



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:22 AM UTC

PDB ID : 1MCO / pdb_00001mco
Title : THREE-DIMENSIONAL STRUCTURE OF A HUMAN IMMUNOGLOBULIN WITH A HINGE DELETION
Authors : Guddat, L.W.; Edmundson, A.B.
Deposited on : 1993-02-25
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

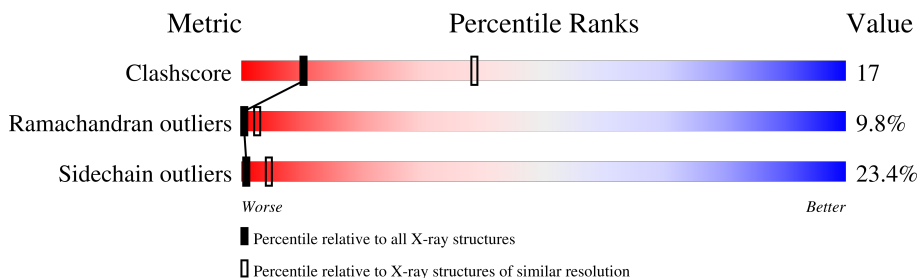
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

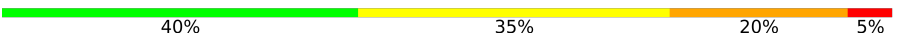
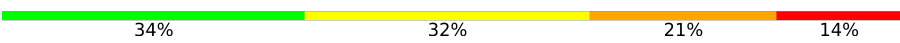
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	L	216	
2	H	428	
3	A	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	A	3	-	-	X	-
3	GUP	A	8	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5041 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 IGG1 MCG INTACT ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1606	999	266	336	5			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	ILE	PHE	conflict	PIR S14675
L	23	THR	SER	conflict	PIR S14675
L	29	VAL	ILE	conflict	PIR S14675
L	31	GLY	ASN	conflict	PIR S14675
L	39	GLN	ARG	conflict	PIR S14675
L	42	ALA	PRO	conflict	PIR S14675
L	48	VAL	LEU	conflict	PIR S14675
L	49	ILE	MET	conflict	PIR S14675
L	54	ASN	THR	conflict	PIR S14675
L	62	ASP	ASN	conflict	PIR S14675
L	94	GLU	ALA	conflict	PIR S14675
L	97	ASP	ASN	conflict	PIR S14675
L	98	ASN	SER	conflict	PIR S14675
L	99	PHE	LEU	conflict	PIR S14675
L	100	VAL	ILE	conflict	PIR S14675
L	103	THR	GLY	conflict	PIR S14675
L	106	LYS	ARG	conflict	PIR S14675
L	107	VAL	LEU	conflict	PIR S14675
L	116	ASN	ALA	conflict	PIR S14675
L	118	THR	SER	conflict	PIR S14675
L	136	GLU	LEU	conflict	PIR S14675
L	156	GLY	SER	conflict	PIR S14675
L	167	LYS	THR	conflict	PIR S14675

- Molecule 2 is a protein called IGG1 MCG INTACT ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	428	Total	C	N	O	S	0	0	0
			3305	2108	551	635	11			

There are 67 discrepancies between the modelled and reference sequences:

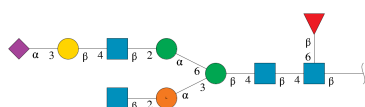
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLN	deletion	GB 243866
H	13	LYS	ARG	conflict	GB 243866
H	16	GLU	GLN	conflict	GB 243866
H	17	ALA	THR	conflict	GB 243866
H	27	ASP	-	insertion	GB 243866
H	28	SER	PHE	conflict	GB 243866
H	29	ILE	THR	conflict	GB 243866
H	30	ASN	PHE	conflict	GB 243866
H	32	ILE	-	insertion	GB 243866
H	33	LEU	ASP	conflict	GB 243866
H	34	TYR	PHE	conflict	GB 243866
H	36	TRP	MET	conflict	GB 243866
H	37	SER	ASN	conflict	GB 243866
H	39	ILE	VAL	conflict	GB 243866
H	45	LYS	ARG	conflict	GB 243866
H	52	TYR	PHE	conflict	GB 243866
H	?	-	ARG	deletion	GB 243866
H	?	-	ASP	deletion	GB 243866
H	54	TYR	LYS	conflict	GB 243866
H	55	TYR	ALA	conflict	GB 243866
H	56	SER	LYS	conflict	GB 243866
H	58	SER	TYR	conflict	GB 243866
H	?	-	THR	deletion	GB 243866
H	?	-	GLU	deletion	GB 243866
H	61	GLY	-	insertion	GB 243866
H	65	LEU	VAL	conflict	GB 243866
H	67	SER	GLY	conflict	GB 243866
H	71	ILE	MET	conflict	GB 243866
H	72	SER	LEU	conflict	GB 243866
H	74	ASN	ASP	conflict	GB 243866
H	81	TYR	SER	conflict	GB 243866
H	82	SER	LEU	conflict	GB 243866
H	83	LYS	ARG	conflict	GB 243866
H	100	VAL	GLU	conflict	GB 243866
H	101	PRO	GLY	conflict	GB 243866
H	102	LEU	HIS	conflict	GB 243866
H	103	VAL	THR	conflict	GB 243866

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Chain	Residue	Modelled	Actual	Comment	Reference
H	104	VAL	ALA	conflict	GB 243866
H	105	ASN	ALA	conflict	GB 243866
H	?	-	PHE	deletion	GB 243866
H	?	-	ASP	deletion	GB 243866
H	?	-	TYR	deletion	GB 243866
H	111	THR	SER	conflict	GB 243866
H	152	GLN	GLU	conflict	GB 243866
H	214	ARG	LYS	conflict	GB 243866
H	?	-	GLU	deletion	GB 243866
H	?	-	PRO	deletion	GB 243866
H	?	-	LYS	deletion	GB 243866
H	?	-	SER	deletion	GB 243866
H	?	-	CYS	deletion	GB 243866
H	?	-	ASP	deletion	GB 243866
H	?	-	LYS	deletion	GB 243866
H	?	-	THR	deletion	GB 243866
H	?	-	HIS	deletion	GB 243866
H	?	-	THR	deletion	GB 243866
H	?	-	CYS	deletion	GB 243866
H	?	-	PRO	deletion	GB 243866
H	?	-	PRO	deletion	GB 243866
H	?	-	CYS	deletion	GB 243866
H	?	-	PRO	deletion	GB 243866
H	257	GLN	GLU	conflict	GB 243866
H	268	GLN	GLU	conflict	GB 243866
H	279	GLN	GLU	conflict	GB 243866
H	297	ASN	ASP	conflict	GB 243866
H	300	ASP	ASN	conflict	GB 243866
H	341	GLU	ASP	conflict	GB 243866
H	343	MET	LEU	conflict	GB 243866

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-L-gulopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



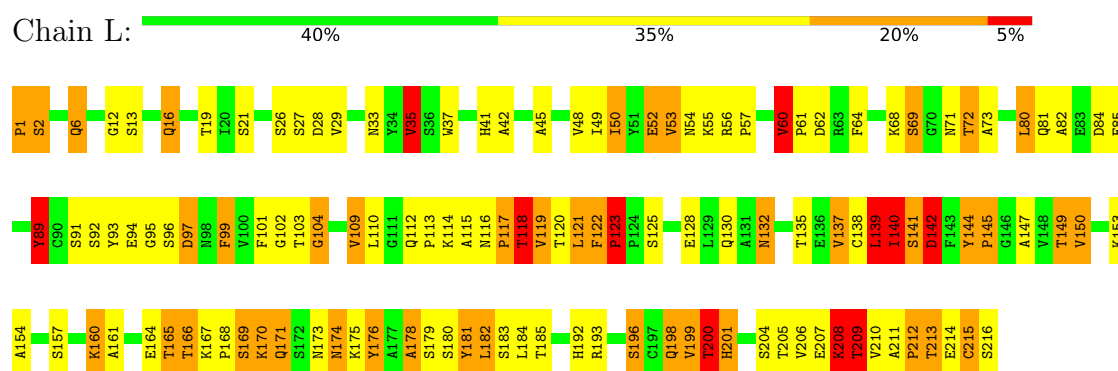
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	10	Total	C	N	O	0	0	0
			130	73	5	52			

3 Residue-property plots

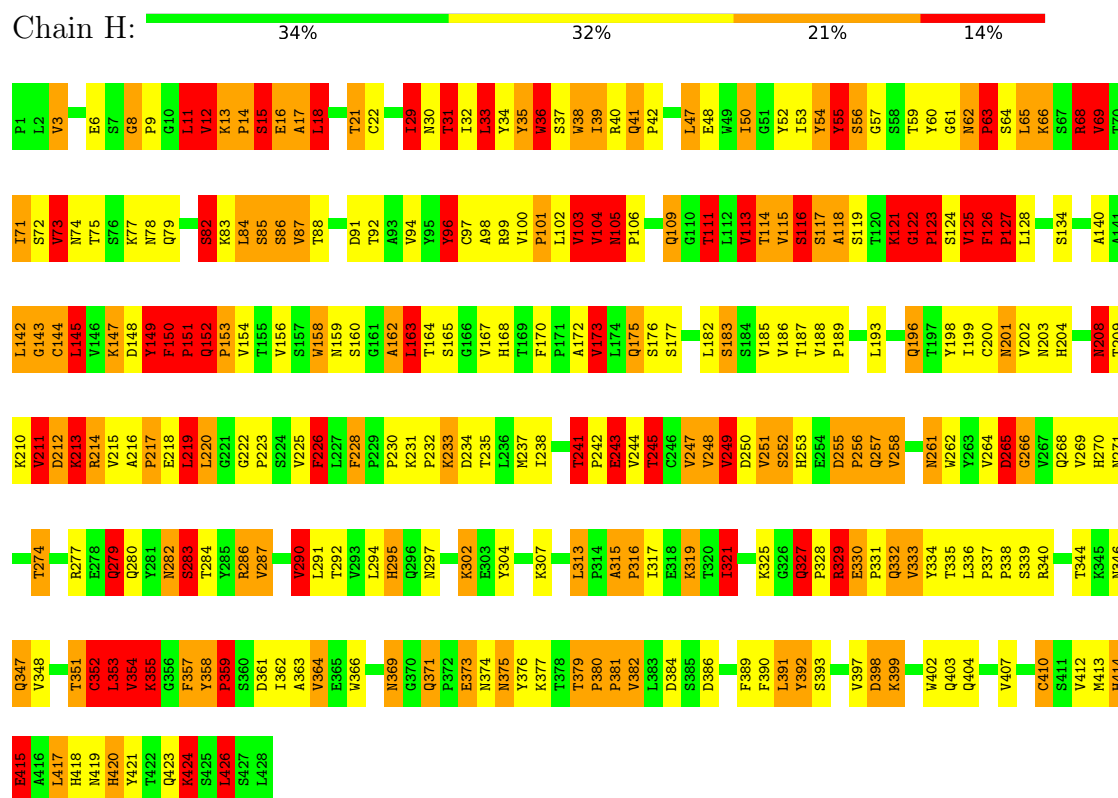
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: IGG1 MCG INTACT ANTIBODY (LIGHT CHAIN)



• Molecule 2: IGG1 MCG INTACT ANTIBODY (HEAVY CHAIN)



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-L-gulopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]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	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.40Å 110.00Å 186.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.232 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5041	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: NAG, SIA, MAN, BMA, GAL, FUL, GUP

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	L	1.25	13/1645 (0.8%)	2.65	148/2242 (6.6%)
2	H	1.48	53/3396 (1.6%)	2.92	390/4641 (8.4%)
All	All	1.41	66/5041 (1.3%)	2.84	538/6883 (7.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
2	H	0	10
All	All	0	12

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	17	ALA	CA-C	12.28	1.68	1.52
2	H	18	LEU	N-CA	11.52	1.59	1.46
2	H	18	LEU	CA-C	11.49	1.67	1.52
2	H	84	LEU	CA-CB	10.00	1.70	1.53
2	H	17	ALA	C-N	9.04	1.45	1.33
2	H	69	VAL	CA-CB	8.70	1.66	1.54
2	H	84	LEU	CB-CG	8.30	1.70	1.53
2	H	85	SER	CA-C	8.30	1.63	1.52
1	L	209	THR	CA-CB	8.25	1.67	1.53
2	H	87	VAL	CA-CB	8.25	1.65	1.54
2	H	321	ILE	CA-CB	8.23	1.62	1.53
2	H	32	ILE	CA-CB	8.16	1.65	1.54
2	H	71	ILE	CA-CB	8.07	1.64	1.53
2	H	17	ALA	C-O	-7.74	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	84	LEU	CA-C	7.69	1.63	1.52
2	H	85	SER	N-CA	7.52	1.55	1.46
2	H	16	GLU	C-N	7.43	1.42	1.33
2	H	295	HIS	CD2-NE2	-7.36	1.29	1.37
2	H	414	HIS	CD2-NE2	-7.25	1.29	1.37
2	H	115	VAL	CA-CB	7.17	1.64	1.54
2	H	86	SER	N-CA	7.14	1.55	1.46
2	H	287	VAL	CA-CB	7.06	1.63	1.54
2	H	199	ILE	CA-CB	6.84	1.63	1.54
2	H	92	THR	CA-CB	6.78	1.61	1.53
1	L	29	VAL	CA-CB	6.75	1.61	1.54
2	H	382	VAL	CA-CB	6.69	1.62	1.54
1	L	213	THR	CA-CB	6.64	1.64	1.53
2	H	269	VAL	CA-CB	6.60	1.62	1.54
2	H	85	SER	CA-CB	6.58	1.64	1.53
2	H	3	VAL	CA-CB	6.48	1.64	1.54
1	L	50	ILE	CA-CB	6.45	1.64	1.54
2	H	50	ILE	CA-CB	6.36	1.62	1.54
2	H	253	HIS	CD2-NE2	-6.27	1.30	1.37
1	L	210	VAL	CA-CB	6.23	1.62	1.54
2	H	204	HIS	CD2-NE2	-6.20	1.31	1.37
2	H	164	THR	CA-CB	6.17	1.61	1.53
1	L	201	HIS	CD2-NE2	-6.15	1.31	1.37
1	L	122	PHE	CA-CB	6.15	1.63	1.53
1	L	192	HIS	CD2-NE2	-6.07	1.31	1.37
1	L	109	VAL	CA-CB	6.05	1.62	1.54
1	L	41	HIS	CD2-NE2	-6.02	1.31	1.37
2	H	84	LEU	C-N	5.96	1.42	1.33
2	H	364	VAL	CA-CB	5.96	1.62	1.54
2	H	88	THR	CA-CB	5.93	1.62	1.53
2	H	284	THR	CA-CB	5.87	1.63	1.53
2	H	75	THR	CA-CB	5.85	1.62	1.53
2	H	270	HIS	CG-ND1	-5.84	1.31	1.38
2	H	104	VAL	CA-CB	5.79	1.62	1.54
2	H	418	HIS	CD2-NE2	-5.72	1.31	1.37
2	H	251	VAL	CA-CB	5.59	1.62	1.54
2	H	16	GLU	CA-C	5.56	1.60	1.52
1	L	28	ASP	CA-C	5.54	1.55	1.52
2	H	235	THR	CA-CB	5.47	1.62	1.53
2	H	94	VAL	CA-CB	5.46	1.59	1.53
2	H	420	HIS	CD2-NE2	-5.46	1.31	1.37
2	H	59	THR	CA-CB	5.45	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	247	VAL	CA-CB	5.43	1.60	1.54
2	H	317	ILE	CA-CB	5.34	1.59	1.53
2	H	168	HIS	CD2-NE2	-5.29	1.32	1.37
2	H	29	ILE	CA-CB	5.27	1.61	1.54
2	H	86	SER	CA-C	5.26	1.59	1.52
1	L	48	VAL	CA-CB	5.23	1.60	1.54
2	H	126	PHE	CA-CB	5.19	1.57	1.53
1	L	200	THR	CA-CB	5.14	1.63	1.53
2	H	355	LYS	CA-CB	5.05	1.61	1.53
2	H	418	HIS	CG-ND1	-5.02	1.32	1.38

All (538) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	17	ALA	O-C-N	-19.37	101.78	123.48
2	H	126	PHE	O-C-N	-17.61	110.70	121.27
2	H	290	VAL	CG1-CB-CG2	-17.11	73.15	110.80
2	H	290	VAL	CA-CB-CG1	-17.04	81.44	110.40
2	H	17	ALA	CA-C-N	16.85	152.86	121.69
2	H	17	ALA	C-N-CA	16.85	152.86	121.69
2	H	126	PHE	CA-CB-CG	-16.38	97.42	113.80
2	H	290	VAL	N-CA-C	15.87	128.91	106.53
1	L	28	ASP	CA-CB-CG	15.27	127.87	112.60
1	L	122	PHE	CA-CB-CG	14.81	128.61	113.80
2	H	329	ARG	N-CA-C	14.24	141.12	110.80
1	L	116	ASN	CA-CB-CG	14.20	126.80	112.60
2	H	84	LEU	N-CA-CB	-13.06	88.42	110.49
2	H	17	ALA	N-CA-CB	-12.79	89.02	111.39
2	H	11	LEU	CD1-CG-CD2	-12.75	82.74	110.80
2	H	247	VAL	CG1-CB-CG2	-12.73	82.80	110.80
2	H	415	GLU	N-CA-C	12.14	136.66	110.80
2	H	354	VAL	CG1-CB-CG2	-12.09	84.20	110.80
2	H	234	ASP	CA-CB-CG	11.90	124.50	112.60
2	H	357	PHE	CA-CB-CG	11.51	125.31	113.80
2	H	84	LEU	CA-C-N	11.42	143.36	121.54
2	H	84	LEU	C-N-CA	11.42	143.36	121.54
2	H	329	ARG	CA-C-O	11.32	136.70	120.51
2	H	18	LEU	CA-C-O	11.31	133.78	120.43
1	L	117	PRO	N-CA-C	11.29	135.73	112.47
2	H	85	SER	CA-C-N	11.08	142.70	121.54
2	H	85	SER	C-N-CA	11.08	142.70	121.54
2	H	264	VAL	CA-C-N	10.92	142.39	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	264	VAL	C-N-CA	10.92	142.39	121.54
2	H	319	LYS	CA-CB-CG	-10.76	92.59	114.10
2	H	355	LYS	CG-CD-CE	-10.62	86.89	111.30
1	L	201	HIS	CA-CB-CG	-10.59	103.21	113.80
1	L	123	PRO	N-CA-C	10.52	123.53	110.70
1	L	168	PRO	N-CA-C	10.45	127.59	110.55
2	H	115	VAL	CA-C-N	10.41	141.42	121.54
2	H	115	VAL	C-N-CA	10.41	141.42	121.54
2	H	264	VAL	O-C-N	10.40	135.63	122.94
1	L	116	ASN	O-C-N	-10.36	112.84	121.44
2	H	16	GLU	O-C-N	-10.22	108.99	122.59
1	L	118	THR	N-CA-C	10.18	132.49	110.80
2	H	84	LEU	CB-CA-C	10.16	130.64	110.42
2	H	103	VAL	CA-CB-CG2	-10.09	93.25	110.40
2	H	16	GLU	CA-C-N	9.96	140.76	121.63
2	H	16	GLU	C-N-CA	9.96	140.76	121.63
2	H	85	SER	O-C-N	-9.94	109.37	122.59
2	H	391	LEU	CD1-CG-CD2	-9.92	88.98	110.80
2	H	290	VAL	CA-CB-CG2	9.89	127.22	110.40
2	H	15	SER	N-CA-C	9.88	131.85	110.80
2	H	126	PHE	CA-C-O	-9.74	110.40	120.63
2	H	105	ASN	CA-CB-CG	9.69	122.29	112.60
2	H	384	ASP	CA-CB-CG	9.65	122.25	112.60
1	L	28	ASP	CA-C-O	-9.60	114.30	119.77
1	L	122	PHE	CA-C-N	9.32	129.99	120.38
1	L	122	PHE	C-N-CA	9.32	129.99	120.38
2	H	204	HIS	CA-CB-CG	9.32	123.12	113.80
2	H	41	GLN	CA-C-N	9.29	126.44	119.66
2	H	41	GLN	C-N-CA	9.29	126.44	119.66
2	H	269	VAL	CG1-CB-CG2	-9.26	90.43	110.80
2	H	414	HIS	CA-C-N	9.25	139.21	121.54
2	H	414	HIS	C-N-CA	9.25	139.21	121.54
2	H	151	PRO	CA-N-CD	-9.16	99.17	112.00
2	H	386	ASP	CA-CB-CG	9.07	121.67	112.60
2	H	287	VAL	CG1-CB-CG2	-8.94	91.14	110.80
1	L	117	PRO	CA-C-N	8.91	138.56	121.54
1	L	117	PRO	C-N-CA	8.91	138.56	121.54
2	H	86	SER	N-CA-C	8.87	129.69	110.80
2	H	241	THR	CA-C-N	8.85	128.99	120.31
2	H	241	THR	C-N-CA	8.85	128.99	120.31
2	H	282	ASN	N-CA-C	8.83	129.60	110.80
2	H	86	SER	CA-CB-OG	8.78	128.65	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	220	LEU	N-CA-C	8.77	129.47	110.80
1	L	185	THR	CA-C-O	-8.72	113.31	121.08
2	H	103	VAL	CG1-CB-CG2	-8.72	91.62	110.80
2	H	103	VAL	CA-CB-CG1	8.69	125.17	110.40
2	H	154	VAL	CG1-CB-CG2	-8.63	91.82	110.80
2	H	103	VAL	O-C-N	-8.59	111.84	122.57
2	H	14	PRO	CA-C-N	8.58	137.93	121.54
2	H	14	PRO	C-N-CA	8.58	137.93	121.54
2	H	62	ASN	CA-C-O	-8.57	111.70	119.75
1	L	112	GLN	CA-C-N	8.56	130.54	119.84
1	L	112	GLN	C-N-CA	8.56	130.54	119.84
2	H	315	ALA	CA-C-N	8.54	130.51	119.84
2	H	315	ALA	C-N-CA	8.54	130.51	119.84
2	H	247	VAL	CA-CB-CG1	8.48	124.82	110.40
2	H	382	VAL	CG1-CB-CG2	-8.42	92.28	110.80
2	H	228	PHE	N-CA-C	8.30	123.12	109.58
2	H	64	SER	N-CA-C	-8.30	93.13	110.80
2	H	265	ASP	N-CA-C	8.29	128.47	110.80
2	H	290	VAL	N-CA-CB	-8.25	102.75	112.40
2	H	269	VAL	CA-C-N	8.16	137.13	121.54
2	H	269	VAL	C-N-CA	8.16	137.13	121.54
1	L	97	ASP	CA-CB-CG	8.12	120.72	112.60
1	L	144	TYR	O-C-N	-8.11	114.39	121.20
1	L	89	TYR	CA-CB-CG	8.10	128.48	113.90
1	L	116	ASN	CA-C-O	-8.08	111.13	120.34
1	L	139	LEU	CB-CA-C	-8.02	97.19	110.19
2	H	344	THR	N-CA-C	-8.00	102.83	112.59
1	L	99	PHE	CA-CB-CG	7.99	121.79	113.80
2	H	264	VAL	N-CA-CB	7.98	120.10	111.00
2	H	14	PRO	N-CA-C	7.93	128.82	112.47
2	H	158	TRP	CA-C-N	7.89	133.96	122.36
2	H	158	TRP	C-N-CA	7.89	133.96	122.36
1	L	72	THR	CA-CB-OG1	-7.88	97.78	109.60
1	L	110	LEU	N-CA-C	7.88	121.69	109.96
2	H	269	VAL	N-CA-C	-7.87	102.77	110.72
1	L	173	ASN	CA-CB-CG	7.87	120.47	112.60
2	H	147	LYS	CG-CD-CE	-7.85	93.24	111.30
2	H	145	LEU	CA-CB-CG	7.84	143.74	116.30
2	H	62	ASN	O-C-N	-7.83	114.33	121.30
1	L	141	SER	O-C-N	7.82	132.34	123.19
2	H	29	ILE	CA-C-N	7.82	136.48	121.54
2	H	29	ILE	C-N-CA	7.82	136.48	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	426	LEU	CD1-CG-CD2	-7.81	93.61	110.80
2	H	241	THR	CB-CA-C	7.78	117.87	110.17
2	H	346	ASN	CA-CB-CG	7.78	120.38	112.60
2	H	333	VAL	CG1-CB-CG2	-7.73	93.79	110.80
2	H	12	VAL	CA-C-O	-7.67	114.12	121.64
2	H	321	ILE	CA-C-O	7.66	130.00	121.04
2	H	62	ASN	CA-C-N	7.62	129.37	119.84
2	H	62	ASN	C-N-CA	7.62	129.37	119.84
2	H	121	LYS	CA-CB-CG	7.59	129.27	114.10
2	H	375	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	L	114	LYS	N-CA-C	7.57	121.72	110.52
2	H	102	LEU	N-CA-C	-7.57	104.58	113.88
2	H	264	VAL	N-CA-C	-7.56	96.66	108.23
2	H	17	ALA	N-CA-C	7.55	120.69	108.76
2	H	91	ASP	CA-CB-CG	7.53	120.13	112.60
2	H	115	VAL	N-CA-CB	-7.53	102.55	112.34
2	H	251	VAL	CA-C-N	7.51	135.89	121.54
2	H	251	VAL	C-N-CA	7.51	135.89	121.54
2	H	18	LEU	O-C-N	-7.51	114.92	123.48
2	H	88	THR	CA-CB-CG2	7.50	123.24	110.50
2	H	274	THR	CA-CB-OG1	-7.50	98.36	109.60
2	H	188	VAL	CA-C-N	7.48	127.53	119.90
2	H	188	VAL	C-N-CA	7.48	127.53	119.90
2	H	212	ASP	CA-CB-CG	7.47	120.07	112.60
2	H	144	CYS	CA-CB-SG	-7.46	97.23	114.40
2	H	109	GLN	N-CA-C	-7.45	103.02	112.93
2	H	282	ASN	CA-C-N	7.45	135.76	121.54
2	H	282	ASN	C-N-CA	7.45	135.76	121.54
2	H	84	LEU	CA-C-O	-7.42	109.90	120.51
2	H	213	LYS	N-CA-C	7.39	120.09	108.79
2	H	79	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	L	140	ILE	CA-CB-CG2	-7.35	98.01	110.50
2	H	243	GLU	N-CA-C	7.33	119.52	108.46
2	H	134	SER	N-CA-C	7.25	120.84	109.96
2	H	41	GLN	OE1-CD-NE2	-7.24	115.36	122.60
2	H	42	PRO	O-C-N	-7.23	117.98	121.31
2	H	88	THR	CA-CB-OG1	-7.22	98.76	109.60
1	L	167	LYS	N-CA-C	7.21	125.74	109.81
2	H	203	ASN	CA-CB-CG	7.20	119.80	112.60
2	H	266	GLY	CA-C-N	7.18	131.64	122.37
2	H	266	GLY	C-N-CA	7.18	131.64	122.37
2	H	36	TRP	CG-CD2-CE3	7.17	141.07	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	355	LYS	CA-CB-CG	7.17	128.44	114.10
2	H	121	LYS	CB-CA-C	-7.16	99.79	110.24
2	H	113	VAL	CA-CB-CG2	-7.15	98.25	110.40
2	H	414	HIS	O-C-N	7.11	131.95	123.27
1	L	201	HIS	CB-CG-CD2	-7.11	121.96	131.20
2	H	17	ALA	CB-CA-C	7.08	123.12	110.16
1	L	214	GLU	CA-C-O	-7.07	111.23	119.64
2	H	186	VAL	CG1-CB-CG2	-7.07	95.26	110.80
2	H	16	GLU	CA-CB-CG	7.06	128.22	114.10
2	H	359	PRO	N-CA-C	7.02	126.94	112.47
2	H	121	LYS	N-CA-C	7.02	120.20	108.13
1	L	115	ALA	N-CA-C	7.01	119.84	108.76
2	H	74	ASN	CA-C-N	7.00	131.33	120.82
2	H	74	ASN	C-N-CA	7.00	131.33	120.82
2	H	376	TYR	CA-CB-CG	7.00	126.50	113.90
2	H	125	VAL	N-CA-C	6.98	120.49	108.90
2	H	353	LEU	CA-C-O	6.97	128.64	120.69
1	L	52	GLU	N-CA-C	6.97	125.65	110.80
1	L	115	ALA	CA-C-N	6.97	130.60	122.52
1	L	115	ALA	C-N-CA	6.97	130.60	122.52
2	H	62	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	L	101	PHE	CA-CB-CG	6.93	120.73	113.80
2	H	337	PRO	N-CA-C	6.92	119.15	110.70
2	H	147	LYS	N-CA-C	6.90	120.76	109.24
1	L	216	SER	N-CA-C	6.88	130.26	111.00
1	L	208	LYS	CA-C-N	6.87	134.66	121.54
1	L	208	LYS	C-N-CA	6.87	134.66	121.54
2	H	241	THR	N-CA-CB	-6.87	99.98	110.07
1	L	154	ALA	CA-C-N	6.86	134.50	123.93
1	L	154	ALA	C-N-CA	6.86	134.50	123.93
2	H	116	SER	N-CA-C	6.86	125.42	110.80
2	H	116	SER	CA-C-N	6.86	134.64	121.54
2	H	116	SER	C-N-CA	6.86	134.64	121.54
2	H	358	TYR	O-C-N	-6.84	115.51	121.32
1	L	141	SER	CA-CB-OG	6.83	124.75	111.10
2	H	65	LEU	CD1-CG-CD2	-6.78	95.88	110.80
2	H	16	GLU	N-CA-CB	-6.78	99.03	110.49
2	H	63	PRO	N-CA-C	6.78	126.44	112.47
2	H	103	VAL	CA-C-O	-6.77	112.32	120.78
1	L	101	PHE	CA-C-N	6.77	127.82	120.44
1	L	101	PHE	C-N-CA	6.77	127.82	120.44
2	H	83	LYS	CA-CB-CG	-6.77	100.57	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	390	PHE	CA-CB-CG	6.74	120.54	113.80
2	H	74	ASN	OD1-CG-ND2	-6.74	115.86	122.60
2	H	381	PRO	N-CA-C	6.73	126.33	112.47
2	H	247	VAL	CA-CB-CG2	-6.70	99.01	110.40
1	L	45	ALA	CA-C-N	6.70	126.61	119.85
1	L	45	ALA	C-N-CA	6.70	126.61	119.85
2	H	212	ASP	O-C-N	-6.70	115.79	123.42
2	H	364	VAL	CG1-CB-CG2	-6.68	96.11	110.80
1	L	206	VAL	N-CA-CB	-6.65	100.53	111.44
2	H	152	GLN	CA-CB-CG	-6.65	100.80	114.10
2	H	329	ARG	CA-CB-CG	6.63	127.36	114.10
1	L	193	ARG	N-CA-C	-6.62	101.43	111.56
1	L	35	VAL	CA-CB-CG1	6.62	121.65	110.40
2	H	250	ASP	CA-CB-CG	6.60	119.20	112.60
2	H	219	LEU	CA-C-N	6.60	134.14	121.54
2	H	219	LEU	C-N-CA	6.60	134.14	121.54
1	L	208	LYS	N-CA-C	6.59	124.83	110.80
2	H	244	VAL	CG1-CB-CG2	-6.58	96.32	110.80
2	H	121	LYS	CA-C-N	6.58	132.20	121.87
2	H	121	LYS	C-N-CA	6.58	132.20	121.87
2	H	291	LEU	CA-C-N	6.56	131.78	122.72
2	H	291	LEU	C-N-CA	6.56	131.78	122.72
2	H	211	VAL	N-CA-C	6.56	117.61	108.23
2	H	255	ASP	CA-C-N	6.54	128.01	119.84
2	H	255	ASP	C-N-CA	6.54	128.01	119.84
2	H	172	ALA	N-CA-C	6.52	118.43	110.41
2	H	31	THR	CA-CB-OG1	-6.51	99.83	109.60
1	L	145	PRO	N-CA-C	6.51	125.88	112.47
1	L	35	VAL	CA-CB-CG2	-6.49	99.37	110.40
2	H	214	ARG	N-CA-C	6.49	124.61	110.80
2	H	371	GLN	CA-C-N	6.48	127.94	119.84
2	H	371	GLN	C-N-CA	6.48	127.94	119.84
1	L	139	LEU	N-CA-C	6.48	119.29	108.73
2	H	338	PRO	N-CA-C	6.45	120.75	111.13
2	H	283	SER	CA-CB-OG	6.44	123.98	111.10
2	H	274	THR	CA-CB-CG2	6.44	121.45	110.50
2	H	87	VAL	CG1-CB-CG2	-6.44	96.64	110.80
2	H	336	LEU	CA-C-N	6.44	127.01	120.38
2	H	336	LEU	C-N-CA	6.44	127.01	120.38
2	H	159	ASN	CA-C-N	6.43	137.51	126.32
2	H	159	ASN	C-N-CA	6.43	137.51	126.32
1	L	117	PRO	CA-N-CD	-6.43	103.00	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	142	ASP	CA-CB-CG	6.43	119.03	112.60
1	L	103	THR	CA-CB-CG2	6.43	121.42	110.50
2	H	258	VAL	CG1-CB-CG2	-6.42	96.67	110.80
1	L	170	LYS	N-CA-C	6.40	124.42	110.80
2	H	380	PRO	CA-C-N	6.39	127.83	119.84
2	H	380	PRO	C-N-CA	6.39	127.83	119.84
2	H	65	LEU	N-CA-CB	-6.38	99.81	110.22
2	H	257	GLN	N-CA-C	6.38	124.38	110.80
1	L	169	SER	O-C-N	6.37	130.53	123.33
1	L	19	THR	CA-C-N	6.37	131.73	122.69
1	L	19	THR	C-N-CA	6.37	131.73	122.69
2	H	382	VAL	CA-CB-CG1	6.36	121.22	110.40
2	H	14	PRO	O-C-N	6.36	131.22	122.64
2	H	371	GLN	OE1-CD-NE2	-6.35	116.25	122.60
2	H	167	VAL	CG1-CB-CG2	-6.35	96.84	110.80
2	H	328	PRO	O-C-N	6.35	131.21	122.64
2	H	62	ASN	CA-CB-CG	6.33	118.93	112.60
2	H	353	LEU	CA-CB-CG	6.32	138.42	116.30
2	H	104	VAL	N-CA-C	-6.31	96.21	109.34
2	H	218	GLU	CA-C-N	6.30	133.58	121.54
2	H	218	GLU	C-N-CA	6.30	133.58	121.54
1	L	119	VAL	O-C-N	-6.30	116.60	122.71
2	H	203	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	H	330	GLU	CA-CB-CG	6.29	126.67	114.10
1	L	6	GLN	CA-C-O	-6.28	114.35	120.19
1	L	50	ILE	CB-CG1-CD1	6.28	126.98	113.80
2	H	185	VAL	CA-CB-CG1	6.27	121.06	110.40
1	L	168	PRO	O-C-N	-6.27	115.95	123.03
1	L	103	THR	CA-CB-OG1	-6.26	100.21	109.60
2	H	390	PHE	N-CA-C	6.25	118.03	108.52
2	H	339	SER	N-CA-C	-6.25	99.02	108.96
2	H	33	LEU	CB-CA-C	-6.24	98.00	110.42
2	H	143	GLY	CA-C-O	6.24	128.07	121.08
2	H	153	PRO	N-CA-C	6.24	125.32	112.47
2	H	313	LEU	CA-C-N	6.22	125.95	119.05
2	H	313	LEU	C-N-CA	6.22	125.95	119.05
2	H	117	SER	CA-C-N	6.21	133.39	121.54
2	H	117	SER	C-N-CA	6.21	133.39	121.54
1	L	144	TYR	CA-C-N	6.18	127.56	119.84
1	L	144	TYR	C-N-CA	6.18	127.56	119.84
2	H	244	VAL	CA-CB-CG2	-6.18	99.90	110.40
1	L	102	GLY	N-CA-C	6.17	119.12	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	241	THR	N-CA-C	6.17	119.80	108.69
2	H	12	VAL	O-C-N	-6.17	116.10	122.95
2	H	62	ASN	N-CA-C	6.16	118.35	109.48
1	L	212	PRO	CA-C-N	6.16	133.30	121.54
1	L	212	PRO	C-N-CA	6.16	133.30	121.54
2	H	150	PHE	CA-C-N	6.14	127.52	119.84
2	H	150	PHE	C-N-CA	6.14	127.52	119.84
1	L	112	GLN	N-CA-C	6.14	128.13	107.32
2	H	113	VAL	CA-CB-CG1	6.13	120.82	110.40
2	H	262	TRP	CG-CD2-CE3	6.13	140.03	133.90
2	H	111	THR	CA-CB-OG1	-6.11	100.44	109.60
1	L	178	ALA	N-CA-C	6.10	119.14	109.81
2	H	13	LYS	CA-CB-CG	6.10	126.30	114.10
2	H	150	PHE	CA-CB-CG	6.10	119.90	113.80
1	L	141	SER	CA-C-N	6.08	133.16	121.54
1	L	141	SER	C-N-CA	6.08	133.16	121.54
1	L	64	PHE	CA-C-O	6.08	127.47	120.60
1	L	113	PRO	N-CA-C	6.07	124.97	112.47
1	L	53	VAL	CA-CB-CG1	6.05	120.69	110.40
1	L	28	ASP	CA-C-N	6.05	128.40	120.60
1	L	28	ASP	C-N-CA	6.05	128.40	120.60
2	H	223	PRO	N-CA-C	6.04	124.91	112.47
2	H	66	LYS	CA-C-N	6.04	133.07	121.54
2	H	66	LYS	C-N-CA	6.04	133.07	121.54
2	H	47	LEU	N-CA-C	6.02	118.99	109.96
2	H	379	THR	OG1-CB-CG2	-6.02	97.27	109.30
2	H	384	ASP	CA-C-N	6.01	128.59	120.65
2	H	384	ASP	C-N-CA	6.01	128.59	120.65
2	H	216	ALA	CA-C-N	6.01	127.35	119.84
2	H	216	ALA	C-N-CA	6.01	127.35	119.84
2	H	189	PRO	N-CA-C	6.00	120.63	111.15
2	H	8	GLY	O-C-N	-5.99	115.78	121.77
2	H	344	THR	CA-CB-CG2	5.98	120.67	110.50
1	L	139	LEU	N-CA-CB	5.98	120.17	110.42
2	H	185	VAL	CA-CB-CG2	-5.97	100.24	110.40
2	H	421	TYR	CA-CB-CG	5.97	124.65	113.90
2	H	233	LYS	N-CA-C	-5.96	105.09	112.90
2	H	244	VAL	CA-CB-CG1	5.96	120.54	110.40
2	H	16	GLU	CB-CG-CD	5.94	122.70	112.60
1	L	53	VAL	CA-CB-CG2	-5.94	100.30	110.40
1	L	33	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	L	167	LYS	CA-C-N	5.94	126.84	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	167	LYS	C-N-CA	5.94	126.84	120.13
1	L	183	SER	CA-C-O	5.94	126.65	120.30
2	H	84	LEU	O-C-N	-5.93	114.70	122.59
2	H	50	ILE	CB-CA-C	-5.93	104.42	110.88
2	H	287	VAL	CA-CB-CG2	5.91	120.45	110.40
2	H	352	CYS	CA-CB-SG	5.89	127.96	114.40
2	H	328	PRO	CA-C-N	5.89	132.80	121.54
2	H	328	PRO	C-N-CA	5.89	132.80	121.54
2	H	348	VAL	CB-CA-C	-5.88	102.91	112.03
1	L	173	ASN	CA-C-N	5.87	131.31	122.68
1	L	173	ASN	C-N-CA	5.87	131.31	122.68
2	H	61	GLY	CA-C-N	5.87	128.63	120.65
2	H	61	GLY	C-N-CA	5.87	128.63	120.65
1	L	209	THR	N-CA-C	5.87	123.30	110.80
1	L	215	CYS	CA-C-N	5.86	132.25	121.70
1	L	215	CYS	C-N-CA	5.86	132.25	121.70
1	L	118	THR	CA-C-O	5.85	128.87	120.51
2	H	332	GLN	OE1-CD-NE2	-5.84	116.76	122.60
2	H	32	ILE	CA-C-N	5.83	132.68	121.54
2	H	32	ILE	C-N-CA	5.83	132.68	121.54
2	H	151	PRO	N-CA-C	5.83	124.47	112.47
2	H	18	LEU	CA-CB-CG	5.83	136.69	116.30
2	H	382	VAL	N-CA-CB	5.83	117.98	110.99
2	H	40	ARG	CA-CB-CG	5.82	125.75	114.10
2	H	165	SER	O-C-N	5.81	129.84	123.27
2	H	175	GLN	N-CA-C	5.81	123.18	110.80
2	H	152	GLN	CA-C-N	5.80	127.09	119.84
2	H	152	GLN	C-N-CA	5.80	127.09	119.84
2	H	31	THR	CA-CB-CG2	5.80	120.36	110.50
2	H	329	ARG	O-C-N	5.80	130.30	122.59
2	H	279	GLN	CA-CB-CG	5.78	125.67	114.10
1	L	109	VAL	CA-CB-CG2	5.77	120.21	110.40
2	H	96	TYR	CA-CB-CG	5.77	124.29	113.90
2	H	163	LEU	N-CA-C	-5.77	98.52	110.80
2	H	399	LYS	CA-CB-CG	5.76	125.63	114.10
1	L	207	GLU	N-CA-C	-5.76	95.66	107.70
2	H	13	LYS	CB-CG-CD	5.76	124.55	111.30
1	L	157	SER	CA-C-N	5.76	126.66	119.98
1	L	157	SER	C-N-CA	5.76	126.66	119.98
2	H	83	LYS	N-CA-C	-5.75	99.81	109.07
1	L	116	ASN	N-CA-C	5.75	121.17	108.64
1	L	210	VAL	CA-C-N	5.75	129.05	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	VAL	C-N-CA	5.75	129.05	120.83
1	L	174	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	L	140	ILE	CA-CB-CG1	5.74	120.16	110.40
2	H	96	TYR	CA-C-O	5.73	127.48	120.60
2	H	152	GLN	OE1-CD-NE2	-5.73	116.87	122.60
2	H	327	GLN	O-C-N	-5.73	114.73	121.32
2	H	274	THR	CA-C-O	5.72	127.28	120.70
2	H	248	VAL	O-C-N	5.72	129.38	123.20
2	H	186	VAL	CA-C-N	5.70	129.99	122.06
2	H	186	VAL	C-N-CA	5.70	129.99	122.06
2	H	68	ARG	CG-CD-NE	5.70	124.53	112.00
2	H	398	ASP	CA-C-N	5.70	127.92	120.28
2	H	398	ASP	C-N-CA	5.70	127.92	120.28
2	H	199	ILE	O-C-N	-5.70	117.05	123.20
1	L	84	ASP	CA-CB-CG	5.68	118.28	112.60
1	L	193	ARG	O-C-N	-5.68	115.79	122.32
2	H	268	GLN	CA-C-N	5.67	128.47	120.42
2	H	268	GLN	C-N-CA	5.67	128.47	120.42
1	L	72	THR	CA-CB-CG2	5.67	120.14	110.50
2	H	145	LEU	CD1-CG-CD2	-5.67	98.33	110.80
2	H	228	PHE	CA-CB-CG	-5.67	108.13	113.80
2	H	199	ILE	CA-CB-CG1	5.66	120.01	110.40
1	L	1	PRO	CA-C-N	5.65	128.89	120.87
1	L	1	PRO	C-N-CA	5.65	128.89	120.87
1	L	209	THR	CA-C-N	5.65	130.00	120.29
1	L	209	THR	C-N-CA	5.65	130.00	120.29
2	H	105	ASN	O-C-N	-5.64	114.84	121.32
1	L	93	TYR	CA-CB-CG	5.63	124.04	113.90
1	L	116	ASN	CA-C-N	5.63	126.88	119.84
1	L	116	ASN	C-N-CA	5.63	126.88	119.84
2	H	414	HIS	CA-C-O	5.63	127.13	120.66
1	L	160	LYS	CA-CB-CG	5.62	125.35	114.10
2	H	77	LYS	CA-C-N	5.62	132.27	121.54
2	H	77	LYS	C-N-CA	5.62	132.27	121.54
1	L	69	SER	CA-C-O	5.61	127.05	120.20
2	H	344	THR	CA-CB-OG1	-5.61	101.19	109.60
1	L	16	GLN	OE1-CD-NE2	-5.59	117.01	122.60
2	H	208	ASN	OD1-CG-ND2	-5.58	117.03	122.60
1	L	183	SER	N-CA-C	5.57	117.50	108.41
2	H	418	HIS	N-CA-C	5.57	120.51	111.37
1	L	160	LYS	N-CA-C	5.55	117.76	107.60
2	H	82	SER	CB-CA-C	-5.55	104.16	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	201	HIS	CB-CG-ND1	5.55	131.02	122.70
2	H	404	GLN	N-CA-C	-5.53	106.53	113.28
2	H	369	ASN	CA-CB-CG	5.53	118.13	112.60
2	H	16	GLU	CA-C-O	-5.53	112.61	120.51
1	L	165	THR	CA-CB-OG1	-5.52	101.32	109.60
2	H	211	VAL	CA-C-O	-5.52	115.92	121.49
2	H	228	PHE	CA-C-N	5.51	126.06	120.38
2	H	228	PHE	C-N-CA	5.51	126.06	120.38
2	H	287	VAL	CA-C-O	5.51	126.12	120.39
2	H	219	LEU	N-CA-C	5.51	122.53	110.80
2	H	249	VAL	N-CA-CB	-5.50	104.82	112.52
1	L	176	TYR	O-C-N	-5.50	116.79	122.94
2	H	111	THR	CA-C-O	5.50	127.04	120.28
2	H	115	VAL	CG1-CB-CG2	-5.48	98.74	110.80
1	L	95	GLY	N-CA-C	-5.47	106.55	112.08
1	L	60	VAL	CA-CB-CG2	5.47	119.69	110.40
2	H	78	ASN	OD1-CG-ND2	-5.46	117.14	122.60
2	H	18	LEU	N-CA-C	5.45	117.38	108.55
2	H	419	ASN	CA-C-N	5.45	129.87	122.07
2	H	419	ASN	C-N-CA	5.45	129.87	122.07
2	H	347	GLN	N-CA-C	5.45	117.28	108.34
2	H	213	LYS	CG-CD-CE	5.44	123.81	111.30
2	H	173	VAL	CA-CB-CG2	-5.44	101.16	110.40
2	H	31	THR	N-CA-CB	-5.43	101.32	110.49
2	H	353	LEU	CD1-CG-CD2	-5.42	98.87	110.80
2	H	366	TRP	CG-CD2-CE3	5.42	139.32	133.90
2	H	173	VAL	CA-CB-CG1	5.41	119.60	110.40
2	H	65	LEU	CB-CA-C	5.41	117.87	111.22
2	H	36	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	L	72	THR	CA-C-O	5.41	126.16	120.54
2	H	380	PRO	CB-CA-C	5.41	117.51	110.92
2	H	115	VAL	N-CA-C	5.40	116.53	107.18
2	H	38	TRP	CG-CD2-CE3	5.39	139.29	133.90
2	H	364	VAL	CA-CB-CG1	5.39	119.57	110.40
1	L	135	THR	CA-CB-OG1	-5.39	101.51	109.60
2	H	33	LEU	N-CA-CB	5.39	119.59	110.49
2	H	271	ASN	CA-C-N	5.38	131.82	121.54
2	H	271	ASN	C-N-CA	5.38	131.82	121.54
2	H	414	HIS	CB-CG-CD2	-5.38	124.20	131.20
2	H	21	THR	CA-CB-OG1	-5.38	101.53	109.60
2	H	73	VAL	N-CA-CB	-5.36	104.36	112.35
2	H	373	GLU	CA-CB-CG	-5.36	103.37	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	60	TYR	CA-C-O	5.36	126.03	120.30
2	H	248	VAL	CA-C-O	5.35	126.03	120.36
2	H	376	TYR	N-CA-C	5.35	117.90	108.75
2	H	361	ASP	CA-CB-CG	5.35	117.95	112.60
2	H	158	TRP	CE2-CD2-CG	-5.34	100.79	107.20
2	H	125	VAL	CA-C-O	-5.34	116.34	121.63
2	H	268	GLN	N-CA-CB	-5.34	101.68	109.95
2	H	122	GLY	N-CA-C	5.33	123.22	112.34
2	H	245	THR	CA-C-O	5.33	126.79	120.66
1	L	185	THR	CA-C-N	5.33	126.50	119.84
1	L	185	THR	C-N-CA	5.33	126.50	119.84
1	L	33	ASN	N-CA-C	-5.33	106.56	113.16
2	H	403	GLN	OE1-CD-NE2	-5.31	117.29	122.60
2	H	69	VAL	N-CA-C	5.30	120.36	109.34
2	H	113	VAL	CA-C-O	5.30	126.89	120.74
2	H	410	CYS	CA-C-O	5.30	127.86	121.66
1	L	209	THR	CA-CB-CG2	5.29	119.50	110.50
1	L	170	LYS	CA-CB-CG	-5.29	103.51	114.10
2	H	252	SER	CA-CB-OG	5.29	121.67	111.10
2	H	148	ASP	CA-CB-CG	5.28	117.88	112.60
1	L	198	GLN	OE1-CD-NE2	-5.28	117.32	122.60
2	H	34	TYR	CA-CB-CG	5.27	123.39	113.90
2	H	294	LEU	CA-C-N	5.27	131.60	121.54
2	H	294	LEU	C-N-CA	5.27	131.60	121.54
1	L	128	GLU	CA-CB-CG	5.25	124.61	114.10
2	H	162	ALA	CA-C-N	5.25	131.57	121.54
2	H	162	ALA	C-N-CA	5.25	131.57	121.54
2	H	417	LEU	CA-C-O	5.24	127.47	121.28
1	L	61	PRO	CA-C-N	5.24	129.06	120.63
1	L	61	PRO	C-N-CA	5.24	129.06	120.63
1	L	82	ALA	CA-C-N	5.24	129.59	120.68
1	L	82	ALA	C-N-CA	5.24	129.59	120.68
2	H	111	THR	CA-CB-CG2	5.24	119.40	110.50
2	H	226	PHE	CA-C-O	5.24	126.61	120.75
2	H	245	THR	N-CA-C	5.24	117.98	109.24
1	L	204	SER	N-CA-C	-5.23	99.23	108.23
2	H	382	VAL	CB-CA-C	-5.23	103.72	110.84
2	H	315	ALA	N-CA-CB	-5.22	100.48	110.61
2	H	125	VAL	CA-C-N	5.22	128.00	122.26
2	H	125	VAL	C-N-CA	5.22	128.00	122.26
2	H	417	LEU	O-C-N	5.21	129.09	123.10
2	H	22	CYS	N-CA-C	5.21	116.90	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	402	TRP	CA-CB-CG	5.21	123.49	113.60
1	L	150	VAL	CA-CB-CG2	5.20	119.24	110.40
2	H	271	ASN	OD1-CG-ND2	-5.19	117.41	122.60
2	H	127	PRO	N-CA-CB	-5.18	97.81	103.25
2	H	379	THR	CA-C-O	-5.18	114.36	119.49
1	L	208	LYS	CA-CB-CG	5.18	124.46	114.10
2	H	104	VAL	CG1-CB-CG2	-5.18	99.41	110.80
2	H	330	GLU	CA-C-N	5.16	125.08	119.76
2	H	330	GLU	C-N-CA	5.16	125.08	119.76
2	H	199	ILE	CA-CB-CG2	-5.15	101.75	110.50
1	L	104	GLY	N-CA-C	5.14	118.70	112.48
2	H	158	TRP	CG-CD2-CE3	5.14	139.04	133.90
1	L	138	CYS	CA-C-O	-5.13	113.12	120.15
2	H	375	ASN	CB-CG-ND2	5.13	124.10	116.40
2	H	175	GLN	CA-CB-CG	-5.13	103.84	114.10
2	H	159	ASN	OD1-CG-ND2	-5.12	117.47	122.60
1	L	2	SER	N-CA-C	-5.12	102.70	110.28
2	H	375	ASN	N-CA-C	5.12	117.75	107.41
2	H	12	VAL	N-CA-C	5.11	116.06	108.65
2	H	85	SER	CA-C-O	-5.11	113.20	120.51
2	H	147	LYS	CA-C-N	5.11	130.64	122.93
2	H	147	LYS	C-N-CA	5.11	130.64	122.93
2	H	212	ASP	N-CA-C	5.10	116.69	108.32
2	H	149	TYR	CA-CB-CG	5.10	123.08	113.90
2	H	222	GLY	CA-C-N	5.09	126.21	119.84
2	H	222	GLY	C-N-CA	5.09	126.21	119.84
2	H	140	ALA	CA-C-O	5.09	126.34	120.14
2	H	196	GLN	CA-C-N	5.09	129.53	122.77
2	H	196	GLN	C-N-CA	5.09	129.53	122.77
2	H	11	LEU	CA-C-N	5.07	129.93	123.03
2	H	11	LEU	C-N-CA	5.07	129.93	123.03
2	H	321	ILE	CB-CG1-CD1	5.07	124.44	113.80
1	L	121	LEU	O-C-N	-5.06	117.19	123.36
1	L	147	ALA	N-CA-C	5.06	115.66	107.32
2	H	282	ASN	CA-CB-CG	-5.06	107.54	112.60
2	H	424	LYS	N-CA-C	-5.05	103.04	110.52
1	L	181	TYR	CA-CB-CG	5.05	123.00	113.90
1	L	182	LEU	CD1-CG-CD2	-5.05	99.68	110.80
2	H	328	PRO	CA-C-O	5.05	129.79	120.60
1	L	210	VAL	N-CA-C	-5.04	104.68	111.44
2	H	167	VAL	CA-C-O	5.03	125.91	120.43
1	L	60	VAL	CA-CB-CG1	-5.02	101.87	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	132	ASN	CA-CB-CG	5.02	117.62	112.60
2	H	292	THR	CA-CB-CG2	5.02	119.03	110.50
1	L	213	THR	OG1-CB-CG2	-5.01	99.27	109.30
2	H	316	PRO	N-CA-C	5.01	122.80	112.47
2	H	165	SER	N-CA-C	-5.00	101.08	109.24
2	H	410	CYS	CA-CB-SG	5.00	125.91	114.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	PHE	Sidechain
2	H	15	SER	Mainchain
2	H	150	PHE	Peptide
2	H	152	GLN	Peptide
2	H	17	ALA	Mainchain
2	H	334	TYR	Sidechain
2	H	358	TYR	Peptide
2	H	380	PRO	Peptide
2	H	54	TYR	Sidechain
2	H	96	TYR	Sidechain
1	L	144	TYR	Sidechain,Peptide

5.2 Too-close contacts [i](#)

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	L	1606	0	1536	49	0
2	H	3305	0	3277	138	0
3	A	130	0	107	22	0
All	All	5041	0	4920	169	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 17.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:139:LEU:HG	2:H:147:LYS:HE3	1.60	0.84
2:H:226:PHE:CD2	3:A:3:BMA:H3	2.15	0.82
1:L:179:SER:HA	2:H:147:LYS:HE2	1.63	0.81
3:A:3:BMA:HO3	3:A:8:GUP:C1	1.94	0.81
2:H:125:VAL:HG21	2:H:211:VAL:HG11	1.63	0.79
2:H:126:PHE:HB3	2:H:145:LEU:HD23	1.63	0.78
2:H:226:PHE:HZ	3:A:9:NAG:H2	1.49	0.77
1:L:125:SER:HB3	2:H:211:VAL:HG13	1.67	0.76
1:L:139:LEU:HD13	2:H:145:LEU:HG	1.66	0.75
2:H:248:VAL:HB	2:H:287:VAL:HG23	1.69	0.72
2:H:50:ILE:HB	2:H:65:LEU:HD23	1.72	0.71
2:H:226:PHE:HD2	3:A:3:BMA:H3	1.53	0.71
2:H:243:GLU:HG3	3:A:6:GAL:H62	1.72	0.71
1:L:145:PRO:HD2	1:L:201:HIS:NE2	2.07	0.70
2:H:333:VAL:HG12	2:H:424:LYS:HB2	1.74	0.69
1:L:179:SER:HA	2:H:147:LYS:CE	2.22	0.68
2:H:158:TRP:HZ3	2:H:198:TYR:HB3	1.58	0.68
2:H:100:VAL:HG13	2:H:103:VAL:O	1.93	0.67
2:H:226:PHE:CZ	3:A:9:NAG:H4	2.30	0.67
1:L:119:VAL:HA	1:L:139:LEU:O	1.94	0.67
2:H:200:CYS:O	2:H:212:ASP:HA	1.95	0.67
3:A:3:BMA:C3	3:A:8:GUP:C1	2.72	0.67
2:H:11:LEU:HD12	2:H:114:THR:HB	1.77	0.66
1:L:179:SER:HA	2:H:147:LYS:NZ	2.11	0.66
2:H:122:GLY:O	2:H:149:TYR:HA	1.95	0.65
2:H:333:VAL:HG22	2:H:354:VAL:HG12	1.79	0.65
1:L:137:VAL:HB	2:H:126:PHE:HE2	1.61	0.65
1:L:179:SER:HA	2:H:147:LYS:HZ3	1.62	0.65
2:H:277:ARG:O	2:H:287:VAL:HA	1.97	0.65
2:H:226:PHE:CZ	3:A:9:NAG:H2	2.32	0.64
2:H:127:PRO:HA	2:H:144:CYS:HA	1.79	0.64
2:H:170:PHE:HB2	2:H:183:SER:HB2	1.78	0.64
1:L:6:GLN:NE2	1:L:104:GLY:H	1.95	0.64
2:H:245:THR:HG23	2:H:290:VAL:HG13	1.81	0.63
2:H:31:THR:HB	2:H:73:VAL:HG11	1.80	0.62
2:H:329:ARG:HB2	2:H:357:PHE:HA	1.82	0.62
2:H:201:ASN:HA	2:H:211:VAL:O	1.99	0.62
2:H:11:LEU:HD22	2:H:118:ALA:HB2	1.82	0.62
2:H:29:ILE:HG23	2:H:30:ASN:H	1.64	0.62
1:L:1:PRO:HB3	2:H:63:PRO:HG3	1.81	0.61
2:H:99:ARG:HH21	2:H:106:PRO:HG2	1.65	0.61
2:H:226:PHE:CE2	3:A:8:GUP:C1	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:357:PHE:O	2:H:389:PHE:HB2	2.04	0.58
1:L:137:VAL:HB	2:H:126:PHE:CE2	2.37	0.58
2:H:128:LEU:HG	2:H:145:LEU:HD22	1.86	0.57
2:H:354:VAL:HG21	2:H:364:VAL:HG21	1.86	0.57
1:L:179:SER:HB2	2:H:175:GLN:HE22	1.69	0.57
2:H:230:PRO:HB3	2:H:243:GLU:H	1.69	0.57
2:H:286:ARG:NH2	3:A:4:MAN:O3	2.38	0.57
2:H:261:ASN:HB2	2:H:307:LYS:HB3	1.85	0.56
1:L:139:LEU:HA	2:H:147:LYS:NZ	2.20	0.56
1:L:179:SER:CB	2:H:175:GLN:HE22	2.19	0.56
2:H:6:GLU:HB3	2:H:111:THR:HB	1.87	0.56
2:H:319:LYS:NZ	3:A:8:GUP:H3	2.21	0.56
2:H:335:THR:HA	2:H:352:CYS:HA	1.88	0.55
1:L:169:SER:HA	1:L:176:TYR:HD2	1.72	0.55
2:H:39:ILE:HG21	2:H:96:TYR:CD2	2.41	0.55
2:H:335:THR:HB	2:H:426:LEU:HD12	1.88	0.55
1:L:119:VAL:HG11	1:L:199:VAL:HG11	1.87	0.55
2:H:65:LEU:HD12	2:H:68:ARG:NH1	2.22	0.55
2:H:160:SER:H	2:H:201:ASN:ND2	2.04	0.55
2:H:249:VAL:HB	3:A:2:NAG:O3	2.07	0.55
3:A:6:GAL:H61	3:A:7:SIA:O1B	2.07	0.54
2:H:335:THR:HG23	2:H:424:LYS:HB3	1.90	0.54
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.90	0.53
1:L:137:VAL:HG11	2:H:124:SER:HB3	1.91	0.53
2:H:198:TYR:HD2	2:H:215:VAL:HG11	1.72	0.53
1:L:97:ASP:HB3	2:H:54:TYR:HB2	1.90	0.53
2:H:226:PHE:HZ	3:A:9:NAG:H4	1.72	0.53
2:H:202:VAL:HB	2:H:211:VAL:HG23	1.90	0.53
2:H:226:PHE:CE2	3:A:3:BMA:H3	2.44	0.53
2:H:304:TYR:HB2	2:H:321:ILE:HG22	1.89	0.53
1:L:149:THR:HB	1:L:200:THR:HG23	1.90	0.52
2:H:38:TRP:HB2	2:H:50:ILE:HG12	1.90	0.52
2:H:35:TYR:HB3	2:H:53:ILE:O	2.09	0.51
2:H:6:GLU:HG2	2:H:21:THR:O	2.10	0.51
2:H:362:ILE:HG12	2:H:391:LEU:HD21	1.92	0.51
2:H:362:ILE:HD11	2:H:364:VAL:HG23	1.93	0.50
3:A:6:GAL:H2	3:A:7:SIA:O1B	2.11	0.50
2:H:38:TRP:CZ2	2:H:82:SER:HB2	2.47	0.50
2:H:62:ASN:O	2:H:66:LYS:N	2.45	0.50
1:L:68:LYS:HA	1:L:73:ALA:HA	1.93	0.50
1:L:80:LEU:HD23	1:L:109:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:PHE:HE2	3:A:8:GUP:C1	2.25	0.50
2:H:121:LYS:H	2:H:150:PHE:HB3	1.77	0.49
2:H:226:PHE:CE1	3:A:9:NAG:H4	2.46	0.49
2:H:331:PRO:HD3	2:H:414:HIS:HD2	1.77	0.49
3:A:3:BMA:O3	3:A:8:GUP:O5	2.27	0.49
2:H:290:VAL:HG12	3:A:7:SIA:O1A	2.13	0.49
1:L:49:ILE:HG22	1:L:60:VAL:HG11	1.95	0.48
2:H:226:PHE:HB3	2:H:228:PHE:CE2	2.48	0.48
1:L:92:SER:O	1:L:99:PHE:HB2	2.13	0.48
2:H:101:PRO:HD3	2:H:106:PRO:HD3	1.94	0.48
2:H:98:ALA:HB1	2:H:104:VAL:HG13	1.96	0.48
1:L:139:LEU:HA	2:H:147:LYS:HZ2	1.78	0.47
1:L:6:GLN:HE22	1:L:89:TYR:HB3	1.79	0.47
2:H:18:LEU:HD21	2:H:113:VAL:HG22	1.96	0.47
2:H:55:TYR:O	2:H:56:SER:HB2	2.14	0.47
2:H:119:SER:HB3	2:H:121:LYS:HE2	1.97	0.47
2:H:243:GLU:HG3	3:A:6:GAL:C6	2.44	0.47
1:L:137:VAL:HA	1:L:181:TYR:HA	1.96	0.47
2:H:392:TYR:HD1	2:H:392:TYR:HA	1.59	0.47
2:H:241:THR:HA	2:H:242:PRO:HD2	1.91	0.46
2:H:279:GLN:HE22	2:H:286:ARG:HB3	1.80	0.46
2:H:381:PRO:HD3	2:H:391:LEU:HD23	1.97	0.46
1:L:120:THR:HB	2:H:126:PHE:HD1	1.80	0.46
1:L:122:PHE:CD2	2:H:127:PRO:HD3	2.51	0.46
1:L:169:SER:O	2:H:173:VAL:HG22	2.16	0.46
2:H:31:THR:HG23	2:H:55:TYR:O	2.16	0.46
2:H:145:LEU:HB2	2:H:182:LEU:O	2.15	0.46
2:H:364:VAL:HG22	2:H:412:VAL:HG13	1.98	0.46
1:L:35:VAL:HG23	1:L:92:SER:OG	2.16	0.46
2:H:156:VAL:HG13	2:H:202:VAL:HG22	1.98	0.46
2:H:297:ASN:O	2:H:302:LYS:HB2	2.16	0.46
2:H:12:VAL:N	2:H:116:SER:H	2.14	0.45
1:L:153:LYS:HD3	1:L:196:SER:HB2	1.97	0.45
2:H:233:LYS:O	2:H:237:MET:HB2	2.16	0.45
1:L:12:GLY:HA2	1:L:16:GLN:OE1	2.16	0.45
1:L:85:GLU:OE2	1:L:109:VAL:HG22	2.16	0.45
2:H:125:VAL:HG11	2:H:211:VAL:HG21	1.99	0.45
1:L:50:ILE:HD13	1:L:56:ARG:HB2	1.99	0.45
1:L:140:ILE:HB	1:L:178:ALA:HB3	1.99	0.45
1:L:179:SER:CA	2:H:147:LYS:HZ3	2.30	0.45
2:H:256:PRO:O	2:H:258:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:GLN:HB2	1:L:175:LYS:O	2.17	0.44
2:H:363:ALA:HB3	2:H:413:MET:HB2	1.99	0.44
2:H:41:GLN:HB2	2:H:47:LEU:HD23	1.99	0.44
2:H:331:PRO:CD	2:H:414:HIS:HD2	2.29	0.44
2:H:99:ARG:HE	2:H:106:PRO:HG2	1.82	0.44
2:H:315:ALA:HA	2:H:316:PRO:HD2	1.73	0.44
2:H:66:LYS:C	2:H:68:ARG:H	2.24	0.44
1:L:37:TRP:HB2	1:L:50:ILE:HB	2.00	0.43
1:L:122:PHE:HD2	2:H:127:PRO:HD3	1.82	0.43
2:H:225:VAL:HG22	2:H:248:VAL:HG22	2.00	0.43
2:H:351:THR:HG22	2:H:352:CYS:H	1.81	0.43
2:H:142:LEU:HD21	2:H:193:LEU:HD11	1.99	0.43
1:L:1:PRO:HD3	2:H:63:PRO:HD2	2.00	0.43
2:H:198:TYR:CD2	2:H:215:VAL:HG11	2.53	0.43
2:H:332:GLN:HB2	2:H:355:LYS:HG3	2.00	0.43
1:L:211:ALA:HA	1:L:212:PRO:HD3	1.84	0.43
2:H:36:TRP:HZ2	2:H:97:CYS:SG	2.42	0.43
1:L:166:THR:HB	2:H:177:SER:CB	2.49	0.43
1:L:27:SER:O	1:L:94:GLU:HA	2.19	0.42
1:L:137:VAL:HG12	1:L:180:SER:O	2.19	0.42
2:H:330:GLU:HA	2:H:331:PRO:HD2	1.92	0.42
2:H:347:GLN:HA	2:H:398:ASP:HA	2.01	0.42
1:L:164:GLU:O	1:L:180:SER:HA	2.20	0.42
2:H:12:VAL:O	2:H:115:VAL:HA	2.19	0.42
2:H:245:THR:HG23	2:H:290:VAL:CG1	2.48	0.42
2:H:415:GLU:C	2:H:417:LEU:H	2.27	0.42
1:L:139:LEU:HD22	1:L:141:SER:HB3	2.02	0.42
2:H:36:TRP:HD1	2:H:37:SER:H	1.66	0.42
2:H:125:VAL:CG1	2:H:211:VAL:HG21	2.50	0.42
2:H:352:CYS:HB3	2:H:393:SER:HB3	2.02	0.42
2:H:36:TRP:CZ2	2:H:97:CYS:SG	3.13	0.42
2:H:126:PHE:CE2	2:H:147:LYS:HD2	2.55	0.42
2:H:65:LEU:HG	2:H:69:VAL:HB	2.02	0.41
2:H:212:ASP:O	2:H:213:LYS:HD2	2.20	0.41
2:H:333:VAL:HA	2:H:353:LEU:O	2.20	0.41
2:H:335:THR:HG22	2:H:352:CYS:HB2	2.02	0.41
1:L:200:THR:HA	1:L:205:THR:HA	2.02	0.41
2:H:128:LEU:O	2:H:143:GLY:N	2.52	0.41
2:H:31:THR:HG23	2:H:55:TYR:C	2.46	0.41
2:H:327:GLN:HE22	2:H:329:ARG:NH1	2.19	0.41
2:H:126:PHE:HB3	2:H:145:LEU:CD2	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:ALA:O	2:H:163:LEU:HB2	2.20	0.40
2:H:255:ASP:N	2:H:256:PRO:HD3	2.35	0.40
2:H:8:GLY:H	2:H:9:PRO:HD3	1.86	0.40
2:H:226:PHE:HZ	3:A:9:NAG:C2	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	214/216 (99%)	164 (77%)	32 (15%)	18 (8%)	0	4
2	H	426/428 (100%)	304 (71%)	77 (18%)	45 (11%)	0	2
All	All	640/644 (99%)	468 (73%)	109 (17%)	63 (10%)	0	2

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	26	SER
1	L	52	GLU
1	L	96	SER
1	L	117	PRO
1	L	123	PRO
1	L	132	ASN
1	L	209	THR
1	L	213	THR
1	L	215	CYS
2	H	15	SER
2	H	29	ILE
2	H	56	SER
2	H	85	SER
2	H	86	SER

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Mol	Chain	Res	Type
2	H	101	PRO
2	H	122	GLY
2	H	151	PRO
2	H	153	PRO
2	H	163	LEU
2	H	208	ASN
2	H	217	PRO
2	H	220	LEU
2	H	251	VAL
2	H	252	SER
2	H	257	GLN
2	H	282	ASN
2	H	283	SER
2	H	359	PRO
1	L	42	ALA
1	L	57	PRO
1	L	118	THR
1	L	142	ASP
1	L	161	ALA
2	H	33	LEU
2	H	116	SER
2	H	219	LEU
2	H	265	ASP
2	H	280	GLN
2	H	295	HIS
2	H	325	LYS
2	H	340	ARG
2	H	369	ASN
1	L	170	LYS
1	L	208	LYS
2	H	104	VAL
2	H	118	ALA
2	H	123	PRO
2	H	152	GLN
1	L	53	VAL
1	L	130	GLN
2	H	55	TYR
2	H	63	PRO
2	H	103	VAL
2	H	117	SER
2	H	68	ARG
2	H	266	GLY

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Mol	Chain	Res	Type
2	H	329	ARG
2	H	256	PRO
2	H	14	PRO
2	H	105	ASN
2	H	127	PRO
2	H	57	GLY
2	H	69	VAL

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	L	181/181 (100%)	144 (80%)	37 (20%)	1	7
2	H	383/383 (100%)	288 (75%)	95 (25%)	1	3
All	All	564/564 (100%)	432 (77%)	132 (23%)	1	4

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	SER
1	L	13	SER
1	L	21	SER
1	L	35	VAL
1	L	54	ASN
1	L	55	LYS
1	L	60	VAL
1	L	62	ASP
1	L	69	SER
1	L	71	ASN
1	L	72	THR
1	L	80	LEU
1	L	81	GLN
1	L	89	TYR
1	L	91	SER
1	L	118	THR

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Mol	Chain	Res	Type
1	L	121	LEU
1	L	123	PRO
1	L	137	VAL
1	L	139	LEU
1	L	140	ILE
1	L	142	ASP
1	L	149	THR
1	L	150	VAL
1	L	160	LYS
1	L	165	THR
1	L	166	THR
1	L	171	GLN
1	L	174	ASN
1	L	182	LEU
1	L	184	LEU
1	L	196	SER
1	L	198	GLN
1	L	199	VAL
1	L	200	THR
1	L	208	LYS
1	L	209	THR
2	H	3	VAL
2	H	11	LEU
2	H	12	VAL
2	H	13	LYS
2	H	16	GLU
2	H	18	LEU
2	H	29	ILE
2	H	31	THR
2	H	33	LEU
2	H	35	TYR
2	H	36	TRP
2	H	39	ILE
2	H	48	GLU
2	H	52	TYR
2	H	55	TYR
2	H	68	ARG
2	H	69	VAL
2	H	71	ILE
2	H	72	SER
2	H	73	VAL
2	H	82	SER

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Mol	Chain	Res	Type
2	H	84	LEU
2	H	87	VAL
2	H	96	TYR
2	H	105	ASN
2	H	109	GLN
2	H	111	THR
2	H	113	VAL
2	H	114	THR
2	H	121	LYS
2	H	123	PRO
2	H	125	VAL
2	H	142	LEU
2	H	145	LEU
2	H	149	TYR
2	H	151	PRO
2	H	152	GLN
2	H	173	VAL
2	H	176	SER
2	H	183	SER
2	H	187	THR
2	H	196	GLN
2	H	201	ASN
2	H	208	ASN
2	H	209	THR
2	H	210	LYS
2	H	211	VAL
2	H	213	LYS
2	H	214	ARG
2	H	217	PRO
2	H	219	LEU
2	H	226	PHE
2	H	231	LYS
2	H	232	PRO
2	H	238	ILE
2	H	241	THR
2	H	243	GLU
2	H	245	THR
2	H	247	VAL
2	H	249	VAL
2	H	261	ASN
2	H	265	ASP
2	H	274	THR

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Mol	Chain	Res	Type
2	H	279	GLN
2	H	283	SER
2	H	286	ARG
2	H	290	VAL
2	H	302	LYS
2	H	313	LEU
2	H	321	ILE
2	H	327	GLN
2	H	329	ARG
2	H	351	THR
2	H	352	CYS
2	H	353	LEU
2	H	354	VAL
2	H	355	LYS
2	H	359	PRO
2	H	371	GLN
2	H	373	GLU
2	H	374	ASN
2	H	375	ASN
2	H	377	LYS
2	H	379	THR
2	H	382	VAL
2	H	392	TYR
2	H	397	VAL
2	H	399	LYS
2	H	407	VAL
2	H	410	CYS
2	H	415	GLU
2	H	420	HIS
2	H	423	GLN
2	H	424	LYS
2	H	426	LEU

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

Mol	Chain	Res	Type
1	L	6	GLN
1	L	98	ASN
1	L	173	ASN
1	L	192	HIS
2	H	109	GLN
2	H	175	GLN

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Mol	Chain	Res	Type
2	H	196	GLN
2	H	201	ASN
2	H	208	ASN
2	H	257	GLN
2	H	279	GLN
2	H	280	GLN
2	H	327	GLN
2	H	332	GLN
2	H	371	GLN
2	H	375	ASN
2	H	403	GLN
2	H	404	GLN
2	H	419	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 ⓘ

10 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$
3	NAG	A	1	2,3	14,14,15	2.35	7 (50%)	17,19,21	4.75	12 (70%)
3	FUL	A	10	3	10,10,11	1.42	1 (10%)	14,14,16	0.82	0
3	NAG	A	2	3	14,14,15	1.59	3 (21%)	17,19,21	3.76	7 (41%)
3	BMA	A	3	3	11,11,12	2.20	4 (36%)	15,15,17	3.93	9 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	A	4	3	11,11,12	1.93	4 (36%)	15,15,17	2.55	5 (33%)
3	NAG	A	5	3	14,14,15	1.63	3 (21%)	17,19,21	3.10	8 (47%)
3	GAL	A	6	3	11,11,12	3.51	8 (72%)	15,15,17	3.81	10 (66%)
3	SIA	A	7	3	20,20,21	2.71	7 (35%)	21,28,31	1.78	5 (23%)
3	GUP	A	8	3	11,11,12	3.91	4 (36%)	15,15,17	4.89	7 (46%)
3	NAG	A	9	3	14,14,15	2.37	5 (35%)	17,19,21	3.06	9 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	2,3	-	3/6/23/26	0/1/1/1
3	FUL	A	10	3	-	-	0/1/1/1
3	NAG	A	2	3	-	3/6/23/26	0/1/1/1
3	BMA	A	3	3	-	1/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	2/6/23/26	0/1/1/1
3	GAL	A	6	3	-	0/2/19/22	0/1/1/1
3	SIA	A	7	3	-	3/18/34/38	0/1/1/1
3	GUP	A	8	3	-	0/2/19/22	0/1/1/1
3	NAG	A	9	3	-	2/6/23/26	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	8	GUP	O5-C1	11.18	1.62	1.43
3	A	7	SIA	C3-C2	8.62	1.66	1.52
3	A	6	GAL	C4-C3	6.19	1.68	1.52
3	A	7	SIA	C6-C5	5.01	1.61	1.53
3	A	6	GAL	O3-C3	4.99	1.55	1.43
3	A	3	BMA	C4-C3	4.62	1.64	1.52
3	A	6	GAL	C4-C5	4.33	1.62	1.53
3	A	8	GUP	C4-C5	4.15	1.61	1.53
3	A	9	NAG	C2-N2	-4.15	1.39	1.46
3	A	1	NAG	C1-C2	4.13	1.58	1.52
3	A	9	NAG	C8-C7	-3.99	1.42	1.50
3	A	6	GAL	C1-C2	3.69	1.61	1.52
3	A	9	NAG	C7-N2	-3.65	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9	NAG	C4-C5	3.48	1.60	1.53
3	A	2	NAG	C3-C2	3.47	1.59	1.52
3	A	1	NAG	C4-C3	3.45	1.61	1.52
3	A	4	MAN	O3-C3	-3.44	1.34	1.43
3	A	5	NAG	C4-C5	3.35	1.60	1.53
3	A	1	NAG	C4-C5	3.21	1.59	1.53
3	A	1	NAG	C2-N2	3.19	1.51	1.46
3	A	6	GAL	O5-C5	3.18	1.49	1.43
3	A	6	GAL	C2-C3	3.13	1.57	1.52
3	A	9	NAG	O7-C7	-3.13	1.16	1.23
3	A	7	SIA	O1B-C1	-2.99	1.21	1.30
3	A	6	GAL	O4-C4	-2.98	1.35	1.43
3	A	6	GAL	C6-C5	2.96	1.61	1.51
3	A	3	BMA	C6-C5	2.96	1.61	1.51
3	A	7	SIA	C9-C8	2.95	1.59	1.52
3	A	2	NAG	O5-C5	2.93	1.49	1.43
3	A	8	GUP	C2-C3	2.92	1.57	1.52
3	A	4	MAN	C4-C3	2.86	1.59	1.52
3	A	10	FUL	C2-C3	2.85	1.56	1.52
3	A	1	NAG	C6-C5	2.85	1.61	1.51
3	A	8	GUP	C1-C2	-2.84	1.45	1.52
3	A	1	NAG	C8-C7	2.80	1.56	1.50
3	A	7	SIA	C3-C4	2.79	1.58	1.52
3	A	4	MAN	O2-C2	2.78	1.49	1.43
3	A	5	NAG	C1-C2	2.75	1.56	1.52
3	A	3	BMA	C4-C5	2.59	1.58	1.53
3	A	3	BMA	C2-C3	2.49	1.56	1.52
3	A	7	SIA	O6-C2	2.37	1.48	1.43
3	A	7	SIA	C8-C7	2.37	1.57	1.53
3	A	1	NAG	O5-C5	-2.23	1.39	1.43
3	A	5	NAG	O5-C5	2.11	1.47	1.43
3	A	2	NAG	C6-C5	2.02	1.58	1.51
3	A	4	MAN	C4-C5	2.02	1.57	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	8	GUP	O6-C6-C5	15.56	164.30	111.33
3	A	1	NAG	C2-N2-C7	12.55	139.72	122.90
3	A	2	NAG	C4-C3-C2	11.51	127.89	111.02
3	A	3	BMA	O3-C3-C4	9.89	133.69	110.38
3	A	1	NAG	C1-C2-N2	8.50	123.83	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	NAG	O3-C3-C4	-7.56	92.54	110.38
3	A	5	NAG	C1-C2-N2	-7.28	98.96	110.43
3	A	9	NAG	O7-C7-N2	6.86	134.10	121.98
3	A	4	MAN	C1-O5-C5	6.70	121.16	112.19
3	A	6	GAL	C1-O5-C5	6.66	121.11	112.19
3	A	5	NAG	C2-N2-C7	6.49	131.60	122.90
3	A	8	GUP	C1-C2-C3	-6.46	100.23	109.64
3	A	3	BMA	C1-O5-C5	6.38	120.74	112.19
3	A	6	GAL	C3-C4-C5	6.21	121.48	110.23
3	A	1	NAG	C3-C4-C5	6.09	121.28	110.23
3	A	6	GAL	C1-C2-C3	5.79	118.08	109.64
3	A	6	GAL	C6-C5-C4	5.53	126.61	113.02
3	A	3	BMA	O5-C1-C2	5.25	123.32	110.79
3	A	1	NAG	C6-C5-C4	5.23	125.85	113.02
3	A	1	NAG	O5-C1-C2	5.13	119.23	111.29
3	A	9	NAG	C8-C7-N2	-4.74	108.26	116.12
3	A	3	BMA	O3-C3-C2	-4.71	100.43	110.05
3	A	5	NAG	O4-C4-C3	-4.59	99.56	110.38
3	A	8	GUP	C6-C5-C4	4.56	124.22	113.02
3	A	8	GUP	O5-C1-C2	-4.51	100.04	110.79
3	A	4	MAN	C2-C3-C4	-4.41	103.10	110.86
3	A	9	NAG	C6-C5-C4	4.21	123.35	113.02
3	A	6	GAL	O2-C2-C3	-4.18	101.48	110.15
3	A	5	NAG	C1-O5-C5	4.12	117.70	112.19
3	A	7	SIA	C6-C5-N5	-4.08	104.39	110.91
3	A	1	NAG	C1-O5-C5	4.02	117.57	112.19
3	A	9	NAG	C1-O5-C5	4.00	117.55	112.19
3	A	9	NAG	C4-C3-C2	-3.84	105.39	111.02
3	A	6	GAL	O3-C3-C4	3.78	119.28	110.38
3	A	8	GUP	O5-C5-C6	3.67	114.81	107.66
3	A	9	NAG	C3-C4-C5	-3.64	103.63	110.23
3	A	7	SIA	C9-C8-C7	3.63	119.56	112.17
3	A	3	BMA	O4-C4-C3	3.48	118.58	110.38
3	A	6	GAL	O4-C4-C5	-3.37	101.02	109.32
3	A	4	MAN	C3-C4-C5	-3.26	104.31	110.23
3	A	6	GAL	C2-C3-C4	-3.26	105.13	110.86
3	A	8	GUP	O2-C2-C3	3.24	116.86	110.15
3	A	2	NAG	C1-O5-C5	3.10	116.34	112.19
3	A	1	NAG	O4-C4-C5	-3.03	101.86	109.32
3	A	1	NAG	O5-C5-C4	-3.03	103.46	110.83
3	A	3	BMA	C6-C5-C4	2.96	120.29	113.02
3	A	2	NAG	C8-C7-N2	2.89	120.91	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	NAG	C1-C2-N2	2.87	114.96	110.43
3	A	9	NAG	O4-C4-C5	2.71	115.99	109.32
3	A	4	MAN	O3-C3-C4	2.71	116.75	110.38
3	A	5	NAG	O5-C1-C2	2.68	115.44	111.29
3	A	1	NAG	C4-C3-C2	-2.63	107.17	111.02
3	A	7	SIA	O8-C8-C9	-2.60	103.12	109.03
3	A	9	NAG	O7-C7-C8	-2.49	117.61	122.05
3	A	8	GUP	C3-C4-C5	2.49	114.75	110.23
3	A	6	GAL	O5-C5-C4	-2.48	104.79	110.83
3	A	3	BMA	C1-C2-C3	2.45	113.22	109.64
3	A	5	NAG	C4-C3-C2	-2.41	107.49	111.02
3	A	7	SIA	C5-N5-C10	2.36	128.63	123.11
3	A	3	BMA	O6-C6-C5	2.30	119.16	111.33
3	A	1	NAG	O4-C4-C3	-2.28	105.00	110.38
3	A	3	BMA	O2-C2-C1	2.25	114.38	109.22
3	A	9	NAG	O5-C5-C4	-2.19	105.50	110.83
3	A	1	NAG	O7-C7-C8	-2.18	118.17	122.05
3	A	5	NAG	C6-C5-C4	2.14	118.28	113.02
3	A	6	GAL	O4-C4-C3	2.13	115.40	110.38
3	A	4	MAN	O4-C4-C5	2.12	114.54	109.32
3	A	2	NAG	O7-C7-C8	-2.11	118.30	122.05
3	A	7	SIA	O6-C2-C3	-2.03	107.83	110.56
3	A	2	NAG	C2-N2-C7	2.02	125.61	122.90
3	A	1	NAG	O3-C3-C2	-2.02	105.20	109.40
3	A	5	NAG	C8-C7-N2	-2.00	112.80	116.12

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C1-C2-N2-C7
3	A	2	NAG	C1-C2-N2-C7
3	A	7	SIA	O1A-C1-C2-O6
3	A	7	SIA	O6-C6-C7-C8
3	A	2	NAG	O5-C5-C6-O6
3	A	5	NAG	O5-C5-C6-O6
3	A	5	NAG	C4-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	A	9	NAG	O5-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6
3	A	3	BMA	O5-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6

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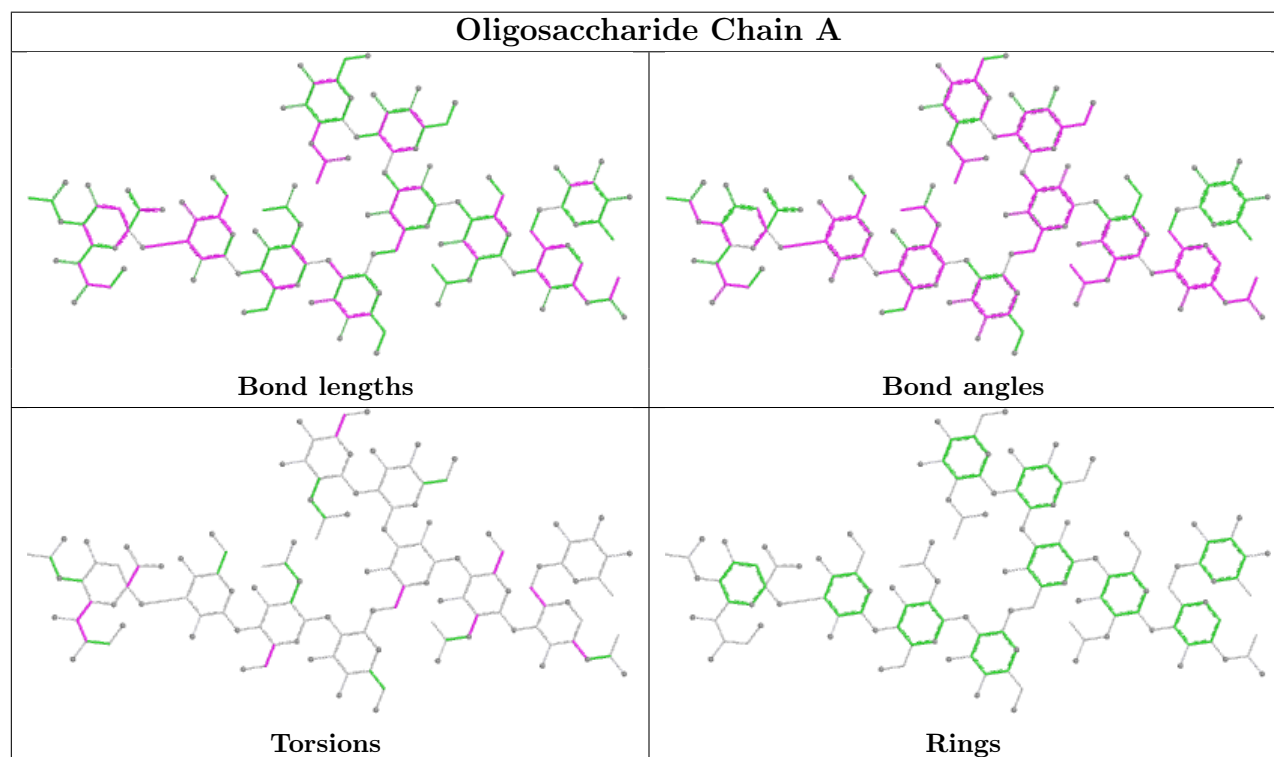
Mol	Chain	Res	Type	Atoms
3	A	9	NAG	C4-C5-C6-O6
3	A	7	SIA	C6-C7-C8-C9

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4	MAN	1	0
3	A	2	NAG	1	0
3	A	8	GUP	6	0
3	A	6	GAL	4	0
3	A	9	NAG	6	0
3	A	3	BMA	6	0
3	A	7	SIA	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 ⓘ

There are no ligands in this entry.

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.