N	2.52	0.41
1:E:27:HIS:H	1:E:287:GLY:CA	2.24	0.41
1:A:342:PRO:HG2	1:A:390:GLY:HA2	2.01	0.41
1:A:342:PRO:HG3	1:A:391:VAL:HG13	2.02	0.41
2:B:71:ALA:HB3	2:B:72:PRO:HD3	2.02	0.41
1:C:4:ILE:O	1:C:6:VAL:N	2.54	0.41
1:C:223:LEU:HD21	1:C:261:GLN:OE1	2.21	0.41
1:C:68:MET:HE2	1:C:255:VAL:HG21	2.03	0.41
1:E:223:LEU:HD21	1:E:261:GLN:OE1	2.21	0.41
1:A:288:HIS:NE2	1:A:424:LEU:HD22	2.35	0.41
1:C:171:PRO:C	1:C:173:SER:N	2.73	0.41
1:E:74:CYS:CB	1:E:75:PRO:CD	2.84	0.41
1:A:312:PHE:O	1:A:396:ILE:HG12	2.21	0.41
1:C:15:MET:CB	1:C:35:ALA:CB	2.99	0.41
1:C:161:ASP:HB3	1:C:164:ARG:NH2	2.35	0.41
1:E:303:VAL:O	1:E:304:SER:OG	2.27	0.41
1:A:258:LEU:HA	1:A:258:LEU:HD23	1.92	0.41
1:A:380:PRO:HB2	1:A:381:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLY:O	1:A:160:THR:O	2.38	0.41
1:A:1:ILE:HG21	1:A:147:GLN:HE22	1.86	0.40
2:B:69:LEU:O	2:B:72:PRO:HD2	2.21	0.40
1:C:146:SER:O	1:C:147:GLN:C	2.60	0.40
1:C:1:ILE:HG21	1:C:147:GLN:HE22	1.87	0.40
1:C:321:THR:CB	1:E:108:PHE:CE1	3.04	0.40
1:E:4:ILE:H	1:E:9:ARG:NH2	2.19	0.40
1:C:312:PHE:O	1:C:396:ILE:HG12	2.21	0.40
1:A:203:TYR:OH	1:A:277:MET:HB3	2.22	0.40
1:C:105:CYS:O	1:C:106:GLY:O	2.39	0.40
1:E:281:LYS:HG2	1:E:281:LYS:O	2.21	0.40
1:A:223:LEU:HD21	1:A:261:GLN:OE1	2.21	0.40
1:A:339:CYS:SG	1:A:340:LYS:N	2.95	0.40
1:C:203:TYR:OH	1:C:277:MET:HB3	2.22	0.40
1:E:298:LEU:HA	1:E:298:LEU:HD23	1.83	0.40
1:A:98:ASP:OD1	1:A:110:LYS:HG2	2.21	0.40
1:A:212:LEU:O	1:A:272:ALA:HB1	2.21	0.40
1:A:331:GLN:HA	1:A:372:SER:O	2.21	0.40
1:A:4:ILE:H	1:A:9:ARG:NH2	2.19	0.40
1:C:314:PHE:HE1	1:C:389:ILE:HD12	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	499/504 (99%)	407 (82%)	61 (12%)	31 (6%)	2	26
1	C	499/504 (99%)	394 (79%)	71 (14%)	34 (7%)	1	24
1	E	499/504 (99%)	407 (82%)	65 (13%)	27 (5%)	2	30
2	B	73/75 (97%)	63 (86%)	7 (10%)	3 (4%)	3	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	73/75 (97%)	63 (86%)	8 (11%)	2 (3%)	6	48
2	F	73/75 (97%)	61 (84%)	9 (12%)	3 (4%)	3	37
All	All	1716/1737 (99%)	1395 (81%)	221 (13%)	100 (6%)	4	28

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	17	GLY
1	A	75	PRO
1	A	78	GLY
1	A	79	GLU
1	A	108	PHE
1	A	147	GLN
1	A	164	ARG
1	A	171	PRO
1	A	172	ASN
1	A	173	SER
1	A	309	THR
1	A	311	ALA
1	A	480	LYS
2	B	2	VAL
1	C	15	MET
1	C	18	GLY
1	C	38	LYS
1	C	101	TRP
1	C	147	GLN
1	C	171	PRO
1	C	172	ASN
1	C	173	SER
1	C	249	HIS
1	C	309	THR
1	C	311	ALA
1	C	348	ASP
1	C	350	GLN
2	D	3	THR
1	E	75	PRO
1	E	77	GLN
1	E	158	HIS
1	E	160	THR
1	E	161	ASP

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Mol	Chain	Res	Type
1	E	171	PRO
1	E	172	ASN
1	E	173	SER
1	E	278	ASP
1	E	309	THR
1	E	311	ALA
1	E	350	GLN
2	F	3	THR
1	A	106	GLY
1	A	146	SER
1	A	160	THR
1	A	162	GLU
1	A	249	HIS
1	A	280	ALA
1	A	352	LEU
1	A	434	VAL
1	A	479	THR
1	C	110	LYS
1	C	146	SER
1	C	156	THR
1	C	160	THR
1	C	422	ALA
1	C	425	GLY
1	C	434	VAL
1	E	76	THR
1	E	78	GLY
1	E	106	GLY
1	E	110	LYS
1	E	317	ILE
1	E	434	VAL
1	E	480	LYS
1	A	4	ILE
1	A	145	GLY
1	A	260	SER
1	A	483	SER
1	C	4	ILE
1	C	106	GLY
1	C	145	GLY
1	C	239	LYS
1	C	260	SER
1	C	384	ASP
1	C	424	LEU

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Mol	Chain	Res	Type
1	C	482	GLY
1	E	4	ILE
1	E	260	SER
1	E	314	PHE
1	A	58	SER
1	A	89	GLN
1	A	250	ALA
1	C	57	ARG
1	C	89	GLN
1	E	58	SER
1	E	89	GLN
1	E	156	THR
1	E	163	ASN
2	F	73	ALA
2	B	3	THR
1	C	158	HIS
1	E	144	HIS
1	C	144	HIS
2	D	2	VAL
2	F	2	VAL
2	B	5	PRO
1	C	302	GLY
1	C	381	PRO
1	A	109	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	221/410 (54%)	220 (100%)	1 (0%)	92	97
1	C	235/410 (57%)	232 (99%)	3 (1%)	76	91
1	E	225/410 (55%)	222 (99%)	3 (1%)	76	91
2	B	25/64 (39%)	25 (100%)	0	100	100
2	D	25/64 (39%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	24/64 (38%)	24 (100%)	0	100	100
All	All	755/1422 (53%)	748 (99%)	7 (1%)	85	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	PHE
1	C	57	ARG
1	C	108	PHE
1	C	382	PHE
1	E	108	PHE
1	E	154	ASN
1	E	339	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	HIS
1	A	147	GLN
1	A	446	HIS
2	B	7	HIS
1	C	144	HIS
1	C	147	GLN
1	C	154	ASN
1	C	399	HIS
1	C	446	HIS
1	C	465	GLN
2	D	7	HIS
2	D	39	ASN
1	E	77	GLN
1	E	144	HIS
1	E	147	GLN
1	E	398	HIS
1	E	446	HIS
2	F	7	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	600	1,3	14,14,15	0.53	0	15,19,21	0.99	0
3	NAG	A	601	3	14,14,15	0.54	0	15,19,21	0.85	1 (6%)
3	NAG	C	600	1,3	14,14,15	0.58	0	15,19,21	0.66	0
3	NAG	C	601	3	14,14,15	0.54	0	15,19,21	0.68	1 (6%)
3	NAG	E	600	1,3	14,14,15	0.76	0	15,19,21	0.84	1 (6%)
3	NAG	E	601	3	14,14,15	0.83	0	15,19,21	0.95	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	600	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	601	3	-	0/6/23/26	0/1/1/1
3	NAG	C	600	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	601	3	-	0/6/23/26	0/1/1/1
3	NAG	E	600	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	601	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	C2-N2-C7	-2.59	119.73	123.11
3	E	601	NAG	C2-N2-C7	-2.38	120.01	123.11
3	E	600	NAG	C2-N2-C7	-2.37	120.02	123.11
3	C	601	NAG	C2-N2-C7	-2.17	120.28	123.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	600	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	NAG	1	0
3	C	600	NAG	9	0
3	C	601	NAG	2	0
3	E	600	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.