



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:45 PM UTC

PDB ID : 1FZC / pdb_00001fzc
Title : CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN WITH TWO DIFFERENT BOUND LIGANDS
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Deposited on : 1998-05-19
Resolution : 2.30 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

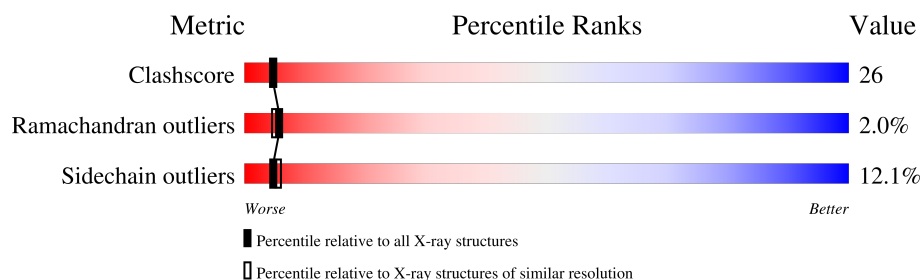
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	
1	D	87	
2	B	328	
2	E	328	
3	C	319	
3	F	319	
4	G	4	
4	H	4	

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Mol	Chain	Length	Quality of chain
5	I	4	 75% 25%
5	J	4	 75% 25%
6	K	2	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called FIBRIN.

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

- Molecule 2 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	0
			2473	1544	434	473	22			
2	E	308	Total	C	N	O	S	0	0	0
			2473	1544	434	473	22			

- Molecule 3 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			
3	F	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	LYS	ILE	conflict	UNP P02679
F	88	LYS	ILE	conflict	UNP P02679

- Molecule 4 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			29	18	7	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			29	18	7	4			

- Molecule 5 is a protein called FIBRIN.

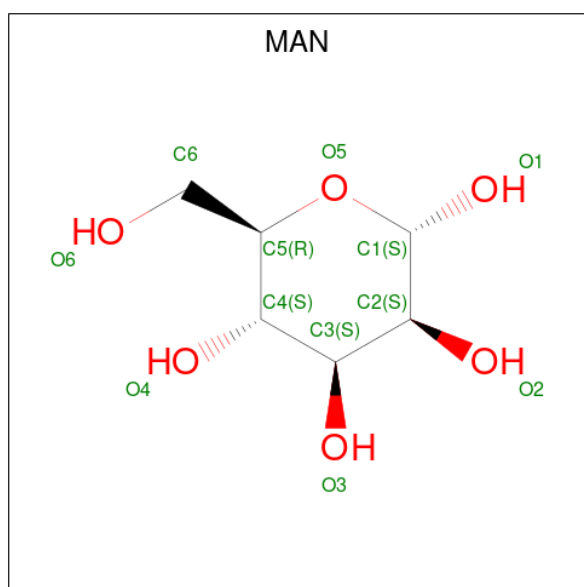
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			32	19	9	4			
5	J	4	Total	C	N	O	0	0	0
			32	19	9	4			

- Molecule 6 is 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
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).

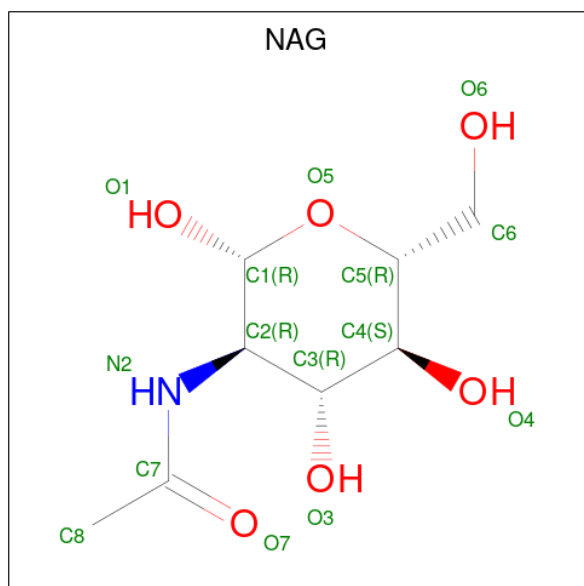


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 10 is water.

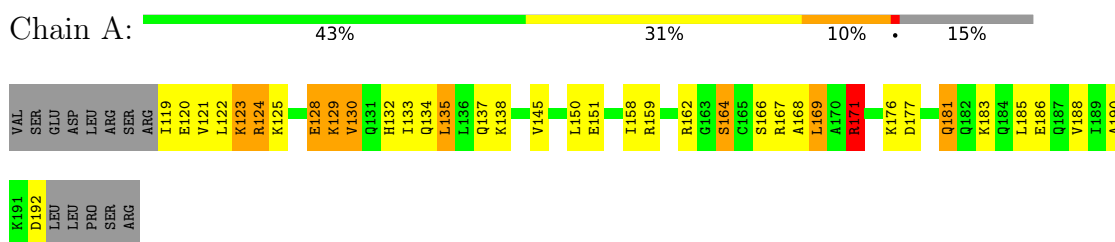
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	15	Total O 15 15	0	0
10	B	123	Total O 123 123	0	0
10	C	72	Total O 72 72	0	0
10	D	16	Total O 16 16	0	0
10	E	118	Total O 118 118	0	0
10	F	83	Total O 83 83	0	0
10	G	1	Total O 1 1	0	0
10	H	1	Total O 1 1	0	0
10	I	1	Total O 1 1	0	0
10	J	1	Total O 1 1	0	0

3 Residue-property plots

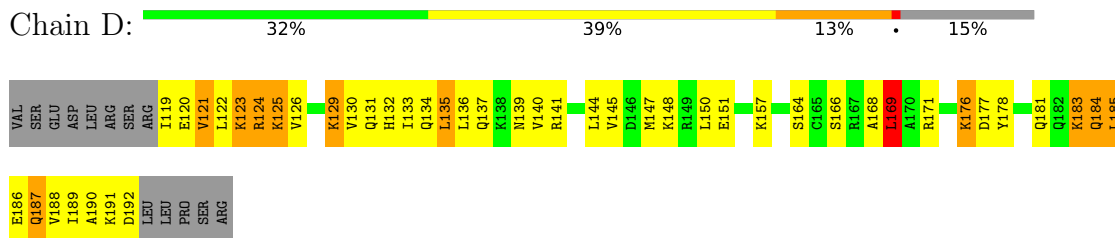
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

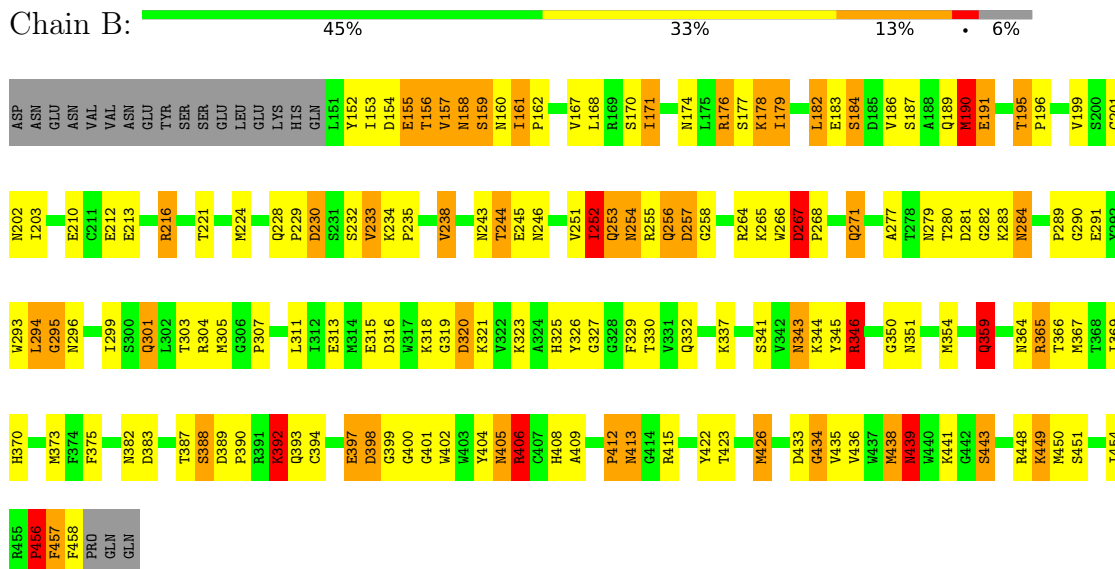
• Molecule 1: FIBRIN



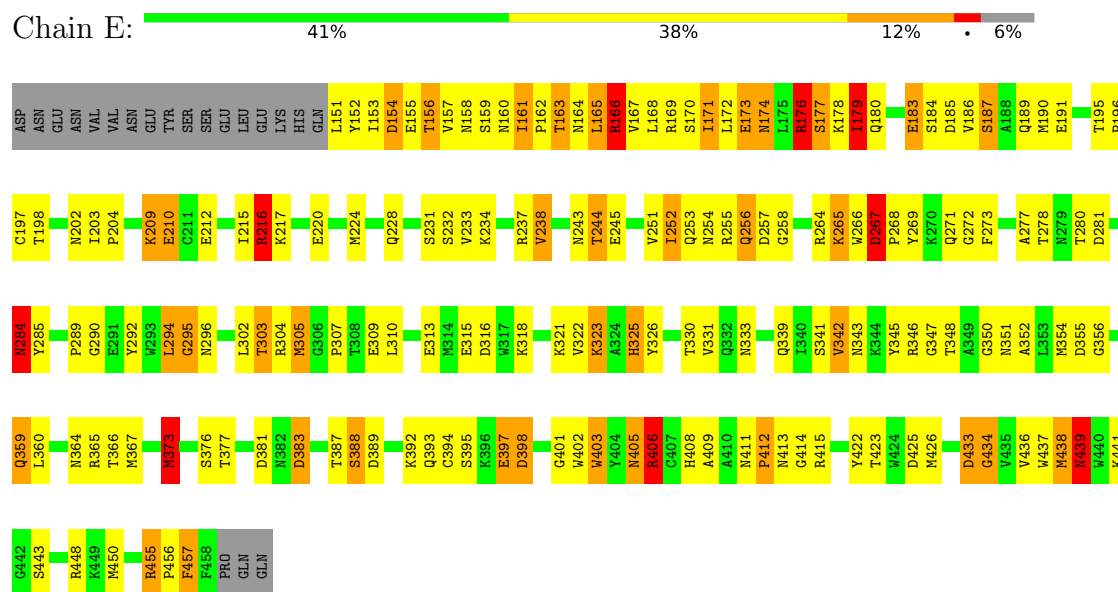
• Molecule 1: FIBRIN



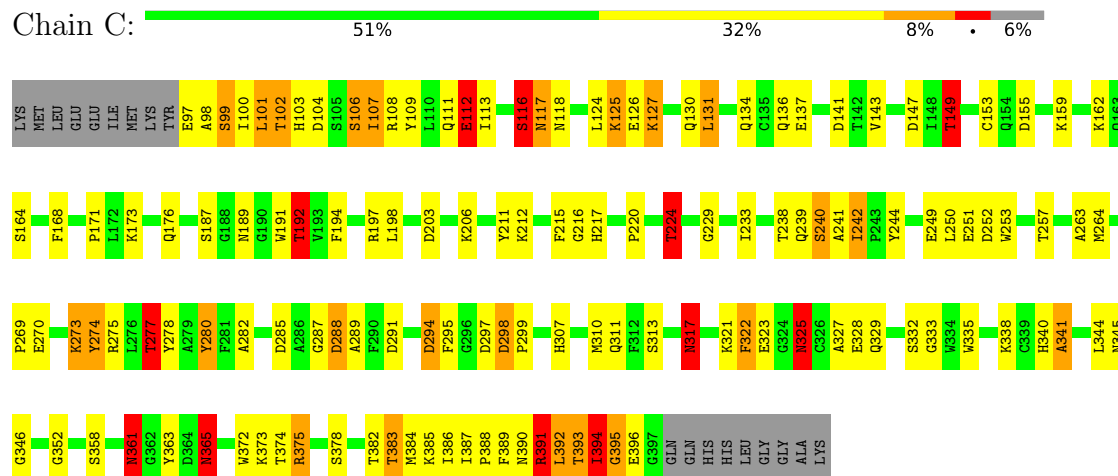
• Molecule 2: FIBRIN



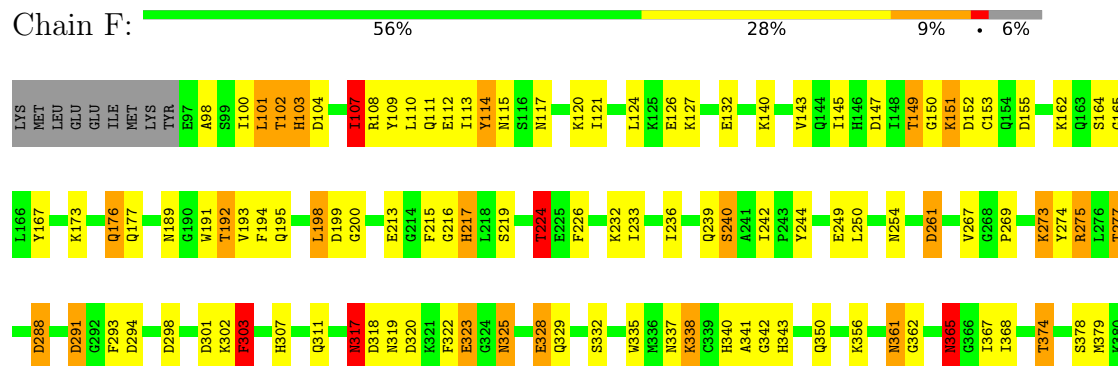
- Molecule 2: FIBRIN



- Molecule 3: FIBRIN



- Molecule 3: FIBRIN





● Molecule 4: FIBRIN



● Molecule 4: FIBRIN



● Molecule 5: FIBRIN



● Molecule 5: FIBRIN



● Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.44Å 95.60Å 113.64Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11594	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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, MAN, 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	0.81	0/609	1.92	12/811 (1.5%)
1	D	0.76	0/609	1.80	15/811 (1.8%)
2	B	1.21	6/2535 (0.2%)	2.30	131/3425 (3.8%)
2	E	1.18	8/2535 (0.3%)	2.34	147/3425 (4.3%)
3	C	0.92	1/2469 (0.0%)	2.08	75/3339 (2.2%)
3	F	0.93	1/2469 (0.0%)	2.00	74/3339 (2.2%)
4	G	0.90	0/30	2.94	3/40 (7.5%)
4	H	1.21	0/30	2.07	1/40 (2.5%)
5	I	1.00	0/33	1.97	1/43 (2.3%)
5	J	1.36	0/33	1.54	0/43
All	All	1.05	16/11352 (0.1%)	2.15	459/15316 (3.0%)

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
3	C	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	295	GLY	N-CA	14.87	1.64	1.45
2	E	295	GLY	N-CA	12.71	1.62	1.45
2	B	434	GLY	N-CA	12.33	1.63	1.45
2	E	258	GLY	N-CA	11.16	1.61	1.45
2	E	290	GLY	N-CA	10.71	1.52	1.44
3	C	274	TYR	N-CA	8.09	1.60	1.46
2	B	258	GLY	N-CA	7.95	1.56	1.45
2	E	350	GLY	CA-C	6.98	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	274	TYR	N-CA	6.63	1.56	1.46
2	E	257	ASP	C-O	5.91	1.29	1.24
2	B	401	GLY	CA-C	5.83	1.56	1.52
2	E	397	GLU	C-N	-5.23	1.26	1.33
2	E	398	ASP	N-CA	5.19	1.52	1.46
2	B	408	HIS	ND1-CE1	5.14	1.37	1.32
2	B	412	PRO	C-O	5.11	1.29	1.23
2	E	434	GLY	N-CA	5.00	1.51	1.45

All (459) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	184	SER	CA-CB-OG	14.07	139.23	111.10
2	E	294	LEU	O-C-N	-13.41	106.52	122.89
3	C	273	LYS	CA-C-N	-13.18	105.37	123.03
3	C	273	LYS	C-N-CA	-13.18	105.37	123.03
2	E	406	ARG	N-CA-C	12.89	128.83	111.30
1	A	167	ARG	CD-NE-CZ	12.84	142.38	124.40
2	B	294	LEU	O-C-N	-12.79	107.59	122.68
3	F	273	LYS	CA-C-N	-11.88	105.77	122.87
3	F	273	LYS	C-N-CA	-11.88	105.77	122.87
4	G	3	ARG	NE-CZ-NH2	-11.80	108.58	119.20
2	E	294	LEU	CA-C-N	-11.65	105.92	121.06
2	E	294	LEU	C-N-CA	-11.65	105.92	121.06
2	B	406	ARG	N-CA-C	11.50	126.94	111.30
2	B	252	ILE	CA-CB-CG2	11.39	129.87	110.50
2	E	406	ARG	O-C-N	-10.82	109.05	122.57
3	C	294	ASP	CA-CB-CG	-10.45	102.15	112.60
2	E	257	ASP	CA-C-N	-10.41	101.02	121.41
2	E	257	ASP	C-N-CA	-10.41	101.02	121.41
2	B	257	ASP	O-C-N	-10.33	112.42	123.26
2	B	267	ASP	CA-CB-CG	-10.27	102.33	112.60
2	B	364	ASN	OD1-CG-ND2	-10.18	112.42	122.60
2	B	412	PRO	CB-CA-C	10.14	124.27	110.98
2	E	405	ASN	O-C-N	-10.08	107.38	122.81
2	B	294	LEU	CA-C-N	-9.99	105.67	121.05
2	B	294	LEU	C-N-CA	-9.99	105.67	121.05
3	F	298	ASP	CA-CB-CG	9.97	122.57	112.60
3	C	126	GLU	CB-CG-CD	9.97	129.55	112.60
2	B	433	ASP	CA-C-N	-9.85	102.10	121.41
2	B	433	ASP	C-N-CA	-9.85	102.10	121.41
2	E	255	ARG	NE-CZ-NH2	9.62	127.86	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	ILE	CB-CA-C	9.53	119.99	110.65
2	E	412	PRO	O-C-N	-9.53	111.38	122.91
3	C	130	GLN	OE1-CD-NE2	-9.49	113.11	122.60
3	F	165	GLY	O-C-N	-9.42	112.56	124.15
2	B	359	GLN	OE1-CD-NE2	9.35	131.95	122.60
3	C	242	ILE	N-CA-CB	-9.33	101.75	111.36
2	E	304	ARG	CD-NE-CZ	9.27	137.38	124.40
2	E	401	GLY	CA-C-O	-9.23	112.08	120.75
2	B	451	SER	CA-CB-OG	9.06	129.23	111.10
2	B	408	HIS	N-CA-C	8.99	121.72	108.60
2	B	350	GLY	CA-C-N	8.96	135.46	122.21
2	B	350	GLY	C-N-CA	8.96	135.46	122.21
3	F	117	ASN	N-CA-C	-8.92	101.50	111.14
2	B	412	PRO	N-CA-C	-8.90	97.22	111.38
2	E	352	ALA	CA-C-O	-8.86	111.42	120.90
2	B	433	ASP	O-C-N	-8.75	110.95	122.59
2	E	252	ILE	CA-CB-CG2	8.72	125.32	110.50
3	C	176	GLN	OE1-CD-NE2	-8.69	113.91	122.60
2	E	183	GLU	CA-C-O	8.66	129.89	120.10
2	E	251	VAL	CA-C-N	8.66	132.11	121.71
2	E	251	VAL	C-N-CA	8.66	132.11	121.71
3	F	165	GLY	CA-C-O	8.65	126.88	120.91
2	B	343	ASN	OD1-CG-ND2	-8.63	113.97	122.60
2	E	228	GLN	OE1-CD-NE2	-8.55	114.05	122.60
3	C	102	THR	CA-C-O	8.54	129.35	119.18
2	B	329	PHE	CA-CB-CG	8.53	122.33	113.80
2	B	351	ASN	OD1-CG-ND2	-8.53	114.07	122.60
2	E	267	ASP	O-C-N	-8.48	113.68	120.38
2	E	267	ASP	CA-CB-CG	-8.45	104.15	112.60
2	B	370	HIS	CA-CB-CG	-8.41	105.39	113.80
2	B	230	ASP	CA-CB-CG	-8.33	104.27	112.60
2	E	356	GLY	CA-C-O	-8.26	115.99	122.52
3	C	395	GLY	N-CA-C	8.22	126.08	112.85
2	E	365	ARG	CD-NE-CZ	8.22	135.90	124.40
2	E	264	ARG	NH1-CZ-NH2	8.15	129.90	119.30
3	C	298	ASP	CA-CB-CG	8.12	120.72	112.60
2	B	409	ALA	N-CA-C	-8.11	103.91	113.88
3	C	125	LYS	CA-C-O	-8.10	110.94	120.10
3	C	285	ASP	CA-CB-CG	8.10	120.70	112.60
3	F	107	ILE	N-CA-C	-8.09	103.00	111.58
1	A	167	ARG	NE-CZ-NH1	8.06	129.56	121.50
2	B	346	ARG	N-CA-CB	8.03	125.45	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	252	ILE	N-CA-CB	-7.99	101.33	112.12
2	E	180	GLN	CA-C-O	7.99	129.20	119.38
2	B	265	LYS	O-C-N	7.95	132.06	122.20
2	B	332	GLN	OE1-CD-NE2	-7.94	114.66	122.60
2	E	393	GLN	OE1-CD-NE2	-7.88	114.72	122.60
2	B	383	ASP	CA-CB-CG	7.82	120.42	112.60
2	E	295	GLY	O-C-N	-7.79	113.80	122.60
2	E	284	ASN	CA-CB-CG	7.79	120.39	112.60
5	I	3	ARG	CD-NE-CZ	7.77	135.27	124.40
3	F	102	THR	CA-C-O	7.75	128.66	119.28
3	F	361	ASN	OD1-CG-ND2	7.75	130.35	122.60
2	B	289	PRO	CA-C-O	-7.74	112.42	121.86
2	E	215	ILE	CA-C-O	-7.73	112.12	120.47
2	B	435	VAL	CA-C-O	7.72	130.43	120.78
2	E	397	GLU	CA-C-O	-7.69	112.73	121.81
2	E	409	ALA	N-CA-C	-7.68	104.52	114.04
2	B	320	ASP	CA-CB-CG	7.62	120.22	112.60
2	E	203	ILE	CA-C-O	-7.60	113.65	119.20
2	B	257	ASP	CA-C-N	-7.59	106.53	121.41
2	B	257	ASP	C-N-CA	-7.59	106.53	121.41
2	B	243	ASN	CA-CB-CG	-7.56	105.04	112.60
2	B	436	VAL	N-CA-C	7.54	120.66	108.97
2	E	325	HIS	CA-CB-CG	7.54	121.34	113.80
3	F	224	THR	N-CA-CB	-7.53	97.67	111.37
2	B	295	GLY	CA-C-N	7.52	131.12	120.28
2	B	295	GLY	C-N-CA	7.52	131.12	120.28
2	B	253	GLN	CB-CG-CD	7.50	125.35	112.60
2	B	252	ILE	N-CA-CB	-7.43	102.08	112.12
3	C	192	THR	CA-C-O	7.43	128.31	120.36
2	B	365	ARG	CD-NE-CZ	7.42	134.79	124.40
2	E	341	SER	CA-C-O	-7.42	111.16	120.28
3	C	287	GLY	CA-C-N	7.41	133.02	122.05
3	C	287	GLY	C-N-CA	7.41	133.02	122.05
2	E	257	ASP	CA-C-O	-7.40	113.03	120.80
2	E	237	ARG	NE-CZ-NH2	7.35	125.82	119.20
3	C	375	ARG	CD-NE-CZ	7.34	134.68	124.40
2	E	184	SER	CB-CA-C	7.34	125.36	110.38
2	E	243	ASN	OD1-CG-ND2	-7.34	115.26	122.60
2	E	436	VAL	N-CA-C	7.33	120.33	108.97
3	F	311	GLN	OE1-CD-NE2	-7.33	115.27	122.60
3	C	220	PRO	O-C-N	-7.32	112.78	122.22
3	C	325	ASN	CA-CB-CG	7.31	119.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	339	GLN	O-C-N	-7.30	114.30	123.06
2	B	246	ASN	CA-CB-CG	-7.30	105.30	112.60
2	B	399	GLY	N-CA-C	7.29	125.80	115.30
2	E	290	GLY	N-CA-C	-7.29	102.75	112.81
2	B	296	ASN	OD1-CG-ND2	-7.27	115.33	122.60
2	E	376	SER	CA-C-O	-7.25	112.63	121.11
2	B	426	MET	CA-C-N	7.22	132.19	121.72
2	B	426	MET	C-N-CA	7.22	132.19	121.72
2	B	375	PHE	CA-C-N	7.21	133.87	122.62
2	B	375	PHE	C-N-CA	7.21	133.87	122.62
3	C	118	ASN	OD1-CG-ND2	-7.20	115.40	122.60
2	B	320	ASP	CA-C-N	7.19	134.74	122.37
2	B	320	ASP	C-N-CA	7.19	134.74	122.37
3	F	277	THR	OG1-CB-CG2	-7.18	94.94	109.30
3	C	203	ASP	O-C-N	-7.18	114.88	123.13
2	E	433	ASP	O-C-N	-7.15	112.42	121.78
2	B	341	SER	CA-C-O	-7.12	112.41	120.32
1	A	167	ARG	CA-C-O	-7.12	113.62	121.23
1	D	145	VAL	CA-C-O	-7.07	113.14	120.71
2	E	203	ILE	O-C-N	7.06	126.97	121.46
2	B	448	ARG	CD-NE-CZ	7.06	134.28	124.40
2	E	203	ILE	N-CA-C	7.05	115.67	107.77
2	E	272	GLY	O-C-N	-7.02	115.57	122.87
2	E	455	ARG	O-C-N	7.01	127.31	121.84
3	F	164	SER	CA-C-O	-7.00	113.93	121.56
3	F	126	GLU	O-C-N	-7.00	114.04	122.22
2	E	289	PRO	CA-C-N	-6.99	115.42	122.69
2	E	289	PRO	C-N-CA	-6.99	115.42	122.69
2	E	405	ASN	CA-C-N	-6.99	112.60	122.46
2	E	405	ASN	C-N-CA	-6.99	112.60	122.46
3	F	215	PHE	CA-C-N	6.98	132.24	121.42
3	F	215	PHE	C-N-CA	6.98	132.24	121.42
3	C	176	GLN	CB-CG-CD	6.98	124.46	112.60
2	E	333	ASN	OD1-CG-ND2	-6.98	115.62	122.60
3	F	365	ASN	OD1-CG-ND2	-6.97	115.63	122.60
2	E	264	ARG	NE-CZ-NH2	-6.95	112.94	119.20
2	E	397	GLU	N-CA-C	-6.95	101.17	110.55
2	E	302	LEU	CA-C-O	-6.93	113.54	120.82
3	C	278	TYR	O-C-N	-6.93	115.50	123.33
2	E	347	GLY	CA-C-N	6.93	134.27	121.52
2	E	347	GLY	C-N-CA	6.93	134.27	121.52
2	B	456	PRO	O-C-N	-6.91	113.31	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	433	ASP	N-CA-C	-6.90	99.52	109.31
2	B	252	ILE	N-CA-C	-6.87	106.80	113.53
3	F	217	HIS	CA-C-N	6.87	132.48	123.00
3	F	217	HIS	C-N-CA	6.87	132.48	123.00
3	C	242	ILE	CA-C-O	-6.85	116.22	120.88
2	E	355	ASP	CA-C-O	-6.84	111.52	119.24
3	C	322	PHE	CA-CB-CG	6.79	120.59	113.80
2	E	381	ASP	N-CA-C	6.79	119.94	107.99
2	B	279	ASN	CA-CB-CG	-6.77	105.83	112.60
2	B	254	ASN	CA-CB-CG	-6.76	105.84	112.60
1	D	164	SER	CB-CA-C	-6.75	98.31	109.65
3	F	267	VAL	CA-C-N	6.74	132.46	121.87
3	F	267	VAL	C-N-CA	6.74	132.46	121.87
2	B	406	ARG	O-C-N	-6.74	114.14	122.57
2	E	359	GLN	OE1-CD-NE2	6.73	129.33	122.60
3	C	332	SER	N-CA-C	6.73	116.93	108.45
2	E	397	GLU	O-C-N	-6.73	115.18	122.85
2	B	190	MET	N-CA-CB	6.72	120.69	110.28
3	C	197	ARG	CA-C-O	-6.71	113.11	120.36
3	C	112	GLU	CB-CG-CD	6.69	123.98	112.60
3	F	288	ASP	CA-C-O	-6.68	114.58	122.13
2	E	243	ASN	CA-C-O	-6.66	112.01	119.67
3	C	329	GLN	OE1-CD-NE2	-6.66	115.94	122.60
2	B	171	ILE	CA-CB-CG2	6.64	121.79	110.50
3	F	302	LYS	CA-C-O	-6.64	113.84	120.82
3	F	114	TYR	CA-C-O	6.64	127.74	120.90
3	C	117	ASN	CA-CB-CG	6.61	119.21	112.60
1	D	141	ARG	CD-NE-CZ	6.60	133.64	124.40
2	E	318	LYS	N-CA-C	-6.59	104.96	114.12
3	C	224	THR	N-CA-CB	-6.57	99.31	111.53
2	B	213	GLU	CB-CG-CD	6.56	123.75	112.60
2	B	265	LYS	CA-C-O	-6.54	113.90	121.82
2	B	271	GLN	CG-CD-NE2	6.54	126.21	116.40
3	C	345	ASN	N-CA-C	-6.53	105.28	112.72
2	E	296	ASN	N-CA-CB	6.52	119.81	110.16
2	E	255	ARG	NE-CZ-NH1	-6.51	114.98	121.50
3	C	361	ASN	OD1-CG-ND2	6.47	129.07	122.60
1	D	129	LYS	N-CA-C	-6.46	105.04	113.12
3	F	328	GLU	CB-CG-CD	-6.41	101.71	112.60
4	G	3	ARG	NH1-CZ-NH2	6.41	127.63	119.30
2	E	198	THR	CA-CB-OG1	-6.40	100.00	109.60
2	B	179	ILE	O-C-N	6.40	128.18	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	THR	CA-C-N	6.36	129.44	120.28
3	C	102	THR	C-N-CA	6.36	129.44	120.28
2	B	449	LYS	O-C-N	6.36	131.02	123.27
1	A	145	VAL	CA-C-O	-6.33	114.46	121.17
2	B	251	VAL	O-C-N	6.33	129.83	122.81
3	F	343	HIS	CA-CB-CG	6.32	120.12	113.80
2	E	412	PRO	CA-C-N	-6.31	113.98	125.66
2	E	412	PRO	C-N-CA	-6.31	113.98	125.66
2	B	337	LYS	CB-CG-CD	6.30	125.80	111.30
2	B	203	ILE	N-CA-C	6.29	114.82	107.77
2	E	437	TRP	CA-C-N	6.29	129.03	120.54
2	E	437	TRP	C-N-CA	6.29	129.03	120.54
2	B	422	TYR	CA-C-O	-6.25	114.54	121.23
2	E	179	ILE	CA-C-O	6.25	127.91	121.41
2	E	267	ASP	CA-C-O	6.24	124.78	118.79
1	A	167	ARG	O-C-N	6.24	130.10	123.42
2	B	304	ARG	NE-CZ-NH2	6.24	124.82	119.20
3	F	302	LYS	O-C-N	6.24	128.50	122.07
2	E	163	THR	N-CA-CB	6.24	119.86	110.19
3	F	329	GLN	CA-C-O	-6.24	113.81	120.42
3	C	131	LEU	O-C-N	-6.24	115.51	122.12
3	F	301	ASP	N-CA-C	6.23	118.59	111.11
3	F	317	ASN	CB-CG-ND2	6.22	125.73	116.40
3	C	365	ASN	CA-C-O	-6.21	112.58	119.78
2	E	342	VAL	CA-C-O	-6.20	115.16	121.67
2	E	395	SER	CA-CB-OG	-6.17	98.75	111.10
3	C	363	TYR	CA-C-O	-6.14	114.13	121.56
2	B	155	GLU	N-CA-C	-6.13	103.22	112.04
3	C	280	TYR	N-CA-C	6.12	118.60	108.99
2	B	301	GLN	CG-CD-NE2	6.12	125.58	116.40
2	E	264	ARG	N-CA-C	6.12	119.13	110.14
1	D	144	LEU	N-CA-C	-6.10	104.54	112.23
2	E	197	CYS	CA-C-O	-6.10	114.46	121.47
3	F	177	GLN	CB-CG-CD	6.09	122.95	112.60
2	E	323	LYS	CA-C-N	6.08	131.39	122.39
2	E	323	LYS	C-N-CA	6.08	131.39	122.39
2	B	405	ASN	CA-C-N	-6.08	113.89	122.46
2	B	405	ASN	C-N-CA	-6.08	113.89	122.46
2	E	281	ASP	CA-CB-CG	6.08	118.68	112.60
2	B	178	LYS	O-C-N	-6.08	115.68	122.12
1	D	135	LEU	CA-C-O	6.07	126.95	120.70
3	F	194	PHE	CA-C-O	6.06	126.33	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	130	GLN	CG-CD-OE1	6.05	132.90	120.80
3	C	289	ALA	CA-C-O	-6.05	111.94	119.38
2	B	307	PRO	O-C-N	-6.04	115.21	122.89
3	F	167	TYR	CA-C-O	-6.04	114.57	121.40
2	E	237	ARG	CD-NE-CZ	-6.03	115.95	124.40
3	F	332	SER	N-CA-C	6.03	116.05	108.45
2	B	238	VAL	N-CA-CB	-6.03	100.16	111.62
2	E	438	MET	O-C-N	6.03	128.36	122.09
2	E	406	ARG	N-CA-CB	-6.02	103.01	111.62
2	B	264	ARG	NE-CZ-NH1	-6.01	115.49	121.50
3	C	194	PHE	CA-CB-CG	6.00	119.80	113.80
2	E	455	ARG	CA-C-O	-6.00	113.13	119.13
2	E	238	VAL	N-CA-CB	-5.99	99.71	112.00
2	E	183	GLU	CB-CG-CD	5.99	122.79	112.60
1	D	169	LEU	CA-C-O	-5.98	114.10	120.92
3	F	193	VAL	CA-C-O	-5.98	113.99	121.11
2	B	264	ARG	NH1-CZ-NH2	5.97	127.06	119.30
2	E	265	LYS	N-CA-C	5.97	118.23	110.53
2	B	433	ASP	CB-CA-C	5.97	122.30	110.42
2	B	161	ILE	N-CA-CB	5.95	114.51	110.52
2	B	271	GLN	OE1-CD-NE2	-5.95	116.65	122.60
3	F	226	PHE	CA-C-N	5.95	131.39	123.00
3	F	226	PHE	C-N-CA	5.95	131.39	123.00
2	B	228	GLN	O-C-N	-5.93	116.13	121.17
2	B	412	PRO	O-C-N	-5.93	115.77	123.06
2	B	230	ASP	N-CA-C	5.92	119.18	108.69
2	E	210	GLU	O-C-N	-5.92	116.88	123.04
2	E	322	VAL	CA-C-N	5.92	131.81	122.21
2	E	322	VAL	C-N-CA	5.92	131.81	122.21
2	B	327	GLY	N-CA-C	-5.91	108.17	114.67
3	F	261	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	134	GLN	N-CA-C	-5.88	105.60	112.89
3	C	375	ARG	NE-CZ-NH1	5.88	127.38	121.50
2	E	278	THR	CA-C-N	5.88	129.10	120.82
2	E	278	THR	C-N-CA	5.88	129.10	120.82
3	F	293	PHE	CA-C-N	-5.87	113.78	122.41
3	F	293	PHE	C-N-CA	-5.87	113.78	122.41
2	E	202	ASN	CA-CB-CG	-5.86	106.74	112.60
2	B	290	GLY	N-CA-C	-5.85	104.73	112.81
2	E	255	ARG	N-CA-CB	5.85	121.61	111.13
3	F	340	HIS	N-CA-C	5.85	117.74	108.79
1	A	150	LEU	CA-C-O	5.84	126.73	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	321	LYS	N-CA-C	5.84	118.63	108.76
3	C	171	PRO	O-C-N	-5.83	115.85	122.91
3	C	238	THR	O-C-N	-5.83	114.64	122.22
2	B	238	VAL	O-C-N	-5.83	116.59	123.00
2	B	184	SER	CA-C-O	-5.82	114.38	120.55
3	C	341	ALA	N-CA-C	-5.80	105.98	114.39
3	C	127	LYS	CA-CB-CG	5.80	125.70	114.10
2	E	216	ARG	NE-CZ-NH2	5.79	124.42	119.20
2	B	397	GLU	N-CA-C	-5.79	100.85	110.17
2	E	411	ASN	CA-CB-CG	5.78	118.38	112.60
3	C	313	SER	CA-C-N	5.76	131.55	122.21
3	C	313	SER	C-N-CA	5.76	131.55	122.21
2	B	406	ARG	CA-C-N	5.76	132.06	121.70
2	B	406	ARG	C-N-CA	5.76	132.06	121.70
3	F	338	LYS	CA-C-N	5.75	132.05	121.70
3	F	338	LYS	C-N-CA	5.75	132.05	121.70
2	E	257	ASP	O-C-N	-5.75	115.50	122.68
2	E	303	THR	CA-C-O	-5.75	113.36	119.97
3	F	114	TYR	N-CA-C	-5.72	104.68	111.03
2	B	319	GLY	CA-C-O	-5.72	112.66	119.06
2	E	285	TYR	CA-C-O	-5.71	114.94	121.40
2	B	438	MET	N-CA-CB	5.71	118.63	110.06
3	C	118	ASN	CA-C-O	5.71	126.60	120.55
2	E	411	ASN	OD1-CG-ND2	-5.71	116.89	122.60
2	E	343	ASN	O-C-N	-5.70	115.37	122.73
3	C	116	SER	CA-CB-OG	-5.69	99.72	111.10
3	C	249	GLU	CB-CG-CD	5.69	122.27	112.60
3	C	311	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	E	273	PHE	CA-CB-CG	5.68	119.48	113.80
3	C	197	ARG	NE-CZ-NH2	-5.67	114.10	119.20
2	E	346	ARG	NE-CZ-NH2	5.64	124.28	119.20
3	F	233	ILE	CA-C-O	5.64	126.82	120.95
2	E	176	ARG	CA-C-O	5.63	126.52	120.55
4	G	3	ARG	CA-CB-CG	5.63	125.36	114.10
2	B	406	ARG	N-CA-CB	-5.62	103.59	111.62
2	E	450	MET	CA-C-O	-5.61	113.64	120.54
2	E	269	TYR	CA-C-O	5.59	126.40	119.97
2	B	290	GLY	CA-C-N	-5.59	114.31	122.19
2	B	290	GLY	C-N-CA	-5.59	114.31	122.19
3	F	198	LEU	CA-C-O	-5.58	112.53	120.51
3	F	275	ARG	CA-C-O	-5.58	114.88	120.96
3	C	274	TYR	N-CA-C	-5.57	99.30	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	364	ASN	CB-CG-ND2	5.57	124.76	116.40
2	E	406	ARG	CD-NE-CZ	5.56	132.19	124.40
3	F	337	ASN	CA-CB-CG	5.56	118.16	112.60
2	E	331	VAL	CA-C-O	-5.55	114.76	120.25
1	D	141	ARG	CA-C-N	5.54	127.71	120.28
1	D	141	ARG	C-N-CA	5.54	127.71	120.28
2	E	414	GLY	O-C-N	-5.54	118.04	122.81
2	E	438	MET	CA-C-O	-5.53	114.98	120.90
2	B	178	LYS	CA-C-O	5.53	126.41	120.55
2	B	439	ASN	OD1-CG-ND2	-5.53	117.08	122.60
2	E	184	SER	N-CA-CB	-5.52	101.79	110.30
2	E	305	MET	CA-CB-CG	5.52	125.15	114.10
3	C	125	LYS	N-CA-CB	5.52	118.72	110.22
1	D	166	SER	CA-C-O	-5.52	114.02	120.20
2	B	369	ILE	CA-C-N	5.51	131.96	122.09
2	B	369	ILE	C-N-CA	5.51	131.96	122.09
2	B	318	LYS	CA-CB-CG	5.50	125.10	114.10
1	A	159	ARG	NE-CZ-NH1	5.50	127.00	121.50
2	B	398	ASP	CA-C-O	-5.47	112.69	120.51
2	B	450	MET	CB-CA-C	5.47	119.14	109.89
3	F	274	TYR	N-CA-C	-5.47	102.04	109.54
2	E	292	TYR	CA-CB-CG	5.47	123.75	113.90
3	F	367	ILE	N-CA-CB	-5.45	106.83	112.28
3	F	254	ASN	CA-C-O	-5.44	113.41	119.34
2	E	348	THR	N-CA-CB	-5.43	102.18	110.33
2	B	426	MET	CA-C-O	5.43	124.79	118.77
3	F	273	LYS	CA-C-O	-5.42	113.45	120.71
3	C	329	GLN	CA-C-O	-5.41	115.12	120.70
2	E	388	SER	N-CA-C	-5.41	107.23	113.88
2	E	433	ASP	CB-CA-C	5.41	126.65	114.16
2	E	360	LEU	CA-C-O	-5.40	115.14	121.46
2	B	176	ARG	CA-C-O	-5.40	114.69	120.42
2	B	456	PRO	CA-C-O	-5.40	110.77	120.60
1	D	171	ARG	CG-CD-NE	5.40	123.87	112.00
2	B	448	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	B	397	GLU	O-C-N	-5.39	116.91	123.10
2	E	434	GLY	CA-C-O	-5.38	117.68	121.88
2	E	408	HIS	N-CA-C	5.38	116.46	108.60
2	E	292	TYR	CA-C-N	5.38	130.35	122.77
2	E	292	TYR	C-N-CA	5.38	130.35	122.77
2	E	412	PRO	CB-CA-C	5.38	118.06	111.12
2	E	185	ASP	CA-CB-CG	-5.38	107.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	192	THR	CA-CB-CG2	5.37	119.64	110.50
2	E	166	ARG	CD-NE-CZ	5.37	131.91	124.40
3	F	274	TYR	O-C-N	5.36	129.25	122.28
2	B	221	THR	CA-C-N	5.35	129.15	121.50
2	B	221	THR	C-N-CA	5.35	129.15	121.50
2	B	332	GLN	O-C-N	-5.35	116.07	122.65
3	F	177	GLN	CG-CD-NE2	5.35	124.42	116.40
3	C	277	THR	OG1-CB-CG2	-5.34	98.61	109.30
2	E	398	ASP	CB-CA-C	5.32	121.01	110.42
2	E	373	MET	N-CA-C	5.32	117.73	110.55
3	F	291	ASP	CA-CB-CG	-5.32	107.28	112.60
3	C	149	THR	N-CA-CB	5.32	119.89	111.43
3	C	164	SER	CA-C-O	-5.32	115.91	121.55
1	D	164	SER	CA-C-O	-5.31	113.32	119.64
2	B	364	ASN	CB-CG-ND2	5.30	124.35	116.40
2	B	365	ARG	O-C-N	5.30	128.58	122.17
2	B	365	ARG	CA-C-O	-5.29	114.89	120.55
2	B	257	ASP	CA-C-O	-5.29	115.77	121.38
3	F	378	SER	CA-C-O	5.29	126.14	120.38
3	F	383	THR	CB-CA-C	5.28	118.82	109.89
2	B	350	GLY	O-C-N	-5.28	115.84	122.70
2	B	443	SER	N-CA-C	5.26	118.86	112.23
2	B	255	ARG	NE-CZ-NH1	5.25	126.75	121.50
2	E	216	ARG	NE-CZ-NH1	-5.25	116.25	121.50
3	C	346	GLY	O-C-N	-5.25	118.29	122.81
2	B	366	THR	CA-C-O	-5.25	114.17	120.10
3	C	215	PHE	CA-C-O	-5.25	115.80	121.36
1	A	171	ARG	CA-C-O	-5.24	115.64	121.51
2	B	400	GLY	O-C-N	5.24	129.51	122.70
3	C	389	PHE	N-CA-C	5.24	117.73	111.71
3	C	277	THR	CA-CB-CG2	5.24	119.40	110.50
2	B	413	ASN	CB-CA-C	5.23	117.94	110.04
2	B	307	PRO	CA-C-O	5.23	127.27	121.36
2	E	198	THR	O-C-N	-5.22	116.82	123.24
2	E	439	ASN	OD1-CG-ND2	-5.22	117.38	122.60
3	C	224	THR	OG1-CB-CG2	5.22	119.74	109.30
2	E	412	PRO	N-CA-C	-5.21	103.26	111.34
3	C	216	GLY	O-C-N	-5.21	117.96	122.91
2	B	405	ASN	O-C-N	-5.20	112.98	122.44
2	E	305	MET	N-CA-CB	5.20	118.55	110.44
3	F	176	GLN	CB-CG-CD	5.18	121.40	112.60
3	F	103	HIS	N-CA-C	-5.17	105.64	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
3	C	386	ILE	O-C-N	5.16	128.89	123.00
3	F	176	GLN	OE1-CD-NE2	-5.16	117.44	122.60
3	F	216	GLY	N-CA-C	-5.16	103.44	112.53
2	E	403	TRP	O-C-N	-5.16	116.26	122.71
2	E	180	GLN	O-C-N	-5.16	115.52	122.43
1	D	169	LEU	CA-CB-CG	5.15	134.33	116.30
2	E	383	ASP	CB-CG-OD2	5.15	130.25	118.40
2	E	204	PRO	N-CA-CB	5.15	107.89	103.31
2	E	425	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	151	GLU	CA-CB-CG	5.14	124.38	114.10
3	C	327	ALA	CA-C-O	-5.13	115.43	120.82
2	B	382	ASN	N-CA-C	-5.12	104.49	111.56
2	E	434	GLY	O-C-N	5.12	127.23	122.47
3	F	303	PHE	CA-CB-CG	5.12	118.92	113.80
3	F	368	ILE	N-CA-C	5.12	117.13	109.20
3	F	177	GLN	CA-C-O	-5.12	115.94	121.87
3	F	277	THR	O-C-N	-5.11	117.14	123.33
1	A	171	ARG	NH1-CZ-NH2	5.11	125.94	119.30
3	C	241	ALA	N-CA-C	5.11	118.29	111.24
3	F	145	ILE	O-C-N	-5.11	117.93	123.14
3	F	381	LYS	N-CA-CB	5.11	121.03	111.53
2	B	392	LYS	CA-CB-CG	-5.10	103.90	114.10
2	B	266	TRP	N-CA-C	5.10	117.23	111.11
2	B	441	LYS	N-CA-C	5.09	120.12	112.94
3	F	329	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	B	422	TYR	O-C-N	5.09	128.86	123.42
3	F	254	ASN	CA-CB-CG	-5.08	107.52	112.60
3	F	261	ASP	CA-C-O	-5.08	115.37	121.11
3	F	374	THR	O-C-N	-5.07	116.82	122.75
2	B	295	GLY	O-C-N	-5.07	113.50	122.82
2	E	310	LEU	CA-C-N	5.06	130.13	123.00
2	E	310	LEU	C-N-CA	5.06	130.13	123.00
2	B	228	GLN	CA-C-O	5.06	127.09	121.22
3	F	319	ASN	N-CA-CB	-5.05	104.21	111.54
2	E	266	TRP	N-CA-C	5.05	117.17	111.11
2	B	182	LEU	CA-C-O	-5.05	114.39	120.10
1	D	184	GLN	N-CA-C	-5.05	104.86	111.02
2	E	377	THR	N-CA-CB	5.05	119.80	111.62
3	C	278	TYR	CA-C-N	5.04	127.48	120.63
3	C	278	TYR	C-N-CA	5.04	127.48	120.63
1	A	181	GLN	OE1-CD-NE2	5.04	127.64	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	337	ASN	CB-CG-ND2	5.03	123.95	116.40
3	C	134	GLN	CB-CG-CD	-5.01	104.08	112.60
3	C	206	LYS	N-CA-CB	-5.01	103.53	111.05
2	E	290	GLY	CA-C-N	5.01	129.26	122.19
2	E	290	GLY	C-N-CA	5.01	129.26	122.19
3	F	323	GLU	CB-CG-CD	5.01	121.12	112.60
3	C	317	ASN	OD1-CG-ND2	-5.00	117.59	122.60
4	H	3	ARG	O-C-N	5.00	127.19	121.94
3	C	288	ASP	N-CA-C	5.00	117.12	109.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	274	TYR	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	608	0	647	32	0
1	D	608	0	649	59	0
2	B	2473	0	2336	127	0
2	E	2473	0	2335	188	0
3	C	2404	0	2249	112	0
3	F	2404	0	2249	136	0
4	G	29	0	32	1	0
4	H	29	0	32	0	0
5	I	32	0	32	0	0
5	J	32	0	32	1	0
6	K	28	0	26	3	0
7	B	11	0	10	2	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	E	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	14	0	13	2	0
10	A	15	0	0	6	0
10	B	123	0	0	18	0
10	C	72	0	0	7	0
10	D	16	0	0	3	0
10	E	118	0	0	5	0
10	F	83	0	0	11	0
10	G	1	0	0	1	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
All	All	11594	0	10655	558	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (558) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:277:THR:HG21	3:F:303:PHE:CD2	1.37	1.59
3:C:277:THR:CG2	3:F:303:PHE:CE2	1.83	1.42
1:A:135:LEU:HD12	10:A:206:HOH:O	1.27	1.34
2:E:423:THR:H	2:E:426:MET:CE	1.40	1.34
2:E:423:THR:N	2:E:426:MET:CE	1.91	1.33
2:E:373:MET:HE2	2:E:405:ASN:CB	1.60	1.29
2:E:373:MET:HE2	2:E:405:ASN:CA	1.63	1.26
1:D:133:ILE:CD1	2:E:161:ILE:HD13	1.65	1.25
3:C:277:THR:HG21	3:F:303:PHE:CG	1.27	1.25
2:B:191:GLU:HG3	10:B:604:HOH:O	1.33	1.24
2:E:422:TYR:CA	2:E:426:MET:HE1	1.68	1.24
3:C:361:ASN:HB3	10:C:604:HOH:O	1.38	1.22
3:C:282:ALA:O	3:C:394:ILE:HD12	1.41	1.18
2:E:162:PRO:HG3	3:F:103:HIS:CE1	1.79	1.17
3:C:277:THR:HG22	3:F:303:PHE:CE2	1.36	1.15
3:C:277:THR:CG2	3:F:303:PHE:CD2	2.07	1.14
1:D:133:ILE:HD11	2:E:161:ILE:HD13	1.17	1.13
2:E:423:THR:N	2:E:426:MET:HE2	1.64	1.10
2:E:423:THR:H	2:E:426:MET:HE3	1.11	1.09
2:E:373:MET:CE	2:E:405:ASN:HA	1.82	1.09
2:E:438:MET:HE3	2:E:443:SER:OG	1.53	1.08
2:E:373:MET:HE2	2:E:405:ASN:HA	1.24	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:422:TYR:HA	2:E:426:MET:CE	1.85	1.06
3:F:98:ALA:HA	3:F:101:LEU:HD12	1.35	1.05
2:E:168:LEU:HA	2:E:171:ILE:HD11	1.37	1.05
2:E:169:ARG:NH2	3:F:109:TYR:HD2	1.54	1.04
3:C:277:THR:CG2	3:F:303:PHE:CG	2.22	1.04
2:B:326:TYR:CE1	2:B:354:MET:HE3	1.93	1.04
2:B:157:VAL:HG12	3:C:100:ILE:HG22	1.40	1.03
2:E:422:TYR:CA	2:E:426:MET:CE	2.36	1.03
3:F:217:HIS:O	3:F:224:THR:HG23	1.60	1.02
2:E:422:TYR:HA	2:E:426:MET:HE1	1.03	1.01
1:D:119:ILE:HD11	1:D:123:LYS:HG3	1.39	1.01
2:E:422:TYR:C	2:E:426:MET:CE	2.35	1.00
2:E:183:GLU:HG3	3:F:124:LEU:HD13	1.39	1.00
2:B:157:VAL:HG12	3:C:100:ILE:CG2	1.92	0.99
3:F:240:SER:OG	3:F:242:ILE:HD11	1.62	0.99
2:B:244:THR:HG21	2:B:313:GLU:OE2	1.63	0.99
3:C:240:SER:C	3:C:242:ILE:HD12	1.86	0.98
10:E:633:HOH:O	5:J:1:GLY:HA2	1.63	0.98
2:E:345:TYR:HB2	2:E:354:MET:HE3	1.44	0.98
3:C:103:HIS:O	3:C:107:ILE:HG22	1.64	0.98
2:B:423:THR:OG1	2:B:426:MET:HE3	1.65	0.97
2:B:326:TYR:CD1	2:B:354:MET:CE	2.48	0.96
2:E:326:TYR:CD2	2:E:354:MET:HE2	2.00	0.96
2:B:224:MET:SD	10:B:707:HOH:O	2.23	0.95
2:E:165:LEU:HD21	3:F:107:ILE:HD12	1.47	0.95
2:E:169:ARG:O	2:E:173:GLU:HG3	1.66	0.94
6:K:1:NAG:O4	6:K:2:NAG:O5	1.83	0.94
2:B:190:MET:SD	10:C:613:HOH:O	2.26	0.94
2:E:169:ARG:NH2	3:F:109:TYR:CD2	2.31	0.94
7:B:501:MAN:H2	6:K:2:NAG:O3	1.70	0.92
2:E:373:MET:HE2	2:E:405:ASN:HB2	1.51	0.91
2:E:224:MET:HE1	10:F:661:HOH:O	1.72	0.90
1:D:126:VAL:O	1:D:130:VAL:HG23	1.71	0.89
1:D:133:ILE:HD11	2:E:161:ILE:CD1	2.01	0.89
2:B:212:GLU:HG3	2:B:216:ARG:NH1	1.86	0.89
3:C:325:ASN:ND2	3:C:328:GLU:H	1.70	0.89
1:D:131:GLN:HG3	1:D:132:HIS:HD2	1.36	0.88
1:D:119:ILE:CD1	1:D:123:LYS:HG3	2.04	0.88
3:F:103:HIS:O	3:F:107:ILE:HG22	1.74	0.88
3:F:114:TYR:HD2	3:F:115:ASN:ND2	1.71	0.87
1:D:133:ILE:CD1	2:E:161:ILE:CD1	2.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:THR:H	2:E:426:MET:HE2	1.25	0.87
3:F:98:ALA:HA	3:F:101:LEU:CD1	2.05	0.86
2:B:257:ASP:O	2:B:291:GLU:OE2	1.94	0.86
2:B:326:TYR:HE1	2:B:354:MET:HE3	1.40	0.86
2:E:169:ARG:HB2	3:F:110:LEU:CD2	2.05	0.86
2:E:345:TYR:HB2	2:E:354:MET:CE	2.06	0.86
3:F:217:HIS:O	3:F:224:THR:CG2	2.22	0.86
3:F:240:SER:OG	3:F:242:ILE:CD1	2.23	0.85
2:B:326:TYR:HD1	2:B:354:MET:CE	1.89	0.85
2:E:326:TYR:HD2	2:E:354:MET:HE2	1.35	0.85
2:E:422:TYR:C	2:E:426:MET:HE1	1.98	0.85
2:B:394:CYS:O	2:B:397:GLU:O	1.94	0.85
2:B:387:THR:HG22	2:B:388:SER:H	1.42	0.84
1:D:119:ILE:HD11	1:D:123:LYS:HE3	1.58	0.84
3:C:149:THR:CG2	3:C:168:PHE:O	2.24	0.84
1:D:157:LYS:HE3	3:F:132:GLU:OE2	1.77	0.84
3:F:239:GLN:O	3:F:242:ILE:HD12	1.77	0.83
3:C:240:SER:OG	3:C:242:ILE:HD11	1.78	0.83
2:E:387:THR:HG21	2:E:392:LYS:HB2	1.57	0.83
1:A:119:ILE:HD11	1:A:123:LYS:HD2	1.60	0.83
2:B:412:PRO:HA	10:B:615:HOH:O	1.78	0.83
3:F:391:ARG:O	3:F:395:GLY:HA3	1.77	0.82
2:E:373:MET:CE	2:E:405:ASN:CB	2.52	0.82
2:B:326:TYR:CD1	2:B:354:MET:HE2	2.13	0.82
2:E:158:ASN:HB2	3:F:100:ILE:HD13	1.62	0.82
2:E:209:LYS:HD2	2:E:305:MET:HE1	1.61	0.81
2:B:326:TYR:HD1	2:B:354:MET:HE2	1.45	0.81
3:C:217:HIS:O	3:C:224:THR:HG23	1.79	0.81
2:E:176:ARG:HE	3:F:120:LYS:NZ	1.80	0.80
2:E:158:ASN:CG	3:F:100:ILE:HD13	2.07	0.80
2:E:169:ARG:HH21	3:F:109:TYR:HD2	0.82	0.80
2:B:326:TYR:CE1	2:B:354:MET:CE	2.63	0.80
2:E:169:ARG:HB2	3:F:110:LEU:HD21	1.64	0.79
1:A:135:LEU:CD1	10:A:203:HOH:O	2.29	0.79
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.62	0.79
2:E:172:LEU:HB3	3:F:113:ILE:CD1	2.12	0.79
2:E:423:THR:N	2:E:426:MET:HE3	1.75	0.79
3:C:340:HIS:O	4:G:1:GLY:N	2.14	0.79
3:F:392:LEU:HG	3:F:393:THR:H	1.47	0.79
2:E:224:MET:HG2	10:E:652:HOH:O	1.81	0.78
2:E:183:GLU:CG	3:F:124:LEU:HD13	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:307:PRO:O	2:E:456:PRO:O	2.01	0.78
2:E:168:LEU:O	2:E:171:ILE:HG12	1.83	0.78
2:E:456:PRO:O	2:E:457:PHE:HB3	1.84	0.78
2:E:169:ARG:NE	3:F:110:LEU:HD21	1.99	0.78
3:C:240:SER:O	3:C:242:ILE:HD12	1.84	0.77
3:C:240:SER:O	3:C:242:ILE:CD1	2.32	0.77
3:F:149:THR:HG22	3:F:150:GLY:H	1.49	0.77
3:C:149:THR:HG22	3:C:168:PHE:O	1.84	0.77
1:D:123:LYS:HZ3	2:E:151:LEU:N	1.83	0.77
2:E:158:ASN:CB	3:F:100:ILE:HD13	2.14	0.76
3:F:176:GLN:NE2	10:F:601:HOH:O	2.17	0.76
1:D:177:ASP:O	1:D:181:GLN:HG3	1.85	0.76
3:C:212:LYS:NZ	3:C:270:GLU:OE1	2.17	0.76
2:E:155:GLU:O	2:E:157:VAL:N	2.18	0.76
2:E:373:MET:HE2	2:E:405:ASN:CG	2.11	0.76
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.67	0.76
2:B:224:MET:CE	2:B:277:ALA:HB3	2.17	0.75
1:D:126:VAL:HG13	2:E:157:VAL:HG22	1.68	0.75
2:E:394:CYS:O	2:E:397:GLU:O	2.04	0.75
3:F:114:TYR:CD2	3:F:115:ASN:ND2	2.53	0.75
3:C:240:SER:C	3:C:242:ILE:CD1	2.60	0.74
3:C:191:TRP:HH2	3:C:393:THR:HG23	1.53	0.74
2:B:156:THR:HG22	2:B:160:ASN:ND2	2.03	0.73
3:F:307:HIS:HE1	3:F:341:ALA:H	1.36	0.73
2:B:252:ILE:HG12	2:B:299:ILE:HG12	1.69	0.73
2:E:172:LEU:HB3	3:F:113:ILE:HD12	1.68	0.73
2:E:212:GLU:HG3	2:E:216:ARG:NH1	2.04	0.72
3:F:195:GLN:OE1	3:F:382:THR:HG22	1.90	0.72
3:C:307:HIS:HE1	3:C:341:ALA:H	1.36	0.72
3:F:392:LEU:HG	3:F:393:THR:N	2.05	0.72
2:E:195:THR:HG22	2:E:196:PRO:HD2	1.70	0.71
3:C:391:ARG:O	3:C:395:GLY:HA3	1.91	0.71
2:B:412:PRO:CA	10:B:615:HOH:O	2.37	0.71
1:D:120:GLU:HA	1:D:124:ARG:HB2	1.72	0.71
2:B:252:ILE:HD11	2:B:454:ILE:CD1	2.20	0.71
2:E:163:THR:O	2:E:166:ARG:N	2.23	0.71
2:E:169:ARG:HE	3:F:110:LEU:HD21	1.55	0.71
3:C:149:THR:HG23	3:C:168:PHE:O	1.91	0.71
3:C:217:HIS:O	3:C:224:THR:CG2	2.38	0.71
1:D:147:MET:HE1	2:E:179:ILE:HG12	1.71	0.71
2:B:373:MET:HE2	2:B:404:TYR:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:195:GLN:OE1	3:F:382:THR:CG2	2.38	0.71
2:B:387:THR:HG22	2:B:388:SER:N	2.05	0.70
1:D:131:GLN:HG3	1:D:132:HIS:CD2	2.26	0.70
1:D:151:GLU:HG3	10:D:201:HOH:O	1.91	0.70
2:E:168:LEU:HA	2:E:171:ILE:CD1	2.20	0.70
2:E:179:ILE:HD11	3:F:121:ILE:HG12	1.73	0.70
3:C:100:ILE:C	3:C:102:THR:H	1.99	0.70
1:D:136:LEU:HB3	2:E:168:LEU:HD23	1.74	0.69
3:F:239:GLN:O	3:F:242:ILE:CD1	2.40	0.69
2:E:456:PRO:O	2:E:457:PHE:CB	2.41	0.69
2:E:176:ARG:HE	3:F:120:LYS:HZ2	1.40	0.69
3:C:189:ASN:OD1	3:C:392:LEU:HB2	1.92	0.68
2:E:323:LYS:HD3	10:E:698:HOH:O	1.94	0.68
3:F:152:ASP:OD2	3:F:244:TYR:OH	2.10	0.68
1:A:135:LEU:HD13	10:A:203:HOH:O	1.94	0.68
3:F:383:THR:HG22	10:F:634:HOH:O	1.93	0.67
3:F:98:ALA:CA	3:F:101:LEU:HD12	2.21	0.67
3:C:153:CYS:SG	3:C:192:THR:HB	2.34	0.67
3:F:100:ILE:O	3:F:102:THR:N	2.25	0.67
2:E:161:ILE:HG21	3:F:103:HIS:ND1	2.10	0.67
2:E:162:PRO:HG3	3:F:103:HIS:HE1	1.50	0.67
2:E:405:ASN:O	2:E:406:ARG:C	2.38	0.67
1:A:120:GLU:HA	1:A:124:ARG:HB2	1.75	0.67
2:B:201:CYS:SG	2:B:224:MET:HE1	2.35	0.67
2:B:415:ARG:O	2:B:434:GLY:HA2	1.95	0.67
2:B:195:THR:HG22	2:B:196:PRO:HD2	1.77	0.67
1:D:140:VAL:HG23	1:D:185:LEU:HD11	1.77	0.67
2:E:387:THR:HG22	2:E:388:SER:N	2.08	0.66
2:B:224:MET:HE3	2:B:277:ALA:HB3	1.76	0.66
3:C:344:LEU:HD13	3:C:382:THR:HG21	1.78	0.66
3:F:100:ILE:C	3:F:102:THR:H	2.04	0.66
2:E:169:ARG:HE	3:F:110:LEU:CD2	2.08	0.66
2:E:161:ILE:CG2	3:F:103:HIS:ND1	2.59	0.66
2:E:326:TYR:CE2	2:E:354:MET:CE	2.79	0.65
3:C:282:ALA:O	3:C:394:ILE:CD1	2.34	0.65
2:E:439:ASN:HD22	2:E:439:ASN:H	1.45	0.65
2:E:294:LEU:O	2:E:295:GLY:C	2.37	0.65
1:A:122:LEU:O	1:A:124:ARG:N	2.29	0.65
3:F:151:LYS:HD2	3:F:155:ASP:OD2	1.96	0.65
2:B:412:PRO:O	2:B:413:ASN:HB2	1.96	0.65
2:B:157:VAL:HG12	3:C:100:ILE:HG21	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:ALA:HA	3:C:101:LEU:HD12	1.79	0.65
2:E:172:LEU:CD2	3:F:114:TYR:HA	2.27	0.65
2:E:326:TYR:CD2	2:E:354:MET:CE	2.78	0.65
3:F:176:GLN:HG3	10:F:668:HOH:O	1.97	0.65
2:E:195:THR:CG2	2:E:196:PRO:HD2	2.26	0.64
3:F:153:CYS:SG	3:F:192:THR:HB	2.38	0.64
3:C:344:LEU:HD13	3:C:382:THR:CG2	2.29	0.64
2:E:373:MET:CE	2:E:405:ASN:HB2	2.25	0.64
2:E:326:TYR:CE2	2:E:354:MET:HE2	2.33	0.63
3:C:100:ILE:O	3:C:102:THR:N	2.28	0.63
2:E:158:ASN:HB2	3:F:100:ILE:HG21	1.80	0.63
2:E:168:LEU:O	2:E:171:ILE:CG1	2.46	0.63
2:E:164:ASN:O	2:E:168:LEU:HD13	1.99	0.63
2:E:168:LEU:CA	2:E:171:ILE:HD11	2.22	0.63
2:E:373:MET:CE	2:E:405:ASN:CG	2.70	0.63
3:C:153:CYS:HB2	3:C:192:THR:HG22	1.81	0.63
3:C:322:PHE:CE1	3:C:323:GLU:HG2	2.33	0.63
3:F:189:ASN:HD22	3:F:391:ARG:HG3	1.64	0.63
2:E:155:GLU:C	2:E:157:VAL:H	2.05	0.62
2:E:183:GLU:HB3	10:F:671:HOH:O	1.99	0.62
3:C:104:ASP:O	3:C:107:ILE:CG2	2.48	0.62
2:E:161:ILE:CB	2:E:162:PRO:HD3	2.29	0.62
2:B:326:TYR:CD1	2:B:354:MET:HE3	2.20	0.62
2:E:315:GLU:OE2	2:E:448:ARG:NH2	2.33	0.62
2:B:252:ILE:CD1	2:B:454:ILE:CD1	2.78	0.61
1:A:164:SER:HB3	3:C:137:GLU:O	2.00	0.61
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.82	0.61
2:E:179:ILE:HD11	3:F:121:ILE:CG1	2.30	0.61
2:B:367:MET:O	2:B:405:ASN:O	2.18	0.61
2:B:252:ILE:HD11	2:B:454:ILE:HD11	1.82	0.61
2:B:438:MET:HE3	2:B:443:SER:OG	2.00	0.61
2:E:172:LEU:HD22	3:F:114:TYR:HA	1.81	0.61
2:E:309:GLU:OE1	2:E:325:HIS:HE1	1.84	0.61
3:C:307:HIS:HD2	3:C:335:TRP:O	1.82	0.61
2:B:252:ILE:CD1	2:B:454:ILE:HG12	2.31	0.61
1:D:148:LYS:NZ	10:D:202:HOH:O	2.33	0.60
2:E:423:THR:OG1	2:E:426:MET:HE2	2.01	0.60
2:B:157:VAL:CG1	3:C:100:ILE:CG2	2.76	0.59
1:D:178:TYR:OH	2:E:178:LYS:HD2	2.02	0.59
3:F:240:SER:C	3:F:242:ILE:HD12	2.27	0.59
3:C:269:PRO:O	3:C:273:LYS:O	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:ASN:HD22	3:C:328:GLU:H	1.49	0.59
1:D:126:VAL:CG1	2:E:157:VAL:HG22	2.32	0.59
3:F:273:LYS:NZ	3:F:317:ASN:HD21	2.00	0.59
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.38	0.59
3:C:136:GLN:NE2	10:C:603:HOH:O	2.28	0.59
3:C:298:ASP:CG	3:C:299:PRO:HD2	2.28	0.59
2:E:422:TYR:HB2	2:E:426:MET:HE3	1.85	0.58
3:F:108:ARG:O	3:F:112:GLU:HG3	2.03	0.58
3:F:191:TRP:HH2	3:F:393:THR:HG1	1.48	0.58
2:B:157:VAL:CG1	3:C:100:ILE:HG22	2.25	0.58
2:B:405:ASN:O	2:B:406:ARG:C	2.45	0.58
3:F:269:PRO:O	3:F:273:LYS:O	2.21	0.58
3:F:307:HIS:CE1	3:F:341:ALA:H	2.20	0.58
2:E:422:TYR:CA	2:E:426:MET:HE3	2.29	0.58
3:F:189:ASN:ND2	3:F:391:ARG:HG3	2.19	0.58
3:C:103:HIS:O	3:C:107:ILE:CG2	2.46	0.57
3:C:189:ASN:ND2	3:C:391:ARG:HG3	2.19	0.57
3:C:189:ASN:OD1	3:C:392:LEU:HD22	2.04	0.57
3:F:191:TRP:CH2	3:F:393:THR:OG1	2.56	0.57
1:A:122:LEU:O	1:A:125:LYS:N	2.38	0.57
2:B:346:ARG:NE	10:B:602:HOH:O	2.33	0.57
2:E:163:THR:O	2:E:166:ARG:HB2	2.04	0.57
2:E:415:ARG:O	2:E:434:GLY:HA2	2.05	0.57
3:F:392:LEU:O	3:F:395:GLY:HA3	2.05	0.57
2:B:190:MET:CE	3:C:131:LEU:HA	2.35	0.57
1:D:190:ALA:O	1:D:192:ASP:N	2.33	0.57
2:E:155:GLU:C	2:E:157:VAL:N	2.62	0.57
2:B:415:ARG:H	2:B:434:GLY:H	1.52	0.57
2:E:326:TYR:CE2	2:E:354:MET:HE3	2.40	0.57
1:D:147:MET:CE	2:E:179:ILE:HG12	2.35	0.57
2:E:162:PRO:CG	3:F:103:HIS:CE1	2.72	0.57
2:E:412:PRO:O	2:E:413:ASN:HB2	2.05	0.57
2:B:212:GLU:HG3	2:B:216:ARG:HH11	1.66	0.56
2:E:387:THR:HG22	2:E:389:ASP:N	2.20	0.56
1:D:147:MET:SD	3:F:121:ILE:HD11	2.45	0.56
2:E:224:MET:HE3	2:E:277:ALA:HB3	1.87	0.56
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.70	0.56
1:D:139:ASN:HB3	3:F:114:TYR:CE1	2.40	0.56
2:B:280:THR:HB	2:B:283:LYS:HG2	1.88	0.56
2:B:456:PRO:O	2:B:457:PHE:HB3	2.06	0.56
2:E:160:ASN:O	2:E:161:ILE:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:O	1:A:125:LYS:HG2	2.06	0.56
3:C:239:GLN:O	3:C:242:ILE:HD12	2.06	0.56
3:C:382:THR:HG22	3:C:383:THR:N	2.20	0.56
2:E:387:THR:CG2	2:E:388:SER:N	2.69	0.56
3:C:322:PHE:CD1	3:C:323:GLU:HG2	2.41	0.55
1:D:133:ILE:HG12	3:F:107:ILE:CD1	2.35	0.55
1:A:171:ARG:NH1	10:A:201:HOH:O	2.28	0.55
1:D:126:VAL:CG2	2:E:157:VAL:HG21	2.36	0.55
2:B:199:VAL:HG23	3:C:141:ASP:HA	1.89	0.55
1:D:133:ILE:HD13	2:E:161:ILE:HD13	1.78	0.55
2:B:229:PRO:HB2	2:B:301:GLN:HE22	1.72	0.54
3:F:318:ASP:C	3:F:318:ASP:OD1	2.50	0.54
1:A:122:LEU:O	1:A:123:LYS:C	2.50	0.54
3:F:383:THR:CG2	10:F:634:HOH:O	2.51	0.54
1:D:136:LEU:HD11	3:F:111:GLN:HG2	1.89	0.54
2:B:457:PHE:O	2:B:458:PHE:O	2.25	0.54
2:E:153:ILE:C	2:E:155:GLU:H	2.16	0.54
2:E:195:THR:HG22	2:E:196:PRO:CD	2.37	0.54
2:E:254:ASN:HD21	2:E:256:GLN:NE2	2.06	0.54
3:F:100:ILE:C	3:F:102:THR:N	2.66	0.54
2:B:224:MET:HE2	2:B:277:ALA:HB3	1.88	0.54
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.89	0.54
3:C:387:ILE:HG12	3:C:388:PRO:HD2	1.89	0.54
2:E:397:GLU:O	2:E:398:ASP:HB2	2.09	0.53
3:F:387:ILE:HG13	3:F:388:PRO:HD2	1.91	0.53
2:E:155:GLU:HG3	2:E:156:THR:H	1.72	0.53
2:E:387:THR:HG21	2:E:392:LYS:CB	2.32	0.53
3:F:325:ASN:HD22	3:F:325:ASN:C	2.16	0.53
3:C:372:TRP:C	3:C:373:LYS:HG2	2.33	0.53
3:F:392:LEU:O	3:F:395:GLY:N	2.42	0.53
2:B:224:MET:CG	10:B:707:HOH:O	2.56	0.53
3:C:100:ILE:C	3:C:102:THR:N	2.66	0.53
1:D:188:VAL:O	1:D:192:ASP:CG	2.52	0.53
3:F:195:GLN:HE22	3:F:382:THR:HG21	1.74	0.53
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.24	0.53
3:C:298:ASP:OD2	3:C:299:PRO:HD2	2.08	0.53
2:E:245:GLU:OE2	2:E:323:LYS:HE3	2.09	0.53
2:E:387:THR:HG22	2:E:389:ASP:H	1.72	0.53
2:B:245:GLU:OE2	2:B:323:LYS:HE2	2.08	0.52
3:C:104:ASP:O	3:C:107:ILE:HG23	2.09	0.52
2:E:160:ASN:O	2:E:163:THR:N	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:LEU:HB3	3:F:113:ILE:HD11	1.87	0.52
2:E:326:TYR:HE2	2:E:354:MET:HE3	1.74	0.52
2:B:191:GLU:CG	10:B:604:HOH:O	2.16	0.52
2:E:169:ARG:HB2	3:F:110:LEU:HD22	1.86	0.52
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.45	0.52
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.09	0.52
2:B:346:ARG:NH2	10:B:602:HOH:O	2.42	0.52
1:D:190:ALA:C	1:D:192:ASP:H	2.17	0.52
2:B:179:ILE:O	2:B:183:GLU:HG3	2.10	0.52
3:F:325:ASN:ND2	3:F:328:GLU:H	2.07	0.52
2:B:183:GLU:HG2	3:C:124:LEU:HD13	1.90	0.52
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.92	0.51
3:F:149:THR:HG22	3:F:150:GLY:N	2.22	0.51
3:F:261:ASP:OD2	3:F:394:ILE:HG12	2.10	0.51
3:C:108:ARG:O	3:C:112:GLU:HG3	2.10	0.51
3:C:107:ILE:CD1	3:C:111:GLN:OE1	2.58	0.51
2:E:284:ASN:C	2:E:284:ASN:HD22	2.19	0.51
3:F:387:ILE:CG1	3:F:388:PRO:HD2	2.41	0.51
2:B:176:ARG:HB2	3:C:117:ASN:HD21	1.74	0.51
3:C:240:SER:O	3:C:242:ILE:HD11	2.08	0.51
3:C:295:PHE:HB3	3:C:375:ARG:NH2	2.25	0.51
1:D:183:LYS:O	1:D:184:GLN:C	2.54	0.51
2:E:373:MET:CE	2:E:405:ASN:CA	2.50	0.51
2:E:351:ASN:HD21	2:E:354:MET:HG3	1.74	0.51
2:B:212:GLU:CG	2:B:216:ARG:NH1	2.69	0.51
2:B:159:SER:C	2:B:162:PRO:HD2	2.36	0.51
2:B:183:GLU:O	3:C:127:LYS:NZ	2.44	0.51
1:D:136:LEU:HD11	3:F:111:GLN:CG	2.41	0.51
1:D:137:GLN:HB3	1:D:189:ILE:HG12	1.92	0.51
2:B:282:GLY:O	2:B:283:LYS:HD2	2.11	0.51
3:C:277:THR:HG23	10:C:668:HOH:O	2.11	0.51
2:B:190:MET:HE3	3:C:131:LEU:HA	1.93	0.50
2:B:295:GLY:HA3	10:B:608:HOH:O	2.12	0.50
3:C:239:GLN:O	3:C:242:ILE:CD1	2.59	0.50
2:E:168:LEU:HD12	2:E:168:LEU:H	1.76	0.50
3:C:275:ARG:HD2	3:F:303:PHE:HE2	1.76	0.50
3:C:310:MET:HE1	3:C:321:LYS:HE2	1.93	0.50
1:A:166:SER:HB3	2:B:195:THR:HB	1.93	0.50
2:B:284:ASN:C	2:B:284:ASN:HD22	2.20	0.50
2:B:230:ASP:O	2:B:233:VAL:N	2.40	0.50
3:C:361:ASN:ND2	10:C:604:HOH:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:GLU:OE1	2:E:325:HIS:CE1	2.65	0.49
2:E:383:ASP:C	2:E:383:ASP:OD1	2.55	0.49
2:B:390:PRO:O	2:B:393:GLN:HG3	2.12	0.49
3:C:97:GLU:C	3:C:99:SER:H	2.20	0.49
1:D:178:TYR:OH	2:E:178:LYS:CD	2.60	0.49
2:E:179:ILE:CD1	3:F:121:ILE:HG12	2.42	0.49
2:E:422:TYR:CB	2:E:426:MET:HE3	2.42	0.49
3:F:273:LYS:HZ2	3:F:317:ASN:HD21	1.58	0.49
2:E:351:ASN:ND2	2:E:354:MET:H	2.10	0.49
2:B:330:THR:HG21	10:B:664:HOH:O	2.13	0.49
3:C:275:ARG:HD2	3:F:303:PHE:CE2	2.48	0.49
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.48	0.49
2:B:186:VAL:O	2:B:190:MET:HG2	2.13	0.49
2:B:412:PRO:CB	10:B:615:HOH:O	2.61	0.49
2:B:456:PRO:O	2:B:457:PHE:CB	2.56	0.49
3:F:356:LYS:HG3	3:F:362:GLY:HA2	1.95	0.49
3:F:379:MET:HE3	3:F:379:MET:HA	1.95	0.49
1:A:169:LEU:H	2:B:189:GLN:NE2	2.11	0.49
3:C:352:GLY:HA2	3:C:378:SER:O	2.13	0.49
1:D:121:VAL:HA	1:D:125:LYS:HG2	1.93	0.49
2:E:183:GLU:HG2	10:F:671:HOH:O	2.13	0.49
9:E:501:NAG:O4	9:J:101:NAG:C1	2.60	0.49
1:A:123:LYS:HB3	1:A:124:ARG:NH2	2.28	0.48
2:B:202:ASN:ND2	2:B:284:ASN:O	2.45	0.48
3:C:106:SER:O	3:C:109:TYR:HB3	2.12	0.48
1:D:151:GLU:OE2	10:D:201:HOH:O	2.20	0.48
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.78	0.48
1:D:147:MET:SD	3:F:121:ILE:CD1	3.01	0.48
2:B:397:GLU:O	2:B:398:ASP:HB2	2.12	0.48
3:F:307:HIS:HD2	3:F:335:TRP:O	1.96	0.48
3:C:192:THR:CG2	10:C:655:HOH:O	2.61	0.48
2:E:152:TYR:C	2:E:154:ASP:N	2.72	0.48
1:A:128:GLU:O	1:A:132:HIS:HD2	1.96	0.48
2:B:254:ASN:HD21	2:B:256:GLN:NE2	2.11	0.48
1:D:120:GLU:C	1:D:122:LEU:H	2.22	0.48
2:E:183:GLU:CG	10:F:671:HOH:O	2.62	0.48
2:B:359:GLN:H	2:B:359:GLN:HE21	1.62	0.48
2:B:155:GLU:HG3	2:B:156:THR:N	2.29	0.48
3:C:104:ASP:C	3:C:107:ILE:HG22	2.37	0.48
1:A:169:LEU:H	2:B:189:GLN:HE22	1.61	0.48
2:E:351:ASN:C	2:E:351:ASN:HD22	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:438:MET:CE	2:E:443:SER:OG	2.43	0.48
2:B:157:VAL:CG1	3:C:100:ILE:HG21	2.43	0.47
2:E:244:THR:HG21	2:E:313:GLU:OE2	2.13	0.47
3:F:392:LEU:O	3:F:393:THR:C	2.57	0.47
1:A:133:ILE:O	1:A:137:GLN:HG3	2.13	0.47
1:A:120:GLU:C	1:A:122:LEU:H	2.23	0.47
2:B:182:LEU:HB2	3:C:124:LEU:HD21	1.95	0.47
2:E:161:ILE:HG22	3:F:103:HIS:ND1	2.29	0.47
3:F:322:PHE:CD1	3:F:338:LYS:HD2	2.49	0.47
1:D:123:LYS:HD3	2:E:154:ASP:OD2	2.14	0.47
1:A:122:LEU:C	1:A:124:ARG:N	2.73	0.47
3:C:273:LYS:NZ	3:C:317:ASN:HD21	2.12	0.47
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.29	0.47
3:F:103:HIS:O	3:F:104:ASP:C	2.56	0.47
1:A:177:ASP:O	1:A:181:GLN:HG3	2.15	0.47
2:B:252:ILE:CD1	2:B:454:ILE:HD13	2.44	0.47
3:C:107:ILE:HD11	3:C:111:GLN:OE1	2.15	0.47
1:D:130:VAL:HA	1:D:133:ILE:HD12	1.96	0.47
1:D:187:GLN:O	1:D:188:VAL:C	2.58	0.47
1:A:129:LYS:HE2	1:A:129:LYS:HA	1.97	0.47
1:D:126:VAL:HG22	2:E:157:VAL:HG21	1.97	0.47
2:B:159:SER:O	2:B:162:PRO:HD2	2.14	0.46
2:B:387:THR:CG2	2:B:388:SER:H	2.22	0.46
2:E:326:TYR:HE2	2:E:354:MET:CE	2.25	0.46
2:E:367:MET:O	2:E:405:ASN:O	2.33	0.46
2:B:229:PRO:O	2:B:305:MET:HE3	2.15	0.46
3:C:191:TRP:CD2	3:C:385:LYS:HE3	2.50	0.46
1:D:119:ILE:HD11	1:D:123:LYS:CG	2.29	0.46
1:D:120:GLU:C	1:D:122:LEU:N	2.74	0.46
1:D:188:VAL:O	1:D:192:ASP:OD1	2.33	0.46
3:F:100:ILE:HA	10:F:605:HOH:O	2.16	0.46
2:B:293:TRP:CD1	2:B:294:LEU:O	2.69	0.46
1:A:130:VAL:O	1:A:134:GLN:HG3	2.15	0.46
3:F:173:LYS:HB2	3:F:173:LYS:HE3	1.68	0.46
3:F:392:LEU:O	3:F:395:GLY:CA	2.64	0.46
1:D:169:LEU:H	2:E:189:GLN:HE22	1.63	0.46
2:E:295:GLY:HA3	10:E:625:HOH:O	2.16	0.46
1:A:190:ALA:C	1:A:192:ASP:H	2.24	0.45
2:B:174:ASN:OD1	2:B:178:LYS:HE2	2.16	0.45
1:D:126:VAL:HG21	2:E:157:VAL:HG21	1.98	0.45
2:E:152:TYR:H	2:E:152:TYR:HD1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:GLU:HG3	2:E:156:THR:N	2.31	0.45
2:E:169:ARG:N	3:F:110:LEU:HD13	2.32	0.45
2:E:402:TRP:CG	2:E:403:TRP:N	2.85	0.45
2:B:267:ASP:N	2:B:268:PRO:CD	2.80	0.45
2:B:316:ASP:OD1	2:B:316:ASP:C	2.60	0.45
2:B:343:ASN:OD1	2:B:344:LYS:HG3	2.16	0.45
3:C:104:ASP:O	3:C:107:ILE:HG22	2.17	0.45
3:C:365:ASN:HD22	3:C:365:ASN:H	1.65	0.45
2:E:316:ASP:OD2	2:E:441:LYS:NZ	2.38	0.45
3:F:365:ASN:HD22	3:F:365:ASN:H	1.63	0.45
3:C:298:ASP:CG	3:C:299:PRO:CD	2.89	0.45
3:F:104:ASP:C	3:F:107:ILE:HG22	2.41	0.45
9:E:501:NAG:H62	9:J:101:NAG:O5	2.17	0.45
3:C:280:TYR:HB3	3:F:275:ARG:NH1	2.32	0.45
1:D:133:ILE:HG12	3:F:107:ILE:HD11	1.97	0.45
2:B:155:GLU:C	2:B:157:VAL:H	2.25	0.44
2:E:217:LYS:HB3	3:F:213:GLU:HG3	1.97	0.44
2:E:267:ASP:O	2:E:271:GLN:HG2	2.17	0.44
3:C:239:GLN:O	3:C:240:SER:C	2.60	0.44
2:E:373:MET:SD	2:E:405:ASN:HB2	2.57	0.44
2:B:330:THR:HG23	10:B:713:HOH:O	2.17	0.44
2:B:190:MET:HE1	3:C:131:LEU:HA	1.98	0.44
3:F:127:LYS:HB3	3:F:127:LYS:HE2	1.69	0.44
2:B:299:ILE:O	2:B:303:THR:HG23	2.18	0.44
2:B:155:GLU:HG3	2:B:156:THR:H	1.83	0.44
3:C:307:HIS:CE1	3:C:341:ALA:H	2.25	0.44
2:E:174:ASN:O	2:E:177:SER:OG	2.35	0.44
2:B:271:GLN:NE2	10:B:613:HOH:O	2.50	0.44
2:E:163:THR:O	2:E:164:ASN:C	2.61	0.44
2:E:167:VAL:O	2:E:168:LEU:C	2.61	0.44
3:F:107:ILE:O	3:F:111:GLN:HG3	2.17	0.44
2:B:252:ILE:CD1	2:B:454:ILE:CG1	2.95	0.44
2:E:153:ILE:O	2:E:155:GLU:N	2.51	0.44
3:C:391:ARG:O	3:C:392:LEU:O	2.36	0.44
2:E:158:ASN:OD1	3:F:100:ILE:CD1	2.66	0.44
2:E:212:GLU:CG	2:E:216:ARG:NH1	2.78	0.44
2:B:212:GLU:CG	2:B:216:ARG:HH11	2.31	0.43
2:E:422:TYR:OH	2:E:433:ASP:O	2.25	0.43
3:F:232:LYS:O	3:F:236:ILE:HG13	2.18	0.43
1:A:119:ILE:O	1:A:120:GLU:C	2.61	0.43
3:C:273:LYS:HD3	3:C:273:LYS:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:ARG:HB2	3:F:110:LEU:CD1	2.48	0.43
3:F:322:PHE:HA	3:F:338:LYS:HD3	1.99	0.43
2:E:183:GLU:CB	10:F:671:HOH:O	2.64	0.43
2:E:397:GLU:O	2:E:398:ASP:CB	2.63	0.43
3:C:107:ILE:HD13	3:C:111:GLN:CD	2.44	0.43
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.19	0.43
2:E:345:TYR:HB2	2:E:354:MET:HE1	1.97	0.43
3:F:391:ARG:O	3:F:392:LEU:O	2.36	0.43
1:D:181:GLN:O	1:D:185:LEU:HB2	2.19	0.43
2:E:172:LEU:HD21	3:F:114:TYR:HA	2.00	0.43
2:E:373:MET:CG	2:E:405:ASN:HB2	2.49	0.43
2:E:422:TYR:CB	2:E:426:MET:CE	2.97	0.43
3:F:103:HIS:O	3:F:107:ILE:N	2.50	0.43
2:B:152:TYR:HD1	2:B:152:TYR:H	1.66	0.43
2:B:234:LYS:HA	2:B:235:PRO:HD3	1.90	0.43
2:B:457:PHE:C	2:B:458:PHE:O	2.61	0.43
7:B:501:MAN:H2	6:K:2:NAG:HO3	1.77	0.43
3:C:263:ALA:O	3:C:264:MET:HB2	2.18	0.43
3:C:394:ILE:HG22	3:C:394:ILE:O	2.19	0.43
2:E:162:PRO:CG	3:F:103:HIS:HE1	2.25	0.43
2:E:186:VAL:CG1	3:F:127:LYS:HE2	2.48	0.43
2:E:455:ARG:HG3	2:E:456:PRO:HD2	2.01	0.43
3:F:153:CYS:H	3:F:192:THR:HG22	1.84	0.43
3:C:211:TYR:CE2	3:C:333:GLY:HA3	2.54	0.42
2:E:153:ILE:C	2:E:155:GLU:N	2.77	0.42
3:F:320:ASP:C	3:F:320:ASP:OD1	2.61	0.42
2:B:190:MET:HE2	2:B:190:MET:HB3	1.69	0.42
3:F:240:SER:HG	3:F:242:ILE:HD11	1.76	0.42
3:C:338:LYS:HG2	10:G:101:HOH:O	2.18	0.42
3:C:322:PHE:CD1	3:C:323:GLU:N	2.87	0.42
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.85	0.42
1:D:176:LYS:HD3	1:D:176:LYS:HA	1.88	0.42
2:E:152:TYR:O	2:E:154:ASP:N	2.52	0.42
3:F:219:SER:OG	3:F:224:THR:HB	2.20	0.42
1:A:171:ARG:CZ	10:A:201:HOH:O	2.67	0.42
2:B:157:VAL:O	3:C:103:HIS:HE1	2.03	0.42
2:B:439:ASN:H	2:B:439:ASN:HD22	1.67	0.42
3:C:155:ASP:O	3:C:159:LYS:HG3	2.20	0.42
1:A:171:ARG:NH2	10:A:201:HOH:O	2.51	0.42
2:B:154:ASP:C	2:B:157:VAL:HG23	2.44	0.42
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:323:GLU:OE2	10:C:601:HOH:O	2.22	0.42
2:E:159:SER:O	2:E:162:PRO:HD2	2.20	0.42
1:A:119:ILE:HD12	1:A:119:ILE:HA	1.86	0.42
2:B:155:GLU:C	2:B:157:VAL:N	2.77	0.42
3:C:112:GLU:O	3:C:116:SER:OG	2.37	0.42
2:B:161:ILE:N	2:B:162:PRO:CD	2.83	0.42
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.85	0.42
2:E:303:THR:HB	2:E:330:THR:HA	2.01	0.42
2:E:373:MET:HE3	2:E:405:ASN:HA	1.89	0.42
3:C:108:ARG:HA	3:C:111:GLN:NE2	2.35	0.41
3:C:252:ASP:OD2	3:C:373:LYS:NZ	2.43	0.41
3:C:338:LYS:O	3:C:338:LYS:CG	2.66	0.41
2:E:163:THR:C	2:E:166:ARG:H	2.25	0.41
2:B:191:GLU:CD	10:B:604:HOH:O	2.58	0.41
2:B:387:THR:HG22	2:B:389:ASP:H	1.85	0.41
1:D:126:VAL:CG2	2:E:157:VAL:CG2	2.98	0.41
2:E:265:LYS:O	2:E:268:PRO:HD2	2.21	0.41
3:F:200:GLY:HA2	10:F:608:HOH:O	2.21	0.41
1:D:186:GLU:O	1:D:187:GLN:C	2.62	0.41
3:F:239:GLN:O	3:F:240:SER:C	2.63	0.41
2:B:346:ARG:CZ	10:B:602:HOH:O	2.67	0.41
2:B:392:LYS:HZ2	2:B:392:LYS:HG2	1.57	0.41
2:E:158:ASN:OD1	3:F:100:ILE:HD13	2.19	0.41
2:B:153:ILE:C	2:B:155:GLU:H	2.29	0.41
2:B:365:ARG:HD2	10:B:661:HOH:O	2.20	0.41
2:B:397:GLU:O	2:B:398:ASP:CB	2.64	0.41
2:E:176:ARG:HH11	2:E:176:ARG:HD3	1.72	0.41
3:C:344:LEU:HD12	3:C:384:MET:SD	2.61	0.41
3:F:307:HIS:CE1	3:F:342:GLY:H	2.38	0.41
3:C:288:ASP:CG	3:C:291:ASP:HB2	2.45	0.41
2:B:311:LEU:HD11	2:B:323:LYS:HG2	2.03	0.41
2:B:325:HIS:O	2:B:345:TYR:HA	2.21	0.41
2:E:152:TYR:O	2:E:153:ILE:C	2.64	0.41
1:A:138:LYS:HA	1:A:138:LYS:HD3	1.94	0.40
2:B:158:ASN:HD22	2:B:158:ASN:HA	1.68	0.40
3:C:229:GLY:O	3:C:233:ILE:HG13	2.22	0.40
2:B:413:ASN:N	10:B:615:HOH:O	2.54	0.40
1:D:133:ILE:CG1	3:F:107:ILE:HD11	2.49	0.40
3:F:249:GLU:HB2	3:F:383:THR:HG23	2.03	0.40
2:B:367:MET:HB2	2:B:406:ARG:HB3	2.04	0.40
2:E:183:GLU:O	2:E:187:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:412:PRO:O	10:E:601:HOH:O	2.22	0.40
1:A:128:GLU:O	1:A:132:HIS:CD2	2.75	0.40
2:B:184:SER:CB	10:B:603:HOH:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/87 (83%)	67 (93%)	3 (4%)	2 (3%)	4	2
1	D	72/87 (83%)	64 (89%)	6 (8%)	2 (3%)	4	2
2	B	306/328 (93%)	286 (94%)	15 (5%)	5 (2%)	7	7
2	E	306/328 (93%)	281 (92%)	21 (7%)	4 (1%)	9	10
3	C	299/319 (94%)	275 (92%)	17 (6%)	7 (2%)	5	4
3	F	299/319 (94%)	276 (92%)	16 (5%)	7 (2%)	5	4
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	2 (100%)	0	0	100	100
5	I	2/4 (50%)	2 (100%)	0	0	100	100
5	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1362/1484 (92%)	1257 (92%)	78 (6%)	27 (2%)	6	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	240	SER
3	C	392	LEU
2	E	156	THR
3	F	101	LEU

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Mol	Chain	Res	Type
3	F	240	SER
3	F	392	LEU
1	A	123	LYS
2	B	457	PHE
3	C	101	LEU
3	C	396	GLU
1	D	191	LYS
2	E	457	PHE
2	E	154	ASP
3	F	198	LEU
2	B	281	ASP
3	C	253	TRP
1	A	121	VAL
2	B	156	THR
2	B	256	GLN
3	C	391	ARG
1	D	187	GLN
2	E	256	GLN
3	F	199	ASP
3	F	396	GLU
2	B	456	PRO
3	C	394	ILE
3	F	394	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	69/82 (84%)	56 (81%)	13 (19%)	1	1
1	D	69/82 (84%)	59 (86%)	10 (14%)	3	3
2	B	266/286 (93%)	237 (89%)	29 (11%)	6	7
2	E	266/286 (93%)	232 (87%)	34 (13%)	4	4
3	C	252/267 (94%)	220 (87%)	32 (13%)	4	5
3	F	252/267 (94%)	227 (90%)	25 (10%)	7	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	3 (100%)	0	100	100
5	I	3/3 (100%)	3 (100%)	0	100	100
5	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1186/1282 (92%)	1042 (88%)	144 (12%)	5	5

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	128	GLU
1	A	129	LYS
1	A	130	VAL
1	A	135	LEU
1	A	162	ARG
1	A	164	SER
1	A	169	LEU
1	A	171	ARG
1	A	176	LYS
1	A	183	LYS
1	A	185	LEU
1	A	186	GLU
2	B	157	VAL
2	B	158	ASN
2	B	159	SER
2	B	168	LEU
2	B	170	SER
2	B	171	ILE
2	B	177	SER
2	B	187	SER
2	B	190	MET
2	B	191	GLU
2	B	195	THR
2	B	210	GLU
2	B	216	ARG
2	B	232	SER
2	B	233	VAL
2	B	238	VAL
2	B	244	THR
2	B	252	ILE
2	B	253	GLN

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Mol	Chain	Res	Type
2	B	267	ASP
2	B	284	ASN
2	B	320	ASP
2	B	321	LYS
2	B	346	ARG
2	B	359	GLN
2	B	388	SER
2	B	392	LYS
2	B	406	ARG
2	B	439	ASN
3	C	99	SER
3	C	106	SER
3	C	107	ILE
3	C	112	GLU
3	C	113	ILE
3	C	116	SER
3	C	125	LYS
3	C	143	VAL
3	C	147	ASP
3	C	149	THR
3	C	162	LYS
3	C	173	LYS
3	C	187	SER
3	C	192	THR
3	C	198	LEU
3	C	224	THR
3	C	244	TYR
3	C	250	LEU
3	C	277	THR
3	C	294	ASP
3	C	297	ASP
3	C	317	ASN
3	C	325	ASN
3	C	358	SER
3	C	361	ASN
3	C	365	ASN
3	C	374	THR
3	C	383	THR
3	C	390	ASN
3	C	391	ARG
3	C	393	THR
3	C	394	ILE

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Mol	Chain	Res	Type
1	D	121	VAL
1	D	123	LYS
1	D	124	ARG
1	D	125	LYS
1	D	129	LYS
1	D	135	LEU
1	D	169	LEU
1	D	176	LYS
1	D	183	LYS
1	D	185	LEU
2	E	161	ILE
2	E	165	LEU
2	E	166	ARG
2	E	170	SER
2	E	171	ILE
2	E	173	GLU
2	E	174	ASN
2	E	176	ARG
2	E	177	SER
2	E	179	ILE
2	E	187	SER
2	E	190	MET
2	E	191	GLU
2	E	209	LYS
2	E	210	GLU
2	E	216	ARG
2	E	220	GLU
2	E	231	SER
2	E	232	SER
2	E	233	VAL
2	E	234	LYS
2	E	238	VAL
2	E	244	THR
2	E	252	ILE
2	E	253	GLN
2	E	267	ASP
2	E	280	THR
2	E	284	ASN
2	E	342	VAL
2	E	359	GLN
2	E	366	THR
2	E	373	MET

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Mol	Chain	Res	Type
2	E	406	ARG
2	E	439	ASN
3	F	107	ILE
3	F	140	LYS
3	F	143	VAL
3	F	147	ASP
3	F	149	THR
3	F	151	LYS
3	F	162	LYS
3	F	192	THR
3	F	224	THR
3	F	250	LEU
3	F	277	THR
3	F	294	ASP
3	F	303	PHE
3	F	317	ASN
3	F	323	GLU
3	F	325	ASN
3	F	350	GLN
3	F	361	ASN
3	F	365	ASN
3	F	374	THR
3	F	382	THR
3	F	383	THR
3	F	390	ASN
3	F	391	ARG
3	F	396	GLU
4	G	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	181	GLN
2	B	158	ASN
2	B	160	ASN
2	B	189	GLN
2	B	256	GLN
2	B	271	GLN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN

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Mol	Chain	Res	Type
2	B	332	GLN
2	B	339	GLN
2	B	351	ASN
2	B	359	GLN
2	B	408	HIS
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	119	GLN
3	C	146	HIS
3	C	177	GLN
3	C	195	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	365	ASN
3	C	390	ASN
1	D	132	HIS
1	D	143	GLN
1	D	187	GLN
2	E	189	GLN
2	E	228	GLN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	351	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	117	ASN
3	F	118	ASN
3	F	119	GLN

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Mol	Chain	Res	Type
3	F	136	GLN
3	F	146	HIS
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	325	ASN
3	F	365	ASN
3	F	390	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 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	$\# Z > 2$
6	NAG	K	1	2,6	14,14,15	1.29	1 (7%)	17,19,21	1.32	3 (17%)
6	NAG	K	2	6	14,14,15	1.33	2 (14%)	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	K	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1	NAG	O7-C7	-4.16	1.13	1.23
6	K	2	NAG	O7-C7	-3.76	1.14	1.23
6	K	2	NAG	C2-N2	2.10	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	C3-C4-C5	2.43	114.64	110.23
6	K	1	NAG	C6-C5-C4	-2.29	107.40	113.02
6	K	1	NAG	C1-O5-C5	2.27	115.22	112.19
6	K	2	NAG	C1-O5-C5	2.23	115.17	112.19

There are no chirality outliers.

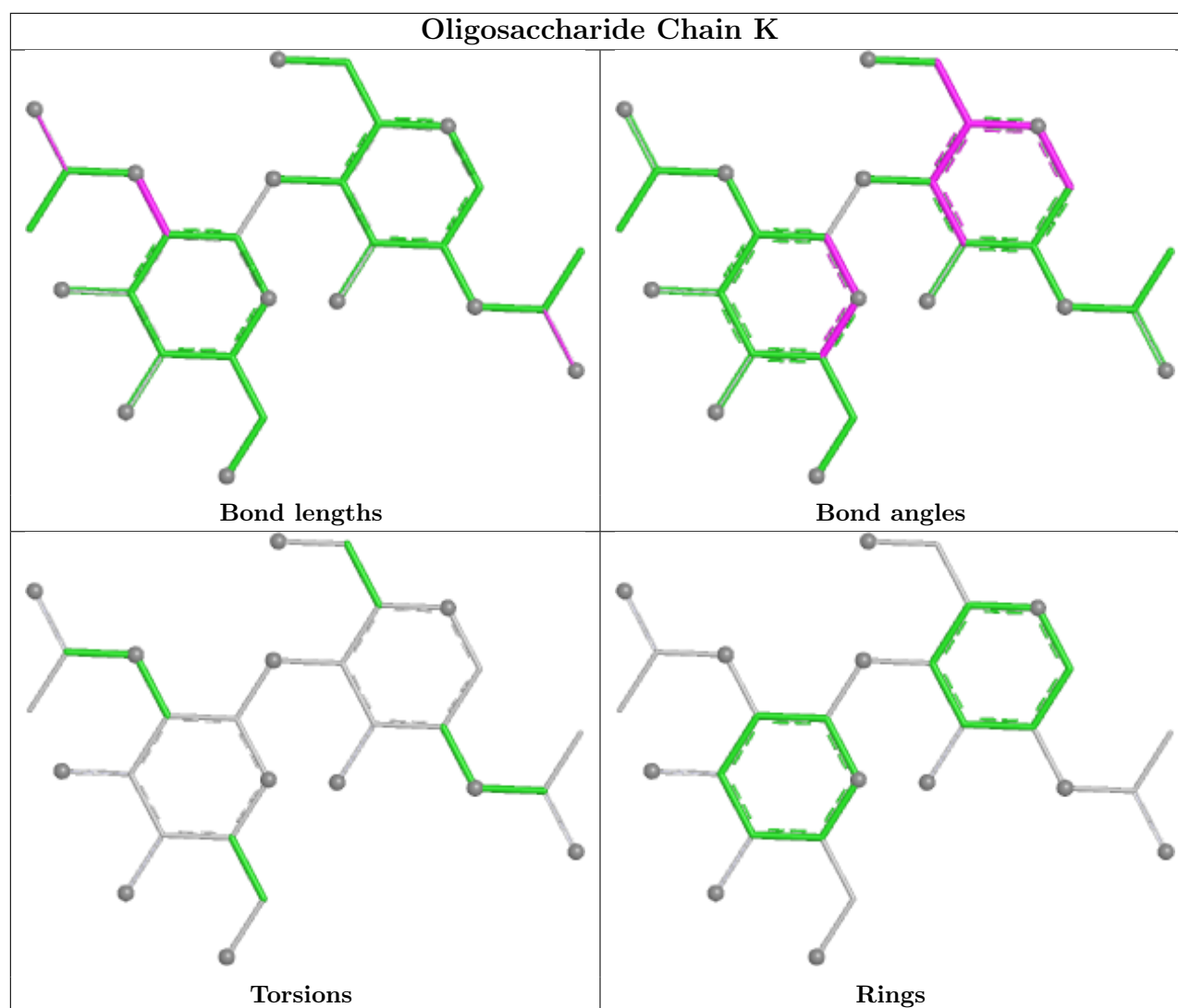
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0
6	K	2	NAG	3	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	NAG	J	101	-	14,14,15	1.30	1 (7%)	17,19,21	1.31	1 (5%)
9	NAG	E	501	2	14,14,15	1.26	1 (7%)	17,19,21	1.87	4 (23%)
7	MAN	B	501	-	11,11,12	1.11	1 (9%)	15,15,17	2.15	4 (26%)

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
9	NAG	J	101	-	-	2/6/23/26	0/1/1/1
9	NAG	E	501	2	-	0/6/23/26	0/1/1/1
7	MAN	B	501	-	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	501	NAG	O7-C7	-3.95	1.14	1.23
9	J	101	NAG	O7-C7	-3.66	1.15	1.23
7	B	501	MAN	O5-C1	-3.15	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	MAN	C1-O5-C5	5.90	120.09	112.19
9	E	501	NAG	O5-C1-C2	-4.89	103.72	111.29
7	B	501	MAN	O5-C1-C2	4.09	120.55	110.79
9	E	501	NAG	C1-O5-C5	3.70	117.15	112.19
9	J	101	NAG	C1-O5-C5	3.53	116.92	112.19
9	E	501	NAG	O3-C3-C2	-2.36	104.50	109.40
7	B	501	MAN	O3-C3-C2	-2.27	105.43	110.05
9	E	501	NAG	O5-C5-C6	-2.17	103.43	107.66
7	B	501	MAN	C1-C2-C3	2.03	112.60	109.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	101	NAG	O5-C5-C6-O6
9	J	101	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	101	NAG	2	0
9	E	501	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	MAN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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.