



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:04 PM UTC

PDB ID : 8API / pdb_00008api
Title : THE S VARIANT OF HUMAN ALPHA1-ANTITRYPSIN, STRUCTURE AND IMPLICATIONS FOR FUNCTION AND METABOLISM
Authors : Loebermann, H.; Tokuoka, R.; Deisenhofer, J.; Huber, R.
Deposited on : 1988-09-08
Resolution : 3.10 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

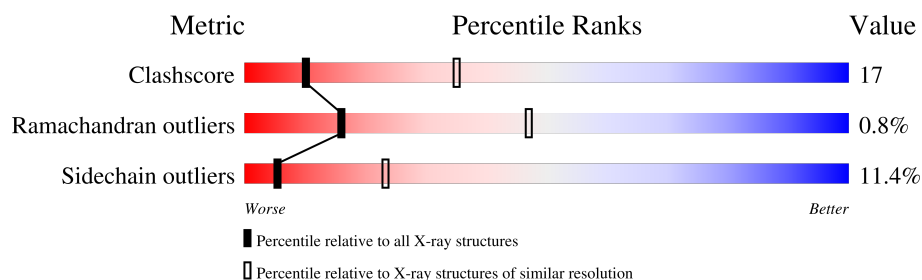
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	347	
2	B	36	
3	C	6	
4	D	2	
4	E	2	

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
4	NAG	E	1	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3286 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.

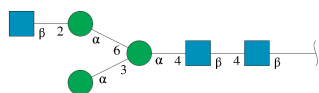
- Molecule 1 is a protein called ALPHA-1 ANTITRYPSIN (CHAIN A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	7	0	0
			2698	1730	442	518	8			

- Molecule 2 is a protein called ALPHA-1 ANTITRYPSIN (CHAIN B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	S	5	0	0
			291	193	46	50	2			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	44	0	0
			75	42	3	30			

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



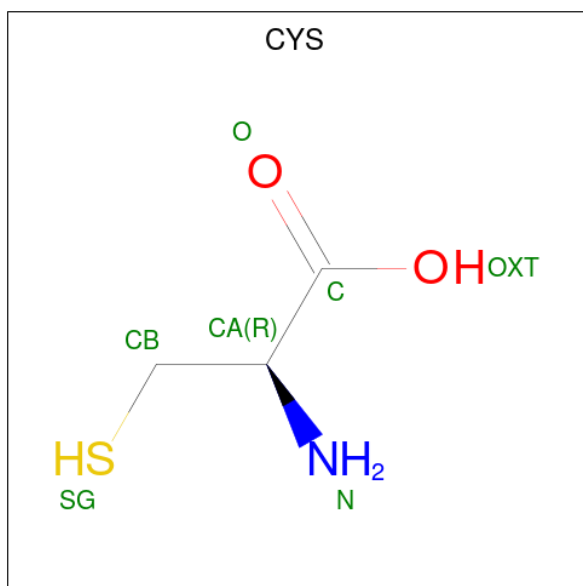
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	14	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 6 is water.

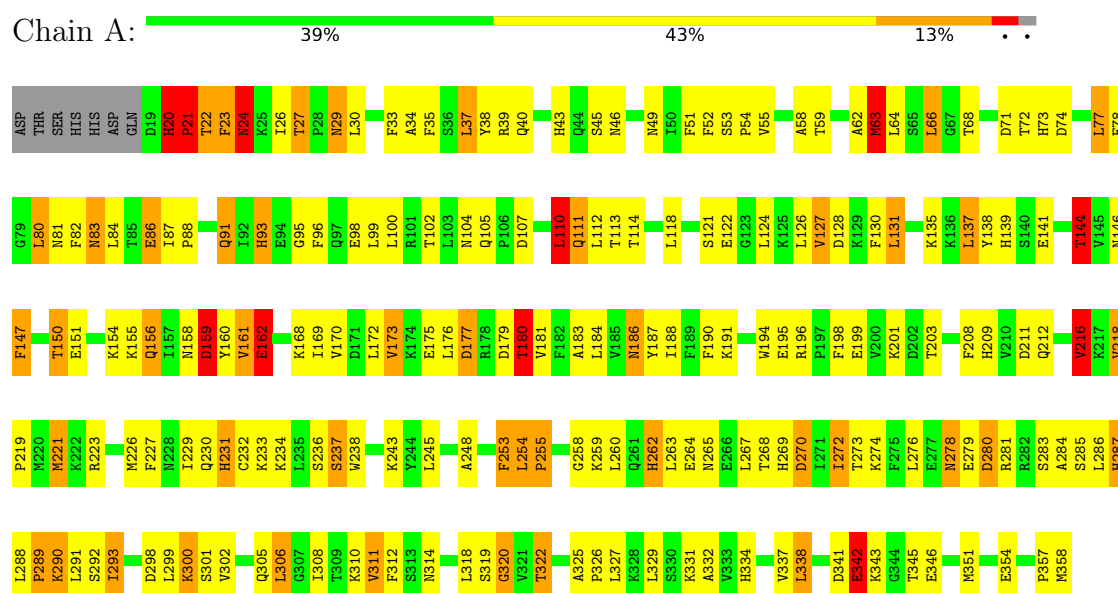
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	137	Total	O	0	0
			137	137		
6	B	22	Total	O	0	0
			22	22		

3 Residue-property plots

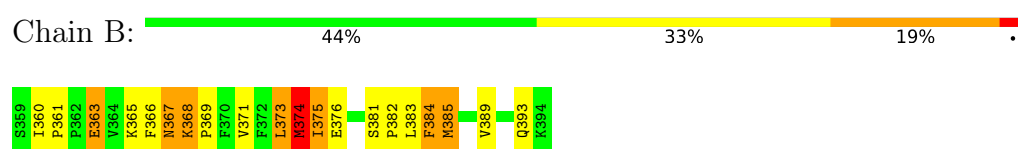
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

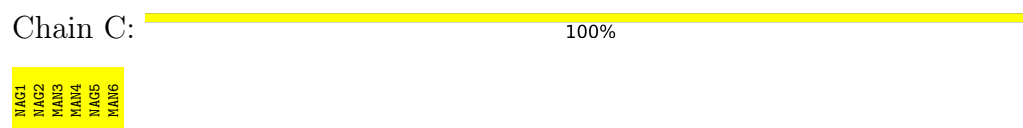
• Molecule 1: ALPHA-1 ANTITRYPSIN (CHAIN A)



• Molecule 2: ALPHA-1 ANTITRYPSIN (CHAIN B)



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain D:  100%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.70Å 119.70Å 216.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3286	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.49	29/2752 (1.1%)	2.04	96/3718 (2.6%)
2	B	1.21	0/299	1.98	8/402 (2.0%)
All	All	1.47	29/3051 (1.0%)	2.03	104/4120 (2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	28

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	HIS	CE1-NE2	11.81	1.44	1.32
1	A	20	HIS	ND1-CE1	11.47	1.44	1.32
1	A	20	HIS	CE1-NE2	10.34	1.42	1.32
1	A	43	HIS	ND1-CE1	9.92	1.42	1.32
1	A	287	HIS	CE1-NE2	9.82	1.42	1.32
1	A	43	HIS	CE1-NE2	9.80	1.42	1.32
1	A	287	HIS	ND1-CE1	9.69	1.42	1.32
1	A	231	HIS	ND1-CE1	9.61	1.42	1.32
1	A	73	HIS	ND1-CE1	9.37	1.42	1.32
1	A	93	HIS	CE1-NE2	9.26	1.41	1.32
1	A	334	HIS	ND1-CE1	9.22	1.41	1.32
1	A	209	HIS	ND1-CE1	9.11	1.41	1.32
1	A	194	TRP	NE1-CE2	-8.92	1.27	1.37
1	A	269	HIS	ND1-CE1	8.88	1.41	1.32
1	A	238	TRP	NE1-CE2	-8.60	1.27	1.37
1	A	139	HIS	CE1-NE2	8.40	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	HIS	ND1-CE1	8.33	1.40	1.32
1	A	139	HIS	ND1-CE1	8.30	1.40	1.32
1	A	73	HIS	CE1-NE2	8.27	1.40	1.32
1	A	93	HIS	ND1-CE1	7.67	1.40	1.32
1	A	262	HIS	CE1-NE2	7.56	1.40	1.32
1	A	269	HIS	CE1-NE2	7.43	1.40	1.32
1	A	209	HIS	CE1-NE2	6.71	1.39	1.32
1	A	334	HIS	CE1-NE2	6.50	1.39	1.32
1	A	180	THR	C-N	-5.97	1.27	1.33
1	A	301	SER	C-N	-5.63	1.26	1.33
1	A	20	HIS	CD2-NE2	5.48	1.43	1.37
1	A	113	THR	C-N	-5.23	1.27	1.33
1	A	52	PHE	C-N	-5.04	1.28	1.33

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ASN	CA-CB-CG	-13.49	99.11	112.60
1	A	162	GLU	N-CA-C	-8.45	102.98	113.38
1	A	237	SER	CA-C-O	-8.08	112.80	121.45
1	A	161	VAL	CA-C-N	-7.47	109.33	122.26
1	A	161	VAL	C-N-CA	-7.47	109.33	122.26
1	A	21	PRO	CA-C-N	7.32	133.95	121.14
1	A	21	PRO	C-N-CA	7.32	133.95	121.14
1	A	24	ASN	CA-CB-CG	-7.32	105.28	112.60
1	A	147	PHE	CA-CB-CG	-7.18	106.62	113.80
1	A	177	ASP	CA-CB-CG	-7.13	105.47	112.60
1	A	186	ASN	CA-CB-CG	-6.95	105.65	112.60
1	A	83	ASN	CA-CB-CG	-6.79	105.81	112.60
1	A	287	HIS	CB-CA-C	-6.68	100.53	110.62
1	A	338	LEU	N-CA-CB	-6.59	99.27	111.53
1	A	280	ASP	CA-CB-CG	-6.49	106.11	112.60
1	A	343	LYS	N-CA-C	-6.49	105.52	113.50
1	A	29	ASN	N-CA-C	-6.46	104.32	111.36
1	A	332	ALA	CA-C-N	-6.45	114.52	123.10
1	A	332	ALA	C-N-CA	-6.45	114.52	123.10
1	A	158	ASN	CA-CB-CG	-6.38	106.22	112.60
1	A	95	GLY	N-CA-C	-6.37	105.09	112.73
1	A	86	GLU	CA-C-N	-6.36	117.31	122.85
1	A	86	GLU	C-N-CA	-6.36	117.31	122.85
1	A	71	ASP	CA-CB-CG	-6.34	106.26	112.60
1	A	322	THR	O-C-N	6.29	130.64	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ASN	CA-CB-CG	-6.23	106.37	112.60
1	A	34	ALA	O-C-N	6.22	128.48	122.07
1	A	100	LEU	O-C-N	6.22	128.50	122.03
1	A	66	LEU	N-CA-CB	-6.17	100.97	110.46
1	A	230	GLN	CB-CG-CD	-6.16	102.12	112.60
1	A	258	GLY	N-CA-C	-6.14	107.22	115.21
2	B	363	GLU	CB-CG-CD	-6.14	102.16	112.60
1	A	34	ALA	N-CA-C	-6.11	104.54	111.07
1	A	212	GLN	CA-C-N	-6.03	115.44	122.14
1	A	212	GLN	C-N-CA	-6.03	115.44	122.14
1	A	292	SER	CB-CA-C	-6.03	99.55	109.80
1	A	95	GLY	O-C-N	6.02	127.97	122.19
1	A	263	LEU	O-C-N	5.98	128.23	122.07
1	A	311	VAL	CA-C-N	-5.95	111.61	122.38
1	A	311	VAL	C-N-CA	-5.95	111.61	122.38
2	B	374	MET	CB-CA-C	-5.95	100.42	110.19
1	A	179	ASP	CA-CB-CG	-5.92	106.68	112.60
1	A	187	TYR	CA-C-O	-5.87	114.75	121.68
1	A	156	GLN	CB-CG-CD	-5.85	102.66	112.60
1	A	160	TYR	N-CA-C	-5.81	104.85	111.07
1	A	51	PHE	CA-CB-CG	-5.80	108.00	113.80
1	A	319	SER	N-CA-C	-5.76	106.02	113.16
1	A	37	LEU	N-CA-C	-5.73	105.11	111.36
1	A	237	SER	CB-CA-C	-5.69	98.17	111.09
1	A	218	VAL	N-CA-CB	-5.68	103.25	111.21
1	A	279	GLU	O-C-N	5.68	130.05	122.26
1	A	248	ALA	N-CA-C	5.67	117.47	108.79
1	A	55	VAL	O-C-N	5.65	127.65	121.83
1	A	233	LYS	N-CA-C	-5.61	105.31	111.82
1	A	286	LEU	CA-C-N	5.61	130.82	122.86
1	A	286	LEU	C-N-CA	5.61	130.82	122.86
1	A	211	ASP	CA-C-N	-5.59	110.67	121.58
1	A	211	ASP	C-N-CA	-5.59	110.67	121.58
1	A	198	PHE	CB-CA-C	-5.57	100.82	110.45
1	A	320	GLY	N-CA-C	-5.55	107.00	115.66
1	A	156	GLN	N-CA-C	-5.54	105.34	111.71
1	A	37	LEU	O-C-N	5.52	128.45	122.15
1	A	270	ASP	O-C-N	5.51	127.97	122.08
2	B	375	ILE	CA-C-N	-5.50	114.43	122.19
2	B	375	ILE	C-N-CA	-5.50	114.43	122.19
1	A	342	GLU	CB-CG-CD	-5.46	103.32	112.60
1	A	38	TYR	O-C-N	5.46	127.76	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TYR	O-C-N	5.45	127.68	122.07
1	A	146	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	96	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	110	LEU	CA-C-N	-5.39	115.29	122.72
1	A	110	LEU	C-N-CA	-5.39	115.29	122.72
1	A	159	ASP	CA-CB-CG	-5.38	107.22	112.60
1	A	341	ASP	CA-C-N	-5.38	111.73	121.14
1	A	341	ASP	C-N-CA	-5.38	111.73	121.14
1	A	300	LYS	CB-CA-C	-5.34	101.61	110.68
1	A	351	MET	N-CA-CB	-5.34	101.66	111.37
2	B	385	MET	CA-C-N	-5.34	115.82	121.48
2	B	385	MET	C-N-CA	-5.34	115.82	121.48
1	A	63	MET	N-CA-CB	5.33	119.37	110.41
1	A	172	LEU	N-CA-C	-5.32	105.40	111.14
1	A	58	ALA	N-CA-C	5.29	116.85	111.14
1	A	312	PHE	CA-C-N	-5.25	113.44	123.32
1	A	312	PHE	C-N-CA	-5.25	113.44	123.32
1	A	33	PHE	O-C-N	5.24	128.50	122.17
1	A	22	THR	N-CA-CB	-5.22	101.89	110.40
1	A	292	SER	N-CA-CB	5.21	119.35	110.71
1	A	194	TRP	O-C-N	5.18	129.21	122.89
1	A	162	GLU	CB-CG-CD	-5.14	103.86	112.60
1	A	253	PHE	CB-CA-C	-5.14	102.60	111.23
1	A	175	GLU	CB-CG-CD	-5.13	103.87	112.60
1	A	55	VAL	N-CA-C	-5.10	105.57	110.72
1	A	337	VAL	CB-CA-C	-5.08	101.91	110.71
1	A	141	GLU	N-CA-CB	-5.07	102.53	110.69
2	B	384	PHE	CA-C-N	-5.06	115.34	122.94
2	B	384	PHE	C-N-CA	-5.06	115.34	122.94
1	A	20	HIS	CA-C-O	-5.06	113.22	120.16
1	A	80	LEU	O-C-N	5.04	129.42	122.46
1	A	155	LYS	CB-CA-C	-5.04	102.90	110.92
1	A	325	ALA	O-C-N	5.04	125.45	121.88
1	A	216	VAL	N-CA-CB	-5.03	101.49	111.91
1	A	173	VAL	CB-CA-C	-5.03	104.86	111.25
1	A	254	LEU	O-C-N	5.02	125.91	121.19
1	A	274	LYS	O-C-N	5.01	127.23	122.07

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LEU	Mainchain
1	A	127	VAL	Mainchain
1	A	144	THR	Mainchain
1	A	159	ASP	Mainchain
1	A	162	GLU	Mainchain
1	A	169	ILE	Mainchain
1	A	180	THR	Mainchain
1	A	183	ALA	Mainchain
1	A	196	ARG	Mainchain
1	A	203	THR	Mainchain
1	A	21	PRO	Peptide,Mainchain
1	A	226	MET	Mainchain
1	A	231	HIS	Mainchain
1	A	237	SER	Mainchain
1	A	24	ASN	Mainchain
1	A	255	PRO	Mainchain
1	A	289	PRO	Mainchain
1	A	290	LYS	Mainchain
1	A	291	LEU	Mainchain
1	A	298	ASP	Peptide,Mainchain
1	A	300	LYS	Mainchain
1	A	308	ILE	Mainchain
1	A	342	GLU	Mainchain
1	A	345	THR	Mainchain
1	A	46	ASN	Sidechain
1	A	63	MET	Mainchain

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	A	2698	0	2689	93	0
2	B	291	0	306	23	0
3	C	75	0	64	0	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	7	0	3	1	0
6	A	137	0	0	0	1
6	B	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3286	0	3112	105	1

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 (105) 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:A:162:GLU:HG3	1:A:170:VAL:HG12	1.67	0.77
1:A:110:LEU:HD11	1:A:190:PHE:HE1	1.52	0.75
1:A:93:HIS:HB3	1:A:137:LEU:HD23	1.69	0.74
1:A:77:LEU:HD23	1:A:84:LEU:HD21	1.69	0.73
1:A:88:PRO:HB2	1:A:91:GLN:HB2	1.70	0.72
1:A:208:PHE:HB2	1:A:218:VAL:HG21	1.73	0.68
1:A:195:GLU:HA	1:A:245:LEU:HD21	1.77	0.65
1:A:195:GLU:HA	1:A:245:LEU:CD2	2.26	0.65
1:A:104:ASN:HD21	1:A:114:THR:H	1.45	0.64
1:A:83:ASN:HD22	1:A:86:GLU:HG3	1.61	0.64
1:A:223:ARG:HB3	1:A:227:PHE:HZ	1.65	0.62
1:A:236:SER:HB2	1:A:262:HIS:HD2	1.63	0.62
1:A:232:CYS:HB3	1:A:234:LYS:HB2	1.82	0.61
1:A:278:ASN:ND2	1:A:280:ASP:HB2	2.16	0.61
1:A:114:THR:HG22	1:A:188:ILE:HB	1.84	0.60
1:A:195:GLU:HG3	1:A:243:LYS:HB2	1.84	0.60
1:A:283:SER:O	2:B:361:PRO:HB3	2.01	0.60
1:A:331:LYS:HB2	1:A:354:GLU:HG2	1.84	0.58
1:A:83:ASN:O	1:A:87:ILE:HG22	2.04	0.58
1:A:49:ASN:H	2:B:393:GLN:HE22	1.51	0.57
1:A:102:THR:HA	1:A:105:GLN:HG3	1.86	0.57
1:A:219:PRO:HG2	1:A:290:LYS:HB3	1.87	0.57
1:A:287:HIS:HB2	2:B:365:LYS:HA	1.86	0.57
1:A:322:THR:HG22	1:A:327:LEU:HD11	1.86	0.56
1:A:255:PRO:HG3	1:A:260:LEU:HD13	1.86	0.56
1:A:63:MET:HE2	1:A:184:LEU:HD11	1.86	0.56
1:A:53:SER:HB2	2:B:384:PHE:CD1	2.42	0.54
2:B:376:GLU:HB2	2:B:383:LEU:HD13	1.89	0.54
1:A:265:ASN:N	1:A:265:ASN:HD22	2.06	0.54
1:A:74:ASP:O	1:A:78:GLU:HB2	2.08	0.54
1:A:37:LEU:HA	1:A:306:LEU:HD11	1.90	0.53
1:A:285:SER:HB3	2:B:363:GLU:HA	1.90	0.53
1:A:130:PHE:HB2	1:A:320:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:ASN:HD22	2:B:368:LYS:HG2	1.73	0.53
1:A:62:ALA:HB1	1:A:138:TYR:OH	2.09	0.53
1:A:23:PHE:HD2	1:A:98:GLU:HB3	1.75	0.52
1:A:181:VAL:HG23	1:A:357:PRO:HD3	1.92	0.52
1:A:49:ASN:H	2:B:393:GLN:NE2	2.07	0.52
1:A:20:HIS:CG	1:A:21:PRO:HD3	2.45	0.51
1:A:24:ASN:HA	1:A:27:THR:HB	1.91	0.51
4:E:1:NAG:H62	4:E:2:NAG:N2	2.24	0.51
2:B:367:ASN:ND2	2:B:368:LYS:HG2	2.25	0.51
1:A:80:LEU:HB3	1:A:82:PHE:HE1	1.76	0.51
1:A:278:ASN:HD21	1:A:280:ASP:HB2	1.77	0.50
1:A:264:GLU:C	1:A:265:ASN:HD22	2.19	0.50
2:B:374:MET:HB2	2:B:384:PHE:HB2	1.94	0.49
1:A:254:LEU:HB2	2:B:366:PHE:CE2	2.48	0.49
1:A:191:LYS:HG3	1:A:346:GLU:HB3	1.95	0.49
1:A:162:GLU:CG	1:A:170:VAL:HG12	2.40	0.48
1:A:173:VAL:HG11	1:A:176:LEU:HD12	1.95	0.48
1:A:35:PHE:O	1:A:39:ARG:HG3	2.13	0.48
1:A:110:LEU:HD11	1:A:190:PHE:CE1	2.39	0.48
1:A:326:PRO:HB2	1:A:358:MET:HE3	1.95	0.48
1:A:199:GLU:HB3	1:A:201:LYS:HD2	1.96	0.47
1:A:208:PHE:HB3	1:A:216:VAL:HG12	1.97	0.47
1:A:284:ALA:HA	2:B:361:PRO:HB2	1.96	0.47
1:A:168:LYS:HD2	1:A:346:GLU:OE1	2.14	0.47
2:B:373:LEU:HD12	2:B:375:ILE:HG13	1.98	0.46
1:A:53:SER:HB2	2:B:384:PHE:CE1	2.50	0.46
1:A:111:GLN:HG3	1:A:191:LYS:HB3	1.98	0.46
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.68	0.46
1:A:284:ALA:HA	2:B:361:PRO:CB	2.45	0.45
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.63	0.45
2:B:367:ASN:HD22	2:B:367:ASN:C	2.25	0.45
1:A:288:LEU:HD12	1:A:289:PRO:HD2	1.98	0.45
1:A:80:LEU:HB3	1:A:82:PHE:CE1	2.52	0.45
2:B:374:MET:O	2:B:383:LEU:HB2	2.17	0.45
1:A:272:ILE:O	1:A:276:LEU:HD13	2.16	0.45
1:A:121:SER:HB2	1:A:147:PHE:HD2	1.82	0.44
2:B:369:PRO:HB3	2:B:389:VAL:HA	2.00	0.44
1:A:150:THR:O	1:A:154:LYS:HB2	2.17	0.44
1:A:268:THR:HG22	1:A:270:ASP:H	1.82	0.44
1:A:63:MET:HB3	1:A:138:TYR:CG	2.52	0.44
1:A:156:GLN:HE21	1:A:156:GLN:HB2	1.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.71	0.44
1:A:177:ASP:HB3	1:A:180:THR:OG1	2.17	0.44
1:A:254:LEU:HD12	1:A:255:PRO:HD2	2.01	0.43
1:A:111:GLN:H	1:A:111:GLN:HG2	1.46	0.43
1:A:72:THR:HG22	1:A:310:LYS:HB3	2.00	0.43
1:A:342:GLU:H	1:A:342:GLU:HG2	1.39	0.43
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.85	0.42
1:A:26:ILE:O	1:A:29:ASN:HB2	2.19	0.42
1:A:107:ASP:HB3	1:A:110:LEU:O	2.19	0.42
1:A:35:PHE:HA	2:B:385:MET:HE1	2.01	0.42
1:A:159:ASP:C	1:A:162:GLU:H	2.27	0.42
1:A:234:LYS:HG3	5:A:395:CYS:SG	2.60	0.42
1:A:281:ARG:HH11	1:A:281:ARG:HD2	1.70	0.42
1:A:53:SER:HA	1:A:54:PRO:HD3	1.76	0.42
1:A:124:LEU:HD23	1:A:126:LEU:HD21	2.02	0.42
1:A:131:LEU:HD21	1:A:135:LYS:HE3	2.02	0.42
1:A:40:GLN:HB3	1:A:302:VAL:HG13	2.00	0.41
2:B:381:SER:HA	2:B:382:PRO:HD2	1.72	0.41
1:A:114:THR:HG22	1:A:188:ILE:CB	2.48	0.41
1:A:122:GLU:HB3	1:A:144:THR:HG22	2.02	0.41
1:A:64:LEU:C	1:A:66:LEU:H	2.29	0.41
1:A:63:MET:HB3	1:A:138:TYR:CD2	2.56	0.41
1:A:285:SER:OG	2:B:363:GLU:HG3	2.21	0.41
1:A:318:LEU:HD13	1:A:327:LEU:HB2	2.02	0.41
1:A:229:ILE:HG21	1:A:229:ILE:HD13	1.84	0.41
2:B:360:ILE:HG21	2:B:360:ILE:HD13	1.81	0.41
1:A:63:MET:HE2	1:A:184:LEU:CD1	2.50	0.40
1:A:253:PHE:O	1:A:255:PRO:HD3	2.21	0.40
1:A:293:ILE:HG21	1:A:293:ILE:HD13	1.86	0.40
1:A:221:MET:HG3	1:A:288:LEU:O	2.20	0.40
2:B:367:ASN:ND2	2:B:367:ASN:C	2.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:612:HOH:O	6:A:612:HOH:O[12_564]	0.71	1.49

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/347 (97%)	317 (94%)	18 (5%)	3 (1%)	14	44
2	B	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
All	All	372/383 (97%)	349 (94%)	20 (5%)	3 (1%)	16	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	81	ASN
1	A	127	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	A	298/305 (98%)	265 (89%)	33 (11%)	6	24
2	B	35/35 (100%)	30 (86%)	5 (14%)	3	14
All	All	333/340 (98%)	295 (89%)	38 (11%)	5	23

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	22	THR
1	A	23	PHE

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Mol	Chain	Res	Type
1	A	27	THR
1	A	45	SER
1	A	59	THR
1	A	68	THR
1	A	77	LEU
1	A	91	GLN
1	A	99	LEU
1	A	110	LEU
1	A	111	GLN
1	A	118	LEU
1	A	128	ASP
1	A	131	LEU
1	A	137	LEU
1	A	144	THR
1	A	150	THR
1	A	151	GLU
1	A	161	VAL
1	A	186	ASN
1	A	216	VAL
1	A	221	MET
1	A	267	LEU
1	A	272	ILE
1	A	273	THR
1	A	293	ILE
1	A	305	GLN
1	A	306	LEU
1	A	311	VAL
1	A	329	LEU
1	A	338	LEU
1	A	342	GLU
2	B	367	ASN
2	B	368	LYS
2	B	371	VAL
2	B	373	LEU
2	B	374	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	97	GLN
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	105	GLN
1	A	109	GLN
1	A	156	GLN
1	A	212	GLN
1	A	228	ASN
1	A	261	GLN
1	A	262	HIS
1	A	265	ASN
2	B	367	ASN
2	B	377	GLN
2	B	378	ASN
2	B	393	GLN

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	C	1	3,1	14,14,15	1.06	2 (14%)	17,19,21	2.08	6 (35%)
3	NAG	C	2	3	14,14,15	1.10	1 (7%)	17,19,21	1.88	3 (17%)
3	MAN	C	3	3	11,11,12	0.88	0	15,15,17	1.66	1 (6%)
3	MAN	C	4	3	11,11,12	1.03	0	15,15,17	2.11	2 (13%)
3	NAG	C	5	3	14,14,15	0.75	0	17,19,21	2.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	C	6	3	11,11,12	0.58	0	15,15,17	1.59	1 (6%)
4	NAG	D	1	4,1	14,14,15	1.07	1 (7%)	17,19,21	1.35	3 (17%)
4	NAG	D	2	4	14,14,15	0.64	0	17,19,21	1.40	2 (11%)
4	NAG	E	1	4,1	14,14,15	1.35	2 (14%)	17,19,21	2.61	8 (47%)
4	NAG	E	2	4	14,14,15	1.18	1 (7%)	17,19,21	1.96	4 (23%)

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	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	1/6/23/26	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	3.97	1.57	1.52
4	E	2	NAG	C1-C2	2.94	1.56	1.52
3	C	2	NAG	C1-C2	2.51	1.55	1.52
4	D	1	NAG	C1-C2	2.26	1.55	1.52
3	C	1	NAG	C1-C2	2.22	1.55	1.52
3	C	1	NAG	C3-C2	2.21	1.57	1.52
4	E	1	NAG	C2-N2	2.20	1.49	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	NAG	C1-O5-C5	7.55	122.30	112.19
3	C	4	MAN	C1-O5-C5	6.61	121.04	112.19
4	E	1	NAG	C1-C2-N2	6.35	120.44	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	6.34	120.69	112.19
3	C	3	MAN	C1-O5-C5	5.83	120.00	112.19
3	C	6	MAN	C1-O5-C5	5.73	119.87	112.19
3	C	1	NAG	C1-O5-C5	5.57	119.65	112.19
4	E	2	NAG	C1-O5-C5	4.99	118.88	112.19
4	E	1	NAG	C2-N2-C7	4.16	128.47	122.90
4	D	2	NAG	C1-O5-C5	4.11	117.70	112.19
4	E	2	NAG	C2-N2-C7	3.76	127.94	122.90
4	E	2	NAG	C1-C2-N2	3.40	115.79	110.43
4	E	1	NAG	O7-C7-N2	3.39	127.97	121.98
4	E	1	NAG	O7-C7-C8	-3.27	116.22	122.05
4	E	1	NAG	O5-C1-C2	-3.15	106.42	111.29
4	D	1	NAG	C1-O5-C5	3.00	116.20	112.19
3	C	1	NAG	C3-C4-C5	2.70	115.13	110.23
3	C	1	NAG	C4-C3-C2	2.70	114.98	111.02
4	E	1	NAG	O5-C5-C6	2.56	112.66	107.66
4	D	1	NAG	O7-C7-N2	2.47	126.35	121.98
4	E	1	NAG	C4-C3-C2	2.46	114.62	111.02
4	D	2	NAG	O5-C1-C2	-2.41	107.56	111.29
3	C	4	MAN	O2-C2-C1	-2.41	103.71	109.22
3	C	2	NAG	O7-C7-N2	2.40	126.23	121.98
4	E	2	NAG	O7-C7-N2	2.35	126.14	121.98
3	C	1	NAG	O7-C7-N2	2.33	126.10	121.98
4	E	1	NAG	C1-O5-C5	2.28	115.24	112.19
3	C	1	NAG	O5-C1-C2	-2.28	107.77	111.29
3	C	5	NAG	O7-C7-N2	2.22	125.91	121.98
3	C	1	NAG	C2-N2-C7	2.19	125.84	122.90
3	C	2	NAG	O7-C7-C8	-2.08	118.34	122.05
4	D	1	NAG	O5-C1-C2	-2.02	108.17	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	1	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

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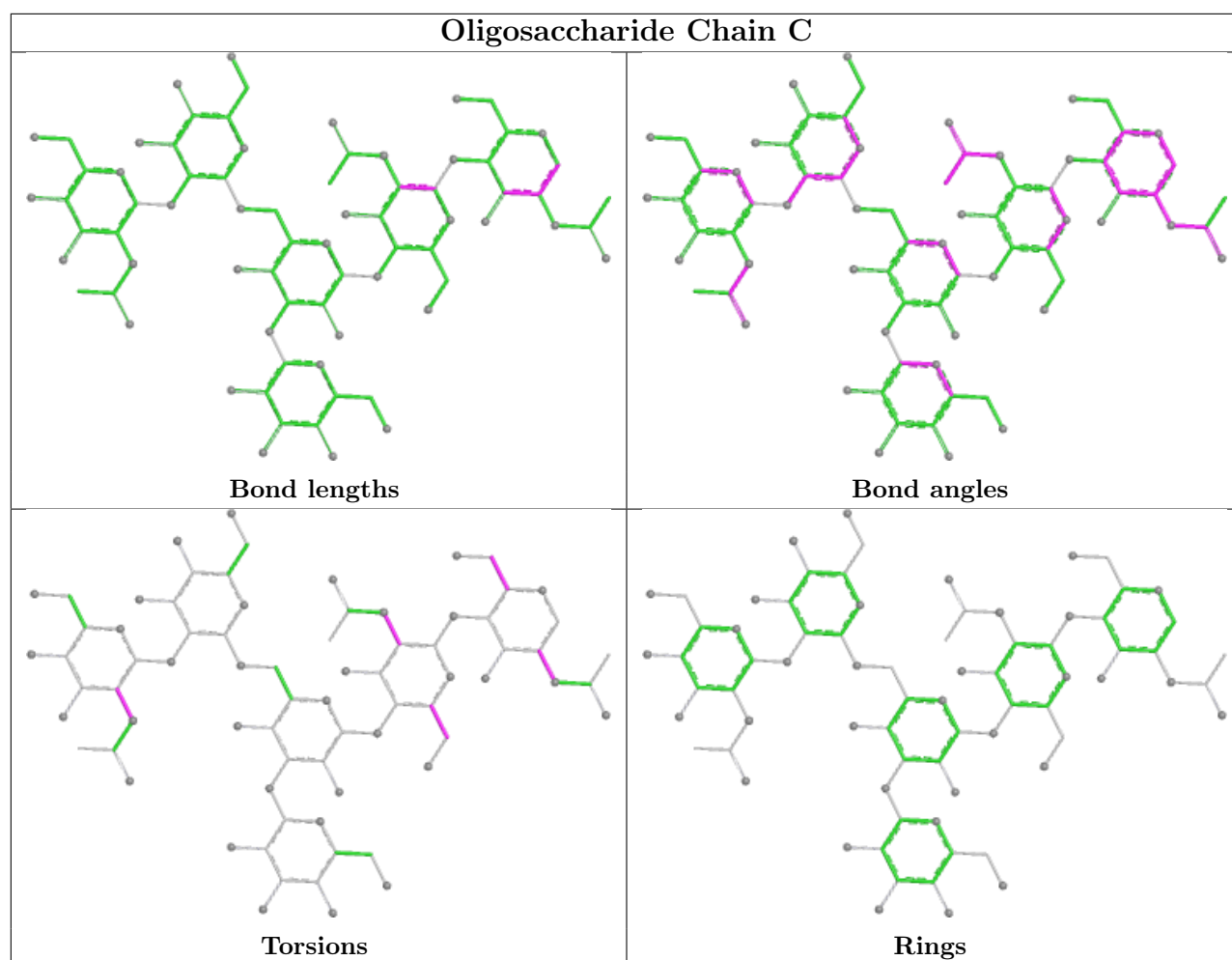
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7
3	C	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7
3	C	5	NAG	C3-C2-N2-C7
4	E	1	NAG	C1-C2-N2-C7

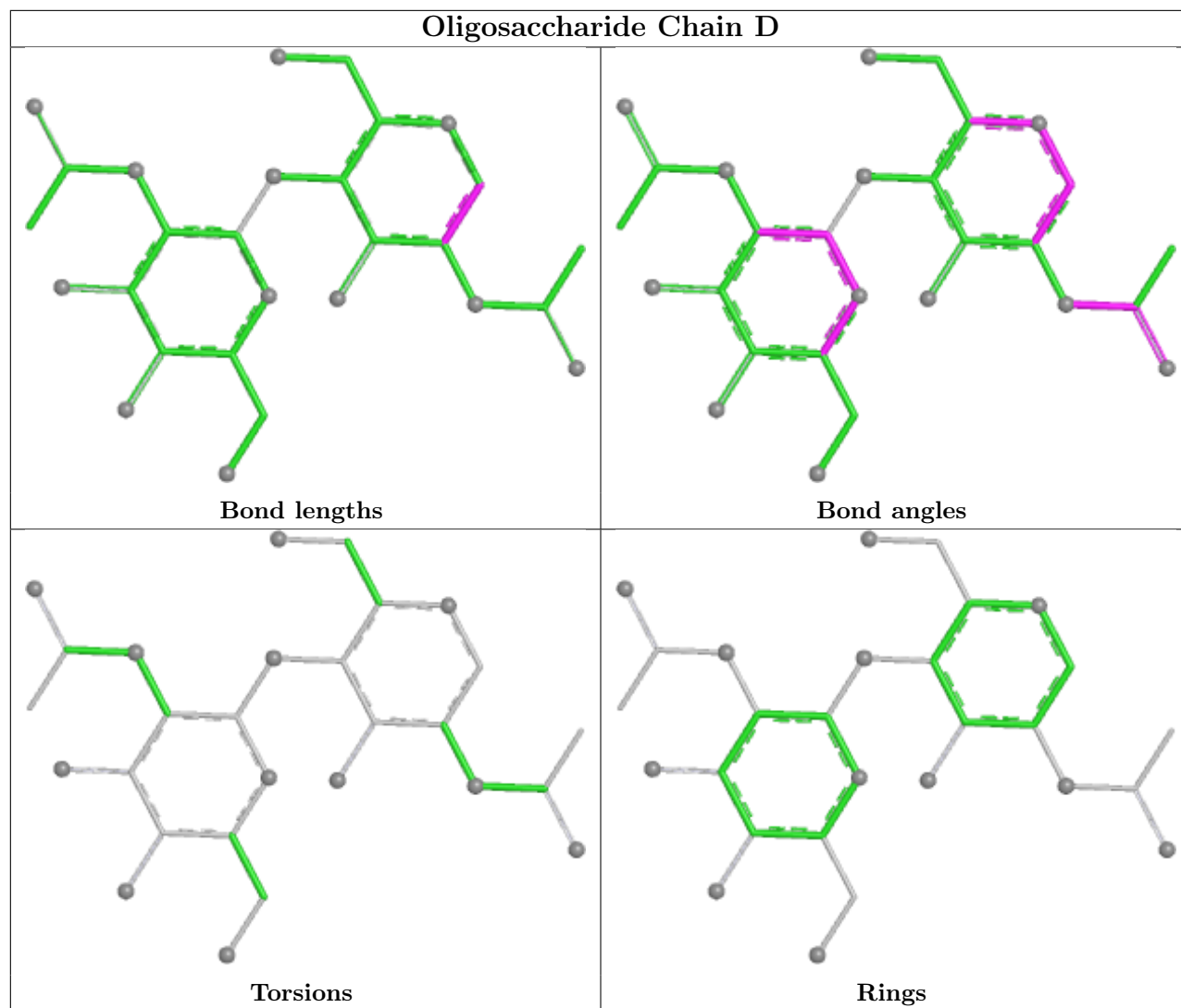
There are no ring outliers.

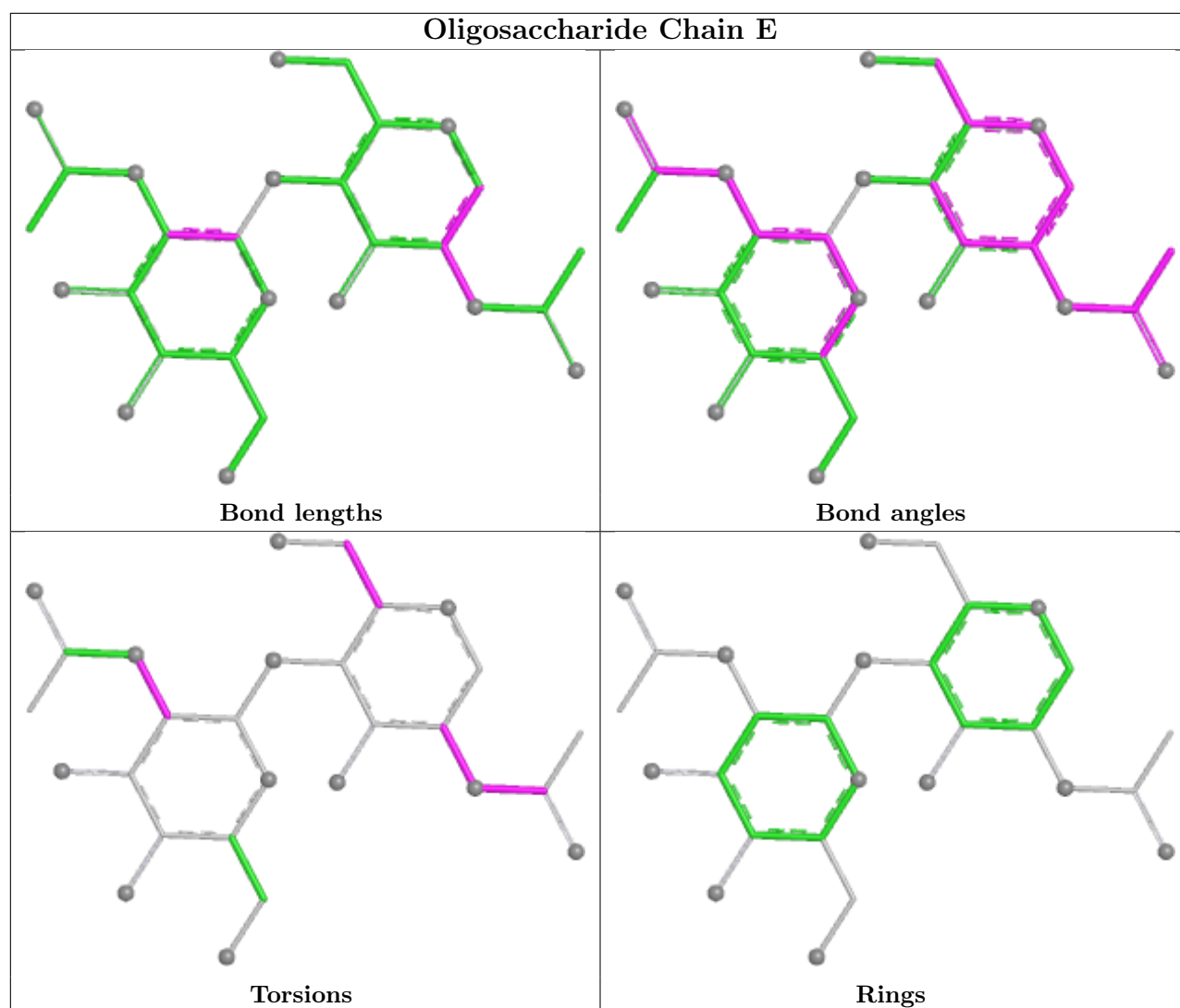
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
4	E	1	NAG	1	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CYS	A	395	1	5,6,6	1.56	1 (20%)	3,7,7	2.58	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYS	A	395	1	-	3/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	395	CYS	CB-CA	3.22	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	395	CYS	CB-CA-C	3.51	113.39	109.89
5	A	395	CYS	OXT-C-O	-2.77	117.79	124.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	395	CYS	N-CA-CB-SG
5	A	395	CYS	C-CA-CB-SG
5	A	395	CYS	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	395	CYS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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.