



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 04:46 PM BST

PDB ID : 1OVW
Title : ENDOGLUCANASE I COMPLEXED WITH NON-HYDROLYSABLE SUB-
STRATE ANALOGUE
Authors : Sulzenbacher, G.; Davies, G.J.; Schulein, M.
Deposited on : 1996-10-17
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

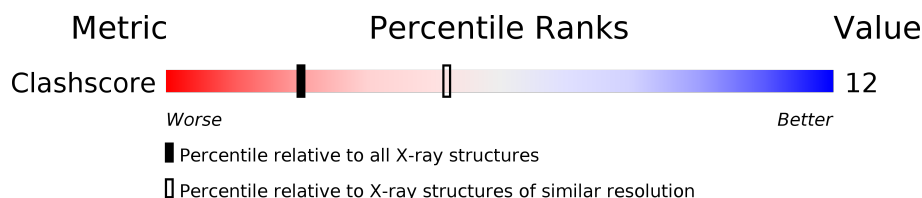
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	141614	3122 (2.70-2.70)

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 on 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	398	 72% 26% •
1	B	398	 69% 28% •
1	C	398	 74% 23% •
1	D	398	 73% 25% •
2	E	3	 100%
2	F	3	 100%
2	G	3	 33% 67%
2	H	3	 33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13412 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 ENDOGLUCANASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	B	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	C	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	D	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			

- Molecule 2 is an oligosaccharide called 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	F	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	G	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	H	3	Total	C	O	S	0	0	0
			34	18	12	4			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

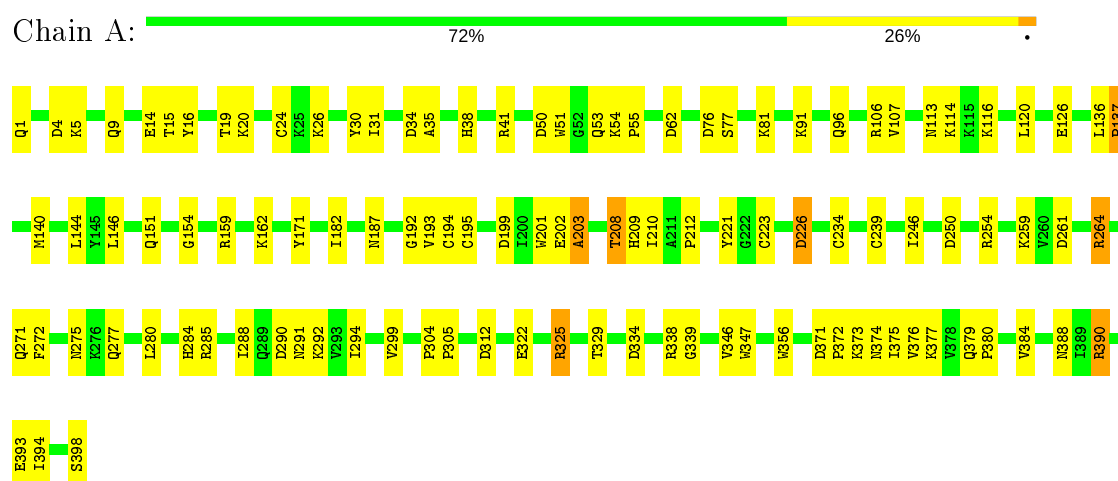
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		
4	B	267	Total	O	0	0
			267	267		
4	C	248	Total	O	0	0
			248	248		
4	D	282	Total	O	0	0
			282	282		

3 Residue-property plots

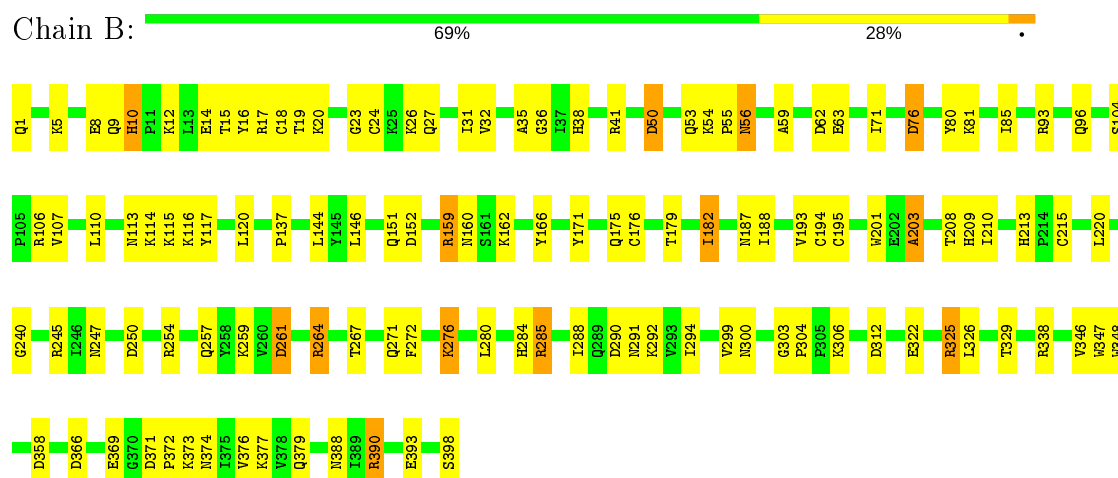
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

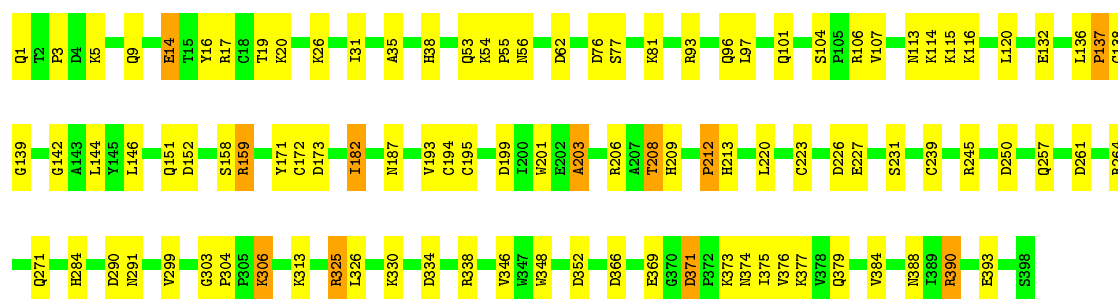


• Molecule 1: ENDOGLUCANASE I



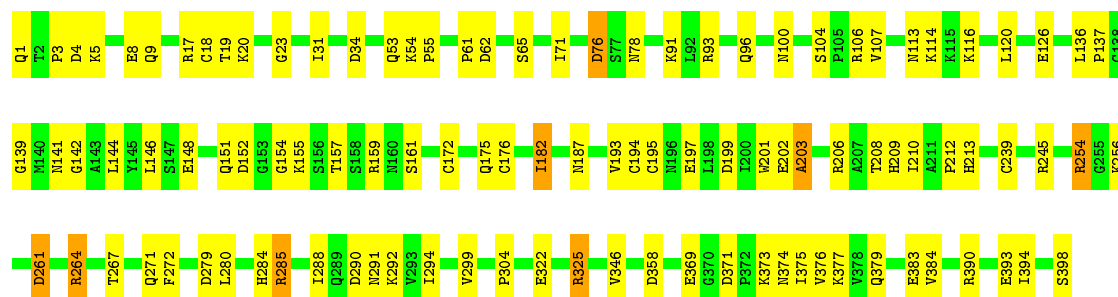
• Molecule 1: ENDOGLUCANASE I





• Molecule 1: ENDOGLUCANASE I

Chain D: 73% 25%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain E: 100%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain F: 100%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain G: 33% 67%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain H: 33% 67%



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	68.16 Å 78.28 Å 142.46 Å 90.00° 96.89° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	89.5 (15.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13412	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: SSG, PCA, NAG, SGC

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	0.64	0/3077	1.54	31/4155 (0.7%)
1	B	0.67	0/3077	1.62	45/4155 (1.1%)
1	C	0.66	0/3077	1.61	49/4155 (1.2%)
1	D	0.67	0/3077	1.57	38/4155 (0.9%)
All	All	0.66	0/12308	1.58	163/16620 (1.0%)

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	ARG	NE-CZ-NH1	21.63	131.11	120.30
1	D	390	ARG	NE-CZ-NH1	18.99	129.80	120.30
1	C	325	ARG	NE-CZ-NH1	17.52	129.06	120.30
1	C	390	ARG	NE-CZ-NH1	16.93	128.77	120.30
1	A	325	ARG	CD-NE-CZ	14.97	144.56	123.60
1	C	93	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	A	390	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	A	226	ASP	CB-CG-OD2	-13.14	106.48	118.30
1	B	93	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	B	264	ARG	NE-CZ-NH2	-11.79	114.40	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	B	325	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	338	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	C	152	ASP	CB-CG-OD1	10.29	127.56	118.30
1	C	352	ASP	CB-CG-OD1	10.24	127.51	118.30
1	A	334	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	B	325	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	B	106	ARG	NE-CZ-NH2	9.78	125.19	120.30
1	B	358	ASP	CB-CG-OD2	9.50	126.85	118.30
1	A	325	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	D	325	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	C	62	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	B	325	ARG	CD-NE-CZ	8.83	135.96	123.60
1	B	17	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	D	285	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	325	ARG	CD-NE-CZ	8.66	135.73	123.60
1	D	325	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	D	264	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	C	250	ASP	CB-CG-OD1	8.59	126.03	118.30
1	A	325	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	D	285	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	D	390	ARG	NH1-CZ-NH2	-8.26	110.31	119.40
1	A	390	ARG	CD-NE-CZ	8.24	135.14	123.60
1	C	159	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	C	17	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	93	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	250	ASP	CB-CG-OD1	7.68	125.21	118.30
1	C	390	ARG	CA-CB-CG	7.59	130.09	113.40
1	B	390	ARG	NH1-CZ-NH2	-7.55	111.10	119.40
1	C	390	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	152	ASP	CB-CG-OD1	7.44	125.00	118.30
1	B	346	VAL	CB-CA-C	-7.42	97.30	111.40
1	A	390	ARG	NH1-CZ-NH2	-7.39	111.27	119.40
1	D	261	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	117	TYR	CB-CG-CD2	7.25	125.35	121.00
1	D	358	ASP	CB-CG-OD1	7.23	124.81	118.30
1	D	261	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	C	325	ARG	CD-NE-CZ	7.20	133.68	123.60
1	D	34	ASP	CB-CG-OD2	7.09	124.68	118.30
1	D	203	ALA	N-CA-CB	-7.05	100.23	110.10
1	D	390	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	312	ASP	CB-CG-OD1	6.90	124.51	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ARG	CA-CB-CG	6.79	128.33	113.40
1	C	17	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	203	ALA	CB-CA-C	-6.66	100.11	110.10
1	C	371	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	346	VAL	CB-CA-C	-6.64	98.78	111.40
1	B	254	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	C	245	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	B	245	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	159	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	106	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	173	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	D	76	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	62	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	338	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	B	254	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	D	104	SER	N-CA-CB	-6.33	101.00	110.50
1	C	226	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	159	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	171	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	B	390	ARG	CA-CB-CG	6.29	127.25	113.40
1	B	56	ASN	CB-CG-OD1	-6.28	109.04	121.60
1	B	261	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	254	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	B	203	ALA	N-CA-CB	-6.15	101.49	110.10
1	D	390	ARG	CA-CB-CG	6.14	126.92	113.40
1	C	203	ALA	N-CA-CB	-6.09	101.57	110.10
1	C	338	ARG	CD-NE-CZ	6.05	132.08	123.60
1	D	245	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	A	264	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	346	VAL	N-CA-CB	5.91	124.50	111.50
1	B	346	VAL	N-CA-CB	5.89	124.47	111.50
1	B	390	ARG	CD-NE-CZ	5.88	131.83	123.60
1	A	62	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	71	ILE	CB-CA-C	-5.85	99.91	111.60
1	A	221	TYR	CB-CG-CD1	5.84	124.51	121.00
1	C	132	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	D	106	ARG	CD-NE-CZ	5.83	131.76	123.60
1	A	346	VAL	CB-CA-C	-5.83	100.33	111.40
1	D	254	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	C	346	VAL	CA-CB-CG2	5.80	119.60	110.90
1	B	152	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	62	ASP	CB-CG-OD1	5.78	123.50	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	30	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	B	80	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	D	182	ILE	CB-CA-C	-5.69	100.21	111.60
1	C	346	VAL	CB-CA-C	-5.69	100.59	111.40
1	C	306	LYS	CA-CB-CG	5.68	125.89	113.40
1	C	152	ASP	OD1-CG-OD2	-5.63	112.60	123.30
1	D	17	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	208	THR	N-CA-CB	5.60	120.94	110.30
1	A	254	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	C	56	ASN	CB-CG-OD1	-5.58	110.44	121.60
1	D	369	GLU	OE1-CD-OE2	-5.56	116.62	123.30
1	A	154	GLY	CA-C-O	-5.52	110.66	120.60
1	D	202	GLU	N-CA-CB	5.51	120.52	110.60
1	D	141	ASN	CA-CB-CG	5.49	125.47	113.40
1	C	206	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	285	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	10	HIS	CA-CB-CG	5.47	122.89	113.60
1	B	312	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	93	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	C	171	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	C	245	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	B	76	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	104	SER	N-CA-CB	-5.42	102.37	110.50
1	C	137	PRO	N-CA-CB	5.41	109.79	103.30
1	C	142	GLY	N-CA-C	-5.40	99.60	113.10
1	B	215	CYS	CA-CB-SG	5.40	123.71	114.00
1	C	334	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	62	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	8	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	B	182	ILE	CB-CA-C	-5.38	100.85	111.60
1	C	3	PRO	N-CA-CB	5.37	109.74	103.30
1	B	306	LYS	CA-CB-CG	5.37	125.20	113.40
1	A	106	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	C	199	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	D	279	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	245	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	C	346	VAL	N-CA-CB	5.32	123.19	111.50
1	A	34	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	B	36	GLY	O-C-N	-5.29	114.24	122.70
1	A	203	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	137	PRO	N-CA-CB	5.28	109.63	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	MET	CA-CB-CG	5.27	122.26	113.30
1	B	245	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	D	17	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	14	GLU	CG-CD-OE2	5.25	128.80	118.30
1	C	182	ILE	CB-CA-C	-5.24	101.13	111.60
1	B	250	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	50	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	208	THR	CA-CB-CG2	-5.20	105.12	112.40
1	A	285	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	138	CYS	CA-CB-SG	5.19	123.35	114.00
1	B	276	LYS	CA-CB-CG	5.19	124.81	113.40
1	D	93	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	D	142	GLY	N-CA-C	-5.17	100.16	113.10
1	C	203	ALA	CB-CA-C	-5.16	102.36	110.10
1	A	30	TYR	CA-CB-CG	-5.16	103.61	113.40
1	D	3	PRO	N-CA-CB	5.15	109.48	103.30
1	A	208	THR	CA-CB-CG2	-5.12	105.24	112.40
1	B	166	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	338	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	148	GLU	CG-CD-OE1	5.07	128.44	118.30
1	C	348	TRP	CA-CB-CG	5.06	123.32	113.70
1	A	171	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	C	104	SER	N-CA-CB	-5.04	102.94	110.50
1	C	212	PRO	N-CA-CB	5.04	109.34	103.30
1	B	390	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	27	GLN	CB-CA-C	-5.03	100.35	110.40
1	A	305	PRO	N-CA-CB	5.01	109.31	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	THR	Mainchain
1	B	15	THR	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	3023	0	2905	79	0
1	B	3023	0	2905	82	0
1	C	3023	0	2905	65	0
1	D	3023	0	2905	65	0
2	E	34	0	30	6	0
2	F	34	0	30	6	0
2	G	34	0	30	4	0
2	H	34	0	29	6	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	275	0	0	13	0
4	B	267	0	0	13	0
4	C	248	0	0	12	0
4	D	282	0	0	9	0
All	All	13412	0	11843	302	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 12.

All (302) 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:D:182:ILE:HG21	4:D:940:HOH:O	1.64	0.95
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.50	0.93
1:D:78:ASN:HB3	4:D:858:HOH:O	1.67	0.93
1:B:203:ALA:HB2	1:B:208:THR:HG23	1.52	0.88
1:D:203:ALA:HB2	1:D:208:THR:HG23	1.55	0.88
1:B:41:ARG:HD3	4:B:584:HOH:O	1.75	0.86
1:C:203:ALA:HB2	1:C:208:THR:HG23	1.56	0.86
1:A:226:ASP:HB2	4:A:632:HOH:O	1.78	0.84
2:H:1:SSG:S4	2:H:2:SGC:H4	2.22	0.79
2:G:1:SSG:S4	2:G:2:SGC:H4	2.22	0.79
1:B:374:ASN:HA	1:B:377:LYS:HD2	1.62	0.79
1:A:19:THR:HA	1:A:393:GLU:HG3	1.64	0.78
2:E:1:SSG:S4	2:E:2:SGC:H4	2.24	0.78
1:A:374:ASN:HA	1:A:377:LYS:HD2	1.65	0.78
1:B:303:GLY:HA3	4:B:627:HOH:O	1.84	0.77
1:A:54:LYS:HB2	1:A:55:PRO:HD2	1.67	0.77
2:F:1:SSG:S4	2:F:2:SGC:H4	2.25	0.76
1:A:182:ILE:HD11	1:A:187:ASN:HA	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HB2	1:B:55:PRO:HD2	1.68	0.75
1:D:374:ASN:HA	1:D:377:LYS:HD2	1.69	0.75
1:C:374:ASN:HA	1:C:377:LYS:HD2	1.69	0.73
1:A:259:LYS:NZ	4:A:653:HOH:O	2.18	0.72
1:C:5:LYS:H	1:C:5:LYS:HD3	1.54	0.71
1:D:182:ILE:HD11	1:D:187:ASN:HA	1.72	0.70
1:D:54:LYS:HB2	1:D:55:PRO:HD2	1.73	0.70
1:D:19:THR:HA	1:D:393:GLU:HG3	1.74	0.70
1:C:14:GLU:HG2	4:C:566:HOH:O	1.90	0.70
1:D:201:TRP:CZ3	1:D:208:THR:HG21	2.27	0.69
1:C:182:ILE:HG23	1:C:193:VAL:HG22	1.75	0.69
1:A:5:LYS:H	1:A:5:LYS:HD3	1.58	0.68
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.29	0.68
1:B:113:ASN:O	1:B:114:LYS:HB2	1.92	0.68
1:D:5:LYS:HD3	1:D:5:LYS:H	1.59	0.67
1:D:116:LYS:HB3	1:D:151:GLN:HG2	1.77	0.67
1:B:19:THR:HA	1:B:393:GLU:HG3	1.74	0.67
1:B:5:LYS:HD3	1:B:5:LYS:H	1.59	0.67
1:D:261:ASP:OD2	1:D:264:ARG:HD3	1.94	0.66
1:B:276:LYS:HB2	4:B:657:HOH:O	1.96	0.66
1:A:116:LYS:HB3	1:A:151:GLN:HG2	1.77	0.66
1:C:182:ILE:HD11	1:C:187:ASN:HA	1.78	0.66
1:C:19:THR:HA	1:C:393:GLU:HG3	1.80	0.64
2:H:1:SSG:S4	2:H:2:SGC:C4	2.86	0.64
1:C:116:LYS:HB3	1:C:151:GLN:HG2	1.80	0.63
2:E:1:SSG:S4	2:E:2:SGC:C4	2.86	0.63
2:G:1:SSG:S4	2:G:2:SGC:C4	2.86	0.63
1:B:116:LYS:HB3	1:B:151:GLN:HG2	1.79	0.63
1:B:261:ASP:OD2	1:B:264:ARG:HD3	1.99	0.62
1:C:201:TRP:CZ3	1:C:208:THR:HG21	2.34	0.62
1:C:113:ASN:O	1:C:114:LYS:HB2	1.99	0.62
1:C:120:LEU:HD12	1:C:146:LEU:HD21	1.81	0.62
1:C:54:LYS:HB2	1:C:55:PRO:HD2	1.82	0.62
1:C:299:VAL:HG11	1:C:304:PRO:HB2	1.80	0.62
1:B:182:ILE:HD11	1:B:187:ASN:HA	1.83	0.61
1:B:182:ILE:HG23	1:B:193:VAL:HG22	1.83	0.61
1:B:96:GLN:HE21	1:B:96:GLN:HA	1.65	0.61
1:C:195:CYS:HA	4:C:576:HOH:O	2.01	0.61
1:B:151:GLN:HB3	4:B:647:HOH:O	2.00	0.60
1:A:261:ASP:OD2	1:A:264:ARG:HD3	2.00	0.60
2:F:1:SSG:S4	2:F:2:SGC:C4	2.88	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ILE:HG13	1:D:187:ASN:HB2	1.83	0.60
1:A:290:ASP:O	1:A:291:ASN:HB2	2.00	0.60
1:A:194:CYS:O	1:A:195:CYS:HB3	2.02	0.59
1:C:182:ILE:HG13	1:C:187:ASN:HB2	1.83	0.59
1:B:54:LYS:HB2	1:B:55:PRO:CD	2.32	0.59
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.37	0.59
1:A:54:LYS:HB2	1:A:55:PRO:CD	2.32	0.59
1:C:231:SER:HB3	4:C:487:HOH:O	2.02	0.58
1:C:96:GLN:HA	1:C:96:GLN:HE21	1.69	0.58
1:D:5:LYS:CD	1:D:5:LYS:H	2.15	0.57
1:C:5:LYS:H	1:C:5:LYS:CD	2.15	0.57
1:B:376:VAL:HA	1:B:379:GLN:O	2.05	0.57
1:B:137:PRO:HB2	4:B:524:HOH:O	2.04	0.57
1:A:5:LYS:H	1:A:5:LYS:CD	2.14	0.57
1:D:96:GLN:HA	1:D:96:GLN:HE21	1.70	0.57
1:C:208:THR:HG22	1:C:209:HIS:H	1.69	0.56
1:A:182:ILE:HG13	1:A:187:ASN:HB2	1.87	0.56
1:C:14:GLU:OE1	1:C:26:LYS:HD2	2.06	0.56
1:C:290:ASP:O	1:C:291:ASN:HB2	2.05	0.56
1:D:376:VAL:HA	1:D:379:GLN:O	2.05	0.56
1:A:151:GLN:HB3	4:A:611:HOH:O	2.06	0.55
1:D:120:LEU:HD12	1:D:146:LEU:HD21	1.87	0.55
1:C:271:GLN:HB2	1:C:284:HIS:HB2	1.89	0.55
1:A:113:ASN:O	1:A:114:LYS:HB2	2.06	0.55
1:D:113:ASN:O	1:D:114:LYS:HB2	2.06	0.55
1:D:54:LYS:HB2	1:D:55:PRO:CD	2.36	0.55
1:B:213:HIS:HE1	2:F:1:SSG:H2	1.70	0.55
1:D:182:ILE:HG23	1:D:193:VAL:HG22	1.88	0.54
1:B:299:VAL:HG11	1:B:304:PRO:HB2	1.89	0.54
1:C:20:LYS:N	1:C:393:GLU:OE2	2.35	0.54
1:D:194:CYS:O	1:D:195:CYS:HB3	2.07	0.54
1:D:256:LYS:HD3	4:D:796:HOH:O	2.06	0.54
1:B:290:ASP:O	1:B:291:ASN:HB2	2.06	0.54
1:A:212:PRO:HD2	1:A:239:CYS:O	2.08	0.54
1:A:137:PRO:HG3	1:A:379:GLN:HB3	1.90	0.53
1:B:371:ASP:OD1	1:B:373:LYS:HB3	2.08	0.53
1:B:288:ILE:CD1	1:B:398:SER:HB2	2.39	0.53
1:D:9:GLN:OE1	1:D:76:ASP:HB2	2.09	0.53
1:A:299:VAL:HG11	1:A:304:PRO:HB2	1.89	0.53
1:A:208:THR:HG22	1:A:209:HIS:H	1.73	0.53
1:B:179:THR:HB	4:B:592:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ARG:NH2	4:C:616:HOH:O	2.35	0.53
1:D:208:THR:HG22	1:D:209:HIS:H	1.74	0.53
1:A:271:GLN:HB2	1:A:284:HIS:HB2	1.90	0.53
1:B:120:LEU:HD12	1:B:146:LEU:HD21	1.91	0.53
1:A:96:GLN:HA	1:A:96:GLN:HE21	1.73	0.52
1:C:388:ASN:OD1	1:C:390:ARG:NH1	2.39	0.52
1:A:388:ASN:OD1	1:A:390:ARG:NH1	2.32	0.52
1:B:388:ASN:OD1	1:B:390:ARG:NH1	2.41	0.52
1:D:137:PRO:HG2	1:D:375:ILE:HG23	1.92	0.52
1:B:159:ARG:HB3	4:B:621:HOH:O	2.09	0.52
1:D:212:PRO:HD2	1:D:239:CYS:O	2.10	0.52
1:C:115:LYS:HE3	4:C:613:HOH:O	2.09	0.52
1:A:14:GLU:OE1	1:A:26:LYS:HD2	2.10	0.52
1:D:137:PRO:HB2	4:D:600:HOH:O	2.10	0.52
1:D:299:VAL:HG11	1:D:304:PRO:HB2	1.92	0.52
1:A:14:GLU:HG2	4:A:569:HOH:O	2.10	0.51
1:B:194:CYS:O	1:B:195:CYS:HB3	2.10	0.51
1:C:194:CYS:O	1:C:195:CYS:HB3	2.10	0.51
1:C:193:VAL:HG13	1:C:220:LEU:HD21	1.93	0.51
1:A:182:ILE:HG23	1:A:193:VAL:HG22	1.93	0.51
1:C:53:GLN:NE2	1:C:54:LYS:O	2.44	0.51
1:A:136:LEU:HD11	1:A:384:VAL:HB	1.92	0.50
1:B:208:THR:HG22	1:B:209:HIS:H	1.74	0.50
1:C:35:ALA:O	1:C:38:HIS:HB2	2.11	0.50
1:D:371:ASP:OD1	1:D:373:LYS:HB3	2.11	0.50
1:A:371:ASP:O	1:A:375:ILE:HG13	2.11	0.50
1:A:53:GLN:NE2	1:A:54:LYS:O	2.44	0.50
1:B:5:LYS:CD	1:B:5:LYS:H	2.19	0.50
1:B:115:LYS:HD2	4:B:614:HOH:O	2.12	0.50
1:A:9:GLN:OE1	1:A:76:ASP:HB2	2.11	0.50
1:A:41:ARG:HD3	4:A:585:HOH:O	2.11	0.50
1:D:290:ASP:O	1:D:291:ASN:HB2	2.11	0.50
1:C:212:PRO:HD2	1:C:239:CYS:O	2.12	0.49
1:C:223:CYS:HB2	1:C:227:GLU:HB2	1.95	0.49
1:D:213:HIS:HE1	2:H:1:SSG:H2	1.76	0.49
1:B:259:LYS:HE3	4:B:634:HOH:O	2.11	0.49
1:B:35:ALA:O	1:B:38:HIS:HB2	2.13	0.49
1:A:16:TYR:CE2	1:A:26:LYS:HG3	2.48	0.49
1:A:380:PRO:HG2	4:A:672:HOH:O	2.12	0.49
1:C:137:PRO:HB2	4:C:524:HOH:O	2.12	0.49
1:A:202:GLU:OE2	2:E:1:SSG:S4	2.71	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HB	1:B:110:LEU:HD11	1.94	0.48
1:B:195:CYS:HA	4:B:572:HOH:O	2.12	0.48
1:A:292:LYS:O	1:A:294:ILE:HD12	2.14	0.48
1:B:182:ILE:HG13	1:B:187:ASN:HB2	1.95	0.48
1:C:144:LEU:C	1:C:144:LEU:HD23	2.34	0.48
1:D:254:ARG:HG3	4:D:500:HOH:O	2.14	0.48
1:D:91:LYS:HE2	4:D:587:HOH:O	2.14	0.48
1:C:376:VAL:HA	1:C:379:GLN:O	2.14	0.48
1:A:159:ARG:NH2	4:A:637:HOH:O	2.47	0.48
1:A:203:ALA:CB	1:A:208:THR:HG23	2.35	0.48
1:B:137:PRO:HG3	1:B:379:GLN:HB3	1.96	0.48
1:C:257:GLN:HB3	4:C:610:HOH:O	2.13	0.48
1:B:14:GLU:OE2	1:B:26:LYS:HB2	2.14	0.47
1:D:100:ASN:ND2	4:D:805:HOH:O	2.47	0.47
1:D:54:LYS:HG2	4:D:860:HOH:O	2.14	0.47
1:A:199:ASP:OD2	2:E:1:SSG:O3	2.33	0.47
1:A:31:ILE:HG23	1:A:107:VAL:HB	1.97	0.47
1:B:213:HIS:CE1	2:F:1:SSG:H2	2.49	0.47
1:D:210:ILE:HD11	1:D:285:ARG:NH1	2.30	0.47
1:B:16:TYR:HB2	1:B:390:ARG:HB3	1.95	0.47
1:B:280:LEU:HD23	1:B:329:THR:CG2	2.45	0.47
1:B:54:LYS:CB	1:B:55:PRO:CD	2.92	0.47
1:A:347:TRP:CE3	2:E:3:SGC:H5	2.50	0.47
1:A:288:ILE:CD1	1:A:398:SER:HB2	2.44	0.47
1:D:144:LEU:HD23	1:D:144:LEU:C	2.35	0.47
1:C:303:GLY:HA3	4:C:611:HOH:O	2.14	0.47
1:A:50:ASP:O	1:A:51:TRP:C	2.54	0.47
1:A:322:GLU:HG3	1:A:325:ARG:HH11	1.80	0.46
1:C:261:ASP:OD2	1:C:264:ARG:HD3	2.15	0.46
1:A:277:GLN:NE2	4:A:606:HOH:O	2.46	0.46
1:B:175:GLN:O	1:B:176:CYS:HB2	2.15	0.46
1:B:247:ASN:HB3	1:B:300:ASN:HB3	1.97	0.46
1:B:288:ILE:HD11	1:B:398:SER:HB2	1.98	0.46
1:A:77:SER:O	1:A:81:LYS:HD2	2.16	0.46
1:A:54:LYS:CB	1:A:55:PRO:CD	2.92	0.46
1:B:9:GLN:OE1	1:B:76:ASP:HB2	2.16	0.46
1:C:313:LYS:HD3	4:C:522:HOH:O	2.15	0.46
1:B:18:CYS:HA	1:B:23:GLY:O	2.15	0.46
1:D:136:LEU:HD11	1:D:384:VAL:HB	1.98	0.46
1:D:175:GLN:O	1:D:176:CYS:HB2	2.16	0.46
1:A:20:LYS:N	1:A:393:GLU:OE2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ASP:O	1:C:375:ILE:HG13	2.16	0.45
1:D:126:GLU:HB2	1:D:394:ILE:HA	1.99	0.45
2:F:1:SSG:O3	2:F:2:SGC:C1	2.64	0.45
1:A:272:PHE:HB3	1:A:280:LEU:HD11	1.97	0.45
1:D:197:GLU:OE1	2:H:2:SGC:O2	2.32	0.45
1:A:137:PRO:HG2	1:A:375:ILE:HG23	1.99	0.45
1:A:371:ASP:OD1	1:A:373:LYS:HB3	2.16	0.45
1:A:54:LYS:CB	1:A:55:PRO:HD2	2.42	0.45
1:B:280:LEU:HD23	1:B:329:THR:HG22	1.98	0.45
2:H:1:SSG:O3	2:H:2:SGC:C1	2.65	0.45
1:A:322:GLU:HG3	1:A:325:ARG:NH1	2.32	0.45
1:A:120:LEU:HD12	1:A:146:LEU:HD21	1.99	0.45
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.82	0.45
1:A:116:LYS:HB3	1:A:151:GLN:CG	2.46	0.45
1:A:91:LYS:HE2	4:A:511:HOH:O	2.17	0.45
1:B:31:ILE:HG23	1:B:107:VAL:HB	1.98	0.45
1:D:31:ILE:HG23	1:D:107:VAL:HB	1.99	0.45
1:B:81:LYS:HE2	1:B:85:ILE:O	2.17	0.45
1:C:54:LYS:CB	1:C:55:PRO:HD2	2.46	0.45
1:D:53:GLN:NE2	1:D:54:LYS:O	2.50	0.45
1:C:9:GLN:OE1	1:C:76:ASP:HB2	2.17	0.44
1:B:325:ARG:NH2	1:B:326:LEU:HD21	2.32	0.44
1:B:20:LYS:N	1:B:393:GLU:OE2	2.44	0.44
1:C:172:CYS:HB3	1:C:193:VAL:HG12	2.00	0.44
1:D:208:THR:HG22	1:D:209:HIS:N	2.32	0.44
1:C:213:HIS:HE1	2:G:1:SSG:H2	1.82	0.44
1:A:246:ILE:HG13	1:A:246:ILE:H	1.70	0.44
1:B:63:GLU:HG2	1:B:160:ASN:HD22	1.83	0.44
1:C:158:SER:OG	1:C:159:ARG:N	2.51	0.44
1:C:371:ASP:OD1	1:C:373:LYS:HB3	2.18	0.44
1:B:257:GLN:HG3	4:B:596:HOH:O	2.16	0.44
1:C:306:LYS:N	1:C:306:LYS:HE2	2.33	0.44
1:C:137:PRO:HG3	1:C:379:GLN:HB3	2.00	0.44
1:D:203:ALA:CB	1:D:208:THR:HG23	2.37	0.44
1:D:18:CYS:HA	1:D:23:GLY:O	2.16	0.44
1:A:16:TYR:HB3	1:A:24:CYS:HB3	1.99	0.44
1:B:193:VAL:HG13	1:B:220:LEU:HD21	1.99	0.44
1:B:208:THR:HG22	1:B:209:HIS:N	2.32	0.44
1:C:81:LYS:HD3	4:C:638:HOH:O	2.18	0.44
1:A:126:GLU:HB2	1:A:394:ILE:HA	1.99	0.44
1:A:19:THR:HA	1:A:393:GLU:CG	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASP:H	1:B:53:GLN:NE2	2.15	0.44
1:D:271:GLN:HB2	1:D:284:HIS:HB2	2.00	0.44
1:D:383:GLU:HG3	4:D:770:HOH:O	2.17	0.44
1:A:20:LYS:H	1:A:393:GLU:CD	2.21	0.43
1:A:210:ILE:HG13	4:A:413:HOH:O	2.17	0.43
1:A:376:VAL:HA	1:A:379:GLN:O	2.18	0.43
1:A:96:GLN:CA	1:A:96:GLN:HE21	2.29	0.43
1:C:19:THR:HA	1:C:393:GLU:CG	2.46	0.43
1:B:366:ASP:CG	1:B:369:GLU:HG2	2.39	0.43
1:C:137:PRO:HG2	1:C:375:ILE:HG23	2.01	0.43
1:D:61:PRO:HD2	1:D:65:SER:HB2	2.00	0.43
1:A:280:LEU:HD23	1:A:329:THR:HG22	2.01	0.43
1:B:203:ALA:CB	1:B:208:THR:HG23	2.38	0.43
1:D:267:THR:HB	1:D:288:ILE:HB	2.00	0.43
1:D:322:GLU:HG3	1:D:325:ARG:NH1	2.34	0.43
1:D:54:LYS:CB	1:D:55:PRO:CD	2.97	0.43
1:B:144:LEU:C	1:B:144:LEU:HD23	2.38	0.43
1:A:144:LEU:C	1:A:144:LEU:HD23	2.40	0.43
1:A:35:ALA:O	1:A:38:HIS:HB2	2.19	0.43
1:A:356:TRP:CZ2	2:E:1:SSG:H5	2.54	0.43
1:D:139:GLY:HA3	1:D:375:ILE:HD11	2.01	0.42
1:A:4:ASP:HB2	1:A:5:LYS:HD3	2.02	0.42
1:B:54:LYS:CB	1:B:55:PRO:HD2	2.42	0.42
1:B:50:ASP:H	1:B:53:GLN:HE21	1.67	0.42
1:C:208:THR:HG22	1:C:209:HIS:N	2.32	0.42
1:C:366:ASP:CG	1:C:369:GLU:HG2	2.40	0.42
1:D:272:PHE:HB3	1:D:280:LEU:HD11	2.02	0.42
2:G:1:SSG:O3	2:G:2:SGC:C1	2.67	0.42
1:A:120:LEU:O	1:A:339:GLY:HA2	2.19	0.42
1:A:192:GLY:HA3	1:A:223:CYS:SG	2.59	0.42
1:C:20:LYS:H	1:C:393:GLU:CD	2.22	0.42
1:B:347:TRP:CE3	2:F:3:SGC:H5	2.54	0.42
1:B:162:LYS:NZ	4:B:532:HOH:O	2.52	0.42
1:B:348:TRP:CE2	1:B:372:PRO:HB3	2.54	0.42
1:C:31:ILE:HG23	1:C:107:VAL:HB	2.01	0.42
1:C:325:ARG:NH2	1:C:326:LEU:HD21	2.33	0.42
1:C:77:SER:HB3	4:C:638:HOH:O	2.19	0.42
1:D:4:ASP:HB3	1:D:71:ILE:CG2	2.49	0.42
1:B:56:ASN:HB3	1:B:59:ALA:HB3	2.00	0.42
1:C:16:TYR:HB2	1:C:390:ARG:HB3	2.01	0.42
1:C:203:ALA:CB	1:C:208:THR:HG23	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LYS:HB2	1:C:55:PRO:CD	2.48	0.42
1:D:172:CYS:HB3	1:D:193:VAL:HG12	2.01	0.42
1:D:292:LYS:O	1:D:294:ILE:HD12	2.19	0.42
1:A:116:LYS:HB3	1:A:116:LYS:HE3	1.88	0.41
1:B:292:LYS:O	1:B:294:ILE:HD12	2.20	0.41
1:B:53:GLN:HE21	1:B:53:GLN:HB3	1.75	0.41
1:D:199:ASP:OD2	2:H:1:SSG:O3	2.38	0.41
1:A:194:CYS:HB3	1:A:234:CYS:SG	2.61	0.41
1:B:12:LYS:HE2	4:B:564:HOH:O	2.20	0.41
1:B:20:LYS:H	1:B:393:GLU:CD	2.24	0.41
1:C:264:ARG:NH2	1:C:290:ASP:OD1	2.53	0.41
1:A:275:ASN:HB2	4:A:665:HOH:O	2.19	0.41
1:B:210:ILE:HD11	1:B:285:ARG:NH1	2.36	0.41
1:B:322:GLU:HG3	1:B:325:ARG:HH11	1.86	0.41
1:D:155:LYS:HA	1:D:161:SER:OG	2.20	0.41
1:B:210:ILE:O	1:B:240:GLY:HA2	2.21	0.41
1:B:16:TYR:HB3	1:B:24:CYS:HB3	2.02	0.41
1:B:271:GLN:HB2	1:B:284:HIS:HB2	2.01	0.41
1:B:53:GLN:NE2	1:B:54:LYS:O	2.54	0.41
1:A:371:ASP:HA	1:A:372:PRO:HD3	1.82	0.41
1:B:267:THR:HB	1:B:288:ILE:HB	2.02	0.41
1:D:374:ASN:O	1:D:375:ILE:C	2.59	0.41
1:D:371:ASP:O	1:D:375:ILE:HG13	2.20	0.41
1:C:136:LEU:HD11	1:C:384:VAL:HB	2.03	0.41
1:B:188:ILE:HG12	1:B:188:ILE:H	1.70	0.41
1:D:20:LYS:N	1:D:393:GLU:OE2	2.51	0.41
1:B:288:ILE:HD12	1:B:398:SER:HB2	2.01	0.40
1:D:154:GLY:O	1:D:157:THR:HG23	2.21	0.40
1:D:288:ILE:CD1	1:D:398:SER:HB2	2.51	0.40
1:B:8:GLU:HG2	1:B:10:HIS:CE1	2.56	0.40
1:C:330:LYS:HB2	4:C:591:HOH:O	2.21	0.40
1:D:54:LYS:CB	1:D:55:PRO:HD2	2.48	0.40
1:A:113:ASN:HB3	4:A:577:HOH:O	2.21	0.40
1:B:272:PHE:HB3	1:B:280:LEU:HD11	2.04	0.40
1:A:41:ARG:HD3	1:A:41:ARG:HH11	1.75	0.40
1:C:97:LEU:HA	1:C:101:GLN:O	2.21	0.40
1:A:162:LYS:NZ	4:A:532:HOH:O	2.54	0.40
1:C:139:GLY:HA3	1:C:375:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	1.23	0	9,10,12	1.77	3 (33%)
1	PCA	D	1	1	7,8,9	1.18	0	9,10,12	1.80	3 (33%)
1	PCA	B	1	1	7,8,9	1.29	0	9,10,12	1.87	2 (22%)
1	PCA	C	1	1	7,8,9	1.41	0	9,10,12	2.28	2 (22%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	OE-CD-CG	-4.61	118.73	126.76
1	B	1	PCA	OE-CD-CG	-4.17	119.48	126.76
1	A	1	PCA	OE-CD-CG	-3.64	120.40	126.76
1	C	1	PCA	O-C-CA	-3.32	116.08	124.78
1	D	1	PCA	OE-CD-CG	-2.99	121.54	126.76
1	D	1	PCA	OE-CD-N	-2.67	118.65	124.86
1	B	1	PCA	OE-CD-N	-2.48	119.08	124.86
1	D	1	PCA	CB-CA-C	-2.42	109.38	112.70
1	A	1	PCA	CA-N-CD	-2.08	106.45	113.58
1	A	1	PCA	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

12 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	$\# Z > 2$
2	SSG	E	1	2	10,12,12	1.91	3 (30%)	11,17,17	2.69	7 (63%)
2	SGC	E	2	2	10,11,12	1.95	2 (20%)	12,15,17	2.69	4 (33%)
2	SGC	E	3	2	10,11,12	0.90	0	12,15,17	1.61	3 (25%)
2	SSG	F	1	2	10,12,12	1.89	2 (20%)	11,17,17	2.19	5 (45%)
2	SGC	F	2	2	10,11,12	1.11	0	12,15,17	2.66	3 (25%)
2	SGC	F	3	2	10,11,12	0.86	0	12,15,17	1.37	2 (16%)
2	SSG	G	1	2	10,12,12	1.97	3 (30%)	11,17,17	2.65	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SGC	G	2	2	10,11,12	1.44	2 (20%)	12,15,17	2.61	3 (25%)
2	SGC	G	3	2	10,11,12	1.12	1 (10%)	12,15,17	1.52	2 (16%)
2	SSG	H	1	2	10,12,12	1.84	2 (20%)	11,17,17	2.50	5 (45%)
2	SGC	H	2	2	10,11,12	1.63	2 (20%)	12,15,17	2.74	3 (25%)
2	SGC	H	3	2	10,11,12	1.36	1 (10%)	12,15,17	1.44	2 (16%)

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
2	SSG	E	1	2	-	0/2/22/22	0/1/1/1
2	SGC	E	2	2	-	0/2/19/22	0/1/1/1
2	SGC	E	3	2	-	0/2/19/22	0/1/1/1
2	SSG	F	1	2	-	0/2/22/22	0/1/1/1
2	SGC	F	2	2	-	0/2/19/22	0/1/1/1
2	SGC	F	3	2	-	1/2/19/22	0/1/1/1
2	SSG	G	1	2	-	0/2/22/22	0/1/1/1
2	SGC	G	2	2	-	0/2/19/22	0/1/1/1
2	SGC	G	3	2	-	0/2/19/22	0/1/1/1
2	SSG	H	1	2	-	0/2/22/22	0/1/1/1
2	SGC	H	2	2	-	0/2/19/22	0/1/1/1
2	SGC	H	3	2	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	SGC	C3-C4	4.38	1.57	1.53
2	H	1	SSG	C1-C2	-4.17	1.46	1.53
2	E	1	SSG	C5-C4	-3.55	1.50	1.53
2	G	1	SSG	C5-C4	-3.47	1.50	1.53
2	F	1	SSG	C5-C4	-3.41	1.50	1.53
2	G	1	SSG	C1-C2	-3.39	1.47	1.53
2	F	1	SSG	C1-C2	-3.35	1.47	1.53
2	H	3	SGC	C5-C4	-3.22	1.50	1.53
2	E	1	SSG	C1-C2	-3.19	1.47	1.53
2	H	2	SGC	C5-C4	-3.11	1.50	1.53
2	G	2	SGC	C5-C4	-3.03	1.50	1.53
2	G	1	SSG	C3-C4	-2.90	1.51	1.53
2	H	2	SGC	O5-C1	-2.88	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	SGC	C5-C4	-2.83	1.50	1.53
2	G	3	SGC	C5-C4	-2.81	1.50	1.53
2	G	2	SGC	O3-C3	-2.33	1.37	1.43
2	E	1	SSG	C3-C4	-2.16	1.51	1.53
2	H	1	SSG	C5-C4	-2.10	1.51	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	SGC	O5-C1-C2	6.61	120.98	110.77
2	H	2	SGC	O5-C1-C2	6.22	120.37	110.77
2	E	2	SGC	O5-C1-C2	6.15	120.26	110.77
2	G	2	SGC	O5-C1-C2	5.94	119.95	110.77
2	E	2	SGC	C1-O5-C5	5.20	119.24	112.19
2	E	1	SSG	O3-C3-C4	5.14	119.67	109.12
2	H	2	SGC	C1-O5-C5	5.08	119.07	112.19
2	G	1	SSG	O3-C3-C4	4.97	119.33	109.12
2	G	2	SGC	C1-O5-C5	4.83	118.74	112.19
2	G	1	SSG	O5-C1-C2	4.57	116.06	110.31
2	H	1	SSG	O3-C3-C4	4.44	118.25	109.12
2	H	1	SSG	O5-C1-C2	4.26	115.67	110.31
2	F	2	SGC	C1-O5-C5	4.07	117.71	112.19
2	E	1	SSG	O5-C1-C2	4.06	115.42	110.31
2	E	3	SGC	O3-C3-C4	4.03	117.39	109.12
2	G	3	SGC	O3-C3-C4	3.78	116.89	109.12
2	F	1	SSG	O3-C3-C4	3.77	116.86	109.12
2	H	3	SGC	O3-C3-C4	3.70	116.72	109.12
2	F	2	SGC	C5-C4-S4	-3.58	101.45	110.16
2	E	2	SGC	C5-C4-S4	-3.53	101.58	110.16
2	H	2	SGC	C5-C4-S4	-3.46	101.75	110.16
2	G	2	SGC	C5-C4-S4	-3.41	101.87	110.16
2	H	1	SSG	C1-O5-C5	-3.16	106.75	112.57
2	F	3	SGC	O3-C3-C4	3.07	115.42	109.12
2	E	1	SSG	C1-O5-C5	-3.03	107.00	112.57
2	F	1	SSG	C1-O5-C5	-2.93	107.18	112.57
2	E	1	SSG	C6-C5-C4	2.92	119.10	112.69
2	G	1	SSG	C6-C5-C4	2.87	119.00	112.69
2	F	1	SSG	O5-C1-C2	2.87	113.92	110.31
2	G	1	SSG	C1-O5-C5	-2.71	107.58	112.57
2	G	3	SGC	O3-C3-C2	-2.53	105.16	109.99
2	H	3	SGC	C1-O5-C5	2.48	115.55	112.19
2	E	1	SSG	O3-C3-C2	-2.39	104.82	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	SSG	C6-C5-C4	2.38	117.92	112.69
2	E	1	SSG	O6-C6-C5	2.34	119.31	111.29
2	G	1	SSG	C1-C2-C3	-2.30	106.04	110.59
2	H	1	SSG	O6-C6-C5	2.26	119.04	111.29
2	F	3	SGC	C1-O5-C5	2.25	115.24	112.19
2	F	1	SSG	C1-C2-C3	-2.16	106.32	110.59
2	E	3	SGC	C1-O5-C5	2.13	115.07	112.19
2	H	1	SSG	C6-C5-C4	2.13	117.36	112.69
2	E	1	SSG	C1-C2-C3	-2.10	106.45	110.59
2	E	3	SGC	O3-C3-C2	-2.04	106.09	109.99
2	E	2	SGC	O2-C2-C1	2.00	113.25	109.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	SGC	C4-C5-C6-O6

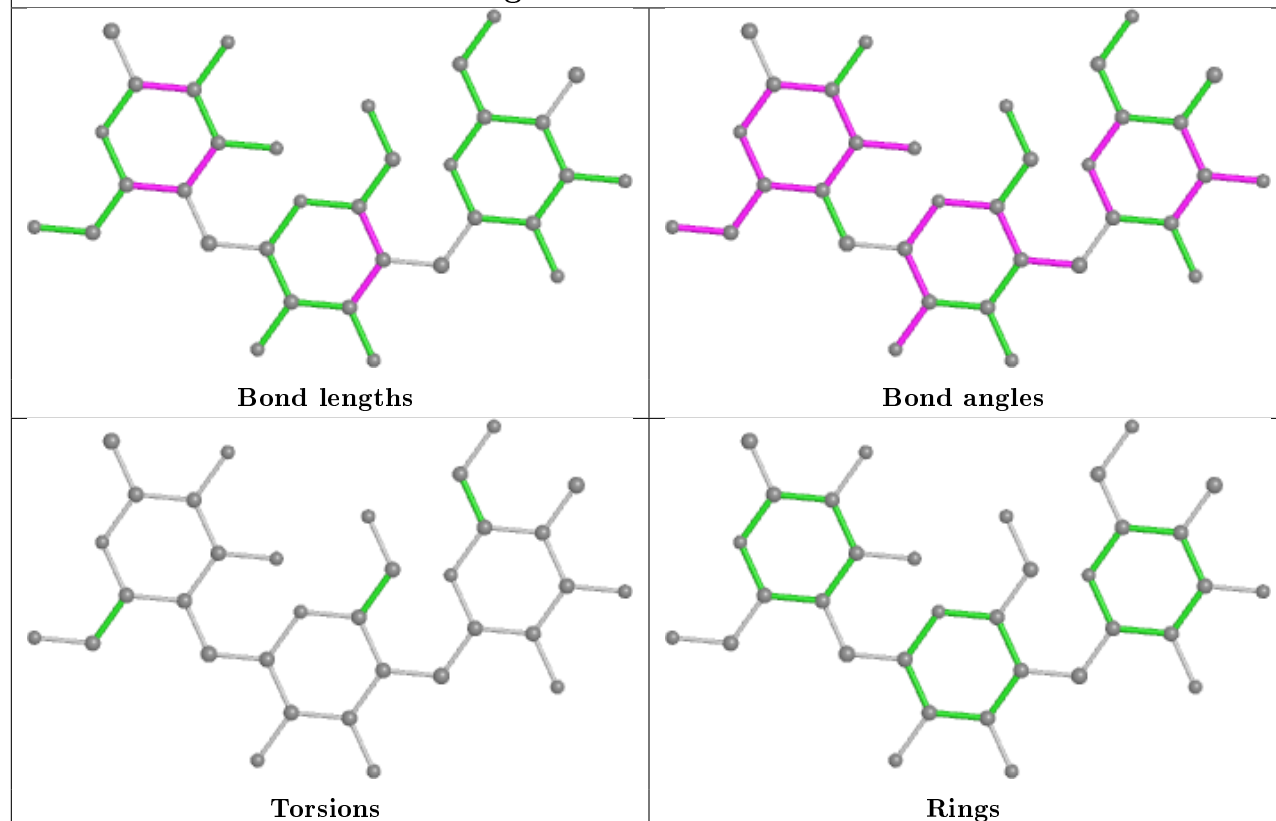
There are no ring outliers.

10 monomers are involved in 22 short contacts:

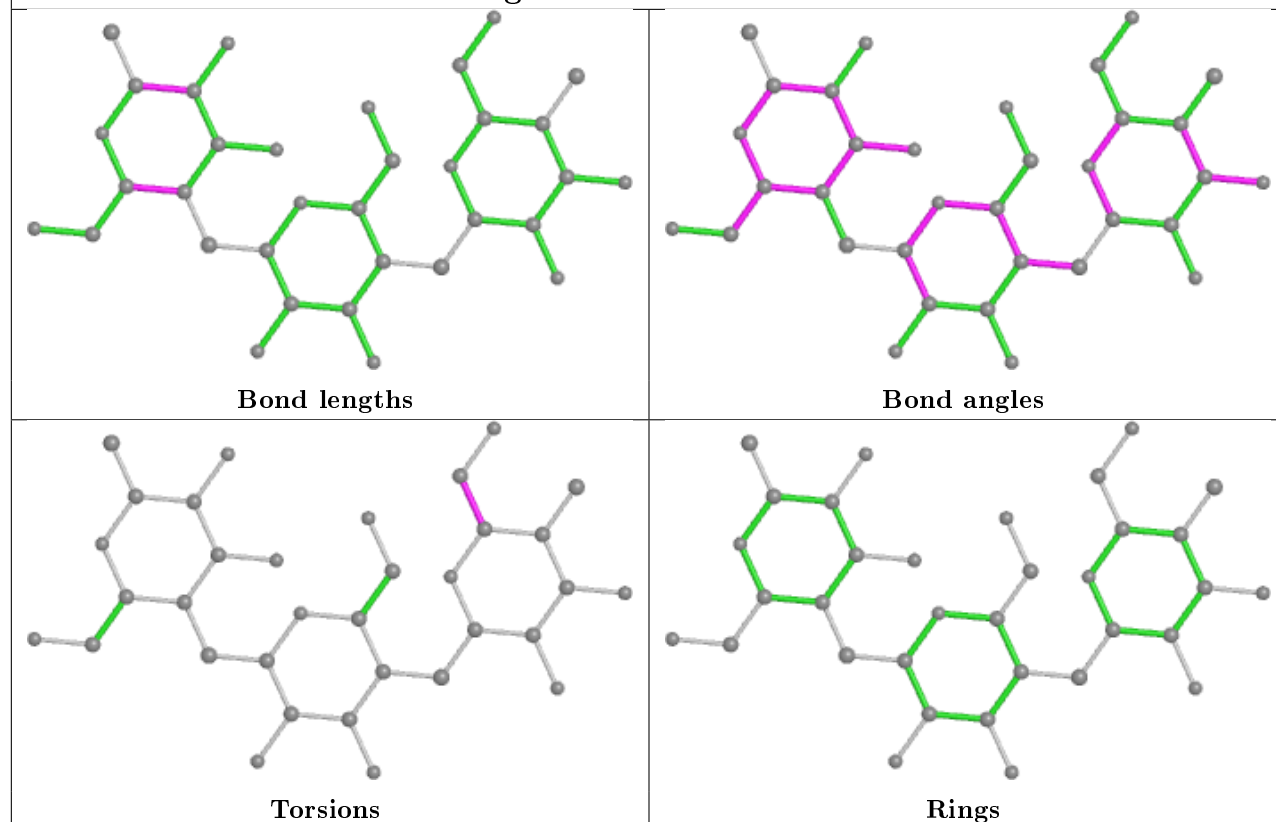
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	SSG	5	0
2	F	2	SGC	3	0
2	E	2	SGC	2	0
2	G	1	SSG	4	0
2	E	1	SSG	5	0
2	G	2	SGC	3	0
2	H	2	SGC	4	0
2	F	3	SGC	1	0
2	E	3	SGC	1	0
2	H	1	SSG	5	0

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

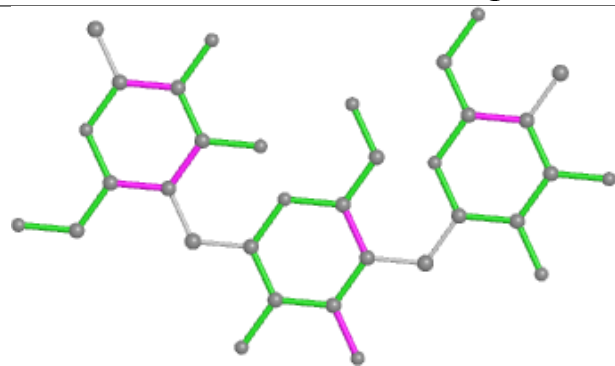
Oligosaccharide Chain E



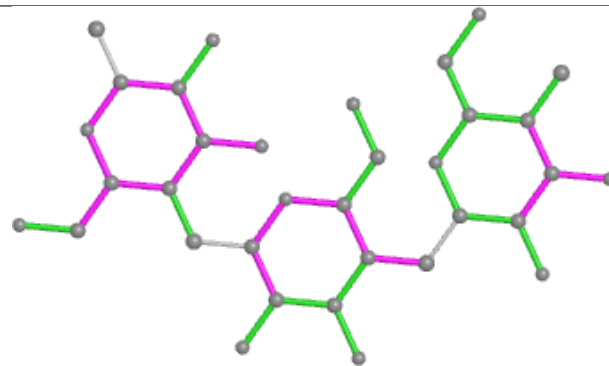
Oligosaccharide Chain F



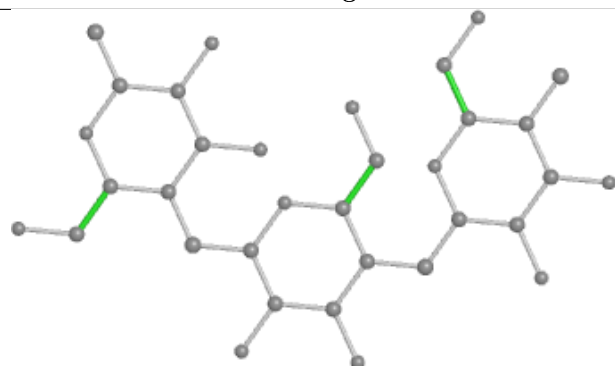
Oligosaccharide Chain G



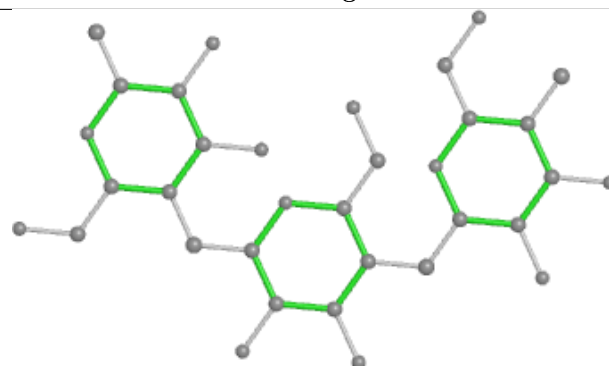
Bond lengths



Bond angles

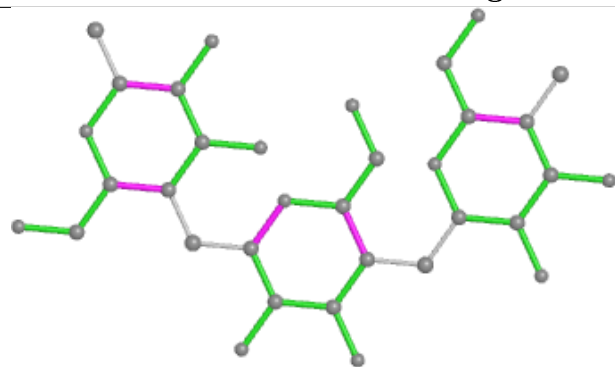


Torsions

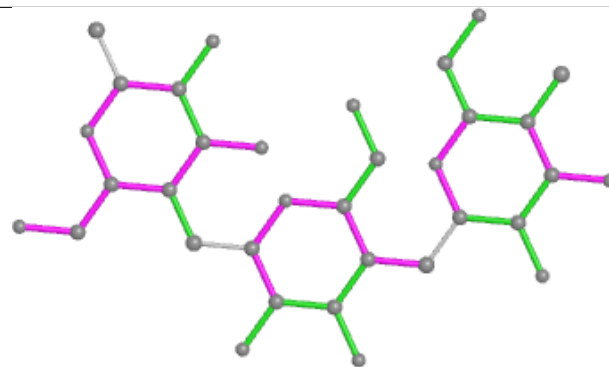


Rings

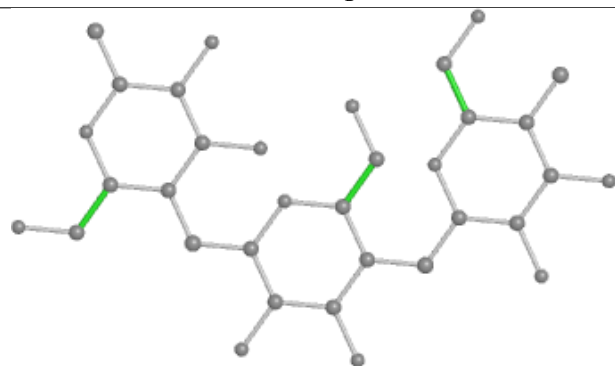
Oligosaccharide Chain H



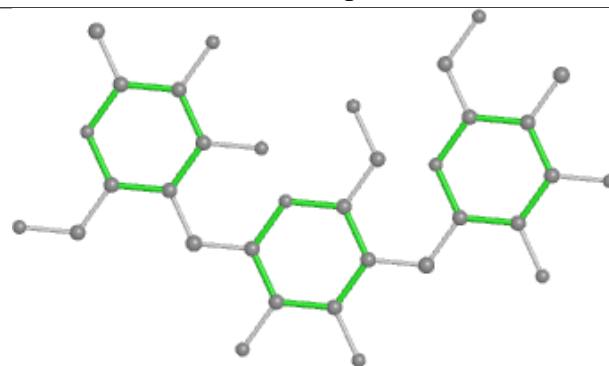
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	400	1	14,14,15	1.26	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	D	399	1	14,14,15	1.34	2 (14%)	17,19,21	2.20	5 (29%)
3	NAG	B	399	1	14,14,15	1.34	2 (14%)	17,19,21	1.75	3 (17%)
3	NAG	A	400	1	14,14,15	1.23	1 (7%)	17,19,21	1.50	3 (17%)
3	NAG	B	400	1	14,14,15	1.20	1 (7%)	17,19,21	1.54	4 (23%)
3	NAG	C	399	1	14,14,15	1.21	1 (7%)	17,19,21	2.10	5 (29%)
3	NAG	A	399	1	14,14,15	1.33	2 (14%)	17,19,21	1.18	1 (5%)
3	NAG	D	400	1	14,14,15	1.15	1 (7%)	17,19,21	1.31	2 (11%)

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	400	1	-	2/6/23/26	0/1/1/1
3	NAG	D	399	1	-	0/6/23/26	0/1/1/1
3	NAG	B	399	1	-	0/6/23/26	0/1/1/1
3	NAG	A	400	1	-	2/6/23/26	0/1/1/1
3	NAG	B	400	1	-	2/6/23/26	0/1/1/1
3	NAG	C	399	1	-	0/6/23/26	0/1/1/1
3	NAG	A	399	1	-	0/6/23/26	0/1/1/1
3	NAG	D	400	1	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	NAG	O7-C7	-3.69	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	399	NAG	O7-C7	-3.68	1.14	1.23
3	A	400	NAG	O7-C7	-3.66	1.15	1.23
3	A	399	NAG	O7-C7	-3.66	1.15	1.23
3	C	399	NAG	O7-C7	-3.51	1.15	1.23
3	B	400	NAG	O7-C7	-3.39	1.15	1.23
3	D	399	NAG	O7-C7	-3.36	1.15	1.23
3	D	400	NAG	O7-C7	-3.25	1.15	1.23
3	D	399	NAG	O5-C1	2.22	1.47	1.43
3	B	399	NAG	O5-C1	2.20	1.47	1.43
3	A	399	NAG	O5-C1	2.11	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	399	NAG	O5-C1-C2	-5.29	102.94	111.29
3	D	399	NAG	C1-O5-C5	-5.01	105.41	112.19
3	B	399	NAG	C1-C2-N2	4.53	118.23	110.49
3	D	399	NAG	O5-C1-C2	-3.89	105.14	111.29
3	C	399	NAG	C1-O5-C5	-3.86	106.96	112.19
3	B	399	NAG	C1-O5-C5	-3.45	107.52	112.19
3	B	400	NAG	O5-C1-C2	-3.40	105.92	111.29
3	D	399	NAG	C2-N2-C7	-3.39	118.07	122.90
3	B	399	NAG	O5-C1-C2	-3.35	105.99	111.29
3	D	399	NAG	C8-C7-N2	-3.34	110.45	116.10
3	C	399	NAG	C8-C7-N2	-3.14	110.79	116.10
3	A	400	NAG	O5-C1-C2	-3.06	106.46	111.29
3	C	400	NAG	C4-C3-C2	-3.01	106.60	111.02
3	C	400	NAG	O5-C1-C2	-2.99	106.57	111.29
3	D	400	NAG	O5-C5-C6	2.92	111.78	107.20
3	C	400	NAG	O6-C6-C5	2.78	120.81	111.29
3	A	400	NAG	O6-C6-C5	2.77	120.78	111.29
3	D	399	NAG	O7-C7-C8	2.58	126.84	122.06
3	B	400	NAG	C4-C3-C2	-2.55	107.29	111.02
3	C	399	NAG	C1-C2-N2	2.49	114.75	110.49
3	A	400	NAG	C4-C3-C2	-2.36	107.56	111.02
3	B	400	NAG	C1-O5-C5	-2.23	109.17	112.19
3	C	399	NAG	O7-C7-C8	2.21	126.16	122.06
3	D	400	NAG	O5-C1-C2	-2.18	107.84	111.29
3	A	399	NAG	C1-O5-C5	-2.09	109.35	112.19
3	B	400	NAG	O4-C4-C5	-2.00	104.32	109.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	400	NAG	O5-C5-C6-O6
3	A	400	NAG	O5-C5-C6-O6
3	C	400	NAG	O5-C5-C6-O6
3	B	400	NAG	O5-C5-C6-O6
3	D	400	NAG	C4-C5-C6-O6
3	B	400	NAG	C4-C5-C6-O6
3	C	400	NAG	C4-C5-C6-O6
3	A	400	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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.