



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:15 PM UTC

PDB ID : 1FZG / pdb_00001fzg
Title : CRYSTAL STRUCTURE OF FRAGMENT D FROM HUMAN FIBRINOGEN WITH THE PEPTIDE LIGAND GLY-HIS-ARG-PRO-AMIDE
Authors : Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on : 1999-01-01
Resolution : 2.50 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

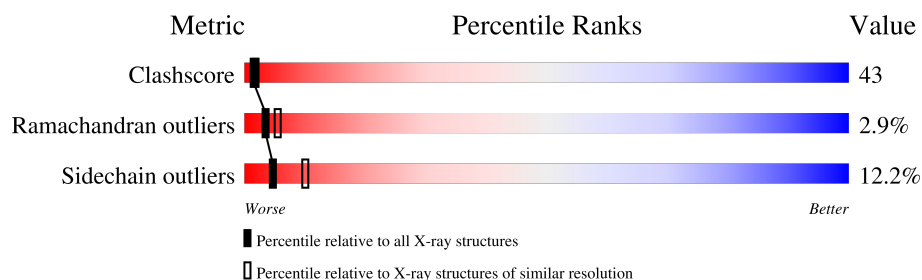
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	15% 33% 22% 7% 23%
1	D	87	17% 21% 18% 6% 38%
2	B	328	29% 41% 17% 5% 8%
2	E	328	35% 38% 16% • 10%
3	C	319	38% 38% 13% • 8%
3	F	319	34% 35% 15% • 11%
4	M	4	50% 25% 25%
4	N	4	25% 25% 25% 25%

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Mol	Chain	Length	Quality of chain
4	S	4	 50%25%25%
4	T	4	 50%50%
5	G	2	 100%
5	H	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	1	-	-	X	-
5	NAG	H	1	-	-	X	-
5	NAG	H	2	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10713 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			546	337	103	103	3			
1	D	54	Total	C	N	O	S	0	0	0
			440	269	84	84	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2427	1515	429	461	22			
2	E	296	Total	C	N	O	S	0	0	0
			2376	1484	420	450	22			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2342	1485	396	450	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	T	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	M	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	N	4	Total	C	N	O	0	0	0
			31	19	9	3			

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



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		
6	C	2	Total	Ca	0	0
			2	2		
6	E	2	Total	Ca	0	0
			2	2		
6	F	2	Total	Ca	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	31	Total	O	0	0
			31	31		
7	C	20	Total	O	0	0
			20	20		
7	D	3	Total	O	0	0
			3	3		
7	E	29	Total	O	0	0
			29	29		
7	F	23	Total	O	0	0
			23	23		

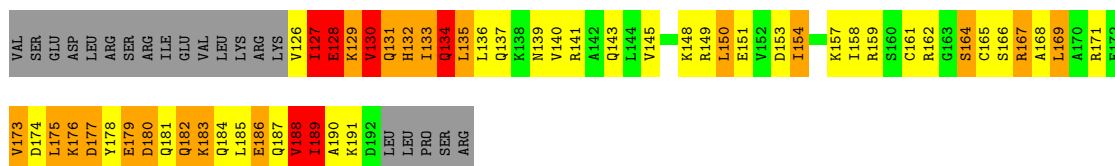
3 Residue-property plots

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

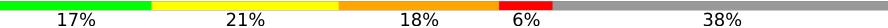
Note EDS was not executed.

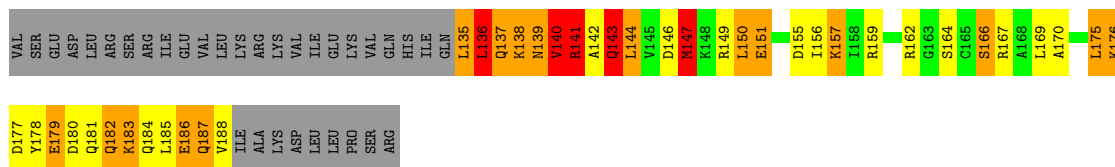
• Molecule 1: FIBRINOGEN

Chain A: 

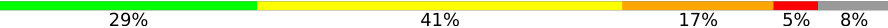


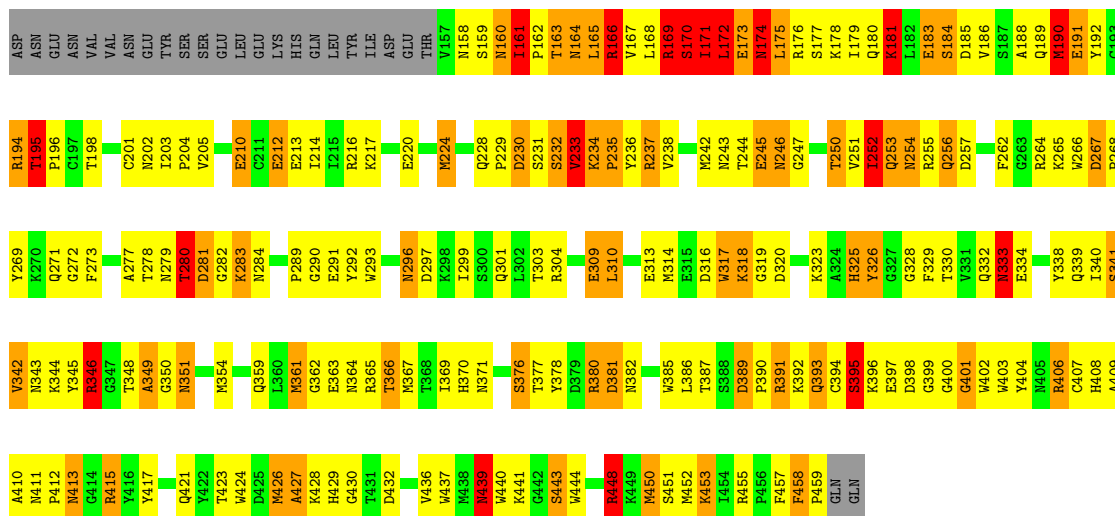
• Molecule 1: FIBRINOGEN

Chain D: 

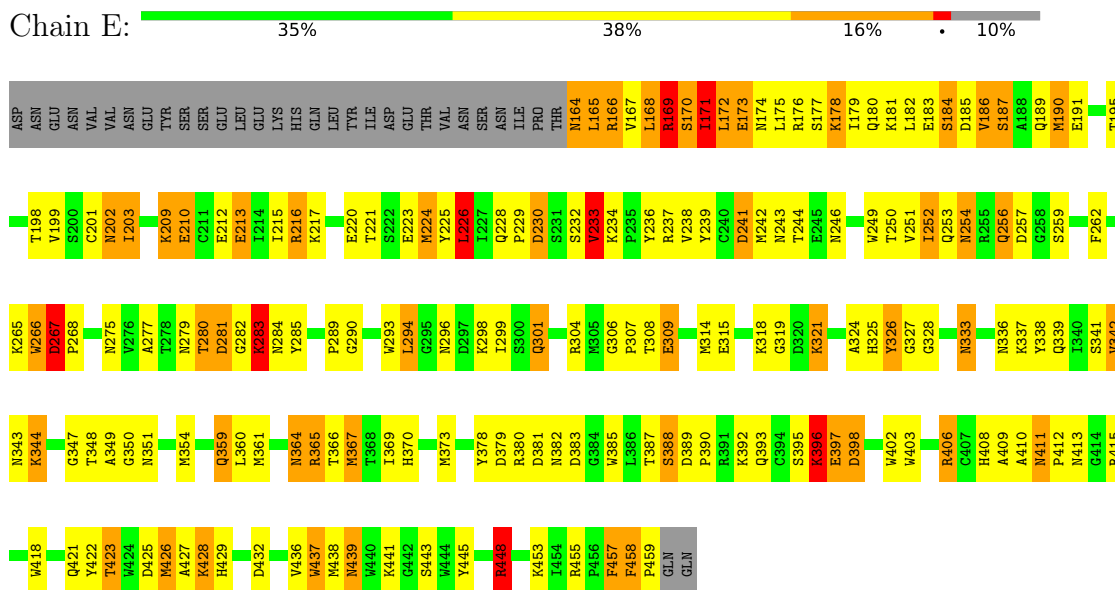


• Molecule 2: FIBRINOGEN

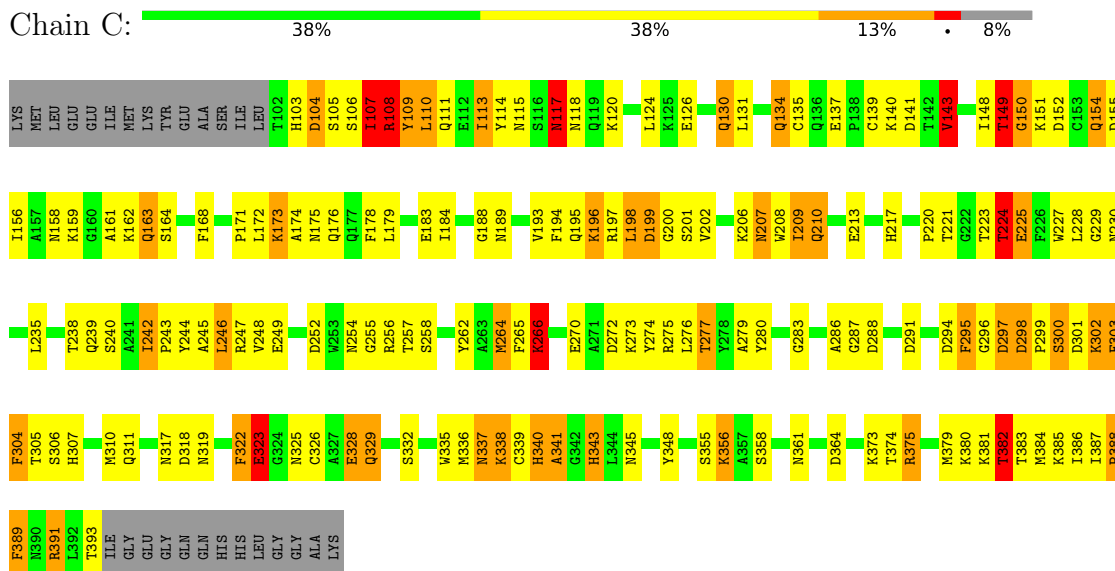
Chain B: 



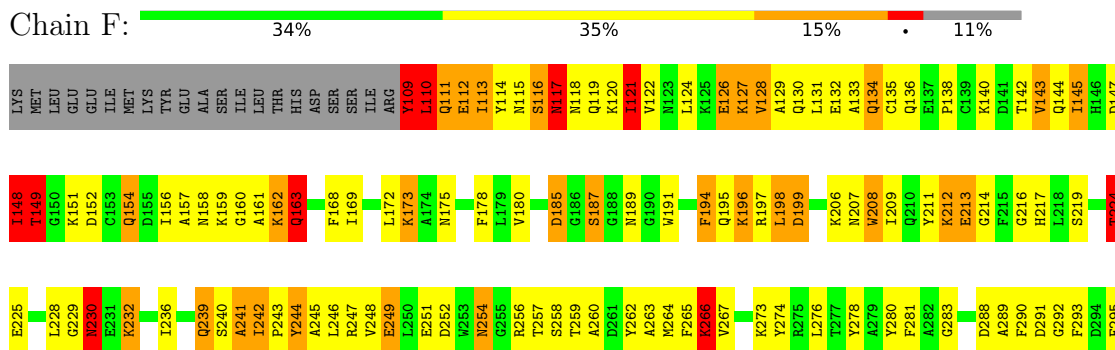
- Molecule 2: FIBRINOGEN

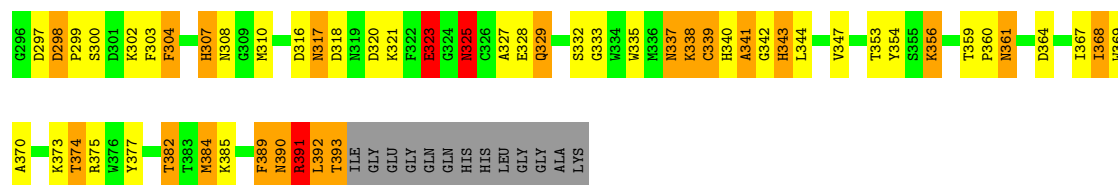


- Molecule 3: FIBRINOGEN



- Molecule 3: FIBRINOGEN





- Molecule 4: FIBRINOGEN

Chain S: 50% 25% 25%



- Molecule 4: FIBRINOGEN

Chain T: 50% 50%



- Molecule 4: FIBRINOGEN

Chain M: 50% 25% 25%



- Molecule 4: FIBRINOGEN

Chain N: 25% 25% 25% 25%



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

Chain G: 100%



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

Chain H: 100%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.80Å 149.40Å 234.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	88.5 (30.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.233 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10713	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	0/547	2.47	35/730 (4.8%)
1	D	0.94	0/440	2.90	33/586 (5.6%)
2	B	1.20	5/2489 (0.2%)	2.65	232/3363 (6.9%)
2	E	1.11	5/2437 (0.2%)	2.60	169/3290 (5.1%)
3	C	1.09	3/2407 (0.1%)	2.40	147/3256 (4.5%)
3	F	1.00	2/2351 (0.1%)	2.27	128/3180 (4.0%)
4	M	1.31	0/32	2.73	2/42 (4.8%)
4	N	1.12	0/32	4.83	4/42 (9.5%)
4	S	1.23	0/32	3.28	3/42 (7.1%)
4	T	1.24	0/32	2.31	2/42 (4.8%)
All	All	1.09	15/10799 (0.1%)	2.52	755/14573 (5.2%)

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
2	B	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	350	GLY	N-CA	11.46	1.57	1.45
3	C	229	GLY	N-CA	9.12	1.56	1.45
3	C	200	GLY	N-CA	8.77	1.58	1.45
2	B	350	GLY	N-CA	8.54	1.54	1.45
3	F	229	GLY	N-CA	8.38	1.55	1.45
2	B	310	LEU	N-CA	-7.16	1.37	1.46
2	B	290	GLY	N-CA	6.52	1.50	1.44
3	F	338	LYS	N-CA	6.19	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	205	VAL	N-CA	-5.66	1.39	1.46
2	E	349	ALA	C-O	5.52	1.31	1.23
3	C	209	ILE	N-CA	-5.28	1.40	1.46
2	E	349	ALA	N-CA	5.24	1.52	1.45
2	E	252	ILE	N-CA	5.17	1.51	1.45
2	B	255	ARG	N-CA	-5.13	1.39	1.46
2	E	349	ALA	C-N	-5.04	1.27	1.33

All (755) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	448	ARG	CD-NE-CZ	35.12	173.56	124.40
1	D	162	ARG	CD-NE-CZ	33.64	171.49	124.40
4	N	3	ARG	CD-NE-CZ	26.91	162.08	124.40
2	E	411	ASN	CA-CB-CG	18.99	131.59	112.60
3	C	134	GLN	OE1-CD-NE2	18.03	140.63	122.60
1	A	159	ARG	CD-NE-CZ	16.38	147.34	124.40
3	C	228	LEU	CA-C-O	-15.94	104.34	121.87
2	E	349	ALA	O-C-N	-15.69	103.35	122.65
2	E	395	SER	CA-C-O	-15.61	103.87	120.42
3	C	318	ASP	CA-CB-CG	14.75	127.35	112.60
2	B	267	ASP	CA-CB-CG	-14.12	98.47	112.60
3	F	228	LEU	CA-C-O	-14.12	106.33	121.87
2	E	349	ALA	CA-C-N	-13.77	108.64	122.27
2	E	349	ALA	C-N-CA	-13.77	108.64	122.27
2	B	243	ASN	CA-CB-CG	-13.35	99.25	112.60
1	D	149	ARG	CD-NE-CZ	12.86	142.40	124.40
2	B	349	ALA	CA-C-O	-12.76	107.27	121.94
2	E	318	LYS	CA-C-O	12.75	132.21	119.08
2	B	349	ALA	CA-C-N	-12.40	110.00	122.27
2	B	349	ALA	C-N-CA	-12.40	110.00	122.27
2	B	252	ILE	CA-CB-CG2	12.30	131.41	110.50
2	E	252	ILE	CA-CB-CG2	12.30	131.41	110.50
4	S	3	ARG	CA-CB-CG	12.25	138.59	114.10
3	C	228	LEU	O-C-N	-12.21	108.47	122.75
4	M	3	ARG	NE-CZ-NH1	-12.01	109.49	121.50
2	B	448	ARG	CD-NE-CZ	11.81	140.94	124.40
2	E	455	ARG	NE-CZ-NH2	-11.74	108.63	119.20
3	C	199	ASP	CA-C-O	-11.41	109.24	121.45
3	F	228	LEU	O-C-N	-11.04	109.83	122.75
2	B	399	GLY	N-CA-C	10.91	129.76	115.47
2	E	392	LYS	CA-C-O	10.85	133.73	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	396	LYS	N-CA-CB	10.73	126.01	110.13
3	C	115	ASN	CA-CB-CG	10.61	123.21	112.60
3	F	194	PHE	CA-CB-CG	10.61	124.41	113.80
2	B	309	GLU	CA-C-N	10.46	137.75	123.00
2	B	309	GLU	C-N-CA	10.46	137.75	123.00
2	E	216	ARG	CD-NE-CZ	10.46	139.04	124.40
2	E	275	ASN	OD1-CG-ND2	10.42	133.02	122.60
2	E	365	ARG	CD-NE-CZ	10.31	138.84	124.40
3	C	375	ARG	NH1-CZ-NH2	10.27	132.65	119.30
1	A	159	ARG	NE-CZ-NH1	10.24	131.74	121.50
2	B	304	ARG	CD-NE-CZ	10.16	138.62	124.40
2	B	349	ALA	O-C-N	-10.15	110.17	122.65
3	C	304	PHE	CA-CB-CG	-10.10	103.70	113.80
2	E	237	ARG	CA-C-N	-10.06	109.33	122.51
2	E	237	ARG	C-N-CA	-10.06	109.33	122.51
3	C	355	SER	CA-C-O	-10.06	110.68	121.45
1	A	159	ARG	NE-CZ-NH2	-9.92	110.28	119.20
3	C	375	ARG	NE-CZ-NH1	-9.90	111.60	121.50
2	B	256	GLN	OE1-CD-NE2	-9.86	112.74	122.60
2	E	409	ALA	N-CA-C	-9.86	101.59	114.31
2	B	400	GLY	O-C-N	9.80	131.50	123.95
1	A	180	ASP	CA-CB-CG	9.69	122.29	112.60
3	F	247	ARG	CA-C-O	-9.68	109.58	120.32
4	S	3	ARG	NE-CZ-NH2	-9.64	110.53	119.20
2	B	439	ASN	OD1-CG-ND2	-9.62	112.98	122.60
2	B	398	ASP	CA-CB-CG	9.52	122.12	112.60
3	F	353	THR	CA-C-O	-9.41	110.19	120.92
2	B	279	ASN	CA-CB-CG	-9.41	103.19	112.60
3	F	262	TYR	CA-C-O	-9.30	110.66	120.70
2	B	237	ARG	CA-C-N	-9.23	110.41	122.51
2	B	237	ARG	C-N-CA	-9.23	110.41	122.51
1	D	183	LYS	N-CA-C	-9.23	101.17	111.14
3	C	117	ASN	CA-CB-CG	9.23	121.83	112.60
2	B	411	ASN	OD1-CG-ND2	9.21	131.81	122.60
2	E	342	VAL	CA-C-O	-9.13	112.08	121.67
3	C	338	LYS	N-CA-C	9.05	123.60	111.30
3	C	248	VAL	CA-C-O	-9.02	110.76	120.59
2	B	409	ALA	N-CA-C	-9.01	102.69	114.31
2	B	399	GLY	CA-C-N	-8.99	114.17	122.17
2	B	399	GLY	C-N-CA	-8.99	114.17	122.17
2	B	318	LYS	CB-CA-C	8.96	125.05	110.09
2	E	275	ASN	CA-CB-CG	-8.95	103.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	421	GLN	CB-CG-CD	8.93	127.79	112.60
3	F	316	ASP	CA-CB-CG	8.91	121.51	112.60
2	B	410	ALA	CA-C-N	-8.90	113.06	122.85
2	B	410	ALA	C-N-CA	-8.90	113.06	122.85
2	B	439	ASN	CA-CB-CG	-8.82	103.78	112.60
2	B	216	ARG	CD-NE-CZ	8.71	136.59	124.40
2	E	349	ALA	CA-C-O	-8.71	111.93	121.94
3	C	117	ASN	CB-CA-C	8.69	127.36	110.67
1	A	167	ARG	CD-NE-CZ	8.69	136.56	124.40
2	B	164	ASN	CA-CB-CG	8.66	121.26	112.60
2	E	443	SER	N-CA-C	8.65	121.86	111.82
2	B	359	GLN	CA-CB-CG	8.64	131.39	114.10
2	E	185	ASP	CA-CB-CG	8.63	121.23	112.60
2	B	166	ARG	CD-NE-CZ	8.60	136.44	124.40
3	F	320	ASP	CA-CB-CG	8.55	121.15	112.60
3	C	126	GLU	CA-CB-CG	8.52	131.15	114.10
2	E	250	THR	CA-C-O	-8.52	110.88	120.43
3	F	254	ASN	CA-CB-CG	8.51	121.11	112.60
2	B	409	ALA	N-CA-CB	8.48	122.18	110.90
3	C	297	ASP	CA-C-O	-8.48	111.82	120.90
1	A	161	CYS	N-CA-C	-8.46	103.10	113.50
2	B	233	VAL	CB-CA-C	-8.41	100.45	111.13
2	B	210	GLU	CA-C-O	-8.40	112.30	121.28
1	A	162	ARG	CD-NE-CZ	8.39	136.15	124.40
2	E	173	GLU	N-CA-C	-8.39	101.04	111.11
2	E	455	ARG	NE-CZ-NH1	8.36	129.86	121.50
2	E	239	TYR	O-C-N	-8.33	113.72	123.22
2	E	327	GLY	CA-C-O	-8.32	111.41	120.40
3	F	129	ALA	CA-C-O	-8.29	111.76	120.55
3	C	111	GLN	CA-CB-CG	8.26	130.62	114.10
1	A	189	ILE	CA-C-O	8.24	128.59	120.27
2	E	262	PHE	CA-CB-CG	-8.23	105.57	113.80
3	C	337	ASN	O-C-N	-8.23	109.94	122.61
2	E	445	TYR	O-C-N	-8.21	112.28	123.12
2	B	232	SER	CA-C-N	8.12	132.95	120.13
2	B	232	SER	C-N-CA	8.12	132.95	120.13
3	F	199	ASP	CA-C-O	-8.10	112.80	121.38
3	C	224	THR	N-CA-CB	-8.05	96.55	111.53
3	F	338	LYS	O-C-N	-8.02	111.92	122.59
2	E	324	ALA	CA-C-O	-7.99	111.70	120.33
2	B	175	LEU	O-C-N	7.97	130.56	122.12
1	D	141	ARG	CD-NE-CZ	7.96	135.55	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	139	CYS	CA-C-O	-7.91	113.17	121.55
2	B	413	ASN	CA-C-O	7.90	128.81	119.56
3	F	292	GLY	CA-C-O	-7.86	116.81	122.23
1	D	155	ASP	CA-CB-CG	7.79	120.39	112.60
3	F	224	THR	N-CA-CB	-7.74	97.68	110.68
2	E	410	ALA	CA-C-N	-7.70	115.50	122.28
2	E	410	ALA	C-N-CA	-7.70	115.50	122.28
1	A	157	LYS	O-C-N	-7.67	112.83	122.27
3	C	134	GLN	CG-CD-OE1	-7.64	105.52	120.80
2	E	370	HIS	CA-CB-CG	-7.63	106.17	113.80
3	F	337	ASN	OD1-CG-ND2	-7.58	115.02	122.60
3	C	208	TRP	CA-C-N	7.57	130.09	120.56
3	C	208	TRP	C-N-CA	7.57	130.09	120.56
2	E	406	ARG	NE-CZ-NH2	-7.56	112.39	119.20
2	B	214	ILE	CA-C-O	-7.55	113.10	120.95
2	E	336	ASN	OD1-CG-ND2	7.53	130.13	122.60
2	B	441	LYS	CA-C-O	-7.51	111.07	119.78
2	E	252	ILE	N-CA-CB	-7.50	97.75	112.75
4	T	2	HIS	CA-CB-CG	-7.50	106.31	113.80
2	E	347	GLY	CA-C-O	7.49	129.78	121.02
2	E	254	ASN	CA-CB-CG	7.47	120.07	112.60
2	E	350	GLY	O-C-N	-7.45	115.80	122.88
2	E	343	ASN	CA-CB-CG	-7.44	105.16	112.60
2	E	344	LYS	O-C-N	-7.43	114.06	122.91
2	E	241	ASP	CA-CB-CG	7.43	120.03	112.60
1	D	157	LYS	CA-C-O	-7.42	112.56	120.42
2	E	282	GLY	CA-C-N	7.41	135.70	121.54
2	E	282	GLY	C-N-CA	7.41	135.70	121.54
3	F	175	ASN	CA-CB-CG	-7.41	105.19	112.60
1	A	149	ARG	CD-NE-CZ	7.40	134.76	124.40
2	B	230	ASP	CA-CB-CG	-7.40	105.20	112.60
1	D	141	ARG	CA-C-O	7.38	129.19	121.07
1	D	159	ARG	NE-CZ-NH2	7.38	125.84	119.20
3	F	323	GLU	N-CA-C	-7.33	103.29	111.28
3	C	135	CYS	N-CA-CB	-7.33	100.55	111.25
1	D	150	LEU	CA-C-N	-7.30	110.95	120.44
1	D	150	LEU	C-N-CA	-7.30	110.95	120.44
3	C	199	ASP	CA-C-N	-7.30	107.10	121.41
3	C	199	ASP	C-N-CA	-7.30	107.10	121.41
3	F	207	ASN	OD1-CG-ND2	-7.30	115.30	122.60
3	C	304	PHE	CA-C-O	-7.29	110.42	119.38
3	C	246	LEU	CA-C-O	-7.28	112.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	152	ASP	CA-C-O	-7.28	113.41	121.05
2	B	421	GLN	O-C-N	-7.26	114.00	122.93
2	E	233	VAL	CB-CA-C	-7.25	100.42	111.08
2	B	252	ILE	CB-CA-C	7.25	117.44	111.06
3	F	117	ASN	OD1-CG-ND2	7.25	129.85	122.60
1	A	165	CYS	CA-CB-SG	-7.22	97.80	114.40
2	B	406	ARG	CA-C-O	7.22	130.84	120.51
2	E	252	ILE	CB-CA-C	7.22	117.41	111.06
2	E	364	ASN	N-CA-C	-7.21	103.42	111.28
4	N	3	ARG	N-CA-CB	7.19	120.64	110.07
3	C	298	ASP	CB-CG-OD2	-7.18	101.88	118.40
2	B	195	THR	CA-CB-OG1	7.17	120.36	109.60
2	B	341	SER	CA-CB-OG	-7.17	96.75	111.10
2	B	264	ARG	CD-NE-CZ	-7.16	114.38	124.40
3	C	266	LYS	CA-C-O	-7.15	112.98	120.99
2	B	453	LYS	CA-C-N	-7.11	113.36	123.03
2	B	453	LYS	C-N-CA	-7.11	113.36	123.03
2	E	395	SER	CA-C-N	-7.11	108.83	120.71
2	E	395	SER	C-N-CA	-7.11	108.83	120.71
2	B	205	VAL	CA-C-O	-7.09	113.33	120.85
2	E	328	GLY	CA-C-O	-7.09	115.41	120.94
3	F	338	LYS	N-CA-C	7.08	125.89	110.80
3	F	228	LEU	CA-C-N	-7.08	110.15	121.05
3	F	228	LEU	C-N-CA	-7.08	110.15	121.05
2	E	321	LYS	CA-CB-CG	7.08	128.26	114.10
2	E	199	VAL	CA-C-N	-7.07	112.34	123.23
2	E	199	VAL	C-N-CA	-7.07	112.34	123.23
2	E	327	GLY	CA-C-N	-7.06	116.85	121.65
2	E	327	GLY	C-N-CA	-7.06	116.85	121.65
2	B	191	GLU	CA-C-O	-7.05	113.44	120.70
1	D	135	LEU	CB-CA-C	7.05	123.50	110.10
2	B	195	THR	CA-C-O	7.03	126.61	119.86
2	B	272	GLY	CA-C-O	-7.03	116.40	121.88
2	B	381	ASP	CB-CA-C	-7.01	100.02	110.67
2	E	246	ASN	CB-CG-ND2	6.99	126.89	116.40
1	D	167	ARG	NE-CZ-NH1	6.96	128.47	121.50
3	C	388	PRO	CB-CA-C	6.96	120.76	111.71
2	B	334	GLU	O-C-N	-6.96	114.90	122.07
3	F	148	ILE	CB-CA-C	-6.95	102.11	111.15
2	E	171	ILE	CA-C-O	6.94	129.46	120.78
2	B	415	ARG	CD-NE-CZ	-6.93	114.69	124.40
2	B	340	ILE	CA-C-N	6.92	132.64	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	ILE	C-N-CA	6.92	132.64	122.39
1	D	166	SER	CA-C-O	-6.92	113.16	120.63
2	B	229	PRO	CA-C-O	6.92	130.06	119.55
2	B	252	ILE	N-CA-CB	-6.90	98.95	112.75
3	F	230	ASN	OD1-CG-ND2	-6.89	115.71	122.60
3	F	127	LYS	N-CA-C	-6.88	103.70	111.07
3	C	207	ASN	CA-C-N	6.88	129.38	120.44
3	C	207	ASN	C-N-CA	6.88	129.38	120.44
3	C	322	PHE	CA-CB-CG	6.85	120.65	113.80
2	B	169	ARG	N-CA-CB	-6.84	98.93	110.49
2	E	294	LEU	CA-C-O	-6.82	113.32	120.55
3	C	247	ARG	CD-NE-CZ	6.82	133.94	124.40
3	F	337	ASN	CA-C-N	-6.80	108.55	121.54
3	F	337	ASN	C-N-CA	-6.80	108.55	121.54
3	C	210	GLN	CG-CD-NE2	6.80	126.60	116.40
2	E	426	MET	N-CA-C	-6.79	105.52	113.88
2	E	181	LYS	CB-CA-C	6.79	122.40	110.85
2	B	237	ARG	NE-CZ-NH1	-6.79	114.72	121.50
1	D	162	ARG	CG-CD-NE	6.78	126.92	112.00
3	F	391	ARG	CA-C-N	-6.77	112.23	123.33
3	F	391	ARG	C-N-CA	-6.77	112.23	123.33
2	E	290	GLY	CA-C-O	-6.76	114.82	122.33
2	B	408	HIS	N-CA-C	6.76	119.14	108.79
2	E	382	ASN	N-CA-C	-6.76	103.11	112.30
2	E	348	THR	CA-C-O	-6.75	110.93	118.69
3	C	318	ASP	CA-C-O	-6.74	112.67	120.49
3	C	198	LEU	CA-C-O	-6.73	110.89	120.51
1	D	137	GLN	N-CA-C	-6.73	104.03	111.36
2	E	427	ALA	O-C-N	-6.72	114.62	122.95
2	B	213	GLU	O-C-N	-6.71	115.01	122.12
2	E	324	ALA	O-C-N	6.70	131.96	123.12
2	B	411	ASN	CB-CG-ND2	-6.69	106.37	116.40
2	B	400	GLY	CA-C-O	-6.68	115.39	121.47
2	B	325	HIS	CE1-NE2-CD2	6.68	115.68	109.00
3	C	323	GLU	N-CA-C	-6.67	104.40	112.54
3	F	307	HIS	CA-CB-CG	-6.66	107.14	113.80
2	B	264	ARG	NE-CZ-NH2	-6.66	113.20	119.20
2	B	396	LYS	N-CA-C	-6.65	104.11	111.36
2	E	233	VAL	N-CA-C	6.65	120.28	109.78
2	B	439	ASN	CA-C-O	-6.64	111.78	119.61
2	B	233	VAL	N-CA-C	6.64	120.05	110.09
3	F	260	ALA	CA-C-O	-6.63	111.02	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	280	THR	OG1-CB-CG2	6.62	122.55	109.30
2	B	436	VAL	N-CA-C	6.62	118.96	108.89
2	E	243	ASN	CA-CB-CG	-6.62	105.98	112.60
3	F	325	ASN	CA-CB-CG	6.62	119.22	112.60
2	E	367	MET	CA-C-N	-6.61	112.29	122.60
2	E	367	MET	C-N-CA	-6.61	112.29	122.60
3	C	328	GLU	N-CA-C	-6.60	104.01	111.14
2	E	186	VAL	CA-C-O	6.60	127.81	120.95
3	C	375	ARG	CD-NE-CZ	-6.59	115.17	124.40
3	F	266	LYS	CA-C-O	-6.59	113.42	121.06
3	C	163	GLN	CA-C-O	6.58	128.23	120.66
4	M	3	ARG	NE-CZ-NH2	6.58	125.12	119.20
2	B	301	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	153	ASP	O-C-N	-6.57	115.16	122.12
2	E	169	ARG	CD-NE-CZ	6.55	133.58	124.40
3	C	280	TYR	CA-C-N	6.55	130.12	120.95
3	C	280	TYR	C-N-CA	6.55	130.12	120.95
2	B	389	ASP	CA-C-N	6.55	127.07	119.47
2	B	389	ASP	C-N-CA	6.55	127.07	119.47
2	B	202	ASN	CA-C-N	-6.55	117.02	123.04
2	B	202	ASN	C-N-CA	-6.55	117.02	123.04
2	B	380	ARG	CD-NE-CZ	-6.54	115.24	124.40
2	E	439	ASN	CB-CG-ND2	6.53	126.19	116.40
2	E	232	SER	CA-C-N	6.53	129.42	120.35
2	E	232	SER	C-N-CA	6.53	129.42	120.35
1	A	189	ILE	N-CA-C	6.51	117.41	107.77
3	C	179	LEU	O-C-N	-6.49	115.44	123.04
2	B	448	ARG	CB-CG-CD	6.45	126.14	111.30
2	E	411	ASN	CB-CA-C	6.45	119.83	110.87
2	E	267	ASP	CA-CB-CG	-6.44	106.16	112.60
3	C	326	CYS	CA-C-N	6.44	128.91	120.28
3	C	326	CYS	C-N-CA	6.44	128.91	120.28
3	C	391	ARG	CG-CD-NE	-6.44	97.83	112.00
3	C	134	GLN	CA-CB-CG	-6.44	101.23	114.10
2	B	173	GLU	N-CA-C	-6.43	104.19	111.07
2	B	262	PHE	CA-CB-CG	-6.43	107.37	113.80
2	B	326	TYR	CA-C-O	-6.43	113.42	120.24
3	C	356	LYS	N-CA-CB	6.42	119.69	110.06
2	B	220	GLU	CG-CD-OE2	-6.41	103.65	118.40
2	B	436	VAL	O-C-N	6.41	129.65	122.98
3	F	214	GLY	O-C-N	-6.41	117.25	122.64
2	B	296	ASN	CA-C-N	-6.41	111.69	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	ASN	C-N-CA	-6.41	111.69	120.28
2	E	392	LYS	O-C-N	-6.40	114.11	122.43
2	B	394	CYS	CA-C-O	6.40	127.20	120.42
2	B	280	THR	CA-CB-CG2	-6.40	99.62	110.50
3	C	175	ASN	CA-CB-CG	6.39	119.00	112.60
2	E	166	ARG	CD-NE-CZ	6.38	133.34	124.40
3	F	368	ILE	CA-C-O	6.38	126.72	121.68
2	B	426	MET	CG-SD-CE	-6.37	86.89	100.90
2	B	252	ILE	CA-C-N	6.37	133.15	121.94
2	B	252	ILE	C-N-CA	6.37	133.15	121.94
3	C	343	HIS	CA-CB-CG	6.36	120.16	113.80
3	C	329	GLN	CA-C-O	-6.36	113.68	120.42
2	B	212	GLU	OE1-CD-OE2	6.36	138.16	122.90
3	C	163	GLN	N-CA-C	6.35	119.84	109.24
2	B	417	TYR	CA-C-O	6.33	127.92	120.58
2	E	413	ASN	O-C-N	-6.33	114.48	122.26
2	E	279	ASN	CA-CB-CG	-6.32	106.28	112.60
1	A	145	VAL	CA-C-O	-6.32	114.15	120.85
2	B	393	GLN	OE1-CD-NE2	-6.32	116.28	122.60
2	B	339	GLN	CA-C-O	-6.31	114.86	121.55
3	C	228	LEU	CA-C-N	-6.31	111.33	121.05
3	C	228	LEU	C-N-CA	-6.31	111.33	121.05
3	F	149	THR	N-CA-CB	6.31	120.40	110.87
3	F	244	TYR	CA-C-O	-6.29	113.99	121.66
2	B	257	ASP	CA-C-O	-6.28	111.53	120.51
2	E	202	ASN	CA-C-O	-6.28	113.59	120.81
2	B	212	GLU	CA-C-O	6.27	127.16	120.70
3	F	135	CYS	N-CA-C	6.26	118.12	109.54
2	B	346	ARG	NE-CZ-NH1	6.25	127.75	121.50
2	E	445	TYR	CA-C-N	6.25	131.08	122.77
2	E	445	TYR	C-N-CA	6.25	131.08	122.77
1	A	129	LYS	N-CA-C	6.25	118.52	110.65
2	E	266	TRP	N-CA-CB	-6.24	100.64	109.94
2	B	273	PHE	CA-CB-CG	6.24	120.04	113.80
3	C	275	ARG	CD-NE-CZ	-6.24	115.66	124.40
2	B	253	GLN	CA-CB-CG	6.24	126.58	114.10
3	C	149	THR	N-CA-CB	6.24	121.08	111.22
2	B	325	HIS	ND1-CE1-NE2	-6.24	102.16	108.40
3	F	247	ARG	O-C-N	6.24	130.61	123.31
1	D	167	ARG	CA-CB-CG	6.24	126.57	114.10
4	S	3	ARG	NE-CZ-NH1	6.24	127.73	121.50
2	E	319	GLY	CA-C-O	-6.23	112.10	119.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	290	PHE	CA-CB-CG	6.23	120.03	113.80
2	B	382	ASN	N-CA-C	-6.22	103.75	113.02
1	A	188	VAL	CA-C-N	-6.22	114.15	122.98
1	A	188	VAL	C-N-CA	-6.22	114.15	122.98
2	B	450	MET	CA-C-O	-6.22	113.09	120.43
2	E	234	LYS	N-CA-CB	-6.22	101.37	110.14
3	F	214	GLY	CA-C-O	6.21	127.11	121.77
3	F	249	GLU	N-CA-CB	6.20	120.30	110.57
2	E	443	SER	CA-C-O	-6.19	112.85	119.97
3	C	202	VAL	O-C-N	6.19	129.86	123.18
3	C	156	ILE	N-CA-C	-6.18	104.72	110.53
2	E	167	VAL	N-CA-CB	6.18	121.42	111.23
1	D	135	LEU	CA-C-O	6.17	131.29	120.80
3	F	163	GLN	CB-CG-CD	6.17	123.08	112.60
3	C	194	PHE	CA-CB-CG	6.16	119.96	113.80
3	C	361	ASN	CA-CB-CG	-6.16	106.44	112.60
2	B	290	GLY	N-CA-C	-6.16	104.14	112.57
3	C	318	ASP	O-C-N	6.15	130.59	123.02
3	F	149	THR	OG1-CB-CG2	6.15	121.60	109.30
2	B	284	ASN	CB-CA-C	6.15	121.03	111.13
1	D	147	MET	N-CA-CB	-6.15	101.06	110.16
2	B	289	PRO	CA-C-N	-6.14	116.97	122.43
2	B	289	PRO	C-N-CA	-6.14	116.97	122.43
3	C	266	LYS	CA-C-N	-6.14	115.58	123.19
3	C	266	LYS	C-N-CA	-6.14	115.58	123.19
3	F	154	GLN	OE1-CD-NE2	-6.13	116.47	122.60
2	E	436	VAL	N-CA-C	6.13	118.48	108.97
2	E	457	PHE	CA-CB-CG	-6.13	107.67	113.80
1	A	164	SER	N-CA-CB	-6.13	100.13	110.49
3	F	337	ASN	CA-CB-CG	6.13	118.73	112.60
2	B	205	VAL	CA-C-N	-6.12	112.53	121.71
2	B	205	VAL	C-N-CA	-6.12	112.53	121.71
2	B	166	ARG	N-CA-C	-6.12	105.12	112.59
2	B	386	LEU	CB-CA-C	6.12	119.44	110.26
3	C	326	CYS	O-C-N	-6.11	115.73	122.09
2	E	283	LYS	N-CA-C	6.11	123.82	110.80
2	B	406	ARG	CD-NE-CZ	6.11	132.95	124.40
2	B	176	ARG	CA-C-O	-6.07	114.44	120.82
3	C	110	LEU	CB-CA-C	6.07	120.35	110.95
2	B	325	HIS	CG-CD2-NE2	-6.06	101.14	107.20
3	F	163	GLN	N-CA-C	6.06	118.26	108.32
4	N	2	HIS	CA-C-O	-6.06	114.57	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	349	ALA	N-CA-C	-6.06	102.72	110.53
2	B	213	GLU	CG-CD-OE1	6.05	132.33	118.40
2	B	400	GLY	N-CA-C	-6.05	102.83	111.42
1	A	137	GLN	N-CA-C	-6.04	104.78	111.36
1	A	173	VAL	CB-CA-C	-6.04	103.30	111.15
2	B	313	GLU	CG-CD-OE1	6.03	132.26	118.40
2	E	277	ALA	N-CA-CB	-6.02	102.23	111.56
2	B	213	GLU	N-CA-CB	-6.01	101.28	110.12
1	A	132	HIS	CA-CB-CG	6.01	119.81	113.80
2	B	391	ARG	N-CA-C	-6.01	104.85	111.82
2	B	272	GLY	N-CA-C	-6.01	104.13	112.18
2	B	301	GLN	CA-C-O	-6.01	114.18	120.55
3	C	348	TYR	CA-C-N	5.99	131.44	123.05
3	C	348	TYR	C-N-CA	5.99	131.44	123.05
1	A	153	ASP	CA-C-O	5.99	126.90	120.55
2	E	349	ALA	N-CA-C	-5.99	102.80	110.53
3	C	279	ALA	CA-C-O	5.98	127.78	120.31
2	E	226	LEU	CB-CA-C	-5.97	99.89	109.75
2	B	455	ARG	NE-CZ-NH1	5.97	127.47	121.50
2	B	233	VAL	CA-C-O	5.96	127.81	121.97
2	E	418	TRP	O-C-N	-5.96	115.62	122.89
3	F	216	GLY	O-C-N	-5.96	117.24	122.90
1	A	157	LYS	CA-CB-CG	5.96	126.02	114.10
3	F	197	ARG	NE-CZ-NH2	-5.95	113.84	119.20
2	B	376	SER	O-C-N	-5.95	115.66	123.16
2	B	232	SER	N-CA-C	-5.94	103.77	111.02
3	F	375	ARG	NE-CZ-NH1	5.94	127.44	121.50
2	B	194	ARG	NE-CZ-NH2	-5.93	113.86	119.20
2	B	279	ASN	OD1-CG-ND2	5.93	128.53	122.60
2	E	250	THR	CA-C-N	-5.93	113.48	121.66
2	E	250	THR	C-N-CA	-5.93	113.48	121.66
2	B	413	ASN	O-C-N	-5.92	115.23	122.34
3	F	207	ASN	N-CA-CB	-5.92	101.42	110.49
3	F	356	LYS	CB-CA-C	5.92	120.62	110.79
3	F	148	ILE	O-C-N	5.92	129.38	122.81
2	E	202	ASN	CA-CB-CG	-5.92	106.68	112.60
3	F	384	MET	N-CA-C	-5.92	98.43	108.26
2	B	395	SER	CA-CB-OG	5.92	122.93	111.10
2	E	321	LYS	CA-C-O	5.92	127.70	120.60
3	F	142	THR	CA-C-O	-5.92	112.10	119.38
2	E	166	ARG	N-CA-C	-5.91	104.72	112.41
2	B	364	ASN	O-C-N	5.91	129.32	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	196	LYS	CA-C-O	-5.90	112.78	119.98
2	E	354	MET	CG-SD-CE	-5.89	87.95	100.90
2	E	169	ARG	CA-CB-CG	5.89	125.88	114.10
3	C	283	GLY	CA-C-N	5.88	130.48	122.54
3	C	283	GLY	C-N-CA	5.88	130.48	122.54
2	E	184	SER	N-CA-CB	-5.87	101.55	110.07
3	C	199	ASP	O-C-N	-5.87	116.35	123.10
3	C	328	GLU	CA-CB-CG	5.87	125.84	114.10
2	B	371	ASN	CA-CB-CG	-5.87	106.73	112.60
1	A	162	ARG	O-C-N	-5.87	115.90	122.12
3	C	134	GLN	CB-CG-CD	-5.87	102.63	112.60
3	C	143	VAL	N-CA-CB	5.87	117.69	111.00
2	B	271	GLN	CB-CG-CD	-5.86	102.63	112.60
2	E	178	LYS	CA-CB-CG	5.86	125.82	114.10
3	C	137	GLU	N-CA-CB	-5.85	102.95	110.03
3	C	255	GLY	N-CA-C	-5.85	107.31	114.92
3	F	169	ILE	CA-C-N	-5.85	115.73	122.52
3	F	169	ILE	C-N-CA	-5.85	115.73	122.52
2	B	166	ARG	NE-CZ-NH1	5.84	127.34	121.50
2	E	443	SER	CA-C-N	-5.83	114.48	123.17
2	E	443	SER	C-N-CA	-5.83	114.48	123.17
3	C	391	ARG	NH1-CZ-NH2	5.83	126.88	119.30
1	D	141	ARG	CA-C-N	5.83	128.34	120.65
1	D	141	ARG	C-N-CA	5.83	128.34	120.65
2	E	220	GLU	CA-C-N	-5.82	113.50	122.87
2	E	220	GLU	C-N-CA	-5.82	113.50	122.87
2	B	316	ASP	CB-CG-OD2	-5.82	105.03	118.40
3	F	361	ASN	CA-CB-CG	-5.82	106.78	112.60
1	D	146	ASP	CA-CB-CG	-5.81	106.79	112.60
2	B	369	ILE	CA-C-O	-5.81	114.46	121.54
2	B	348	THR	CA-CB-OG1	-5.80	100.91	109.60
3	C	178	PHE	CA-CB-CG	5.80	119.60	113.80
2	E	415	ARG	NH1-CZ-NH2	5.80	126.84	119.30
3	F	280	TYR	O-C-N	-5.80	117.72	123.46
2	E	237	ARG	CD-NE-CZ	5.79	132.51	124.40
2	B	399	GLY	O-C-N	-5.79	114.99	122.34
2	B	289	PRO	CA-C-O	-5.79	114.61	121.67
3	C	164	SER	CA-C-O	-5.79	114.83	121.19
2	B	317	TRP	CA-C-N	-5.78	113.00	122.54
2	B	317	TRP	C-N-CA	-5.78	113.00	122.54
3	F	148	ILE	CA-C-O	-5.78	114.26	120.85
2	B	333	ASN	N-CA-C	5.77	118.80	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	413	ASN	N-CA-CB	-5.77	102.13	110.56
2	B	194	ARG	NE-CZ-NH1	5.77	127.27	121.50
3	F	145	ILE	N-CA-CB	-5.76	103.41	111.25
2	E	191	GLU	CG-CD-OE2	-5.76	105.15	118.40
3	F	121	ILE	O-C-N	-5.76	115.37	122.57
2	B	176	ARG	N-CA-C	-5.76	104.91	111.07
3	C	287	GLY	CA-C-N	5.75	130.06	122.06
3	C	287	GLY	C-N-CA	5.75	130.06	122.06
2	E	421	GLN	CB-CA-C	5.75	119.48	109.65
3	F	341	ALA	N-CA-C	-5.74	107.27	114.56
2	E	406	ARG	NE-CZ-NH1	5.74	127.24	121.50
2	E	257	ASP	OD1-CG-OD2	-5.74	109.14	122.90
3	C	193	VAL	CA-C-O	-5.73	113.97	120.74
3	F	389	PHE	CA-CB-CG	5.72	119.52	113.80
3	C	143	VAL	CA-CB-CG2	5.71	120.11	110.40
3	C	174	ALA	N-CA-C	5.71	118.56	110.50
2	E	448	ARG	CB-CG-CD	5.71	124.44	111.30
2	B	320	ASP	O-C-N	-5.71	115.79	122.81
3	F	109	TYR	CA-CB-CG	5.71	124.18	113.90
2	E	359	GLN	CA-CB-CG	5.71	125.51	114.10
2	B	166	ARG	N-CA-CB	5.70	120.05	110.92
2	B	341	SER	N-CA-C	5.70	117.73	108.26
3	F	169	ILE	CA-C-O	-5.70	115.02	121.75
2	E	290	GLY	N-CA-C	-5.69	104.78	112.57
2	B	455	ARG	CD-NE-CZ	-5.68	116.44	124.40
1	D	182	GLN	CA-C-O	5.68	125.08	118.77
3	C	364	ASP	CA-C-N	-5.68	113.58	122.49
3	C	364	ASP	C-N-CA	-5.68	113.58	122.49
2	B	271	GLN	CB-CA-C	-5.67	98.81	110.38
2	B	165	LEU	N-CA-CB	5.67	119.16	110.60
3	C	183	GLU	CA-C-N	-5.67	115.72	123.14
3	C	183	GLU	C-N-CA	-5.67	115.72	123.14
3	C	280	TYR	O-C-N	-5.66	117.36	123.42
3	F	389	PHE	N-CA-C	5.66	117.45	111.28
2	B	247	GLY	CA-C-O	-5.66	114.55	122.58
3	F	389	PHE	N-CA-CB	-5.65	101.81	110.12
3	F	249	GLU	CA-C-O	-5.65	114.22	120.38
2	E	199	VAL	CA-C-O	-5.65	116.04	121.63
2	B	250	THR	CA-CB-CG2	5.64	120.10	110.50
1	D	143	GLN	CA-C-N	-5.64	113.10	120.44
1	D	143	GLN	C-N-CA	-5.64	113.10	120.44
2	E	203	ILE	CA-C-O	5.64	127.51	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	ALA	N-CA-CB	-5.64	102.82	111.56
2	B	192	TYR	CA-C-O	-5.63	113.89	120.20
3	C	134	GLN	CA-C-N	5.63	131.56	123.17
3	C	134	GLN	C-N-CA	5.63	131.56	123.17
3	C	141	ASP	CA-C-N	-5.63	111.31	120.72
3	C	141	ASP	C-N-CA	-5.63	111.31	120.72
3	F	333	GLY	N-CA-C	-5.63	99.84	113.18
1	A	127	ILE	CA-C-O	-5.63	113.75	120.78
3	C	380	LYS	CA-C-O	5.63	126.87	120.00
2	E	423	THR	CA-C-O	5.63	127.41	121.33
2	E	321	LYS	CG-CD-CE	5.62	124.23	111.30
3	F	143	VAL	N-CA-CB	5.62	117.78	111.21
3	F	138	PRO	CA-C-O	-5.62	114.39	122.31
2	E	439	ASN	OD1-CG-ND2	-5.61	116.99	122.60
3	F	343	HIS	CA-CB-CG	5.61	119.41	113.80
2	B	457	PHE	O-C-N	-5.61	115.13	122.59
2	E	213	GLU	CG-CD-OE1	5.61	131.30	118.40
2	B	401	GLY	N-CA-C	-5.61	100.38	111.31
3	F	136	GLN	OE1-CD-NE2	-5.61	116.99	122.60
2	B	325	HIS	CA-CB-CG	5.60	119.40	113.80
2	E	246	ASN	CA-CB-CG	-5.60	107.00	112.60
2	B	255	ARG	CD-NE-CZ	5.59	132.23	124.40
1	A	128	GLU	CB-CG-CD	5.59	122.10	112.60
3	C	340	HIS	CA-C-O	-5.59	115.46	121.38
2	E	306	GLY	N-CA-C	-5.58	100.95	112.34
2	B	271	GLN	CA-C-O	-5.58	113.20	119.79
2	B	334	GLU	CA-C-N	5.58	132.20	121.54
2	B	334	GLU	C-N-CA	5.58	132.20	121.54
3	C	188	GLY	CA-C-N	-5.57	113.45	121.42
3	C	188	GLY	C-N-CA	-5.57	113.45	121.42
2	B	264	ARG	CA-CB-CG	-5.57	102.96	114.10
2	B	452	MET	CA-C-N	-5.57	113.85	122.59
2	B	452	MET	C-N-CA	-5.57	113.85	122.59
2	B	370	HIS	CA-CB-CG	-5.57	108.23	113.80
2	B	341	SER	N-CA-CB	-5.56	101.70	110.77
2	B	411	ASN	CA-CB-CG	5.56	118.16	112.60
4	N	3	ARG	O-C-N	5.56	126.42	121.19
3	F	180	VAL	N-CA-CB	5.56	119.77	112.60
4	T	3	ARG	N-CA-CB	5.55	119.03	111.20
2	E	250	THR	O-C-N	5.55	129.51	123.13
3	F	232	LYS	CG-CD-CE	5.55	124.07	111.30
3	C	224	THR	CA-CB-CG2	5.55	119.93	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	319	GLY	O-C-N	-5.54	116.39	122.65
2	E	318	LYS	O-C-N	-5.54	114.56	122.04
2	B	181	LYS	CA-CB-CG	5.53	125.16	114.10
3	F	304	PHE	CA-CB-CG	-5.53	108.27	113.80
3	F	128	VAL	CB-CA-C	-5.52	104.80	112.04
2	B	254	ASN	CA-CB-CG	-5.52	107.08	112.60
2	E	382	ASN	CB-CG-ND2	5.52	124.68	116.40
3	C	301	ASP	CA-CB-CG	-5.51	107.09	112.60
3	F	229	GLY	CA-C-N	5.51	127.93	120.38
3	F	229	GLY	C-N-CA	5.51	127.93	120.38
2	B	171	ILE	CB-CG1-CD1	5.51	125.37	113.80
2	E	432	ASP	N-CA-CB	5.51	118.28	110.46
2	E	304	ARG	CD-NE-CZ	5.51	132.11	124.40
2	B	174	ASN	OD1-CG-ND2	5.50	128.10	122.60
1	A	154	ILE	O-C-N	5.50	127.49	121.83
1	D	155	ASP	O-C-N	-5.49	116.16	122.09
3	C	389	PHE	CA-CB-CG	5.49	119.29	113.80
3	F	208	TRP	CA-C-O	5.49	126.78	120.90
3	C	134	GLN	CA-C-O	5.49	125.69	119.27
3	C	297	ASP	O-C-N	5.49	127.80	122.09
3	F	337	ASN	O-C-N	-5.48	115.30	122.59
3	C	277	THR	CA-C-O	-5.47	113.97	120.43
2	B	341	SER	CB-CA-C	-5.47	101.71	110.14
3	F	207	ASN	O-C-N	-5.47	115.42	122.20
2	B	190	MET	O-C-N	-5.46	116.33	122.12
2	E	226	LEU	CA-C-O	-5.46	114.48	120.43
3	C	311	GLN	CA-C-O	-5.46	115.54	121.87
2	B	406	ARG	O-C-N	-5.45	115.34	122.59
3	C	382	THR	N-CA-CB	-5.45	101.40	111.53
2	B	246	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	D	179	GLU	N-CA-C	-5.43	105.00	111.03
2	B	426	MET	N-CA-CB	5.43	118.51	110.53
1	D	146	ASP	CA-C-N	5.43	128.00	120.29
1	D	146	ASP	C-N-CA	5.43	128.00	120.29
2	B	292	TYR	CA-C-N	5.43	130.42	122.77
2	B	292	TYR	C-N-CA	5.43	130.42	122.77
2	B	444	TRP	CA-CB-CG	-5.43	103.29	113.60
2	E	259	SER	O-C-N	5.42	129.94	122.46
3	C	286	ALA	N-CA-C	-5.42	106.63	113.18
3	F	247	ARG	NE-CZ-NH1	-5.42	116.08	121.50
2	B	440	TRP	O-C-N	-5.41	114.31	122.20
2	B	359	GLN	N-CA-C	-5.40	106.53	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	354	TYR	CA-C-O	-5.40	115.41	121.40
2	B	224	MET	CA-C-N	-5.39	113.76	122.82
2	B	224	MET	C-N-CA	-5.39	113.76	122.82
3	F	321	LYS	CA-C-N	5.38	130.67	122.65
3	F	321	LYS	C-N-CA	5.38	130.67	122.65
2	B	220	GLU	CA-C-N	-5.38	113.49	122.64
2	B	220	GLU	C-N-CA	-5.38	113.49	122.64
3	F	175	ASN	OD1-CG-ND2	5.38	127.98	122.60
3	F	246	LEU	CA-C-O	-5.37	114.83	120.80
3	F	111	GLN	N-CA-C	-5.37	106.68	113.18
2	E	187	SER	N-CA-CB	-5.37	102.22	110.01
2	B	163	THR	CA-C-N	5.37	128.87	120.82
2	B	163	THR	C-N-CA	5.37	128.87	120.82
2	E	190	MET	O-C-N	-5.36	116.55	122.07
2	B	236	TYR	CA-C-N	5.36	130.03	122.09
2	B	236	TYR	C-N-CA	5.36	130.03	122.09
3	C	391	ARG	NE-CZ-NH2	-5.36	114.37	119.20
3	C	108	ARG	CD-NE-CZ	5.36	131.90	124.40
2	E	230	ASP	CA-CB-CG	-5.36	107.24	112.60
2	E	181	LYS	N-CA-CB	-5.36	102.23	110.16
3	C	311	GLN	OE1-CD-NE2	5.35	127.95	122.60
2	B	457	PHE	CA-C-O	-5.35	112.86	120.51
2	E	408	HIS	N-CA-C	5.35	116.97	108.79
2	B	370	HIS	CA-C-O	5.34	125.28	119.24
3	C	197	ARG	CA-CB-CG	5.34	124.79	114.10
3	F	337	ASN	CB-CG-ND2	5.34	124.42	116.40
1	A	127	ILE	N-CA-C	5.34	120.45	109.34
1	A	165	CYS	CA-C-O	-5.34	115.42	121.72
2	B	278	THR	CA-C-O	5.34	127.25	121.06
3	F	267	VAL	CB-CA-C	5.33	118.52	110.63
3	C	150	GLY	CA-C-N	5.33	127.42	120.28
3	C	150	GLY	C-N-CA	5.33	127.42	120.28
1	A	186	GLU	CA-C-O	-5.32	115.22	120.70
3	C	356	LYS	CA-CB-CG	5.32	124.74	114.10
2	E	457	PHE	O-C-N	-5.31	115.52	122.59
2	E	437	TRP	N-CA-CB	5.30	119.75	111.64
3	C	257	THR	OG1-CB-CG2	-5.30	98.70	109.30
2	B	235	PRO	O-C-N	-5.29	116.45	123.01
2	B	213	GLU	CB-CG-CD	5.29	121.59	112.60
3	C	154	GLN	CA-C-N	5.29	127.63	120.38
3	C	154	GLN	C-N-CA	5.29	127.63	120.38
3	C	306	SER	CA-CB-OG	-5.29	100.52	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	225	GLU	CA-CB-CG	-5.28	103.55	114.10
2	E	326	TYR	N-CA-CB	5.28	118.98	110.65
2	B	318	LYS	CA-CB-CG	5.27	124.65	114.10
2	E	333	ASN	CA-CB-CG	-5.27	107.33	112.60
3	C	108	ARG	N-CA-CB	5.27	119.39	110.49
2	E	344	LYS	CA-C-O	5.27	128.62	122.03
3	C	258	SER	CA-C-O	-5.27	115.64	121.33
2	B	411	ASN	CA-C-N	5.26	124.93	119.56
2	B	411	ASN	C-N-CA	5.26	124.93	119.56
2	B	269	TYR	CA-C-O	5.26	126.02	119.97
2	E	309	GLU	CA-C-N	5.26	130.84	122.74
2	E	309	GLU	C-N-CA	5.26	130.84	122.74
3	C	299	PRO	N-CA-C	-5.26	106.87	114.18
3	F	248	VAL	O-C-N	-5.25	117.20	123.03
2	E	396	LYS	N-CA-C	-5.25	105.00	111.40
3	F	134	GLN	N-CA-C	-5.25	106.65	113.16
2	E	239	TYR	CB-CA-C	5.24	118.39	109.80
3	F	212	LYS	CG-CD-CE	-5.24	99.26	111.30
3	F	318	ASP	OD1-CG-OD2	-5.23	110.34	122.90
3	F	329	GLN	CA-C-O	-5.23	113.96	119.97
3	F	280	TYR	CA-C-O	5.23	126.85	121.10
3	F	332	SER	O-C-N	5.23	129.47	122.73
1	A	186	GLU	N-CA-C	-5.22	105.50	111.14
2	E	321	LYS	CA-C-N	-5.22	115.40	122.92
2	E	321	LYS	C-N-CA	-5.22	115.40	122.92
2	B	247	GLY	O-C-N	5.22	128.43	123.05
2	E	237	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	A	149	ARG	NE-CZ-NH1	-5.22	116.28	121.50
3	F	110	LEU	CA-C-N	5.21	131.75	121.58
3	F	110	LEU	C-N-CA	5.21	131.75	121.58
3	F	339	CYS	CA-C-O	-5.21	111.94	120.80
3	F	224	THR	CA-CB-CG2	5.21	119.35	110.50
3	C	176	GLN	CA-CB-CG	5.21	124.51	114.10
3	C	383	THR	CA-C-O	-5.21	114.35	120.60
2	B	440	TRP	CA-C-O	5.20	126.08	119.78
3	F	185	ASP	N-CA-C	-5.20	102.78	110.48
2	B	395	SER	CA-C-N	-5.20	112.91	120.29
2	B	395	SER	C-N-CA	-5.20	112.91	120.29
2	E	448	ARG	N-CA-C	-5.20	105.06	111.40
2	B	334	GLU	CB-CA-C	5.19	119.03	110.88
2	B	194	ARG	N-CA-C	-5.19	106.46	112.89
3	F	133	ALA	N-CA-C	-5.19	106.21	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	239	GLN	OE1-CD-NE2	5.18	127.78	122.60
3	F	317	ASN	CA-CB-CG	5.18	117.78	112.60
3	C	201	SER	O-C-N	-5.17	115.32	122.46
2	E	164	ASN	CB-CG-ND2	5.17	124.16	116.40
3	F	274	TYR	N-CA-CB	-5.17	104.13	111.84
3	F	298	ASP	O-C-N	5.17	125.47	121.85
3	C	264	MET	CA-C-N	5.17	128.90	121.50
3	C	264	MET	C-N-CA	5.17	128.90	121.50
2	E	301	GLN	CA-CB-CG	5.16	124.43	114.10
3	C	341	ALA	N-CA-C	-5.16	108.01	114.56
2	B	228	GLN	CA-C-N	5.16	124.95	119.28
2	B	228	GLN	C-N-CA	5.16	124.95	119.28
3	F	266	LYS	CB-CA-C	5.16	121.01	109.56
2	B	170	SER	N-CA-C	-5.16	104.73	111.02
2	B	351	ASN	OD1-CG-ND2	-5.15	117.45	122.60
2	E	257	ASP	CA-C-O	-5.15	113.14	120.51
3	F	390	ASN	CA-CB-CG	-5.15	107.45	112.60
2	E	448	ARG	CG-CD-NE	5.15	123.32	112.00
2	E	216	ARG	CA-C-O	5.14	125.71	119.38
3	F	274	TYR	CA-C-N	5.14	128.41	121.05
3	F	274	TYR	C-N-CA	5.14	128.41	121.05
2	B	272	GLY	CA-C-N	5.14	130.59	121.80
2	B	272	GLY	C-N-CA	5.14	130.59	121.80
2	E	289	PRO	CA-C-N	-5.14	117.86	122.43
2	E	289	PRO	C-N-CA	-5.14	117.86	122.43
2	B	344	LYS	CA-C-O	5.14	128.45	122.03
2	B	364	ASN	CB-CG-ND2	-5.13	108.70	116.40
3	C	302	LYS	CA-C-O	-5.13	115.11	120.55
1	A	177	ASP	CA-CB-CG	-5.13	107.47	112.60
3	F	246	LEU	CA-C-N	-5.13	114.84	122.74
3	F	246	LEU	C-N-CA	-5.13	114.84	122.74
2	E	237	ARG	N-CA-C	5.13	118.07	110.48
2	B	242	MET	CA-C-O	-5.12	113.57	119.56
2	B	350	GLY	O-C-N	-5.12	118.02	122.88
3	C	295	PHE	CA-CB-CG	5.12	118.92	113.80
3	C	117	ASN	N-CA-C	-5.12	105.88	111.82
1	D	170	ALA	O-C-N	-5.12	117.05	123.04
3	F	213	GLU	CA-C-O	-5.12	113.75	119.79
3	C	373	LYS	CA-C-O	-5.12	115.76	121.23
3	F	126	GLU	CA-C-O	-5.12	113.62	119.60
3	C	379	MET	O-C-N	-5.11	116.77	122.75
1	D	156	ILE	O-C-N	-5.11	116.90	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	ASP	CA-C-O	5.10	127.81	120.51
2	E	337	LYS	N-CA-CB	-5.10	104.24	111.84
3	C	104	ASP	CA-CB-CG	5.10	117.70	112.60
2	E	373	MET	N-CA-C	5.10	117.10	110.53
1	A	130	VAL	CA-C-O	5.09	127.15	120.78
2	B	195	THR	OG1-CB-CG2	-5.09	99.11	109.30
2	B	334	GLU	CA-CB-CG	-5.09	103.92	114.10
3	C	229	GLY	N-CA-C	5.09	121.05	112.85
3	C	300	SER	O-C-N	-5.08	116.24	122.34
2	B	342	VAL	CA-C-O	-5.08	115.39	121.28
3	F	327	ALA	CA-C-N	-5.08	113.53	120.44
3	F	327	ALA	C-N-CA	-5.08	113.53	120.44
2	E	308	THR	CA-C-O	-5.08	114.68	120.32
3	F	267	VAL	O-C-N	-5.08	117.78	123.26
3	C	126	GLU	CB-CG-CD	5.08	121.23	112.60
3	C	332	SER	N-CA-CB	-5.08	103.22	111.24
2	B	329	PHE	CA-CB-CG	5.07	118.87	113.80
2	B	245	GLU	CA-C-N	-5.07	116.28	125.66
2	B	245	GLU	C-N-CA	-5.07	116.28	125.66
2	B	448	ARG	N-CA-C	-5.07	105.46	111.69
3	F	241	ALA	CA-C-N	-5.07	112.75	122.13
3	F	241	ALA	C-N-CA	-5.07	112.75	122.13
1	A	169	LEU	N-CA-CB	-5.06	102.31	109.85
2	E	365	ARG	CA-C-O	5.06	125.86	120.24
2	B	448	ARG	NE-CZ-NH1	5.06	126.56	121.50
3	C	196	LYS	CG-CD-CE	5.05	122.91	111.30
2	B	393	GLN	CB-CG-CD	5.04	121.18	112.60
3	C	345	ASN	N-CA-C	-5.04	106.44	112.59
2	E	341	SER	CA-C-N	-5.04	114.71	122.68
2	E	341	SER	C-N-CA	-5.04	114.71	122.68
1	D	151	GLU	CA-CB-CG	-5.04	104.02	114.10
3	C	310	MET	CA-C-O	-5.04	115.13	120.92
3	F	145	ILE	CA-C-O	-5.03	115.14	120.48
2	E	344	LYS	CA-C-N	5.03	128.62	121.42
2	E	344	LYS	C-N-CA	5.03	128.62	121.42
3	C	303	PHE	CA-CB-CG	5.03	118.83	113.80
2	E	418	TRP	CA-CB-CG	-5.03	104.04	113.60
3	F	347	VAL	CA-CB-CG2	-5.03	101.85	110.40
1	D	151	GLU	O-C-N	5.03	127.25	122.07
3	C	300	SER	CA-C-N	5.02	131.13	121.54
3	C	300	SER	C-N-CA	5.02	131.13	121.54
2	B	196	PRO	CA-C-O	-5.02	115.89	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	441	LYS	CA-C-O	-5.02	113.96	119.78
1	D	139	ASN	CA-C-O	-5.01	115.55	121.07
3	F	180	VAL	CB-CA-C	-5.01	104.32	111.19
3	F	228	LEU	N-CA-C	-5.01	103.87	110.43
2	B	452	MET	CG-SD-CE	5.01	111.92	100.90
2	B	283	LYS	CA-C-N	-5.01	115.20	122.86
2	B	283	LYS	C-N-CA	-5.01	115.20	122.86
3	F	239	GLN	CB-CG-CD	-5.01	104.09	112.60
2	E	246	ASN	OD1-CG-ND2	-5.00	117.60	122.60
2	B	224	MET	CG-SD-CE	-5.00	89.90	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	427	ALA	Mainchain

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	546	0	573	112	0
1	D	440	0	456	114	0
2	B	2427	0	2295	170	0
2	E	2376	0	2243	226	0
3	C	2342	0	2188	155	6
3	F	2287	0	2136	234	5
4	M	31	0	32	5	0
4	N	31	0	32	9	0
4	S	31	0	32	7	0
4	T	31	0	32	5	0
5	G	28	0	25	10	0
5	H	28	0	25	11	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	B	31	0	0	10	0
7	C	20	0	0	2	0
7	D	3	0	0	2	0
7	E	29	0	0	8	0
7	F	23	0	0	2	1
All	All	10713	0	10069	891	6

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 43.

All (891) 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)
2:E:172:LEU:HD11	3:F:114:TYR:CD2	1.31	1.59
3:C:104:ASP:HA	3:C:107:ILE:CD1	1.33	1.53
2:E:171:ILE:CG2	2:E:172:LEU:CD2	1.86	1.50
2:E:171:ILE:CG2	2:E:172:LEU:HD23	1.08	1.49
1:A:179:GLU:C	1:A:183:LYS:HE3	1.36	1.48
3:F:109:TYR:N	3:F:112:GLU:CB	1.78	1.46
2:E:378:TYR:CG	2:E:396:LYS:HE2	1.54	1.42
2:E:176:ARG:HB2	3:F:117:ASN:OD1	1.20	1.33
2:B:361:MET:HB2	5:G:1:NAG:C8	1.56	1.33
2:E:172:LEU:CD1	3:F:114:TYR:CD2	2.11	1.31
3:C:265:PHE:O	3:C:266:LYS:HD2	1.16	1.31
5:G:1:NAG:O3	5:G:2:NAG:N2	1.64	1.27
1:A:180:ASP:HA	1:A:183:LYS:CD	1.62	1.27
1:D:138:LYS:O	1:D:141:ARG:HB3	1.27	1.27
1:D:140:VAL:HG12	3:F:114:TYR:CE2	1.70	1.26
1:A:188:VAL:HG22	2:B:165:LEU:CD2	1.66	1.24
1:D:138:LYS:O	1:D:141:ARG:CB	1.85	1.24
3:C:298:ASP:OD1	3:C:300:SER:N	1.70	1.23
2:E:171:ILE:CG2	2:E:172:LEU:H	1.44	1.23
2:B:230:ASP:O	2:B:233:VAL:HG23	1.34	1.21
3:F:109:TYR:N	3:F:112:GLU:CG	2.03	1.21
3:F:149:THR:HG22	3:F:168:PHE:O	1.42	1.20
3:F:217:HIS:O	3:F:224:THR:HG23	1.38	1.20
3:C:103:HIS:O	3:C:106:SER:OG	1.60	1.17
3:C:265:PHE:O	3:C:266:LYS:CD	1.92	1.17
1:D:178:TYR:O	1:D:182:GLN:HG2	1.43	1.17
1:D:179:GLU:HB3	1:D:183:LYS:NZ	1.59	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:O	1:A:131:GLN:NE2	1.78	1.16
5:H:1:NAG:C6	5:H:2:NAG:C1	2.22	1.16
5:H:1:NAG:H62	5:H:2:NAG:O5	1.44	1.16
1:D:188:VAL:HG22	2:E:165:LEU:HD11	1.23	1.15
2:B:165:LEU:HB3	7:B:498:HOH:O	1.42	1.15
2:E:230:ASP:O	2:E:233:VAL:HG23	1.47	1.14
1:A:180:ASP:N	1:A:183:LYS:HE3	1.63	1.14
1:A:180:ASP:CA	1:A:183:LYS:HD2	1.77	1.14
3:F:185:ASP:OD2	3:F:187:SER:HB2	1.43	1.14
2:E:179:ILE:HD12	3:F:117:ASN:HB2	1.30	1.14
1:D:188:VAL:CG2	2:E:165:LEU:HD11	1.77	1.13
2:B:361:MET:CB	5:G:1:NAG:H82	1.77	1.13
5:H:1:NAG:H62	5:H:2:NAG:C1	1.77	1.12
1:A:133:ILE:O	1:A:135:LEU:N	1.82	1.12
1:A:179:GLU:C	1:A:183:LYS:CE	2.20	1.12
2:E:176:ARG:CB	3:F:117:ASN:OD1	1.98	1.12
2:E:381:ASP:HB2	2:E:393:GLN:HE22	1.13	1.12
1:A:134:GLN:O	1:A:135:LEU:HD22	1.49	1.11
3:C:104:ASP:HA	3:C:107:ILE:HD13	1.12	1.10
2:E:168:LEU:HB3	7:E:44:HOH:O	1.50	1.10
3:C:104:ASP:CA	3:C:107:ILE:CD1	2.28	1.10
2:E:169:ARG:NH1	2:E:173:GLU:OE2	1.82	1.10
1:D:140:VAL:CG1	3:F:114:TYR:HE2	1.63	1.09
1:D:179:GLU:C	1:D:183:LYS:HE3	1.77	1.09
2:E:179:ILE:HD12	3:F:117:ASN:CB	1.81	1.09
3:F:109:TYR:N	3:F:112:GLU:HB2	1.63	1.08
2:B:165:LEU:CB	7:B:498:HOH:O	1.99	1.08
1:D:166:SER:HB3	2:E:195:THR:HG23	1.32	1.06
2:E:179:ILE:CD1	3:F:117:ASN:O	2.03	1.06
2:E:381:ASP:HB2	2:E:393:GLN:NE2	1.69	1.05
3:F:109:TYR:N	3:F:112:GLU:HB3	1.68	1.05
1:A:180:ASP:HA	1:A:183:LYS:HD2	1.36	1.05
3:C:109:TYR:O	3:C:113:ILE:HD13	1.55	1.05
3:C:104:ASP:CA	3:C:107:ILE:HD13	1.87	1.04
2:E:171:ILE:HG23	2:E:172:LEU:CD2	1.82	1.04
1:A:134:GLN:O	1:A:135:LEU:CD2	2.05	1.04
2:E:171:ILE:HG21	2:E:172:LEU:HD23	1.08	1.04
2:E:378:TYR:CD1	2:E:396:LYS:HE2	1.93	1.04
3:C:173:LYS:HE2	3:C:238:THR:O	1.57	1.04
2:E:176:ARG:HA	3:F:117:ASN:HB3	1.04	1.04
2:E:385:TRP:HD1	2:E:406:ARG:NH1	1.55	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:O	2:B:171:ILE:N	1.91	1.04
1:D:179:GLU:C	1:D:183:LYS:CE	2.31	1.04
2:E:176:ARG:HA	3:F:117:ASN:CB	1.87	1.03
3:F:149:THR:CG2	3:F:168:PHE:O	2.06	1.03
3:C:104:ASP:HA	3:C:107:ILE:HD12	1.36	1.03
2:B:230:ASP:O	2:B:233:VAL:CG2	2.06	1.03
2:E:385:TRP:CD1	2:E:406:ARG:NH1	2.27	1.03
1:D:147:MET:SD	3:F:121:ILE:HD11	1.99	1.02
2:E:378:TYR:CD1	2:E:396:LYS:CE	2.43	1.02
1:D:179:GLU:HB3	1:D:183:LYS:CE	1.88	1.02
1:A:188:VAL:HG22	2:B:165:LEU:HD21	1.02	1.02
2:E:381:ASP:CB	2:E:393:GLN:HE22	1.71	1.02
3:F:217:HIS:O	3:F:224:THR:CG2	2.06	1.02
3:C:105:SER:O	3:C:108:ARG:HG3	1.57	1.01
1:A:188:VAL:CG2	2:B:165:LEU:HD21	1.90	1.01
2:E:378:TYR:CG	2:E:396:LYS:CE	2.43	1.01
2:E:171:ILE:CG2	2:E:172:LEU:N	2.16	1.01
2:E:171:ILE:HG22	2:E:172:LEU:H	0.88	1.00
2:E:172:LEU:HD11	3:F:114:TYR:CE2	1.97	1.00
2:B:160:ASN:C	2:B:162:PRO:HD2	1.86	1.00
2:B:323:LYS:HE2	7:B:488:HOH:O	1.59	0.99
2:E:209:LYS:HG3	2:E:213:GLU:OE1	1.60	0.99
1:A:180:ASP:CA	1:A:183:LYS:CD	2.35	0.99
1:A:133:ILE:C	1:A:135:LEU:H	1.71	0.99
1:A:148:LYS:HE3	1:A:182:GLN:HE22	1.23	0.98
2:E:171:ILE:HG22	2:E:172:LEU:N	1.74	0.98
2:E:176:ARG:CA	3:F:117:ASN:HB3	1.93	0.98
3:F:111:GLN:HE21	3:F:112:GLU:HG2	1.29	0.98
3:F:160:GLY:O	3:F:162:LYS:HE2	1.63	0.97
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.47	0.97
3:C:265:PHE:C	3:C:266:LYS:HD3	1.88	0.97
2:B:169:ARG:O	2:B:173:GLU:HG2	1.64	0.97
2:B:361:MET:HB2	5:G:1:NAG:H82	0.99	0.97
2:E:385:TRP:CH2	4:N:3:ARG:HD2	2.00	0.97
1:A:143:GLN:CD	3:C:117:ASN:HD21	1.72	0.97
3:C:265:PHE:C	3:C:266:LYS:CD	2.38	0.96
1:D:188:VAL:CG1	2:E:165:LEU:HD21	1.96	0.96
1:D:140:VAL:HG12	3:F:114:TYR:HE2	0.80	0.95
1:A:179:GLU:O	1:A:183:LYS:CD	2.13	0.95
3:F:109:TYR:CA	3:F:112:GLU:HG3	1.95	0.95
3:F:298:ASP:OD1	3:F:300:SER:OG	1.85	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:ILE:HG22	2:E:172:LEU:HD23	0.97	0.95
2:B:381:ASP:OD2	7:B:477:HOH:O	1.84	0.95
3:F:117:ASN:HD22	3:F:118:ASN:N	1.65	0.95
2:B:169:ARG:NH1	2:B:173:GLU:CD	2.24	0.94
2:E:171:ILE:HG23	2:E:172:LEU:HD22	1.47	0.93
1:D:179:GLU:CB	1:D:183:LYS:NZ	2.31	0.93
3:C:105:SER:C	3:C:108:ARG:HG3	1.93	0.93
2:E:179:ILE:HD13	3:F:117:ASN:O	1.67	0.93
2:E:190:MET:SD	3:F:134:GLN:NE2	2.42	0.92
1:D:188:VAL:CG2	2:E:165:LEU:HD21	1.98	0.92
5:H:1:NAG:H62	5:H:2:NAG:C5	2.00	0.92
3:F:109:TYR:N	3:F:112:GLU:HG3	1.84	0.92
1:A:143:GLN:CD	3:C:117:ASN:ND2	2.28	0.91
2:E:169:ARG:NH1	2:E:173:GLU:CD	2.27	0.91
2:E:179:ILE:HD12	3:F:117:ASN:CA	2.01	0.91
2:E:171:ILE:HG22	2:E:172:LEU:CD2	1.74	0.91
3:C:217:HIS:O	3:C:224:THR:HG23	1.71	0.91
1:D:135:LEU:O	1:D:138:LYS:N	2.03	0.91
2:E:423:THR:OG1	2:E:425:ASP:OD1	1.87	0.90
1:A:143:GLN:OE1	3:C:117:ASN:ND2	2.02	0.90
3:F:325:ASN:ND2	3:F:328:GLU:H	1.69	0.90
1:A:180:ASP:N	1:A:183:LYS:CE	2.31	0.90
1:D:166:SER:HB3	2:E:195:THR:CG2	2.00	0.90
2:E:252:ILE:HD12	2:E:299:ILE:HG12	1.53	0.90
1:A:180:ASP:OD1	1:A:183:LYS:NZ	2.05	0.90
3:C:307:HIS:HD2	3:C:335:TRP:O	1.53	0.90
3:F:109:TYR:CB	3:F:112:GLU:HG3	2.02	0.90
1:A:179:GLU:O	1:A:183:LYS:HD2	1.72	0.89
2:B:265:LYS:HE3	2:B:378:TYR:OH	1.70	0.89
1:D:188:VAL:HG22	2:E:165:LEU:CD1	2.02	0.89
1:D:177:ASP:OD2	2:E:178:LYS:NZ	2.06	0.89
2:E:315:GLU:OE2	2:E:448:ARG:NH1	2.06	0.89
1:A:188:VAL:CG2	2:B:165:LEU:CD2	2.47	0.89
2:E:172:LEU:CD1	3:F:114:TYR:HD2	1.65	0.88
2:E:172:LEU:HD11	3:F:114:TYR:HD2	1.07	0.88
5:H:1:NAG:O6	5:H:2:NAG:H5	1.73	0.88
2:E:385:TRP:HD1	2:E:406:ARG:HH11	1.15	0.88
1:D:175:LEU:O	1:D:178:TYR:N	2.06	0.88
1:D:179:GLU:O	1:D:183:LYS:HD2	1.71	0.88
2:E:169:ARG:HH12	2:E:173:GLU:CD	1.81	0.88
1:A:148:LYS:HE3	1:A:182:GLN:NE2	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:GLU:OE1	3:F:120:LYS:HD3	1.74	0.88
1:D:179:GLU:CB	1:D:183:LYS:HZ2	1.88	0.87
2:B:169:ARG:HH12	2:B:173:GLU:CD	1.81	0.87
1:D:180:ASP:N	1:D:183:LYS:HZ2	1.72	0.86
1:A:180:ASP:HA	1:A:183:LYS:HD3	1.57	0.86
3:F:185:ASP:OD2	3:F:187:SER:CB	2.23	0.86
2:E:396:LYS:O	2:E:398:ASP:N	2.07	0.86
1:A:143:GLN:NE2	3:C:117:ASN:ND2	2.23	0.86
2:E:230:ASP:O	2:E:233:VAL:CG2	2.23	0.86
1:A:134:GLN:C	1:A:135:LEU:HD23	2.01	0.85
2:E:168:LEU:O	2:E:170:SER:N	2.09	0.85
1:D:147:MET:SD	3:F:121:ILE:CD1	2.64	0.85
2:B:161:ILE:O	2:B:164:ASN:HB3	1.76	0.85
2:E:168:LEU:O	2:E:169:ARG:C	2.20	0.85
2:B:181:LYS:HE2	2:B:185:ASP:OD2	1.76	0.85
3:F:116:SER:O	3:F:119:GLN:N	2.09	0.85
2:B:333:ASN:HD22	2:B:333:ASN:H	1.22	0.85
2:E:179:ILE:CD1	3:F:117:ASN:HB2	2.07	0.84
2:B:333:ASN:H	2:B:333:ASN:ND2	1.70	0.84
3:C:240:SER:OG	3:C:242:ILE:CD1	2.25	0.84
3:F:189:ASN:OD1	3:F:391:ARG:HG3	1.77	0.84
1:A:180:ASP:C	1:A:183:LYS:HD2	2.02	0.84
1:A:181:GLN:HE22	2:B:174:ASN:ND2	1.76	0.84
1:A:186:GLU:O	1:A:189:ILE:N	2.08	0.84
2:B:415:ARG:NE	7:B:495:HOH:O	2.02	0.83
3:F:240:SER:OG	3:F:242:ILE:HG13	1.78	0.83
1:A:169:LEU:HD23	1:A:171:ARG:HD2	1.59	0.83
1:D:179:GLU:CA	1:D:183:LYS:HE3	2.09	0.83
2:E:378:TYR:CB	2:E:396:LYS:HE2	2.09	0.82
3:C:209:ILE:H	3:C:209:ILE:HD12	1.44	0.82
3:C:329:GLN:HE22	4:S:3:ARG:HD2	1.42	0.82
2:E:212:GLU:OE2	2:E:216:ARG:HD3	1.80	0.81
1:A:180:ASP:HA	1:A:183:LYS:CE	2.10	0.81
2:E:397:GLU:O	2:E:398:ASP:CG	2.24	0.81
3:C:217:HIS:O	3:C:224:THR:CG2	2.28	0.81
3:F:160:GLY:C	3:F:162:LYS:HE2	2.05	0.81
2:B:161:ILE:O	2:B:164:ASN:CB	2.28	0.80
2:E:381:ASP:CB	2:E:393:GLN:NE2	2.35	0.80
2:E:378:TYR:CD1	2:E:396:LYS:HE3	2.15	0.79
1:A:134:GLN:HG3	1:A:135:LEU:HD23	1.62	0.79
2:E:168:LEU:O	2:E:171:ILE:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ARG:HD3	3:F:113:ILE:HG23	1.62	0.79
1:A:140:VAL:HG11	2:B:172:LEU:HD21	1.65	0.79
3:C:296:GLY:O	7:C:408:HOH:O	1.99	0.79
3:C:104:ASP:HA	3:C:107:ILE:HD11	1.60	0.79
3:F:109:TYR:HB2	3:F:112:GLU:HG3	1.64	0.79
2:B:159:SER:HB2	2:B:162:PRO:HG3	1.65	0.79
2:B:179:ILE:O	2:B:183:GLU:HG2	1.83	0.78
3:F:122:VAL:O	3:F:126:GLU:HG2	1.81	0.78
2:E:385:TRP:CZ2	4:N:3:ARG:HD2	2.18	0.78
2:B:385:TRP:CZ3	4:M:3:ARG:NH1	2.51	0.78
1:A:131:GLN:HA	1:A:134:GLN:HG3	1.62	0.78
3:C:206:LYS:HD2	3:C:210:GLN:OE1	1.82	0.78
1:A:180:ASP:CA	1:A:183:LYS:CE	2.62	0.78
2:B:166:ARG:NH2	3:C:106:SER:CB	2.46	0.78
1:A:131:GLN:HA	1:A:134:GLN:CG	2.14	0.78
1:D:188:VAL:HG21	2:E:165:LEU:HD21	1.67	0.77
1:A:178:TYR:O	1:A:182:GLN:HG2	1.84	0.77
2:E:458:PHE:HB3	2:E:459:PRO:HD3	1.67	0.77
2:E:172:LEU:HD12	3:F:114:TYR:HA	1.64	0.77
3:F:161:ALA:O	3:F:162:LYS:HE2	1.85	0.77
1:D:140:VAL:N	3:F:114:TYR:OH	2.18	0.77
2:E:422:TYR:HA	2:E:426:MET:HE3	1.67	0.77
5:H:1:NAG:C6	5:H:2:NAG:C5	2.62	0.77
2:B:406:ARG:O	4:M:2:HIS:HA	1.84	0.77
1:A:134:GLN:C	1:A:135:LEU:CD2	2.57	0.77
3:F:148:ILE:HG22	3:F:156:ILE:HG12	1.67	0.77
2:B:415:ARG:NH2	7:B:495:HOH:O	2.17	0.76
3:F:209:ILE:HD12	3:F:209:ILE:H	1.50	0.76
2:E:179:ILE:CD1	3:F:117:ASN:C	2.58	0.76
3:C:329:GLN:NE2	4:S:3:ARG:HH11	1.83	0.76
3:F:117:ASN:ND2	3:F:118:ASN:N	2.34	0.76
1:A:127:ILE:HD12	1:A:130:VAL:HG23	1.66	0.76
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.85	0.76
3:F:307:HIS:HD2	3:F:335:TRP:O	1.69	0.76
1:D:188:VAL:HG11	2:E:165:LEU:HD21	1.67	0.75
5:H:1:NAG:O6	5:H:2:NAG:C1	2.33	0.75
1:D:139:ASN:C	1:D:141:ARG:N	2.44	0.75
2:E:422:TYR:HA	2:E:426:MET:CE	2.17	0.74
1:D:140:VAL:CG1	2:E:172:LEU:HD21	2.17	0.74
1:D:179:GLU:HB3	1:D:183:LYS:HZ1	1.49	0.74
2:E:171:ILE:HG21	2:E:172:LEU:CD2	1.81	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:GLU:HB3	1:D:183:LYS:HE3	1.68	0.74
3:F:178:PHE:CE1	3:F:232:LYS:HG2	2.22	0.74
2:B:161:ILE:N	2:B:162:PRO:HD2	2.00	0.74
3:F:110:LEU:HB2	3:F:111:GLN:NE2	2.01	0.74
2:B:439:ASN:H	2:B:439:ASN:HD22	1.33	0.73
1:A:179:GLU:C	1:A:183:LYS:CD	2.60	0.73
3:F:263:ALA:C	3:F:264:MET:HE2	2.11	0.73
2:B:428:LYS:HG2	2:B:429:HIS:CD2	2.22	0.73
2:E:171:ILE:O	2:E:174:ASN:N	2.22	0.73
1:D:177:ASP:O	1:D:181:GLN:HB2	1.89	0.73
3:F:304:PHE:O	3:F:337:ASN:O	2.05	0.73
1:A:179:GLU:HB2	1:A:183:LYS:HE3	1.69	0.72
3:C:149:THR:HG23	3:C:168:PHE:O	1.88	0.72
1:D:186:GLU:O	1:D:187:GLN:C	2.31	0.72
3:C:294:ASP:OD1	7:C:408:HOH:O	2.06	0.72
2:E:397:GLU:O	2:E:398:ASP:OD1	2.06	0.72
1:D:180:ASP:N	1:D:183:LYS:NZ	2.36	0.72
1:A:181:GLN:NE2	2:B:174:ASN:ND2	2.37	0.72
2:B:166:ARG:C	2:B:168:LEU:H	1.98	0.72
3:C:240:SER:OG	3:C:242:ILE:HG13	1.89	0.72
1:A:151:GLU:HG2	1:A:173:VAL:HG13	1.71	0.72
1:D:188:VAL:CG2	2:E:165:LEU:CD1	2.62	0.71
3:C:104:ASP:CB	3:C:107:ILE:HD13	2.20	0.71
2:E:172:LEU:HD12	3:F:114:TYR:CD2	2.22	0.71
5:G:1:NAG:O3	5:G:2:NAG:C7	2.39	0.71
3:C:307:HIS:HE1	3:C:341:ALA:H	1.39	0.71
1:A:143:GLN:HE22	3:C:117:ASN:ND2	1.86	0.71
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.91	0.71
1:D:151:GLU:HG3	2:E:182:LEU:HD21	1.71	0.71
1:A:179:GLU:O	1:A:183:LYS:CE	2.38	0.71
1:D:139:ASN:O	1:D:140:VAL:C	2.33	0.70
3:F:244:TYR:H	3:F:266:LYS:HE2	1.57	0.70
2:E:265:LYS:HE3	2:E:378:TYR:OH	1.91	0.70
3:F:310:MET:SD	3:F:337:ASN:HB2	2.31	0.70
2:B:171:ILE:O	2:B:174:ASN:HB2	1.90	0.70
2:B:428:LYS:HG2	2:B:429:HIS:NE2	2.07	0.70
3:C:195:GLN:OE1	3:C:382:THR:CG2	2.40	0.70
1:A:134:GLN:O	1:A:135:LEU:HD23	1.90	0.70
3:F:337:ASN:O	3:F:338:LYS:C	2.31	0.70
2:E:390:PRO:O	2:E:393:GLN:HG3	1.92	0.70
3:C:307:HIS:CD2	3:C:335:TRP:O	2.42	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:VAL:HG11	2:E:172:LEU:HD21	1.72	0.69
1:D:175:LEU:CD2	1:D:175:LEU:H	2.05	0.69
3:C:195:GLN:OE1	3:C:382:THR:HG22	1.92	0.69
5:H:1:NAG:C6	5:H:2:NAG:H5	2.23	0.69
1:A:179:GLU:CA	1:A:183:LYS:HE3	2.21	0.69
1:D:138:LYS:O	1:D:141:ARG:HB2	1.90	0.69
3:F:111:GLN:CD	3:F:111:GLN:H	2.01	0.69
3:C:107:ILE:HD12	3:C:107:ILE:H	1.58	0.69
1:A:166:SER:OG	2:B:195:THR:HG23	1.92	0.68
3:F:244:TYR:H	3:F:266:LYS:CE	2.06	0.68
3:F:392:LEU:C	3:F:393:THR:OG1	2.33	0.68
1:A:131:GLN:O	1:A:135:LEU:HG	1.94	0.68
1:A:179:GLU:HB2	1:A:183:LYS:CE	2.24	0.68
1:D:135:LEU:O	1:D:138:LYS:CB	2.42	0.68
2:B:393:GLN:O	2:B:397:GLU:HG3	1.94	0.68
2:B:361:MET:HB2	5:G:1:NAG:H81	1.70	0.68
3:F:111:GLN:NE2	3:F:112:GLU:HG2	2.05	0.68
3:F:117:ASN:ND2	3:F:118:ASN:H	1.92	0.67
1:D:179:GLU:O	1:D:183:LYS:CD	2.43	0.67
2:E:381:ASP:OD2	2:E:393:GLN:NE2	2.27	0.67
3:F:114:TYR:HD1	3:F:115:ASN:OD1	1.75	0.67
1:A:130:VAL:O	1:A:134:GLN:N	2.25	0.67
3:F:307:HIS:HE1	3:F:341:ALA:H	1.41	0.67
3:F:291:ASP:OD2	3:F:302:LYS:NZ	2.27	0.67
3:F:195:GLN:OE1	3:F:382:THR:HG22	1.94	0.67
1:D:179:GLU:C	1:D:183:LYS:HD2	2.18	0.67
3:F:151:LYS:HE2	3:F:172:LEU:HD21	1.76	0.67
3:F:161:ALA:O	3:F:162:LYS:CE	2.42	0.67
2:B:432:ASP:OD2	2:B:443:SER:HB3	1.95	0.67
3:C:240:SER:HG	3:C:242:ILE:HD12	1.60	0.67
2:E:169:ARG:N	7:E:44:HOH:O	2.28	0.67
3:C:149:THR:HG22	3:C:150:GLY:H	1.59	0.67
1:D:179:GLU:CB	1:D:183:LYS:HE3	2.26	0.66
2:E:171:ILE:HG23	2:E:172:LEU:N	2.07	0.66
3:F:240:SER:OG	3:F:242:ILE:CG1	2.42	0.66
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.31	0.66
2:B:458:PHE:H	2:B:459:PRO:HD2	1.59	0.66
2:E:176:ARG:NH1	3:F:113:ILE:HG12	2.10	0.66
1:D:139:ASN:O	1:D:141:ARG:N	2.28	0.66
3:F:224:THR:HG22	7:F:411:HOH:O	1.95	0.66
1:A:188:VAL:HG22	2:B:165:LEU:CG	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:LYS:HD3	3:F:132:GLU:HG3	1.77	0.66
2:B:406:ARG:N	2:B:407:CYS:HA	2.11	0.65
3:F:240:SER:HG	3:F:242:ILE:HG13	1.61	0.65
2:B:362:GLY:O	2:B:366:THR:HG23	1.96	0.65
2:E:385:TRP:CD1	2:E:406:ARG:HH11	2.00	0.65
3:C:104:ASP:CA	3:C:107:ILE:HD12	2.14	0.65
3:C:240:SER:OG	3:C:242:ILE:CG1	2.45	0.65
1:D:179:GLU:C	1:D:183:LYS:CD	2.68	0.65
1:D:175:LEU:O	1:D:178:TYR:HB2	1.97	0.65
2:E:168:LEU:O	2:E:171:ILE:HB	1.96	0.65
2:E:169:ARG:O	2:E:170:SER:C	2.40	0.65
1:A:130:VAL:HG23	1:A:131:GLN:OE1	1.97	0.65
3:C:130:GLN:O	3:C:134:GLN:HG3	1.97	0.65
3:C:195:GLN:HE22	3:C:382:THR:HG21	1.62	0.65
3:C:304:PHE:O	3:C:337:ASN:O	2.14	0.65
3:F:340:HIS:CE1	4:T:1:GLY:N	2.65	0.65
1:D:166:SER:CB	2:E:195:THR:CG2	2.75	0.64
2:B:415:ARG:CZ	7:B:495:HOH:O	2.38	0.64
3:C:323:GLU:H	3:C:323:GLU:CD	2.03	0.64
1:D:138:LYS:O	1:D:141:ARG:CA	2.46	0.64
2:E:411:ASN:OD1	7:E:11:HOH:O	2.15	0.64
3:F:273:LYS:HZ2	3:F:317:ASN:HD21	1.45	0.64
2:B:332:GLN:O	2:B:338:TYR:HA	1.96	0.64
1:D:183:LYS:O	1:D:186:GLU:HB2	1.97	0.64
7:E:40:HOH:O	5:H:1:NAG:H61	1.98	0.64
3:F:196:LYS:HD2	3:F:198:LEU:CD2	2.27	0.64
2:B:432:ASP:CB	2:B:443:SER:HB2	2.28	0.64
2:B:439:ASN:H	2:B:439:ASN:ND2	1.95	0.64
2:E:176:ARG:HH11	3:F:113:ILE:HG23	1.63	0.64
3:F:241:ALA:O	3:F:243:PRO:CD	2.45	0.64
3:F:172:LEU:H	3:F:239:GLN:NE2	1.96	0.63
2:E:176:ARG:HG3	3:F:117:ASN:H	1.62	0.63
3:F:161:ALA:O	3:F:162:LYS:NZ	2.32	0.63
1:A:179:GLU:CB	1:A:183:LYS:HE3	2.27	0.63
2:E:171:ILE:O	2:E:174:ASN:HB2	1.97	0.63
2:E:176:ARG:NH1	3:F:113:ILE:CG2	2.61	0.63
3:F:263:ALA:HB1	3:F:264:MET:HE1	1.80	0.63
1:A:179:GLU:C	1:A:183:LYS:HD2	2.23	0.63
2:B:161:ILE:CG1	2:B:164:ASN:OD1	2.46	0.63
2:B:168:LEU:O	2:B:170:SER:N	2.31	0.63
2:E:179:ILE:HD11	3:F:117:ASN:O	1.94	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:203:ILE:CD1	3:F:145:ILE:HD11	2.29	0.63
2:E:179:ILE:HG21	3:F:120:LYS:HB3	1.80	0.63
2:B:161:ILE:N	2:B:162:PRO:CD	2.62	0.63
2:B:217:LYS:HD3	3:C:213:GLU:CD	2.24	0.63
3:C:173:LYS:HB3	3:C:235:LEU:HD22	1.79	0.63
2:E:230:ASP:HB3	2:E:233:VAL:HG22	1.81	0.63
1:A:180:ASP:O	1:A:183:LYS:HD2	1.99	0.62
3:C:184:ILE:HA	3:C:189:ASN:O	1.98	0.62
3:C:103:HIS:CE1	3:C:106:SER:HB3	2.34	0.62
3:F:241:ALA:O	3:F:243:PRO:HD3	1.99	0.62
1:D:138:LYS:O	1:D:141:ARG:N	2.33	0.62
1:D:179:GLU:CB	1:D:183:LYS:CE	2.70	0.62
3:C:148:ILE:HD12	3:C:161:ALA:HB2	1.82	0.62
2:E:422:TYR:CA	2:E:426:MET:HE3	2.29	0.62
3:F:249:GLU:OE1	3:F:385:LYS:NZ	2.33	0.62
2:B:397:GLU:OE1	4:M:3:ARG:NH1	2.33	0.62
3:F:110:LEU:HB2	3:F:111:GLN:HE22	1.63	0.62
3:F:209:ILE:H	3:F:209:ILE:CD1	2.11	0.62
1:D:166:SER:CB	2:E:195:THR:HG23	2.19	0.61
1:A:127:ILE:HB	1:A:130:VAL:CG2	2.30	0.61
1:A:130:VAL:C	1:A:134:GLN:HG2	2.25	0.61
2:B:265:LYS:O	2:B:268:PRO:HD2	2.00	0.61
3:F:195:GLN:OE1	3:F:382:THR:CG2	2.48	0.61
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.82	0.61
3:C:209:ILE:H	3:C:209:ILE:CD1	2.12	0.61
1:D:143:GLN:O	1:D:147:MET:HB2	1.99	0.61
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.65	0.61
1:A:143:GLN:NE2	3:C:117:ASN:HD21	1.90	0.61
2:E:378:TYR:CD2	2:E:396:LYS:HE2	2.28	0.61
1:A:179:GLU:O	1:A:183:LYS:CG	2.48	0.61
2:B:158:ASN:O	2:B:160:ASN:ND2	2.33	0.61
3:C:322:PHE:CZ	4:S:3:ARG:HG2	2.36	0.61
2:E:176:ARG:CA	3:F:117:ASN:CB	2.67	0.61
3:F:244:TYR:HB2	3:F:266:LYS:HE2	1.82	0.61
3:F:263:ALA:HB1	3:F:264:MET:CE	2.31	0.61
1:A:127:ILE:O	1:A:129:LYS:N	2.34	0.60
3:C:221:THR:O	3:C:223:THR:HG23	2.01	0.60
1:D:178:TYR:O	1:D:182:GLN:CG	2.35	0.60
3:F:329:GLN:NE2	4:T:3:ARG:HH21	1.99	0.60
3:C:298:ASP:OD1	3:C:300:SER:CA	2.48	0.60
1:D:180:ASP:HA	1:D:183:LYS:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:O	1:A:183:LYS:HG3	2.02	0.60
2:E:179:ILE:CD1	3:F:121:ILE:HG13	2.31	0.60
2:E:236:TYR:CG	2:E:298:LYS:HE2	2.36	0.60
3:F:323:GLU:H	3:F:323:GLU:CD	2.08	0.60
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.15	0.60
3:F:149:THR:HG23	3:F:168:PHE:O	2.00	0.60
2:B:166:ARG:NH2	3:C:106:SER:HB2	2.15	0.60
3:C:240:SER:HG	3:C:242:ILE:CD1	2.13	0.60
2:E:381:ASP:CG	2:E:393:GLN:NE2	2.60	0.60
1:A:131:GLN:NE2	1:A:132:HIS:N	2.49	0.60
1:A:175:LEU:O	1:A:179:GLU:HG3	2.02	0.60
2:B:161:ILE:HG12	2:B:164:ASN:HB3	1.84	0.60
1:D:175:LEU:H	1:D:175:LEU:HD22	1.66	0.60
2:E:176:ARG:NH1	3:F:113:ILE:HG23	2.16	0.60
2:E:172:LEU:CD1	3:F:114:TYR:CG	2.82	0.60
1:A:131:GLN:NE2	1:A:132:HIS:H	1.99	0.60
1:A:139:ASN:HB3	3:C:114:TYR:CE2	2.37	0.59
1:D:179:GLU:HB2	1:D:183:LYS:HZ2	1.65	0.59
3:C:106:SER:C	3:C:108:ARG:N	2.57	0.59
2:E:172:LEU:HD12	3:F:114:TYR:CA	2.32	0.59
3:F:195:GLN:HE22	3:F:382:THR:HG21	1.66	0.59
1:A:134:GLN:HG3	1:A:135:LEU:CD2	2.32	0.59
3:F:160:GLY:O	3:F:162:LYS:CE	2.43	0.59
3:F:161:ALA:C	3:F:162:LYS:HE2	2.27	0.59
3:F:199:ASP:O	3:F:225:GLU:OE2	2.20	0.59
1:A:186:GLU:O	1:A:187:GLN:C	2.45	0.59
1:A:188:VAL:HG13	2:B:165:LEU:CD2	2.31	0.59
2:B:309:GLU:OE1	2:B:325:HIS:HE1	1.85	0.59
3:F:178:PHE:CZ	3:F:232:LYS:HG2	2.37	0.59
3:F:254:ASN:OD1	3:F:256:ARG:NH2	2.31	0.59
3:F:264:MET:HE2	3:F:264:MET:N	2.17	0.59
5:G:1:NAG:HO3	5:G:2:NAG:HN2	1.47	0.59
3:C:322:PHE:CZ	4:S:3:ARG:CG	2.86	0.59
2:E:176:ARG:CA	3:F:117:ASN:OD1	2.51	0.58
2:E:283:LYS:HG2	2:E:285:TYR:CE1	2.38	0.58
3:F:219:SER:N	3:F:224:THR:HG21	2.18	0.58
2:B:175:LEU:O	2:B:179:ILE:HG13	2.03	0.58
3:F:111:GLN:NE2	3:F:111:GLN:H	2.02	0.58
2:B:169:ARG:NH1	2:B:173:GLU:OE1	2.35	0.58
2:B:179:ILE:HG21	3:C:120:LYS:HB3	1.86	0.58
2:B:179:ILE:CD1	3:C:117:ASN:HB2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:179:ILE:CD1	3:F:117:ASN:CA	2.76	0.58
2:B:169:ARG:HH11	2:B:173:GLU:CD	2.11	0.58
2:B:432:ASP:OD2	2:B:443:SER:CB	2.51	0.58
2:E:221:THR:OG1	2:E:223:GLU:OE2	2.22	0.58
1:D:188:VAL:HG21	2:E:165:LEU:CD2	2.33	0.57
2:E:169:ARG:HH11	2:E:169:ARG:HB3	1.69	0.57
2:E:182:LEU:HB3	3:F:124:LEU:HD21	1.85	0.57
3:F:157:ALA:O	3:F:159:LYS:N	2.38	0.57
3:C:325:ASN:C	3:C:325:ASN:HD22	2.12	0.57
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.85	0.57
3:F:189:ASN:OD1	3:F:391:ARG:CG	2.52	0.57
1:A:127:ILE:HD12	1:A:130:VAL:CG2	2.34	0.57
2:B:166:ARG:C	2:B:168:LEU:N	2.62	0.57
2:B:201:CYS:CB	2:B:224:MET:HE1	2.35	0.57
3:C:172:LEU:H	3:C:239:GLN:NE2	2.03	0.57
2:B:361:MET:HB2	5:G:1:NAG:C7	2.31	0.57
3:C:249:GLU:OE2	3:C:385:LYS:NZ	2.36	0.57
2:B:238:VAL:HG21	2:B:250:THR:HG23	1.87	0.57
1:D:188:VAL:CG2	2:E:165:LEU:CD2	2.77	0.57
1:D:144:LEU:HD23	2:E:175:LEU:HD21	1.87	0.56
2:E:176:ARG:HH11	3:F:113:ILE:HG12	1.70	0.56
2:E:280:THR:O	2:E:281:ASP:C	2.48	0.56
2:E:309:GLU:OE1	2:E:325:HIS:CE1	2.58	0.56
2:E:428:LYS:HG2	2:E:429:HIS:CD2	2.40	0.56
3:F:329:GLN:HE22	4:T:3:ARG:HE	1.53	0.56
1:D:169:LEU:H	2:E:189:GLN:HE22	1.53	0.56
3:F:109:TYR:N	3:F:112:GLU:CD	2.63	0.56
3:F:303:PHE:HE2	3:F:304:PHE:CZ	2.24	0.56
2:B:168:LEU:O	2:B:169:ARG:C	2.48	0.56
1:D:179:GLU:C	1:D:183:LYS:NZ	2.63	0.56
2:E:184:SER:O	2:E:187:SER:HB3	2.06	0.56
3:F:109:TYR:N	3:F:112:GLU:OE1	2.37	0.56
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.88	0.56
1:A:169:LEU:H	2:B:189:GLN:NE2	2.04	0.55
2:B:395:SER:HB2	2:B:404:TYR:HE2	1.71	0.55
3:C:338:LYS:N	3:C:339:CYS:HA	2.21	0.55
2:B:171:ILE:O	2:B:174:ASN:N	2.38	0.55
1:A:175:LEU:H	1:A:175:LEU:CD2	2.19	0.55
2:E:172:LEU:HD12	3:F:114:TYR:CB	2.35	0.55
3:F:162:LYS:H	3:F:163:GLN:NE2	2.03	0.55
1:D:180:ASP:HA	1:D:183:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:LYS:CE	2:B:185:ASP:OD2	2.52	0.55
1:D:179:GLU:O	1:D:183:LYS:HE3	2.04	0.55
3:F:298:ASP:OD1	3:F:300:SER:N	2.33	0.55
2:B:174:ASN:O	2:B:177:SER:N	2.39	0.55
2:E:252:ILE:HD13	2:E:294:LEU:CD2	2.36	0.55
1:A:166:SER:CB	2:B:195:THR:HG23	2.37	0.55
2:B:161:ILE:HG12	2:B:164:ASN:OD1	2.05	0.55
1:A:188:VAL:HG13	2:B:165:LEU:HD23	1.89	0.55
1:D:140:VAL:O	1:D:144:LEU:HB2	2.07	0.55
1:D:188:VAL:CG1	2:E:165:LEU:CD2	2.79	0.54
3:F:249:GLU:CD	3:F:385:LYS:NZ	2.65	0.54
2:B:423:THR:OG1	2:B:426:MET:HG3	2.07	0.54
3:C:105:SER:CA	3:C:108:ARG:HG3	2.36	0.54
1:A:150:LEU:HD21	3:C:124:LEU:HD23	1.89	0.54
3:F:196:LYS:HD2	3:F:198:LEU:HD23	1.88	0.54
3:C:106:SER:C	3:C:108:ARG:H	2.15	0.54
3:F:160:GLY:O	3:F:162:LYS:HG2	2.07	0.54
1:D:141:ARG:CZ	7:D:72:HOH:O	2.56	0.54
1:D:188:VAL:CB	2:E:165:LEU:HD21	2.37	0.54
2:B:169:ARG:NH1	2:B:173:GLU:OE2	2.29	0.54
1:D:183:LYS:O	1:D:185:LEU:N	2.41	0.54
3:F:172:LEU:HB2	3:F:239:GLN:HB2	1.89	0.54
2:B:169:ARG:HH11	2:B:169:ARG:HG2	1.72	0.54
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.42	0.54
2:E:169:ARG:O	2:E:173:GLU:HG2	2.08	0.54
2:B:231:SER:O	2:B:232:SER:C	2.51	0.54
2:B:351:ASN:CG	2:B:354:MET:HB2	2.33	0.54
2:E:309:GLU:OE1	2:E:325:HIS:HE1	1.91	0.53
3:F:109:TYR:HB2	3:F:112:GLU:CG	2.34	0.53
3:F:325:ASN:ND2	3:F:328:GLU:N	2.48	0.53
3:C:131:LEU:O	3:C:134:GLN:N	2.34	0.53
2:E:307:PRO:HB2	2:E:457:PHE:HB3	1.90	0.53
3:F:160:GLY:C	3:F:162:LYS:CE	2.80	0.53
3:C:245:ALA:HB2	3:C:389:PHE:HD1	1.73	0.53
3:C:337:ASN:O	3:C:338:LYS:C	2.51	0.53
1:A:128:GLU:C	1:A:129:LYS:HD3	2.34	0.53
3:F:116:SER:O	3:F:118:ASN:N	2.42	0.53
2:B:439:ASN:ND2	2:B:439:ASN:N	2.56	0.53
2:E:172:LEU:O	2:E:173:GLU:C	2.50	0.53
2:E:360:LEU:HD13	4:N:2:HIS:HB3	1.91	0.53
3:C:196:LYS:HD2	3:C:198:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:VAL:HG13	2:E:165:LEU:HD21	1.85	0.53
2:E:388:SER:O	2:E:390:PRO:HD3	2.09	0.53
5:G:1:NAG:O3	5:G:2:NAG:C2	2.56	0.53
3:C:240:SER:OG	3:C:242:ILE:HD11	2.08	0.53
1:D:139:ASN:C	1:D:141:ARG:H	2.13	0.53
1:D:180:ASP:N	1:D:183:LYS:CE	2.72	0.53
3:F:160:GLY:HA2	3:F:162:LYS:HE3	1.91	0.53
1:A:127:ILE:O	1:A:128:GLU:C	2.52	0.53
1:D:180:ASP:CA	1:D:183:LYS:HD2	2.38	0.53
2:B:190:MET:SD	3:C:134:GLN:NE2	2.82	0.52
2:B:201:CYS:HB3	2:B:224:MET:HE1	1.91	0.52
3:C:106:SER:O	3:C:108:ARG:N	2.42	0.52
2:E:254:ASN:HD21	2:E:256:GLN:NE2	2.07	0.52
3:F:109:TYR:CA	3:F:112:GLU:HB2	2.37	0.52
3:F:392:LEU:C	3:F:393:THR:HG1	2.14	0.52
1:A:154:ILE:O	1:A:158:ILE:HG13	2.09	0.52
2:B:159:SER:HB2	2:B:162:PRO:CG	2.36	0.52
1:D:135:LEU:O	1:D:138:LYS:HB3	2.09	0.52
3:F:109:TYR:C	3:F:112:GLU:HB2	2.34	0.52
1:A:133:ILE:C	1:A:135:LEU:N	2.38	0.52
2:B:191:GLU:CD	2:B:194:ARG:HE	2.16	0.52
5:H:1:NAG:O6	5:H:2:NAG:C5	2.52	0.52
2:E:172:LEU:CD2	2:E:172:LEU:H	2.22	0.52
3:F:112:GLU:C	3:F:114:TYR:N	2.67	0.52
2:B:161:ILE:HG12	2:B:164:ASN:CB	2.40	0.52
2:B:280:THR:O	2:B:281:ASP:C	2.51	0.52
3:C:149:THR:CG2	3:C:168:PHE:O	2.56	0.52
1:D:179:GLU:C	1:D:183:LYS:HZ2	2.16	0.52
1:A:140:VAL:CG1	2:B:172:LEU:HD21	2.37	0.52
2:B:361:MET:CB	5:G:1:NAG:C8	2.50	0.52
3:C:322:PHE:CE2	4:S:3:ARG:HG2	2.44	0.52
1:D:188:VAL:HG21	2:E:165:LEU:CG	2.40	0.52
3:C:104:ASP:HB2	3:C:107:ILE:HD13	1.90	0.52
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.56	0.52
2:E:333:ASN:ND2	2:E:333:ASN:H	2.06	0.52
2:B:179:ILE:HD12	3:C:117:ASN:HB2	1.91	0.52
2:B:180:GLN:HA	2:B:183:GLU:CG	2.39	0.52
1:D:188:VAL:HG11	2:E:165:LEU:CD2	2.39	0.52
2:B:363:GLU:HA	2:B:366:THR:HG23	1.92	0.51
2:E:174:ASN:O	2:E:177:SER:N	2.43	0.51
3:F:116:SER:O	3:F:117:ASN:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:281:PHE:CE2	3:F:283:GLY:HA2	2.45	0.51
2:B:395:SER:HB2	2:B:404:TYR:CE2	2.45	0.51
3:F:152:ASP:OD2	3:F:244:TYR:OH	2.21	0.51
1:A:166:SER:HG	2:B:195:THR:HG23	1.74	0.51
2:B:165:LEU:HB2	7:B:498:HOH:O	1.83	0.51
3:C:303:PHE:HE2	3:C:304:PHE:CZ	2.28	0.51
2:E:169:ARG:HH11	2:E:173:GLU:CD	2.16	0.51
7:E:40:HOH:O	4:N:4:PRO:HB3	2.10	0.51
1:A:132:HIS:NE2	3:C:107:ILE:HG22	2.24	0.51
3:F:160:GLY:O	3:F:161:ALA:C	2.53	0.51
1:D:180:ASP:H	1:D:183:LYS:HZ2	1.56	0.51
2:E:230:ASP:HB3	2:E:233:VAL:CG2	2.40	0.51
3:C:338:LYS:O	3:C:338:LYS:HG2	2.10	0.51
3:F:217:HIS:O	3:F:224:THR:HG21	2.04	0.51
3:C:254:ASN:OD1	3:C:256:ARG:NH2	2.45	0.51
1:A:127:ILE:HD12	1:A:131:GLN:OE1	2.11	0.50
2:E:228:GLN:NE2	2:E:233:VAL:O	2.44	0.50
2:E:388:SER:O	2:E:390:PRO:CD	2.59	0.50
2:B:303:THR:HB	2:B:330:THR:HA	1.93	0.50
1:D:147:MET:SD	3:F:121:ILE:HD13	2.50	0.50
2:E:439:ASN:H	2:E:439:ASN:ND2	2.08	0.50
3:F:110:LEU:N	3:F:112:GLU:HG3	2.26	0.50
2:B:161:ILE:O	2:B:164:ASN:N	2.45	0.50
2:B:238:VAL:HG21	2:B:250:THR:CG2	2.41	0.50
2:E:249:TRP:HB3	2:E:453:LYS:HB3	1.93	0.50
3:F:263:ALA:CB	3:F:264:MET:CE	2.89	0.50
1:A:166:SER:N	2:B:195:THR:O	2.42	0.50
3:F:263:ALA:CB	3:F:264:MET:HE2	2.42	0.50
3:F:325:ASN:HD22	3:F:328:GLU:H	1.54	0.50
1:A:174:ASP:OD2	1:A:177:ASP:HB2	2.12	0.50
2:B:310:LEU:HB3	2:B:326:TYR:HB2	1.93	0.50
3:F:370:ALA:HA	3:F:373:LYS:O	2.12	0.50
2:E:378:TYR:CE1	2:E:396:LYS:CE	2.95	0.49
3:F:109:TYR:C	3:F:112:GLU:HG3	2.36	0.49
1:A:132:HIS:CD2	3:C:107:ILE:CG2	2.95	0.49
2:E:171:ILE:HG22	2:E:172:LEU:CG	2.38	0.49
2:B:265:LYS:HE3	2:B:378:TYR:CZ	2.48	0.49
2:E:179:ILE:HD12	3:F:117:ASN:C	2.28	0.49
3:F:112:GLU:O	3:F:114:TYR:N	2.45	0.49
1:A:188:VAL:CG1	2:B:165:LEU:HD23	2.42	0.49
2:B:166:ARG:NH2	3:C:106:SER:OG	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:GLN:O	3:C:158:ASN:N	2.41	0.49
2:E:422:TYR:C	2:E:426:MET:HE3	2.37	0.49
3:F:209:ILE:HD12	3:F:209:ILE:N	2.24	0.49
1:A:143:GLN:HE22	3:C:117:ASN:HD22	1.58	0.49
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.48	0.49
3:F:224:THR:HG22	7:F:429:HOH:O	2.12	0.49
3:C:104:ASP:C	3:C:106:SER:N	2.70	0.49
2:B:385:TRP:CH2	4:M:3:ARG:NH1	2.74	0.49
1:D:139:ASN:O	1:D:142:ALA:N	2.46	0.49
2:E:385:TRP:CE2	4:N:3:ARG:HG3	2.47	0.49
2:E:423:THR:OG1	2:E:426:MET:HG3	2.13	0.49
3:C:172:LEU:CD1	3:C:239:GLN:HE21	2.25	0.48
3:C:244:TYR:H	3:C:266:LYS:HZ3	1.60	0.48
3:F:116:SER:OG	3:F:117:ASN:N	2.46	0.48
3:F:124:LEU:O	3:F:128:VAL:HG23	2.13	0.48
2:B:174:ASN:O	2:B:178:LYS:N	2.38	0.48
2:E:178:LYS:O	2:E:179:ILE:C	2.56	0.48
2:E:367:MET:HG3	4:N:2:HIS:HB2	1.95	0.48
1:D:176:LYS:HG3	1:D:180:ASP:OD1	2.12	0.48
2:E:174:ASN:O	2:E:175:LEU:C	2.56	0.48
2:E:267:ASP:CB	2:E:268:PRO:HD3	2.43	0.48
1:D:183:LYS:C	1:D:185:LEU:H	2.21	0.48
2:E:201:CYS:CB	2:E:224:MET:HE1	2.43	0.48
3:F:157:ALA:C	3:F:159:LYS:N	2.69	0.48
2:B:168:LEU:C	2:B:170:SER:N	2.71	0.48
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.46	0.48
2:B:161:ILE:HG12	2:B:164:ASN:CG	2.39	0.48
2:B:367:MET:SD	2:B:406:ARG:HG2	2.54	0.48
2:E:203:ILE:HD13	3:F:145:ILE:HD11	1.96	0.48
2:E:361:MET:O	2:E:364:ASN:HB2	2.13	0.48
3:F:172:LEU:HG	3:F:239:GLN:HE21	1.78	0.48
2:E:251:VAL:HG22	2:E:453:LYS:HG2	1.96	0.48
2:E:265:LYS:O	2:E:268:PRO:HD2	2.14	0.48
2:B:161:ILE:O	2:B:164:ASN:HB2	2.12	0.48
2:B:402:TRP:CG	2:B:403:TRP:N	2.82	0.48
3:C:264:MET:HE3	3:F:308:ASN:ND2	2.28	0.48
1:D:180:ASP:CA	1:D:183:LYS:CD	2.91	0.48
3:C:243:PRO:HA	3:C:266:LYS:NZ	2.28	0.48
1:D:135:LEU:O	1:D:137:GLN:N	2.47	0.48
1:D:183:LYS:O	1:D:186:GLU:N	2.30	0.48
2:E:383:ASP:C	2:E:383:ASP:OD1	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:173:LYS:NZ	3:F:173:LYS:HB3	2.28	0.47
1:A:176:LYS:HA	1:A:176:LYS:HZ2	1.79	0.47
1:A:187:GLN:O	1:A:189:ILE:N	2.47	0.47
2:B:281:ASP:OD1	2:B:282:GLY:N	2.47	0.47
1:D:176:LYS:O	1:D:177:ASP:C	2.56	0.47
2:E:314:MET:HE1	2:E:437:TRP:CD2	2.48	0.47
3:F:162:LYS:N	3:F:163:GLN:NE2	2.63	0.47
2:B:376:SER:O	2:B:401:GLY:HA2	2.14	0.47
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.80	0.47
2:E:252:ILE:CD1	2:E:299:ILE:HG12	2.37	0.47
3:F:178:PHE:CD1	3:F:232:LYS:HG2	2.49	0.47
2:B:186:VAL:HG13	3:C:131:LEU:HD22	1.96	0.47
3:C:322:PHE:HE2	3:C:329:GLN:NE2	2.12	0.47
3:F:157:ALA:C	3:F:159:LYS:H	2.23	0.47
1:A:131:GLN:N	1:A:134:GLN:HG2	2.30	0.47
2:B:413:ASN:HB2	7:B:483:HOH:O	2.14	0.47
2:E:179:ILE:HG21	3:F:120:LYS:CB	2.44	0.47
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.13	0.47
2:E:172:LEU:HD12	3:F:114:TYR:CG	2.50	0.47
2:E:252:ILE:HD13	2:E:294:LEU:HD22	1.95	0.47
2:B:427:ALA:O	2:B:428:LYS:C	2.58	0.47
3:C:387:ILE:HD11	3:C:391:ARG:HG2	1.97	0.47
3:F:252:ASP:OD2	3:F:256:ARG:HB2	2.14	0.47
2:E:458:PHE:CB	2:E:459:PRO:HD3	2.38	0.46
7:E:40:HOH:O	4:N:4:PRO:CB	2.63	0.46
3:F:325:ASN:HD22	3:F:325:ASN:C	2.23	0.46
2:B:296:ASN:O	2:B:297:ASP:C	2.56	0.46
3:F:265:PHE:CE2	3:F:276:LEU:CD1	2.98	0.46
1:A:183:LYS:C	1:A:185:LEU:H	2.23	0.46
1:D:144:LEU:CD2	2:E:175:LEU:HD21	2.46	0.46
2:E:428:LYS:HE3	2:E:428:LYS:HB2	1.78	0.46
2:B:432:ASP:HB2	2:B:443:SER:HB2	1.95	0.46
1:D:140:VAL:CG1	3:F:114:TYR:CE2	2.56	0.46
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.16	0.46
1:D:176:LYS:HA	1:D:179:GLU:HB2	1.96	0.46
1:D:186:GLU:O	1:D:188:VAL:N	2.48	0.46
1:A:169:LEU:H	2:B:189:GLN:HE22	1.61	0.46
2:B:362:GLY:O	2:B:366:THR:CG2	2.63	0.46
1:D:179:GLU:O	1:D:183:LYS:CE	2.59	0.46
1:D:176:LYS:C	1:D:178:TYR:N	2.72	0.46
2:E:385:TRP:CD1	2:E:406:ARG:HH12	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:359:THR:HB	3:F:360:PRO:HD2	1.98	0.46
3:C:252:ASP:CG	3:C:256:ARG:HB2	2.41	0.46
1:D:175:LEU:O	1:D:176:LYS:C	2.58	0.46
2:B:252:ILE:HG13	2:B:299:ILE:HG12	1.97	0.46
3:C:276:LEU:C	3:C:277:THR:HG23	2.40	0.45
1:A:188:VAL:CG2	2:B:165:LEU:HD23	2.41	0.45
3:F:236:ILE:O	3:F:239:GLN:HG2	2.15	0.45
2:B:314:MET:HE1	2:B:437:TRP:CG	2.51	0.45
3:C:143:VAL:HB	3:C:220:PRO:CG	2.46	0.45
1:D:169:LEU:H	2:E:189:GLN:NE2	2.13	0.45
3:F:374:THR:HG23	3:F:377:TYR:HB2	1.98	0.45
1:A:143:GLN:NE2	3:C:117:ASN:HD22	2.10	0.45
2:B:251:VAL:HG22	2:B:453:LYS:HG2	1.97	0.45
2:E:439:ASN:H	2:E:439:ASN:HD22	1.62	0.45
3:F:252:ASP:OD1	3:F:256:ARG:N	2.47	0.45
3:F:265:PHE:CE2	3:F:276:LEU:HD11	2.52	0.45
1:D:141:ARG:NH2	7:D:72:HOH:O	2.50	0.45
2:B:162:PRO:O	2:B:163:THR:C	2.59	0.45
3:C:272:ASP:HB2	3:F:299:PRO:HB2	1.99	0.45
1:D:137:GLN:O	1:D:138:LYS:C	2.60	0.45
3:F:114:TYR:O	3:F:117:ASN:ND2	2.50	0.45
3:C:173:LYS:HB3	3:C:235:LEU:CD2	2.46	0.45
3:F:303:PHE:CE2	3:F:304:PHE:CZ	3.04	0.45
2:B:389:ASP:O	2:B:392:LYS:N	2.46	0.45
3:C:375:ARG:HH11	3:C:375:ARG:HD2	1.35	0.45
2:E:198:THR:HA	3:F:140:LYS:O	2.17	0.45
2:E:385:TRP:CZ2	4:N:3:ARG:CD	2.97	0.45
3:F:343:HIS:O	3:F:367:ILE:HA	2.17	0.45
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.82	0.45
2:E:360:LEU:CD1	4:N:2:HIS:HB3	2.47	0.45
2:E:176:ARG:NH1	3:F:113:ILE:HG21	2.32	0.45
2:E:411:ASN:N	2:E:412:PRO:HD3	2.31	0.45
3:F:109:TYR:HB2	3:F:112:GLU:CD	2.42	0.45
3:F:127:LYS:O	3:F:130:GLN:N	2.50	0.45
3:F:249:GLU:CD	3:F:385:LYS:HZ3	2.23	0.45
3:F:307:HIS:CE1	3:F:342:GLY:H	2.34	0.45
3:C:155:ASP:O	3:C:159:LYS:HG3	2.17	0.44
3:C:243:PRO:CB	3:C:264:MET:HG3	2.47	0.44
3:C:273:LYS:HD2	3:C:319:ASN:CG	2.41	0.44
3:C:388:PRO:O	3:C:391:ARG:HB2	2.17	0.44
2:E:293:TRP:HZ2	2:E:296:ASN:HD21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:HIS:CD2	3:C:107:ILE:HG22	2.52	0.44
2:B:406:ARG:N	2:B:407:CYS:CA	2.79	0.44
1:D:135:LEU:O	1:D:136:LEU:C	2.59	0.44
1:D:176:LYS:HD3	1:D:179:GLU:OE1	2.16	0.44
2:E:381:ASP:OD1	2:E:381:ASP:C	2.60	0.44
3:C:243:PRO:HB3	3:C:264:MET:HG3	1.98	0.44
3:F:148:ILE:HG21	3:F:156:ILE:HG23	1.98	0.44
3:F:289:ALA:HB3	3:F:369:TRP:CE2	2.52	0.44
2:B:254:ASN:O	2:B:291:GLU:HA	2.17	0.44
3:C:173:LYS:CE	3:C:238:THR:O	2.48	0.44
1:D:188:VAL:CG2	2:E:165:LEU:CG	2.95	0.44
1:A:143:GLN:OE1	3:C:117:ASN:CG	2.60	0.44
2:B:198:THR:HA	3:C:140:LYS:O	2.18	0.44
2:B:317:TRP:CE2	2:B:448:ARG:HB2	2.52	0.44
3:F:161:ALA:HB1	3:F:163:GLN:NE2	2.33	0.44
3:F:264:MET:O	3:F:278:TYR:HA	2.16	0.44
3:F:392:LEU:N	3:F:392:LEU:HD23	2.32	0.44
1:A:131:GLN:N	1:A:131:GLN:CD	2.76	0.44
2:B:245:GLU:O	2:B:246:ASN:HB2	2.18	0.44
2:B:266:TRP:CE3	2:B:380:ARG:HG2	2.52	0.44
2:B:328:GLY:O	2:B:342:VAL:HA	2.17	0.44
3:F:212:LYS:HA	3:F:230:ASN:HB2	1.99	0.44
4:T:2:HIS:CD2	4:T:4:PRO:HG3	2.52	0.44
3:C:105:SER:O	3:C:108:ARG:CG	2.47	0.44
2:E:176:ARG:CB	3:F:117:ASN:HB3	2.46	0.44
1:A:180:ASP:HA	1:A:183:LYS:NZ	2.32	0.44
2:B:458:PHE:N	2:B:459:PRO:HD2	2.26	0.44
3:C:297:ASP:O	3:C:298:ASP:C	2.60	0.44
2:E:168:LEU:C	2:E:170:SER:N	2.75	0.44
2:E:226:LEU:HA	2:E:226:LEU:HD12	1.82	0.44
2:E:423:THR:N	2:E:426:MET:HE3	2.33	0.44
3:F:304:PHE:CD1	3:F:338:LYS:HD3	2.53	0.44
3:C:105:SER:HA	3:C:108:ARG:HG3	2.00	0.43
3:C:143:VAL:HB	3:C:220:PRO:HG2	1.99	0.43
3:C:172:LEU:H	3:C:239:GLN:HE21	1.65	0.43
2:E:252:ILE:HD13	2:E:294:LEU:HD23	2.00	0.43
2:E:402:TRP:CG	2:E:403:TRP:N	2.86	0.43
1:A:129:LYS:N	1:A:129:LYS:HD3	2.32	0.43
1:A:131:GLN:CA	1:A:134:GLN:CG	2.92	0.43
2:B:169:ARG:NH1	2:B:169:ARG:HG2	2.33	0.43
3:C:307:HIS:CE1	3:C:341:ALA:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:LEU:CD2	2:E:172:LEU:N	2.81	0.43
3:F:157:ALA:O	3:F:158:ASN:C	2.60	0.43
2:B:345:TYR:CG	2:B:346:ARG:N	2.87	0.43
3:C:150:GLY:HA3	3:C:155:ASP:OD2	2.18	0.43
3:C:198:LEU:HA	3:C:381:LYS:HG2	2.00	0.43
3:C:246:LEU:HA	3:C:386:ILE:HG22	2.01	0.43
2:E:180:GLN:OE1	2:E:180:GLN:HA	2.18	0.43
3:F:185:ASP:CG	3:F:187:SER:H	2.26	0.43
3:C:336:MET:HE1	3:C:343:HIS:CD2	2.54	0.43
2:E:236:TYR:CD1	2:E:298:LYS:HE2	2.54	0.43
3:F:109:TYR:CA	3:F:112:GLU:CG	2.69	0.43
3:F:338:LYS:N	3:F:339:CYS:HA	2.34	0.43
2:E:215:ILE:HD12	2:E:242:MET:HB3	1.99	0.43
3:C:264:MET:HE2	3:C:264:MET:HB2	1.89	0.43
3:F:206:LYS:HB2	3:F:211:TYR:CE2	2.54	0.43
5:H:1:NAG:HO6	5:H:2:NAG:H5	1.80	0.43
2:B:184:SER:O	2:B:188:ALA:N	2.43	0.43
3:C:209:ILE:HD12	3:C:209:ILE:N	2.23	0.43
3:F:389:PHE:O	3:F:391:ARG:N	2.52	0.43
3:F:390:ASN:OD1	3:F:391:ARG:N	2.52	0.43
1:A:187:GLN:C	1:A:189:ILE:N	2.77	0.42
1:D:135:LEU:O	1:D:138:LYS:CA	2.67	0.42
2:E:171:ILE:HG22	2:E:172:LEU:CB	2.49	0.42
3:F:122:VAL:O	3:F:126:GLU:CG	2.62	0.42
3:F:254:ASN:HB2	3:F:256:ARG:NH2	2.33	0.42
3:F:307:HIS:HE1	3:F:342:GLY:H	1.66	0.42
3:F:392:LEU:O	3:F:393:THR:CB	2.67	0.42
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.16	0.42
1:D:139:ASN:C	3:F:114:TYR:OH	2.63	0.42
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.54	0.42
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.18	0.42
2:B:351:ASN:OD1	2:B:354:MET:HB2	2.20	0.42
3:C:104:ASP:O	3:C:105:SER:C	2.61	0.42
1:A:127:ILE:HB	1:A:130:VAL:HG22	2.01	0.42
3:C:172:LEU:HD13	3:C:239:GLN:HE21	1.84	0.42
2:E:217:LYS:HG2	3:F:213:GLU:HG3	2.01	0.42
3:F:148:ILE:CG2	3:F:156:ILE:HG23	2.48	0.42
3:F:390:ASN:OD1	3:F:390:ASN:C	2.62	0.42
1:A:175:LEU:H	1:A:175:LEU:HD22	1.82	0.42
2:B:180:GLN:O	2:B:183:GLU:HG3	2.20	0.42
2:B:280:THR:HG22	2:B:281:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:CD	7:E:58:HOH:O	2.68	0.42
3:F:298:ASP:CG	3:F:299:PRO:HD2	2.44	0.42
2:B:402:TRP:CG	2:B:403:TRP:H	2.37	0.42
3:C:207:ASN:OD1	3:C:207:ASN:C	2.62	0.42
3:C:273:LYS:HD2	3:C:319:ASN:ND2	2.35	0.42
2:E:209:LYS:HB3	2:E:229:PRO:HA	2.01	0.42
3:F:307:HIS:CE1	3:F:341:ALA:H	2.29	0.42
2:B:161:ILE:HB	2:B:164:ASN:HB2	2.02	0.42
3:C:171:PRO:O	3:C:172:LEU:C	2.63	0.42
3:C:264:MET:HA	3:C:266:LYS:HE2	2.01	0.42
3:C:340:HIS:CE1	4:S:1:GLY:N	2.88	0.42
2:E:423:THR:HG23	2:E:426:MET:HE3	2.01	0.42
2:B:377:THR:C	2:B:395:SER:OG	2.63	0.42
3:C:131:LEU:O	3:C:134:GLN:HB2	2.19	0.42
2:E:379:ASP:O	2:E:380:ARG:HB2	2.18	0.42
2:B:166:ARG:HH22	3:C:103:HIS:CD2	2.38	0.42
2:B:180:GLN:HA	2:B:183:GLU:HG3	2.02	0.42
2:E:301:GLN:NE2	7:E:62:HOH:O	2.44	0.42
3:C:243:PRO:HA	3:C:266:LYS:HZ1	1.85	0.41
3:F:230:ASN:HD22	3:F:230:ASN:HA	1.68	0.41
2:B:385:TRP:CZ2	4:M:3:ARG:HG3	2.54	0.41
2:B:234:LYS:HA	2:B:235:PRO:HD3	1.88	0.41
2:B:424:TRP:O	2:B:430:GLY:HA2	2.19	0.41
1:D:183:LYS:C	1:D:185:LEU:N	2.78	0.41
1:D:188:VAL:HG22	2:E:165:LEU:HD21	1.92	0.41
2:E:402:TRP:CG	2:E:403:TRP:H	2.37	0.41
2:B:244:THR:O	2:B:245:GLU:C	2.62	0.41
1:D:143:GLN:O	1:D:144:LEU:C	2.61	0.41
2:E:169:ARG:O	2:E:171:ILE:N	2.53	0.41
3:F:389:PHE:C	3:F:391:ARG:N	2.78	0.41
2:B:282:GLY:O	2:B:283:LYS:HD2	2.21	0.41
3:C:270:GLU:HB2	3:C:274:TYR:CZ	2.56	0.41
3:C:295:PHE:HE2	3:C:305:THR:HG21	1.85	0.41
3:C:322:PHE:CZ	4:S:3:ARG:HG3	2.55	0.41
2:E:224:MET:HG2	2:E:225:TYR:N	2.36	0.41
2:E:389:ASP:HA	2:E:390:PRO:HD2	1.76	0.41
3:C:151:LYS:HD3	3:C:172:LEU:HD11	2.02	0.41
3:C:189:ASN:OD1	3:C:391:ARG:HG3	2.21	0.41
2:E:367:MET:HB2	2:E:406:ARG:HB3	2.03	0.41
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.19	0.41
3:C:325:ASN:C	3:C:325:ASN:ND2	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:154:GLN:OE1	3:F:189:ASN:HA	2.21	0.41
3:F:258:SER:C	3:F:259:THR:CG2	2.94	0.41
3:F:293:PHE:HB3	3:F:295:PHE:CE2	2.56	0.41
2:B:201:CYS:HB3	2:B:224:MET:CE	2.50	0.41
2:E:369:ILE:HD13	2:E:369:ILE:HG21	1.86	0.41
3:F:245:ALA:HB2	3:F:389:PHE:HD1	1.85	0.41
1:A:188:VAL:CB	2:B:165:LEU:HD21	2.49	0.41
2:B:389:ASP:HA	2:B:390:PRO:HD2	1.67	0.41
3:C:106:SER:O	3:C:107:ILE:C	2.63	0.41
2:E:213:GLU:OE2	2:E:217:LYS:HE3	2.21	0.41
3:F:131:LEU:O	3:F:134:GLN:N	2.49	0.41
3:F:172:LEU:H	3:F:239:GLN:HE21	1.66	0.41
3:F:185:ASP:C	3:F:187:SER:H	2.29	0.41
3:F:364:ASP:OD1	4:T:1:GLY:HA3	2.21	0.41
1:A:127:ILE:C	1:A:129:LYS:N	2.79	0.41
1:D:150:LEU:O	1:D:151:GLU:C	2.61	0.41
1:D:186:GLU:O	1:D:188:VAL:C	2.64	0.41
2:E:437:TRP:O	2:E:438:MET:C	2.64	0.41
3:F:194:PHE:CZ	3:F:384:MET:HE2	2.56	0.41
2:B:237:ARG:NE	7:B:494:HOH:O	2.34	0.40
2:B:309:GLU:OE1	2:B:325:HIS:CE1	2.68	0.40
3:C:249:GLU:OE2	3:C:385:LYS:HE2	2.20	0.40
1:D:147:MET:HG2	2:E:175:LEU:HD22	2.03	0.40
2:E:182:LEU:O	2:E:186:VAL:HG23	2.21	0.40
2:E:338:TYR:O	2:E:339:GLN:C	2.62	0.40
2:E:359:GLN:OE1	2:E:359:GLN:N	2.51	0.40
3:F:208:TRP:HB3	3:F:209:ILE:HD12	2.03	0.40
1:A:148:LYS:CE	1:A:182:GLN:NE2	2.74	0.40
3:C:199:ASP:O	3:C:225:GLU:OE2	2.40	0.40
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.20	0.40
2:E:378:TYR:CD2	2:E:396:LYS:CE	2.98	0.40
3:C:249:GLU:OE2	3:C:385:LYS:CE	2.69	0.40
3:C:276:LEU:C	3:C:277:THR:CG2	2.93	0.40
1:D:175:LEU:O	1:D:178:TYR:CB	2.67	0.40
1:A:166:SER:HB3	2:B:195:THR:HG23	2.03	0.40
1:A:183:LYS:C	1:A:185:LEU:N	2.79	0.40
3:F:389:PHE:C	3:F:391:ARG:H	2.29	0.40
2:B:345:TYR:OH	2:B:349:ALA:O	2.38	0.40
3:C:172:LEU:HD12	3:C:239:GLN:NE2	2.36	0.40
3:C:246:LEU:HB3	3:C:262:TYR:HB2	2.03	0.40
2:E:179:ILE:HD13	3:F:121:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:LEU:CB	3:F:124:LEU:HD21	2.49	0.40
2:E:202:ASN:HB2	2:E:284:ASN:O	2.21	0.40
2:E:241:ASP:OD2	2:E:244:THR:OG1	2.25	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:THR:OG1	3:F:328:GLU:OE2[4_466]	1.16	1.04
3:C:375:ARG:NH2	3:F:361:ASN:OD1[4_466]	1.42	0.78
3:C:375:ARG:N	7:F:426:HOH:O[4_466]	1.52	0.68
3:C:374:THR:OG1	3:F:328:GLU:CD[4_466]	1.80	0.40
3:C:295:PHE:O	3:F:329:GLN:OE1[4_466]	2.01	0.19
3:C:374:THR:CB	3:F:328:GLU:CG[4_466]	2.17	0.03

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	65/87 (75%)	52 (80%)	6 (9%)	7 (11%)	0	0
1	D	52/87 (60%)	39 (75%)	8 (15%)	5 (10%)	0	0
2	B	301/328 (92%)	273 (91%)	19 (6%)	9 (3%)	3	5
2	E	294/328 (90%)	262 (89%)	23 (8%)	9 (3%)	3	5
3	C	290/319 (91%)	265 (91%)	24 (8%)	1 (0%)	36	55
3	F	283/319 (89%)	261 (92%)	16 (6%)	6 (2%)	5	9
4	M	2/4 (50%)	2 (100%)	0	0	100	100
4	N	2/4 (50%)	2 (100%)	0	0	100	100
4	S	2/4 (50%)	2 (100%)	0	0	100	100
4	T	2/4 (50%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1293/1484 (87%)	1160 (90%)	96 (7%)	37 (3%)	3 5

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	190	ALA
2	B	169	ARG
2	B	171	ILE
2	B	281	ASP
2	E	169	ARG
2	E	171	ILE
2	E	281	ASP
2	E	283	LYS
2	E	397	GLU
2	E	398	ASP
3	F	112	GLU
1	A	127	ILE
1	A	128	GLU
1	A	191	LYS
2	B	160	ASN
2	E	168	LEU
3	F	116	SER
1	A	184	GLN
2	B	172	LEU
1	D	140	VAL
1	D	184	GLN
1	D	187	GLN
2	E	458	PHE
3	F	117	ASN
3	F	110	LEU
2	B	161	ILE
2	B	256	GLN
2	B	458	PHE
1	D	136	LEU
1	D	138	LYS
2	E	256	GLN
1	A	188	VAL
3	F	113	ILE
3	C	107	ILE
2	B	167	VAL
3	F	121	ILE

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	62/82 (76%)	45 (73%)	17 (27%)	0	1
1	D	50/82 (61%)	40 (80%)	10 (20%)	1	2
2	B	261/286 (91%)	229 (88%)	32 (12%)	4	10
2	E	254/286 (89%)	228 (90%)	26 (10%)	7	15
3	C	246/267 (92%)	222 (90%)	24 (10%)	7	16
3	F	239/267 (90%)	213 (89%)	26 (11%)	6	13
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	S	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	T	3/3 (100%)	3 (100%)	0	100	100
All	All	1124/1282 (88%)	987 (88%)	137 (12%)	5	10

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	130	VAL
1	A	131	GLN
1	A	133	ILE
1	A	134	GLN
1	A	135	LEU
1	A	136	LEU
1	A	141	ARG
1	A	150	LEU
1	A	164	SER
1	A	167	ARG
1	A	175	LEU
1	A	176	LYS
1	A	179	GLU
1	A	182	GLN
1	A	183	LYS

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Mol	Chain	Res	Type
1	A	189	ILE
2	B	161	ILE
2	B	166	ARG
2	B	170	SER
2	B	172	LEU
2	B	174	ASN
2	B	181	LYS
2	B	183	GLU
2	B	184	SER
2	B	190	MET
2	B	195	THR
2	B	233	VAL
2	B	234	LYS
2	B	252	ILE
2	B	253	GLN
2	B	267	ASP
2	B	280	THR
2	B	318	LYS
2	B	333	ASN
2	B	341	SER
2	B	343	ASN
2	B	346	ARG
2	B	361	MET
2	B	365	ARG
2	B	366	THR
2	B	387	THR
2	B	391	ARG
2	B	395	SER
2	B	439	ASN
2	B	443	SER
2	B	448	ARG
2	B	450	MET
2	B	451	SER
3	C	107	ILE
3	C	108	ARG
3	C	109	TYR
3	C	110	LEU
3	C	113	ILE
3	C	117	ASN
3	C	118	ASN
3	C	130	GLN
3	C	143	VAL

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Mol	Chain	Res	Type
3	C	149	THR
3	C	162	LYS
3	C	163	GLN
3	C	173	LYS
3	C	224	THR
3	C	242	ILE
3	C	266	LYS
3	C	302	LYS
3	C	317	ASN
3	C	323	GLU
3	C	328	GLU
3	C	356	LYS
3	C	358	SER
3	C	382	THR
3	C	393	THR
1	D	136	LEU
1	D	140	VAL
1	D	141	ARG
1	D	143	GLN
1	D	144	LEU
1	D	147	MET
1	D	164	SER
1	D	175	LEU
1	D	176	LYS
1	D	186	GLU
2	E	164	ASN
2	E	165	LEU
2	E	166	ARG
2	E	169	ARG
2	E	170	SER
2	E	171	ILE
2	E	172	LEU
2	E	209	LYS
2	E	210	GLU
2	E	224	MET
2	E	226	LEU
2	E	233	VAL
2	E	238	VAL
2	E	253	GLN
2	E	267	ASP
2	E	280	THR
2	E	321	LYS

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Mol	Chain	Res	Type
2	E	342	VAL
2	E	344	LYS
2	E	365	ARG
2	E	366	THR
2	E	387	THR
2	E	388	SER
2	E	396	LYS
2	E	428	LYS
2	E	448	ARG
3	F	109	TYR
3	F	117	ASN
3	F	143	VAL
3	F	144	GLN
3	F	147	ASP
3	F	148	ILE
3	F	149	THR
3	F	162	LYS
3	F	163	GLN
3	F	173	LYS
3	F	187	SER
3	F	198	LEU
3	F	224	THR
3	F	230	ASN
3	F	242	ILE
3	F	266	LYS
3	F	297	ASP
3	F	323	GLU
3	F	325	ASN
3	F	356	LYS
3	F	368	ILE
3	F	374	THR
3	F	382	THR
3	F	391	ARG
3	F	392	LEU
3	F	393	THR
4	S	3	ARG
4	N	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	160	ASN

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Mol	Chain	Res	Type
2	B	174	ASN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	333	ASN
2	B	339	GLN
2	B	351	ASN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	117	ASN
3	C	118	ASN
3	C	123	ASN
3	C	130	GLN
3	C	136	GLN
3	C	146	HIS
3	C	163	GLN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	329	GLN
2	E	174	ASN
2	E	189	GLN
2	E	256	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	333	ASN
2	E	351	ASN
2	E	393	GLN
2	E	411	ASN
2	E	429	HIS
2	E	439	ASN
3	F	111	GLN
3	F	119	GLN

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Mol	Chain	Res	Type
3	F	123	ASN
3	F	144	GLN
3	F	163	GLN
3	F	176	GLN
3	F	177	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	G	1	5,2	14,14,15	1.26	1 (7%)	17,19,21	4.25	7 (41%)
5	NAG	G	2	5	14,14,15	1.55	2 (14%)	17,19,21	4.85	6 (35%)
5	NAG	H	1	5,2	14,14,15	1.34	1 (7%)	17,19,21	2.09	7 (41%)
5	NAG	H	2	5	14,14,15	1.42	2 (14%)	17,19,21	2.25	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	NAG	O7-C7	-3.92	1.14	1.23
5	H	1	NAG	O7-C7	-3.88	1.14	1.23
5	G	2	NAG	O5-C1	3.65	1.49	1.43
5	G	1	NAG	O7-C7	-3.40	1.15	1.23
5	G	2	NAG	O7-C7	-3.17	1.16	1.23
5	H	2	NAG	C2-N2	2.86	1.51	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2	NAG	C1-O5-C5	-12.59	95.31	112.19
5	G	1	NAG	C3-C4-C5	9.35	127.19	110.23
5	G	2	NAG	C1-C2-N2	9.31	125.10	110.43
5	G	2	NAG	O5-C1-C2	-9.23	97.01	111.29
5	G	1	NAG	C4-C3-C2	-8.74	98.21	111.02
5	G	1	NAG	O4-C4-C3	-7.32	93.12	110.38
5	G	2	NAG	C3-C4-C5	6.38	121.81	110.23
5	G	1	NAG	C1-C2-N2	5.63	119.31	110.43
5	H	2	NAG	C1-O5-C5	-5.12	105.32	112.19
5	G	1	NAG	C2-N2-C7	-4.45	116.94	122.90
5	G	1	NAG	C1-O5-C5	-4.09	106.71	112.19
5	H	2	NAG	C1-C2-N2	-3.75	104.52	110.43
5	G	1	NAG	O3-C3-C2	3.56	116.80	109.40
5	H	1	NAG	O4-C4-C3	3.55	118.75	110.38
5	H	2	NAG	C4-C3-C2	3.47	116.11	111.02
5	H	1	NAG	C1-C2-N2	-3.47	104.97	110.43
5	H	1	NAG	O5-C5-C4	-3.31	102.76	110.83
5	H	2	NAG	O5-C5-C4	-3.19	103.06	110.83
5	H	1	NAG	O7-C7-C8	3.16	127.69	122.05
5	G	2	NAG	C6-C5-C4	2.65	119.53	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C4-C3-C2	2.59	114.81	111.02
5	H	1	NAG	C3-C4-C5	-2.38	105.91	110.23
5	H	2	NAG	O5-C5-C6	2.19	111.93	107.66
5	G	2	NAG	O4-C4-C3	-2.13	105.36	110.38
5	H	2	NAG	O5-C1-C2	-2.02	108.16	111.29
5	H	1	NAG	O7-C7-N2	-2.02	118.41	121.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

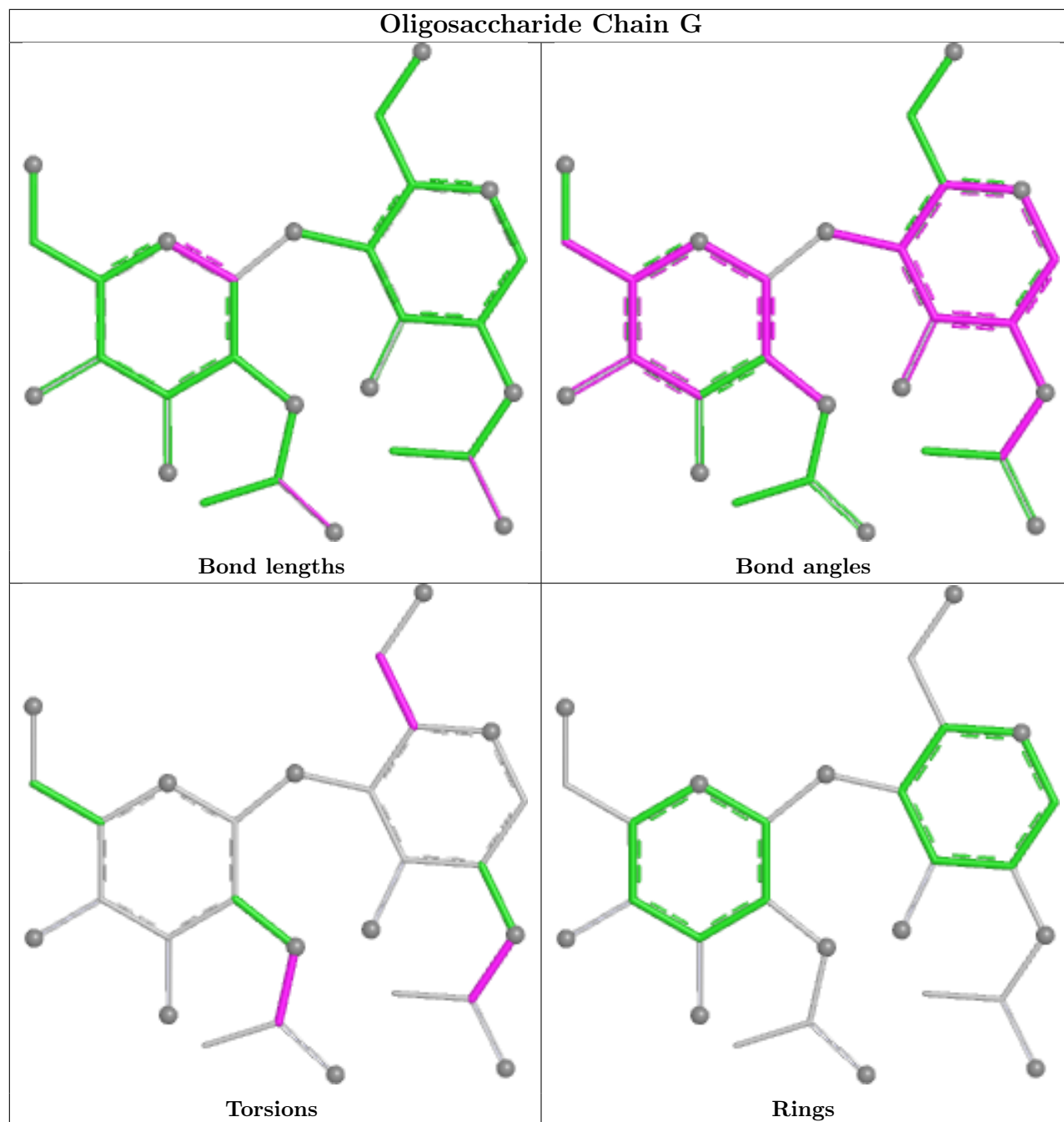
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C8-C7-N2-C2
5	H	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O7-C7-N2-C2
5	G	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C3-C2-N2-C7
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2

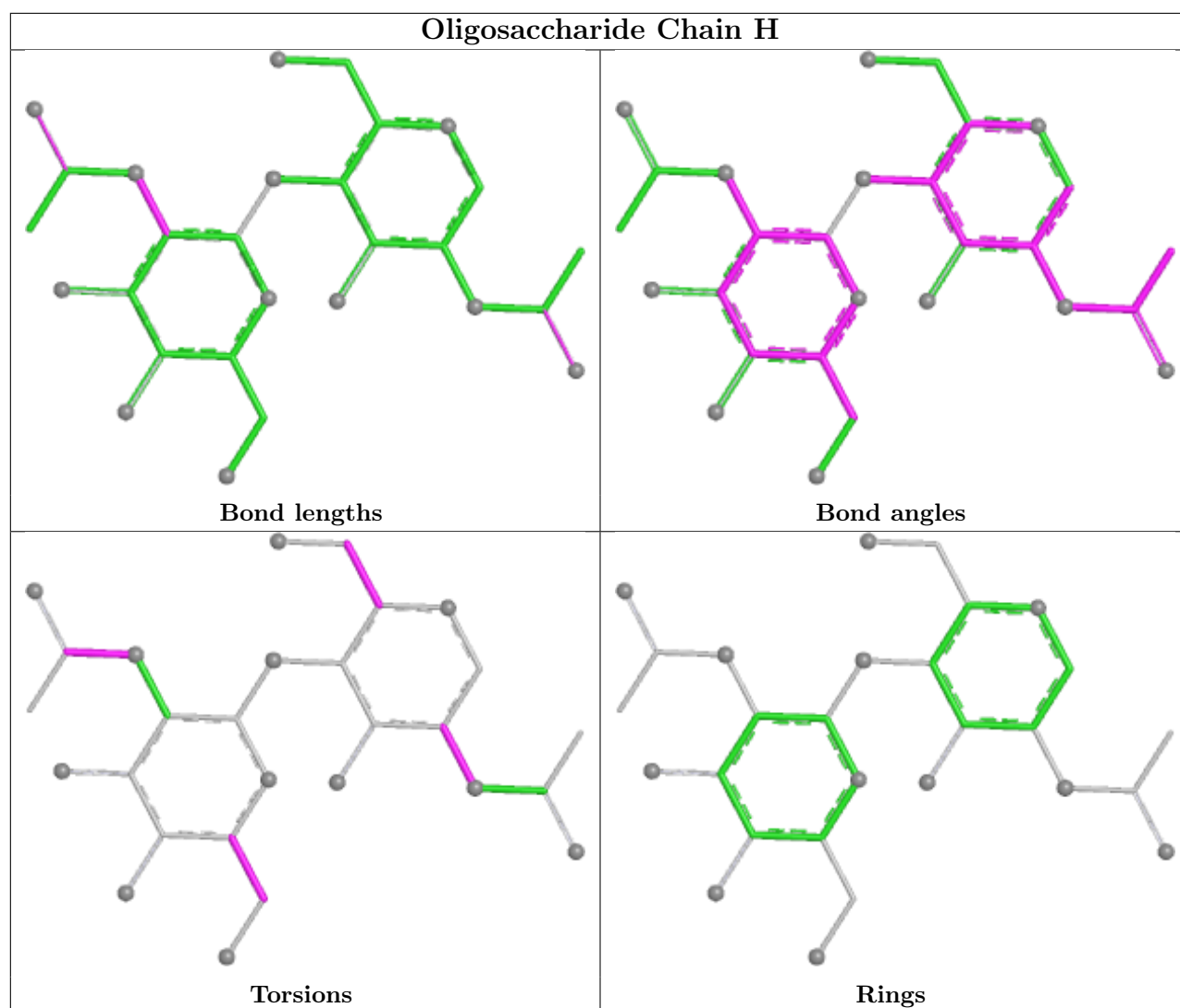
There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	11	0
5	H	2	NAG	10	0
5	G	2	NAG	4	0
5	G	1	NAG	10	0

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





5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.