Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 01:42 PM EDT

PDB ID	:	1G1Y
Title	:	CRYSTAL STRUCTURE OF ALPHA-AMYLASE II (TVAII) FROM THERMOACTINOMYCES VULGARIS R-47 AND BETA-CYCLODEXTRIN COMPLEX
Authors	:	Kondo, S.; Ohtaki, A.; Tonozuka, T.; Sakano, Y.; Kamitori, S.
Deposited on	:	2000-10-16
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

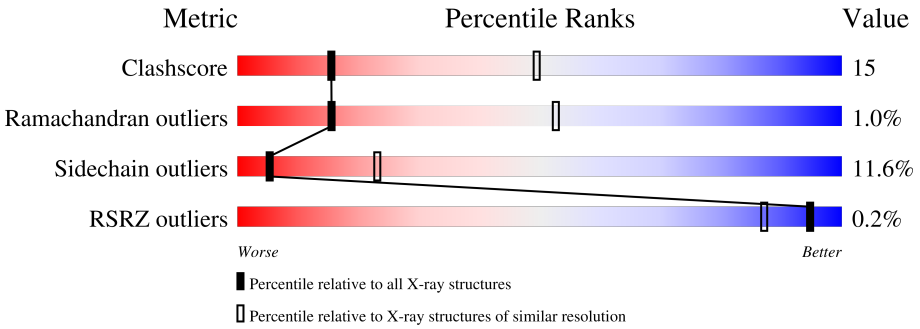
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	59% 31% 9%
1	B	585	56% 35% 8%
2	C	7	57% 43%
2	D	7	71% 29%

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
2	GLC	C	3	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10221 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.

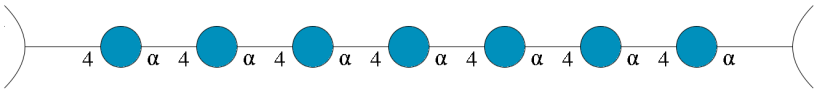
- Molecule 1 is a protein called ALPHA-AMYLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4772	3054	831	872	15			
1	B	585	Total	C	N	O	S	0	0	0
			4772	3054	831	872	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	GLU	engineered mutation	UNP Q08751
B	354	ALA	GLU	engineered mutation	UNP Q08751

- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total	C	O	0	0	0
			77	42	35			
2	D	7	Total	C	O	0	0	0
			77	42	35			

- Molecule 3 is water.

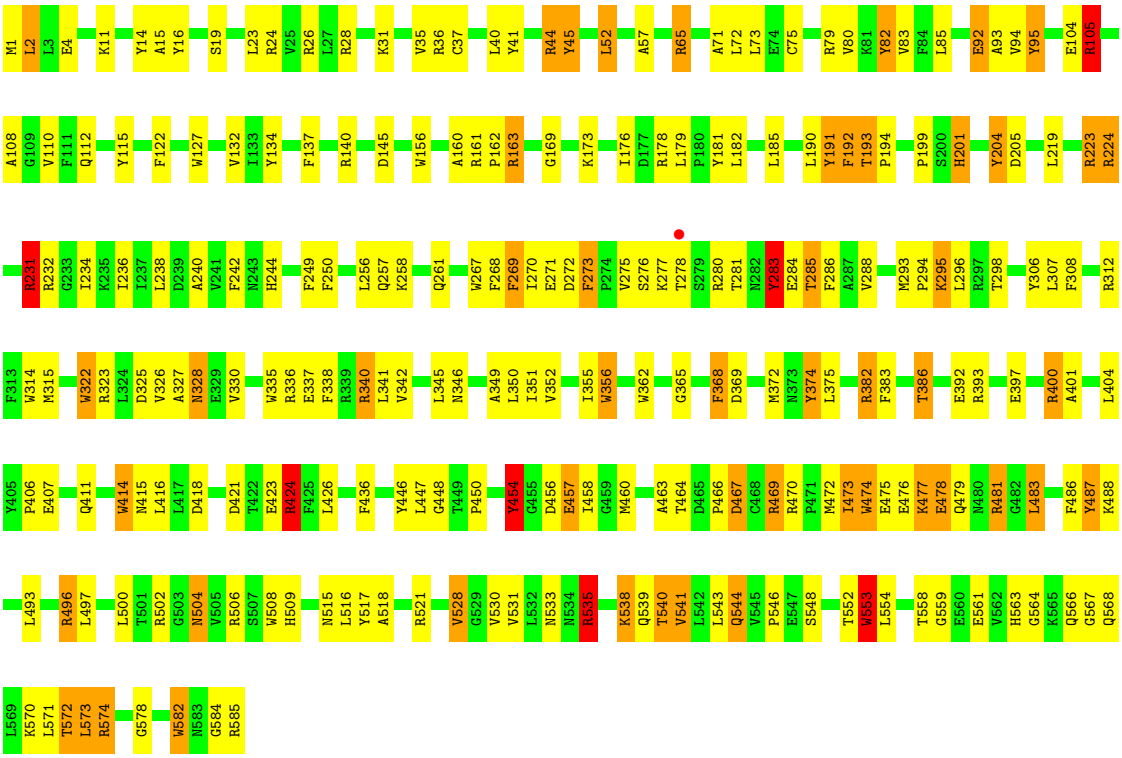
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	264	Total	O	0	0
			264	264		
3	B	259	Total	O	0	0
			259	259		

3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

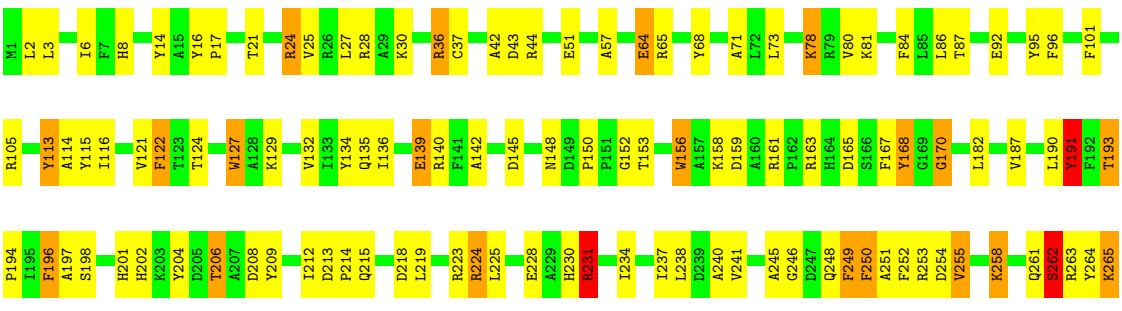
• Molecule 1: ALPHA-AMYLASE II

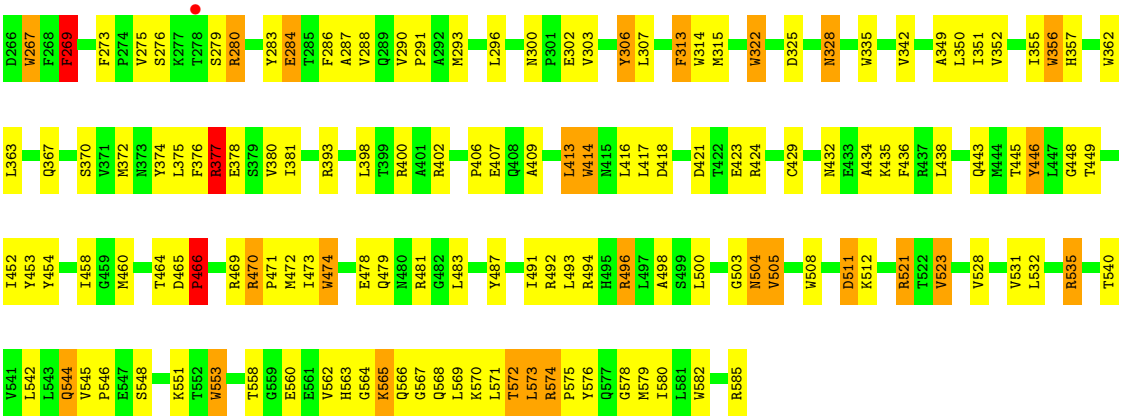
Chain A:



• Molecule 1: ALPHA-AMYLASE II

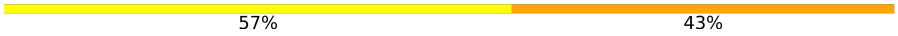
Chain B:





- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain C:



- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.12Å 117.66Å 113.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.00) 92.4 (8.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.191 , 0.260 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 120.0	EDS
L-test for twinning[1]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10221	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.95	1/4902 (0.0%)	1.69	98/6636 (1.5%)
1	B	0.95	0/4902	1.73	107/6636 (1.6%)
All	All	0.95	1/9804 (0.0%)	1.71	205/13272 (1.5%)

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	24
1	B	0	17
All	All	0	41

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	TRP	CD1-NE1	-5.42	1.28	1.38

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	TRP	NE1-CE2-CZ2	-11.28	118.00	130.40
1	B	127	TRP	CD1-CG-CD2	10.60	114.78	106.30
1	A	356	TRP	CD1-CG-CD2	10.39	114.61	106.30
1	B	156	TRP	NE1-CE2-CZ2	-10.36	119.00	130.40
1	A	336	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	A	127	TRP	CD1-CG-CD2	9.60	113.98	106.30
1	A	322	TRP	CD1-CG-CD2	9.60	113.98	106.30
1	A	582	TRP	CD1-CG-CD2	9.54	113.93	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	356	TRP	CD1-CG-CD2	9.29	113.73	106.30
1	B	474	TRP	CD1-CG-CD2	9.25	113.70	106.30
1	B	414	TRP	CD1-CG-CD2	9.15	113.62	106.30
1	A	356	TRP	CE2-CD2-CG	-9.15	99.98	107.30
1	A	335	TRP	CD1-CG-CD2	9.09	113.57	106.30
1	B	481	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	A	474	TRP	CD1-CG-CD2	9.00	113.50	106.30
1	B	508	TRP	CD1-CG-CD2	8.94	113.45	106.30
1	B	322	TRP	CD1-CG-CD2	8.88	113.40	106.30
1	B	335	TRP	CD1-CG-CD2	8.88	113.40	106.30
1	B	356	TRP	CB-CG-CD1	-8.79	115.57	127.00
1	A	362	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	B	582	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	A	336	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	356	TRP	CG-CD2-CE3	8.37	141.43	133.90
1	A	356	TRP	CB-CG-CD1	-8.35	116.15	127.00
1	B	560	GLU	N-CA-C	8.30	133.42	111.00
1	A	156	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	A	496	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	314	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A	335	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	A	508	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	B	356	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	B	156	TRP	CG-CD2-CE3	-7.95	126.74	133.90
1	B	267	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	582	TRP	NE1-CE2-CZ2	-7.91	121.69	130.40
1	B	553	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	B	574	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	585	ARG	N-CA-C	-7.84	89.84	111.00
1	B	362	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	A	553	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	B	262	SER	N-CA-CB	-7.73	98.90	110.50
1	B	377	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	314	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	B	322	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	B	127	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	322	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	B	558	THR	CA-C-N	7.55	131.29	116.20
1	B	267	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	414	TRP	CD1-CG-CD2	7.45	112.26	106.30
1	B	127	TRP	CG-CD1-NE1	-7.45	102.65	110.10
1	A	582	TRP	CG-CD1-NE1	-7.41	102.69	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	414	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	B	36	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	356	TRP	CG-CD1-NE1	-7.31	102.79	110.10
1	A	553	TRP	CD1-CG-CD2	7.31	112.15	106.30
1	B	377	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	B	393	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	A	267	TRP	CD1-CG-CD2	7.23	112.09	106.30
1	A	582	TRP	CG-CD2-CE3	-7.21	127.41	133.90
1	B	335	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A	362	TRP	CE2-CD2-CG	-7.18	101.55	107.30
1	B	191	TYR	CB-CG-CD2	-7.16	116.70	121.00
1	B	156	TRP	CD1-CG-CD2	7.11	111.98	106.30
1	A	414	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	B	314	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	B	280	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	127	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	B	474	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	A	582	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	314	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	A	508	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	A	156	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	B	553	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	B	209	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	178	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	481	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	582	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	A	267	TRP	CE2-CD2-CG	-6.66	101.98	107.30
1	B	224	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	474	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	127	TRP	CG-CD1-NE1	-6.62	103.48	110.10
1	B	356	TRP	CG-CD2-CE3	6.61	139.85	133.90
1	B	156	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	B	508	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	B	566	GLN	N-CA-CB	6.57	122.43	110.60
1	A	322	TRP	CG-CD1-NE1	-6.52	103.58	110.10
1	A	362	TRP	CB-CG-CD1	-6.52	118.52	127.00
1	B	553	TRP	CG-CD2-CE3	6.49	139.74	133.90
1	B	582	TRP	CG-CD1-NE1	-6.48	103.62	110.10
1	A	276	SER	N-CA-C	-6.47	93.54	111.00
1	A	362	TRP	CG-CD1-NE1	-6.46	103.64	110.10
1	B	356	TRP	CG-CD1-NE1	-6.45	103.65	110.10
1	A	44	ARG	NE-CZ-NH1	6.44	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	258	LYS	N-CA-C	6.42	128.34	111.00
1	B	315	MET	CA-CB-CG	-6.42	102.39	113.30
1	B	224	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	315	MET	CG-SD-CE	-6.41	89.95	100.20
1	B	508	TRP	CG-CD1-NE1	-6.39	103.71	110.10
1	A	232	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	574	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	21	THR	CA-CB-CG2	-6.30	103.58	112.40
1	A	553	TRP	CB-CG-CD1	-6.30	118.81	127.00
1	A	65	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	535	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	B	105	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	178	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	335	TRP	NE1-CE2-CZ2	-6.17	123.61	130.40
1	B	481	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	558	THR	N-CA-C	6.15	127.62	111.00
1	A	280	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	414	TRP	NE1-CE2-CZ2	-6.12	123.67	130.40
1	B	362	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	B	414	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	B	511	ASP	N-CA-CB	-6.08	99.65	110.60
1	A	418	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	362	TRP	CE2-CD2-CG	-6.06	102.45	107.30
1	A	474	TRP	CG-CD1-NE1	-6.02	104.08	110.10
1	B	322	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	B	474	TRP	CG-CD1-NE1	-6.00	104.10	110.10
1	B	269	PHE	N-CA-C	-5.97	94.88	111.00
1	A	558	THR	CA-C-N	5.96	128.12	116.20
1	B	335	TRP	CG-CD1-NE1	-5.95	104.16	110.10
1	B	558	THR	N-CA-C	5.93	127.03	111.00
1	B	413	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	335	TRP	CB-CG-CD1	-5.90	119.33	127.00
1	A	543	LEU	CA-CB-CG	5.87	128.79	115.30
1	B	156	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	B	267	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	A	199	PRO	N-CA-C	5.85	127.30	112.10
1	B	306	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	A	559	GLY	O-C-N	-5.80	113.42	122.70
1	A	224	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	335	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	B	64	GLU	CA-CB-CG	5.72	125.99	113.40
1	A	481	ARG	NE-CZ-NH1	5.72	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	585	ARG	CA-CB-CG	5.70	125.95	113.40
1	A	105	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	179	LEU	CA-C-N	5.67	132.98	117.10
1	A	362	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	B	367	GLN	N-CA-C	5.66	126.28	111.00
1	B	267	TRP	CB-CG-CD1	-5.66	119.65	127.00
1	B	424	ARG	CB-CG-CD	-5.64	96.94	111.60
1	A	314	TRP	CG-CD1-NE1	-5.62	104.47	110.10
1	A	469	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	466	PRO	N-CA-C	5.58	126.61	112.10
1	B	512	LYS	N-CA-CB	-5.54	100.63	110.60
1	A	156	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	B	580	ILE	N-CA-C	-5.53	96.07	111.00
1	A	400	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	340	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	173	LYS	CA-CB-CG	5.50	125.51	113.40
1	B	335	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	A	325	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	492	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	553	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	B	542	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	568	GLN	CA-CB-CG	5.42	125.33	113.40
1	B	218	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	26	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	325	ASP	O-C-N	5.40	131.34	122.70
1	A	336	ARG	CB-CG-CD	-5.40	97.56	111.60
1	B	498	ALA	CB-CA-C	-5.40	102.00	110.10
1	B	574	ARG	CA-CB-CG	5.40	125.27	113.40
1	A	508	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	283	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	B	313	PHE	CB-CG-CD1	-5.37	117.04	120.80
1	B	68	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	B	572	THR	CA-C-N	5.34	128.94	117.20
1	B	267	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	A	108	ALA	CB-CA-C	-5.30	102.15	110.10
1	B	496	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	506	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	574	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	1	MET	N-CA-C	-5.25	96.81	111.00
1	B	78	LYS	CG-CD-CE	-5.25	96.16	111.90
1	B	322	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	A	386	THR	CA-CB-CG2	5.23	119.72	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	566	GLN	N-CA-CB	5.22	119.99	110.60
1	A	322	TRP	CB-CG-CD1	-5.21	120.23	127.00
1	B	127	TRP	CB-CG-CD1	-5.21	120.23	127.00
1	A	104	GLU	N-CA-C	-5.18	97.02	111.00
1	B	414	TRP	CB-CG-CD1	-5.17	120.28	127.00
1	B	225	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	191	TYR	N-CA-C	-5.14	97.12	111.00
1	B	267	TRP	NE1-CE2-CZ2	-5.14	124.75	130.40
1	B	362	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	B	574	ARG	N-CA-CB	-5.12	101.38	110.60
1	B	121	VAL	CA-CB-CG1	5.12	118.58	110.90
1	B	36	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	252	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	A	454	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	B	14	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	B	466	PRO	CA-C-N	5.08	128.38	117.20
1	B	521	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	127	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	B	92	GLU	CB-CA-C	-5.06	100.28	110.40
1	A	288	VAL	N-CA-C	5.06	124.65	111.00
1	A	559	GLY	CA-C-N	5.04	128.28	117.20
1	B	291	PRO	N-CA-CB	-5.03	97.06	102.60
1	A	392	GLU	CA-CB-CG	-5.03	102.34	113.40
1	A	231	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	105	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	113	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	368	PHE	CB-CG-CD1	-5.01	117.29	120.80
1	A	424	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	92	GLU	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	LYS	Peptide
1	A	115	TYR	Sidechain
1	A	134	TYR	Sidechain
1	A	14	TYR	Sidechain
1	A	16	TYR	Sidechain
1	A	163	ARG	Sidechain
1	A	181	TYR	Sidechain
1	A	192	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	204	TYR	Sidechain
1	A	250	PHE	Sidechain
1	A	269	PHE	Peptide
1	A	28	ARG	Sidechain
1	A	283	TYR	Sidechain
1	A	374	TYR	Sidechain
1	A	382	ARG	Sidechain
1	A	400	ARG	Sidechain
1	A	45	TYR	Sidechain
1	A	454	TYR	Sidechain
1	A	487	TYR	Sidechain
1	A	502	ARG	Sidechain
1	A	548	SER	Peptide
1	A	65	ARG	Sidechain
1	A	82	TYR	Sidechain
1	A	95	TYR	Sidechain
1	B	113	TYR	Sidechain
1	B	165	ASP	Peptide
1	B	168	TYR	Sidechain
1	B	196	PHE	Sidechain
1	B	231	ARG	Sidechain
1	B	264	TYR	Sidechain
1	B	28	ARG	Sidechain
1	B	377	ARG	Sidechain
1	B	400	ARG	Sidechain
1	B	402	ARG	Sidechain
1	B	446	TYR	Sidechain
1	B	453	TYR	Sidechain
1	B	454	TYR	Sidechain
1	B	487	TYR	Sidechain
1	B	535	ARG	Sidechain
1	B	576	TYR	Sidechain
1	B	95	TYR	Sidechain

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	4772	0	4606	135	0
1	B	4772	0	4606	149	0
2	C	77	0	63	11	0
2	D	77	0	63	5	0
3	A	264	0	0	2	0
3	B	259	0	0	4	0
All	All	10221	0	9338	282	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 15.

All (282) 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:B:296:LEU:HD13	1:B:307:LEU:HD11	1.52	0.89
1:A:533:ASN:HB2	1:A:573:LEU:HD13	1.56	0.86
1:B:328:ASN:HB3	1:B:355:ILE:HG13	1.58	0.84
1:B:255:VAL:HG12	1:B:262:SER:HB2	1.59	0.83
2:D:3:GLC:O3	2:D:4:GLC:O2	1.96	0.83
1:B:548:SER:HB2	1:B:585:ARG:HH22	1.45	0.82
1:B:258:LYS:HB3	1:B:261:GLN:HB2	1.64	0.79
1:A:23:LEU:HD22	1:A:80:VAL:HG11	1.65	0.79
1:A:328:ASN:HB3	1:A:355:ILE:HG12	1.65	0.78
1:B:182:LEU:HD13	1:B:190:LEU:HD11	1.65	0.78
1:B:571:LEU:HD22	1:B:579:MET:SD	2.26	0.77
1:B:370:SER:HB2	1:B:413:LEU:HA	1.66	0.76
1:A:326:VAL:HG22	2:C:3:GLC:H61	1.67	0.76
1:B:500:LEU:HD23	1:B:521:ARG:HG3	1.68	0.75
1:A:312:ARG:HG2	1:A:345:LEU:HD11	1.70	0.72
1:A:269:PHE:HB2	1:A:284:GLU:HB2	1.70	0.72
1:A:132:VAL:HG13	1:A:450:PRO:HB2	1.72	0.71
1:B:42:ALA:HB3	1:B:81:LYS:HE2	1.72	0.71
1:A:475:GLU:HB2	1:A:478:GLU:HG3	1.70	0.71
1:B:300:ASN:HB3	1:B:303:VAL:HG23	1.71	0.71
1:A:286:PHE:CE1	2:C:4:GLC:H62	2.26	0.70
1:A:516:LEU:HD22	1:A:541:VAL:HG11	1.72	0.69
1:A:122:PHE:CD2	1:A:365:GLY:HA2	2.28	0.69
1:B:429:CYS:SG	1:B:435:LYS:HB2	2.33	0.69
1:A:85:LEU:HD13	1:A:95:TYR:CE1	2.28	0.68
1:A:355:ILE:HD11	1:A:368:PHE:HE1	1.57	0.67
1:B:142:ALA:O	1:B:170:GLY:HA2	1.93	0.67
1:B:139:GLU:O	1:B:170:GLY:HA3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PHE:HE2	1:A:296:LEU:HD23	1.60	0.67
1:A:52:LEU:HD11	1:A:105:ARG:NH2	2.10	0.67
1:A:272:ASP:HB2	1:A:283:TYR:HB3	1.77	0.66
1:A:283:TYR:CE1	1:A:294:PRO:HB3	2.31	0.66
1:B:148:ASN:HB2	1:B:215:GLN:O	1.96	0.66
1:A:454:TYR:OH	1:A:469:ARG:HA	1.95	0.65
1:B:267:TRP:HE1	1:B:302:GLU:HG3	1.61	0.64
1:B:249:PHE:CE1	1:B:306:TYR:HE1	2.15	0.64
1:A:533:ASN:OD1	1:A:535:ARG:HB2	1.99	0.62
1:B:544:GLN:HE22	1:B:568:GLN:HE22	1.46	0.62
1:A:257:GLN:HG3	1:A:258:LYS:HG3	1.81	0.61
1:B:132:VAL:HG21	1:B:491:ILE:HG23	1.83	0.61
1:B:414:TRP:HD1	1:B:449:THR:HB	1.66	0.61
1:B:269:PHE:HB2	1:B:284:GLU:HB2	1.83	0.61
1:A:538:LYS:HB2	1:A:574:ARG:HA	1.83	0.61
1:A:552:THR:O	1:A:553:TRP:HD1	1.82	0.61
1:B:156:TRP:CZ3	1:B:168:TYR:HB3	2.36	0.61
1:B:17:PRO:HB3	1:B:116:ILE:HG23	1.82	0.60
1:B:27:LEU:HD13	1:B:37:CYS:SG	2.42	0.60
1:A:44:ARG:HD2	1:A:112:GLN:OE1	2.03	0.59
1:A:356:TRP:HE1	2:C:3:GLC:C2	2.15	0.59
1:A:162:PRO:HD3	1:A:470:ARG:HG2	1.83	0.59
1:B:286:PHE:HZ	2:D:3:GLC:H62	1.67	0.59
1:A:337:GLU:HG2	1:A:340:ARG:NH2	2.17	0.59
1:B:27:LEU:HD12	1:B:84:PHE:CD2	2.38	0.59
1:B:504:ASN:HD22	1:B:504:ASN:H	1.50	0.59
1:A:190:LEU:HD13	1:A:234:ILE:CG2	2.33	0.58
1:B:156:TRP:HZ3	1:B:168:TYR:HB3	1.67	0.58
1:A:244:HIS:HD2	1:A:293:MET:HB3	1.70	0.57
1:A:57:ALA:HA	1:A:71:ALA:HB2	1.86	0.57
1:A:190:LEU:HD13	1:A:234:ILE:HG23	1.87	0.57
1:B:267:TRP:NE1	1:B:302:GLU:HG3	2.18	0.57
1:A:249:PHE:CZ	1:A:306:TYR:HE1	2.22	0.57
1:B:503:GLY:HA2	1:B:523:VAL:HG13	1.86	0.57
1:A:242:PHE:HE2	1:A:338:PHE:CE1	2.23	0.57
1:B:191:TYR:HA	1:B:237:ILE:O	2.05	0.56
1:B:241:VAL:HG12	1:B:325:ASP:HB3	1.87	0.56
1:B:372:MET:SD	1:B:414:TRP:HE3	2.29	0.56
1:A:372:MET:SD	1:A:414:TRP:HE3	2.29	0.56
1:A:479:GLN:OE1	1:A:481:ARG:NH2	2.38	0.56
1:B:148:ASN:HA	3:B:1385:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:HD12	1:B:190:LEU:HG	1.88	0.56
1:A:122:PHE:CG	1:A:365:GLY:HA2	2.40	0.55
1:B:44:ARG:HA	1:B:81:LYS:HD3	1.87	0.55
1:A:268:PHE:O	1:A:270:ILE:HG12	2.06	0.55
1:B:245:ALA:O	1:B:293:MET:HA	2.07	0.55
1:B:460:MET:SD	1:B:473:ILE:HG13	2.46	0.55
1:B:356:TRP:HE1	2:D:3:GLC:H2	1.72	0.55
1:A:286:PHE:CZ	2:C:4:GLC:H62	2.42	0.55
1:A:24:ARG:HD2	1:A:407:GLU:OE2	2.07	0.54
1:A:295:LYS:HB2	1:A:295:LYS:NZ	2.22	0.54
1:A:176:ILE:HD13	1:A:224:ARG:HD3	1.90	0.54
1:A:411:GLN:HG2	1:A:447:LEU:HD11	1.88	0.54
1:B:263:ARG:HD3	3:B:1411:HOH:O	2.06	0.54
1:A:483:LEU:O	1:A:486:PHE:HB3	2.07	0.54
1:B:228:GLU:HG3	1:B:231:ARG:HH21	1.73	0.54
1:B:544:GLN:NE2	1:B:568:GLN:HE22	2.05	0.54
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.43	0.53
1:B:255:VAL:HG12	1:B:262:SER:CB	2.36	0.53
1:A:240:ALA:HB2	1:A:322:TRP:HE3	1.72	0.53
1:A:249:PHE:HZ	1:A:306:TYR:HE1	1.54	0.53
1:B:44:ARG:CD	1:B:114:ALA:HA	2.39	0.53
1:B:122:PHE:HE2	1:B:363:LEU:O	1.92	0.53
1:A:415:ASN:HD21	1:A:448:GLY:HA3	1.74	0.52
1:B:250:PHE:CG	1:B:251:ALA:N	2.76	0.52
1:B:429:CYS:SG	1:B:435:LYS:CB	2.96	0.52
1:B:474:TRP:HA	1:B:479:GLN:HE21	1.73	0.52
1:A:286:PHE:HA	3:A:1521:HOH:O	2.09	0.52
1:B:521:ARG:HB2	1:B:528:VAL:HG13	1.91	0.52
1:B:458:ILE:HD12	1:B:460:MET:HG3	1.91	0.52
1:B:246:GLY:O	1:B:249:PHE:HB3	2.11	0.51
1:B:531:VAL:HG21	1:B:571:LEU:HD13	1.93	0.51
1:A:193:THR:HB	1:A:194:PRO:HD2	1.93	0.51
1:A:295:LYS:HB2	1:A:295:LYS:HZ2	1.74	0.51
1:B:24:ARG:HD2	1:B:407:GLU:OE2	2.11	0.51
1:B:140:ARG:HG3	1:B:469:ARG:O	2.10	0.51
1:B:342:VAL:HG12	1:B:349:ALA:HB3	1.92	0.51
1:B:356:TRP:CE3	1:B:374:TYR:HB3	2.46	0.51
1:B:500:LEU:CD2	1:B:521:ARG:HG3	2.41	0.51
1:B:417:LEU:HG	1:B:443:GLN:NE2	2.26	0.50
1:A:327:ALA:HB1	1:A:368:PHE:HZ	1.75	0.50
1:B:134:TYR:HD1	1:B:187:VAL:HG11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:VAL:HG13	1:B:567:GLY:O	2.11	0.50
1:A:182:LEU:HD13	1:A:190:LEU:HD11	1.94	0.50
1:A:185:LEU:HD22	1:A:457:GLU:HG2	1.92	0.50
1:B:140:ARG:NH1	1:B:168:TYR:HD2	2.10	0.50
1:B:167:PHE:CZ	1:B:201:HIS:HB2	2.46	0.50
1:A:249:PHE:HZ	1:A:306:TYR:CE1	2.30	0.50
1:A:493:LEU:HD12	1:A:496:ARG:HH11	1.77	0.50
1:A:140:ARG:HG2	1:A:469:ARG:O	2.13	0.49
1:A:382:ARG:HA	1:A:386:THR:OG1	2.12	0.49
1:A:516:LEU:HD11	1:A:539:GLN:NE2	2.27	0.49
1:A:2:LEU:HD23	1:B:2:LEU:HD11	1.95	0.49
1:B:445:THR:HB	1:B:500:LEU:HD22	1.94	0.49
1:B:446:TYR:HE1	1:B:505:VAL:HG21	1.77	0.49
1:A:350:LEU:HG	1:A:352:VAL:HG23	1.95	0.49
1:A:509:HIS:O	1:A:517:TYR:HA	2.12	0.49
1:B:249:PHE:CZ	1:B:306:TYR:HE1	2.31	0.49
1:A:242:PHE:HB3	1:A:307:LEU:HD13	1.93	0.49
1:A:421:ASP:O	1:A:464:THR:HG23	2.11	0.49
1:B:377:ARG:HG3	1:B:378:GLU:N	2.28	0.49
1:A:185:LEU:HD11	1:A:487:TYR:HB3	1.95	0.49
1:A:281:THR:HG22	1:A:285:THR:HG21	1.95	0.49
1:B:156:TRP:CZ2	1:B:471:PRO:HB3	2.48	0.49
1:B:521:ARG:HB2	1:B:528:VAL:CG1	2.42	0.49
1:B:153:THR:HA	1:B:167:PHE:O	2.14	0.48
1:B:432:ASN:OD1	1:B:434:ALA:HB3	2.13	0.48
1:B:8:HIS:CE1	1:B:25:VAL:HG13	2.48	0.48
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.95	0.48
1:A:24:ARG:HH11	1:A:72:LEU:HD13	1.77	0.48
1:A:326:VAL:CG2	2:C:3:GLC:H61	2.41	0.48
1:A:356:TRP:NE1	2:C:3:GLC:C2	2.77	0.48
1:B:300:ASN:OD1	1:B:302:GLU:HG2	2.13	0.48
1:B:127:TRP:HH2	1:B:237:ILE:HD11	1.78	0.48
1:A:356:TRP:HE1	2:C:3:GLC:C1	2.26	0.48
1:A:112:GLN:HE21	1:B:357:HIS:HB3	1.78	0.48
1:A:518:ALA:HA	1:A:530:VAL:O	2.13	0.48
1:B:565:LYS:NZ	1:B:565:LYS:HB3	2.29	0.48
1:A:268:PHE:CE2	1:A:296:LEU:HD23	2.45	0.48
1:B:196:PHE:HB2	1:B:206:THR:HG22	1.96	0.47
1:A:415:ASN:ND2	1:A:448:GLY:HA3	2.30	0.47
1:A:544:GLN:HA	1:A:567:GLY:O	2.14	0.47
1:B:250:PHE:CE2	1:B:251:ALA:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ILE:HG21	1:B:478:GLU:O	2.14	0.47
1:A:283:TYR:HE1	1:A:294:PRO:HB3	1.78	0.47
1:B:78:LYS:O	1:B:115:TYR:HA	2.14	0.47
1:A:458:ILE:HD13	1:A:473:ILE:HG12	1.95	0.47
1:A:95:TYR:CE2	1:A:105:ARG:HB2	2.50	0.47
1:B:202:HIS:O	1:B:202:HIS:ND1	2.48	0.47
1:B:458:ILE:HD13	1:B:473:ILE:HB	1.97	0.47
1:B:546:PRO:HG3	1:B:553:TRP:CH2	2.50	0.47
1:A:474:TRP:HA	1:A:479:GLN:HE21	1.79	0.47
1:A:137:PHE:HD1	1:A:140:ARG:HB2	1.79	0.47
1:A:342:VAL:HG11	1:A:351:ILE:HD11	1.97	0.47
1:A:137:PHE:HB3	1:A:454:TYR:CE2	2.50	0.47
1:A:436:PHE:HZ	1:A:456:ASP:HB3	1.79	0.47
1:A:201:HIS:CE1	1:A:469:ARG:HH11	2.33	0.46
1:B:161:ARG:HA	1:B:161:ARG:HD3	1.76	0.46
1:B:540:THR:OG1	1:B:572:THR:HG23	2.15	0.46
1:A:185:LEU:HA	1:A:488:LYS:HG2	1.96	0.46
1:A:401:ALA:O	1:A:404:LEU:HB2	2.15	0.46
1:A:328:ASN:HD22	1:A:328:ASN:H	1.63	0.46
1:A:328:ASN:HD22	1:A:328:ASN:N	2.13	0.46
1:A:355:ILE:HD11	1:A:368:PHE:CE1	2.44	0.46
1:B:544:GLN:HE22	1:B:568:GLN:NE2	2.12	0.46
1:A:563:HIS:HD2	1:A:570:LYS:O	1.99	0.46
1:B:423:GLU:CD	1:B:423:GLU:H	2.19	0.46
1:B:448:GLY:O	1:B:494:ARG:NH2	2.49	0.46
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.97	0.46
1:B:465:ASP:HA	1:B:466:PRO:HA	1.70	0.46
1:B:546:PRO:HG3	1:B:553:TRP:HH2	1.81	0.46
1:A:137:PHE:HA	1:A:193:THR:OG1	2.15	0.46
1:B:224:ARG:HA	1:B:224:ARG:NE	2.31	0.46
1:B:452:ILE:HD11	1:B:491:ILE:HD11	1.96	0.46
1:A:275:VAL:HG22	3:A:1330:HOH:O	2.14	0.46
1:B:376:PHE:O	1:B:380:VAL:HG22	2.16	0.46
1:B:531:VAL:O	1:B:578:GLY:HA2	2.15	0.45
1:A:41:TYR:CB	1:A:82:TYR:HB3	2.46	0.45
1:A:516:LEU:HD11	1:A:539:GLN:HE21	1.80	0.45
1:A:582:TRP:CZ2	1:A:584:GLY:HA2	2.51	0.45
1:B:124:THR:OG1	1:B:129:LYS:HE3	2.17	0.45
1:B:134:TYR:HB2	1:B:187:VAL:HG21	1.99	0.45
1:B:493:LEU:HD23	1:B:493:LEU:HA	1.79	0.45
1:B:378:GLU:HG3	3:B:1471:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLN:NE2	1:B:357:HIS:HB3	2.31	0.45
1:B:3:LEU:HD13	1:B:101:PHE:CG	2.51	0.45
1:B:6:ILE:HD13	1:B:86:LEU:HD13	1.99	0.45
1:B:73:LEU:HD23	1:B:80:VAL:HG21	1.99	0.45
1:B:193:THR:HB	1:B:194:PRO:HD2	1.99	0.45
1:A:269:PHE:CD2	1:A:295:LYS:HG3	2.51	0.45
1:B:287:ALA:H	1:B:290:VAL:HG22	1.82	0.45
1:B:446:TYR:CE1	1:B:505:VAL:HG21	2.52	0.45
1:B:212:ILE:HG22	1:B:213:ASP:N	2.32	0.45
1:B:548:SER:HB2	1:B:585:ARG:NH2	2.23	0.45
1:A:244:HIS:CD2	1:A:293:MET:HB3	2.51	0.45
1:A:308:PHE:HB3	1:A:341:LEU:HD22	1.99	0.45
1:A:356:TRP:CZ2	2:C:3:GLC:O2	2.59	0.45
1:A:393:ARG:O	1:A:397:GLU:HG3	2.16	0.45
1:A:231:ARG:HH11	1:A:231:ARG:HD3	1.66	0.44
1:A:401:ALA:HA	1:A:404:LEU:HD13	1.99	0.44
1:B:197:ALA:HB3	1:B:208:ASP:HB3	1.99	0.44
1:A:500:LEU:HD21	1:A:528:VAL:HG21	2.00	0.44
1:B:470:ARG:HE	1:B:471:PRO:HG2	1.82	0.44
2:C:6:GLC:HO6	2:C:7:GLC:C1	2.31	0.44
1:A:327:ALA:HB1	1:A:368:PHE:CZ	2.52	0.44
1:A:75:CYS:SG	1:A:80:VAL:HB	2.57	0.44
1:A:223:ARG:HB3	1:A:223:ARG:NH1	2.32	0.44
1:A:504:ASN:O	1:A:521:ARG:HA	2.17	0.44
1:A:446:TYR:CG	1:A:447:LEU:N	2.86	0.44
1:B:122:PHE:HB2	3:B:1120:HOH:O	2.17	0.44
1:B:429:CYS:SG	1:B:436:PHE:N	2.91	0.44
1:A:41:TYR:HB3	1:A:82:TYR:HB3	2.00	0.44
1:A:160:ALA:O	1:A:470:ARG:HD2	2.17	0.44
1:A:540:THR:HA	1:A:572:THR:HA	2.00	0.44
1:A:477:LYS:N	1:A:477:LYS:HD2	2.33	0.43
1:A:204:TYR:CZ	2:C:4:GLC:H2	2.54	0.43
1:A:356:TRP:HE1	2:C:3:GLC:H2	1.82	0.43
1:A:242:PHE:HE2	1:A:338:PHE:HE1	1.64	0.43
1:A:424:ARG:HD3	1:A:460:MET:O	2.19	0.43
1:B:540:THR:HA	1:B:572:THR:HA	1.99	0.43
1:B:531:VAL:HG21	1:B:571:LEU:CD1	2.49	0.43
1:B:574:ARG:HG2	1:B:575:PRO:HD2	2.00	0.43
1:B:553:TRP:CD1	1:B:553:TRP:N	2.85	0.43
1:A:15:ALA:HA	1:A:24:ARG:O	2.18	0.43
1:B:240:ALA:HB2	1:B:322:TRP:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG12	1:A:95:TYR:N	2.33	0.43
1:A:57:ALA:CA	1:A:71:ALA:HB2	2.49	0.43
1:A:531:VAL:O	1:A:578:GLY:HA2	2.18	0.43
1:B:16:TYR:CE2	1:B:406:PRO:HA	2.53	0.42
1:B:276:SER:O	1:B:283:TYR:HE1	2.02	0.42
1:B:202:HIS:O	1:B:202:HIS:CG	2.73	0.42
1:B:363:LEU:HD22	1:B:409:ALA:HB1	2.01	0.42
1:B:350:LEU:HG	1:B:352:VAL:HG23	2.01	0.42
1:A:45:TYR:HD1	1:A:79:ARG:NH2	2.17	0.42
1:A:95:TYR:CD2	1:A:105:ARG:HA	2.55	0.42
1:B:44:ARG:HD2	1:B:114:ALA:HA	2.02	0.42
1:A:192:PHE:HE2	1:A:236:ILE:HG13	1.85	0.42
1:A:463:ALA:H	1:A:467:ASP:HB3	1.84	0.42
1:B:36:ARG:HB3	1:B:87:THR:HB	2.02	0.42
1:B:438:LEU:HD12	1:B:438:LEU:HA	1.84	0.42
1:A:497:LEU:HD13	1:A:528:VAL:HG11	2.01	0.41
1:B:249:PHE:HE1	1:B:306:TYR:HE1	1.65	0.41
1:A:546:PRO:HG2	1:A:553:TRP:CZ2	2.55	0.41
1:B:27:LEU:HD12	1:B:84:PHE:CE2	2.55	0.41
1:B:219:LEU:HD21	1:B:313:PHE:HZ	1.85	0.41
1:B:84:PHE:HB2	1:B:96:PHE:HB3	2.01	0.41
1:B:573:LEU:HD23	1:B:573:LEU:H	1.84	0.41
1:B:148:ASN:O	1:B:215:GLN:HA	2.20	0.41
1:B:573:LEU:HD23	1:B:573:LEU:N	2.35	0.41
1:B:27:LEU:HD11	1:B:86:LEU:HD21	2.02	0.41
1:B:213:ASP:OD1	1:B:215:GLN:HG2	2.19	0.41
1:B:254:ASP:O	1:B:258:LYS:HB2	2.20	0.41
1:B:262:SER:O	1:B:265:LYS:HG3	2.21	0.41
1:A:85:LEU:HD11	1:A:93:ALA:HB1	2.03	0.41
1:A:273:PHE:HD1	1:A:273:PHE:HA	1.62	0.41
1:B:249:PHE:O	1:B:253:ARG:HG3	2.20	0.41
1:B:250:PHE:CD2	1:B:251:ALA:N	2.89	0.41
1:B:351:ILE:HD13	1:B:351:ILE:HG21	1.87	0.41
1:A:219:LEU:HD13	1:A:219:LEU:HA	1.87	0.41
1:B:563:HIS:ND1	1:B:570:LYS:O	2.54	0.41
1:A:23:LEU:HD23	1:A:73:LEU:HD12	2.02	0.40
1:B:17:PRO:HB3	1:B:116:ILE:CG2	2.51	0.40
1:A:346:ASN:HB3	1:A:349:ALA:HB2	2.02	0.40
1:B:204:TYR:CD2	2:D:4:GLC:H4	2.56	0.40
1:B:267:TRP:HE1	1:B:302:GLU:CG	2.33	0.40
1:A:40:LEU:HD12	1:A:83:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD12	1:A:369:ASP:OD2	2.22	0.40
1:A:383:PHE:HE1	1:A:515:ASN:OD1	2.03	0.40
1:B:64:GLU:HG3	1:B:65:ARG:HG3	2.03	0.40
1:B:356:TRP:CD1	2:D:3:GLC:C1	3.04	0.40
1:B:574:ARG:HG2	1:B:574:ARG:HH11	1.86	0.40
1:A:4:GLU:HG2	1:B:65:ARG:HB3	2.03	0.40
1:A:285:THR:OG1	1:A:286:PHE:N	2.54	0.40
1:B:574:ARG:CG	1:B:575:PRO:HD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	533 (91%)	47 (8%)	3 (0%)	29	68
1	B	583/585 (100%)	533 (91%)	41 (7%)	9 (2%)	10	42
All	All	1166/1170 (100%)	1066 (91%)	88 (8%)	12 (1%)	15	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	PRO
1	B	170	GLY
1	B	193	THR
1	B	262	SER
1	B	562	VAL
1	A	169	GLY
1	A	298	THR
1	B	275	VAL
1	B	288	VAL
1	B	564	GLY

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Mol	Chain	Res	Type
1	B	152	GLY
1	A	564	GLY

5.3.2 Protein sidechains (i)

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	492/492 (100%)	432 (88%)	60 (12%)	5 21
1	B	492/492 (100%)	438 (89%)	54 (11%)	6 25
All	All	984/984 (100%)	870 (88%)	114 (12%)	5 23

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	19	SER
1	A	31	LYS
1	A	35	VAL
1	A	36	ARG
1	A	37	CYS
1	A	52	LEU
1	A	92	GLU
1	A	105	ARG
1	A	110	VAL
1	A	145	ASP
1	A	161	ARG
1	A	163	ARG
1	A	191	TYR
1	A	193	THR
1	A	201	HIS
1	A	205	ASP
1	A	223	ARG
1	A	231	ARG
1	A	238	LEU
1	A	256	LEU

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Mol	Chain	Res	Type
1	A	261	GLN
1	A	271	GLU
1	A	273	PHE
1	A	277	LYS
1	A	278	THR
1	A	285	THR
1	A	295	LYS
1	A	323	ARG
1	A	328	ASN
1	A	330	VAL
1	A	374	TYR
1	A	375	LEU
1	A	406	PRO
1	A	416	LEU
1	A	423	GLU
1	A	424	ARG
1	A	426	LEU
1	A	457	GLU
1	A	466	PRO
1	A	467	ASP
1	A	472	MET
1	A	473	ILE
1	A	476	GLU
1	A	477	LYS
1	A	478	GLU
1	A	483	LEU
1	A	504	ASN
1	A	528	VAL
1	A	535	ARG
1	A	538	LYS
1	A	540	THR
1	A	541	VAL
1	A	544	GLN
1	A	553	TRP
1	A	554	LEU
1	A	561	GLU
1	A	571	LEU
1	A	572	THR
1	A	573	LEU
1	B	24	ARG
1	B	30	LYS
1	B	43	ASP

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Mol	Chain	Res	Type
1	B	51	GLU
1	B	122	PHE
1	B	135	GLN
1	B	139	GLU
1	B	145	ASP
1	B	158	LYS
1	B	159	ASP
1	B	163	ARG
1	B	191	TYR
1	B	198	SER
1	B	206	THR
1	B	214	PRO
1	B	223	ARG
1	B	230	HIS
1	B	231	ARG
1	B	238	LEU
1	B	248	GLN
1	B	249	PHE
1	B	250	PHE
1	B	255	VAL
1	B	265	LYS
1	B	269	PHE
1	B	273	PHE
1	B	279	SER
1	B	280	ARG
1	B	284	GLU
1	B	328	ASN
1	B	375	LEU
1	B	377	ARG
1	B	381	ILE
1	B	398	LEU
1	B	416	LEU
1	B	418	ASP
1	B	421	ASP
1	B	464	THR
1	B	466	PRO
1	B	470	ARG
1	B	472	MET
1	B	483	LEU
1	B	496	ARG
1	B	504	ASN
1	B	505	VAL

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Mol	Chain	Res	Type
1	B	511	ASP
1	B	523	VAL
1	B	532	LEU
1	B	535	ARG
1	B	544	GLN
1	B	551	LYS
1	B	565	LYS
1	B	569	LEU
1	B	573	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	201	HIS
1	A	215	GLN
1	A	244	HIS
1	A	248	GLN
1	A	328	ASN
1	A	443	GLN
1	A	563	HIS
1	B	215	GLN
1	B	243	ASN
1	B	248	GLN
1	B	257	GLN
1	B	328	ASN
1	B	367	GLN
1	B	411	GLN
1	B	504	ASN
1	B	544	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

14 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	GLC	C	1	2	11,11,12	0.82	0	15,15,17	0.90	1 (6%)
2	GLC	C	2	2	11,11,12	0.91	1 (9%)	15,15,17	2.00	2 (13%)
2	GLC	C	3	2	11,11,12	0.78	0	15,15,17	2.04	2 (13%)
2	GLC	C	4	2	11,11,12	0.61	0	15,15,17	0.66	0
2	GLC	C	5	2	11,11,12	0.68	0	15,15,17	0.87	1 (6%)
2	GLC	C	6	2	11,11,12	0.90	0	15,15,17	0.84	1 (6%)
2	GLC	C	7	2	11,11,12	0.85	0	15,15,17	1.22	3 (20%)
2	GLC	D	1	2	11,11,12	0.76	0	15,15,17	1.25	2 (13%)
2	GLC	D	2	2	11,11,12	0.70	0	15,15,17	1.08	1 (6%)
2	GLC	D	3	2	11,11,12	0.79	0	15,15,17	1.49	1 (6%)
2	GLC	D	4	2	11,11,12	0.54	0	15,15,17	1.61	2 (13%)
2	GLC	D	5	2	11,11,12	0.60	0	15,15,17	2.19	3 (20%)
2	GLC	D	6	2	11,11,12	0.79	0	15,15,17	0.96	1 (6%)
2	GLC	D	7	2	11,11,12	0.72	0	15,15,17	1.66	3 (20%)

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	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	2/2/19/22	0/1/1/1
2	GLC	C	7	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	5	2	-	2/2/19/22	0/1/1/1
2	GLC	D	6	2	-	1/2/19/22	0/1/1/1
2	GLC	D	7	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	O4-C4	2.12	1.48	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5	GLC	O4-C4-C3	-7.35	93.35	110.35
2	C	3	GLC	O4-C4-C5	-6.79	92.44	109.30
2	C	2	GLC	O4-C4-C3	-5.95	96.58	110.35
2	D	7	GLC	O4-C4-C3	-4.84	99.16	110.35
2	D	4	GLC	O4-C4-C3	-4.60	99.71	110.35
2	D	3	GLC	O4-C4-C3	-4.21	100.61	110.35
2	C	2	GLC	O4-C4-C5	4.00	119.24	109.30
2	D	4	GLC	O4-C4-C5	-3.39	100.88	109.30
2	D	5	GLC	O4-C4-C5	-3.30	101.10	109.30
2	D	1	GLC	O4-C4-C5	3.05	116.87	109.30
2	D	2	GLC	O4-C4-C3	-2.70	104.11	110.35
2	C	7	GLC	O4-C4-C5	-2.65	102.71	109.30
2	D	7	GLC	C1-O5-C5	2.64	115.77	112.19
2	C	7	GLC	C1-O5-C5	2.63	115.76	112.19
2	C	5	GLC	C1-O5-C5	2.58	115.68	112.19
2	C	6	GLC	C1-O5-C5	2.54	115.64	112.19
2	D	7	GLC	O4-C4-C5	-2.54	102.98	109.30
2	D	6	GLC	C1-O5-C5	2.52	115.61	112.19
2	D	5	GLC	C1-O5-C5	2.50	115.58	112.19
2	C	1	GLC	C1-O5-C5	2.31	115.32	112.19
2	D	1	GLC	C1-O5-C5	2.26	115.26	112.19
2	C	7	GLC	O4-C4-C3	-2.16	105.34	110.35
2	C	3	GLC	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	GLC	C4-C5-C6-O6
2	C	6	GLC	O5-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	D	7	GLC	C4-C5-C6-O6
2	D	7	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	7	GLC	C4-C5-C6-O6
2	D	5	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	D	6	GLC	C4-C5-C6-O6
2	D	5	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6

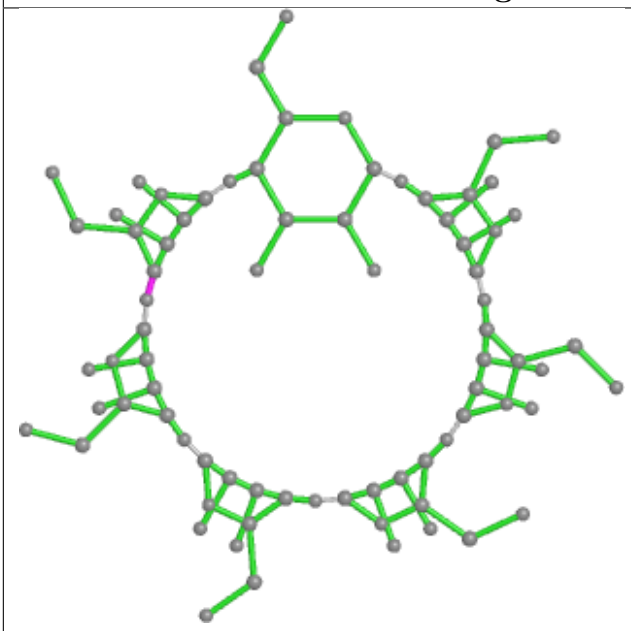
There are no ring outliers.

6 monomers are involved in 16 short contacts:

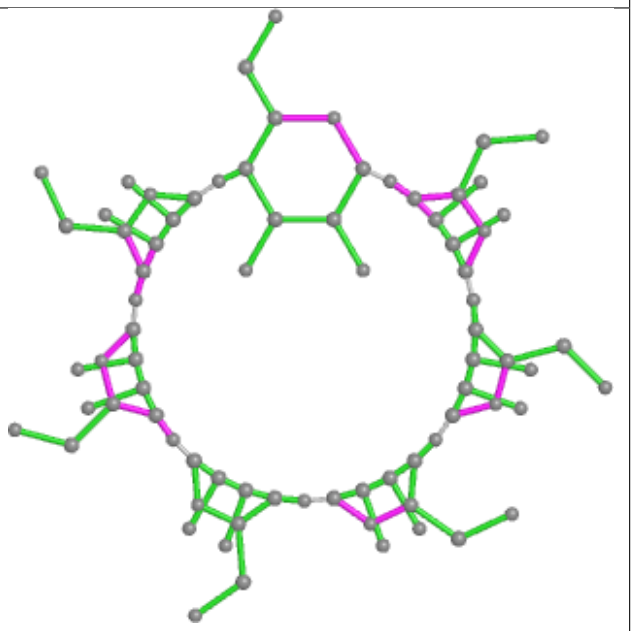
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	GLC	1	0
2	C	7	GLC	1	0
2	D	3	GLC	4	0
2	C	3	GLC	7	0
2	C	4	GLC	3	0
2	D	4	GLC	2	0

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

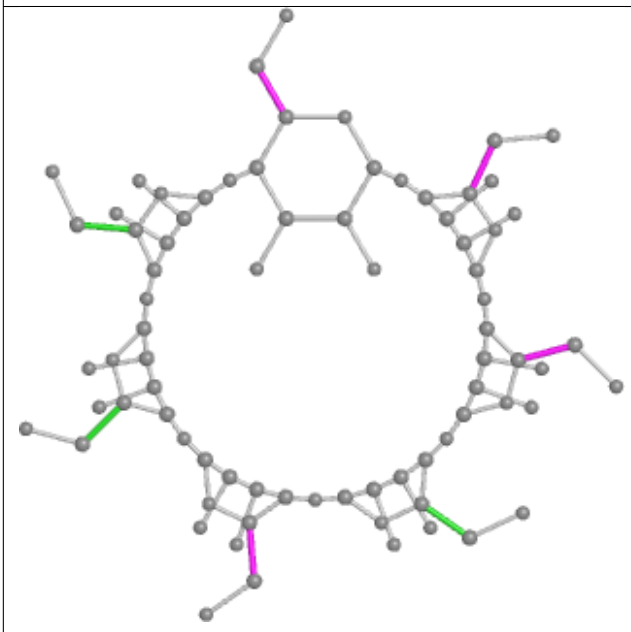
Oligosaccharide Chain C



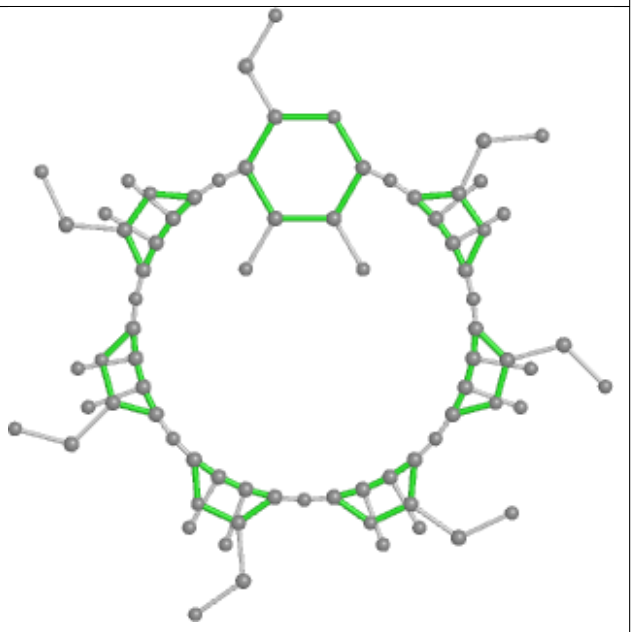
Bond lengths



Bond angles

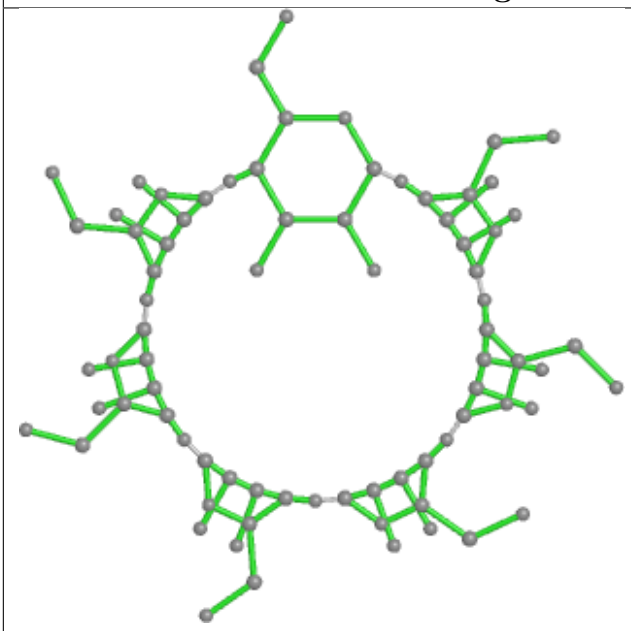


Torsions

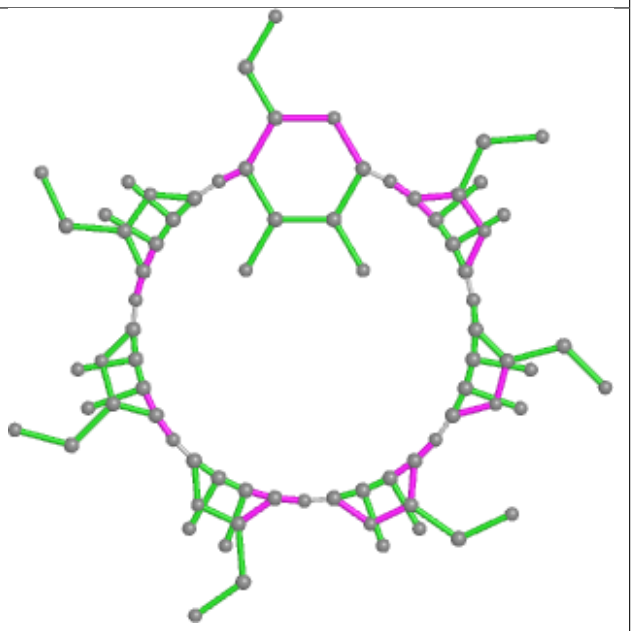


Rings

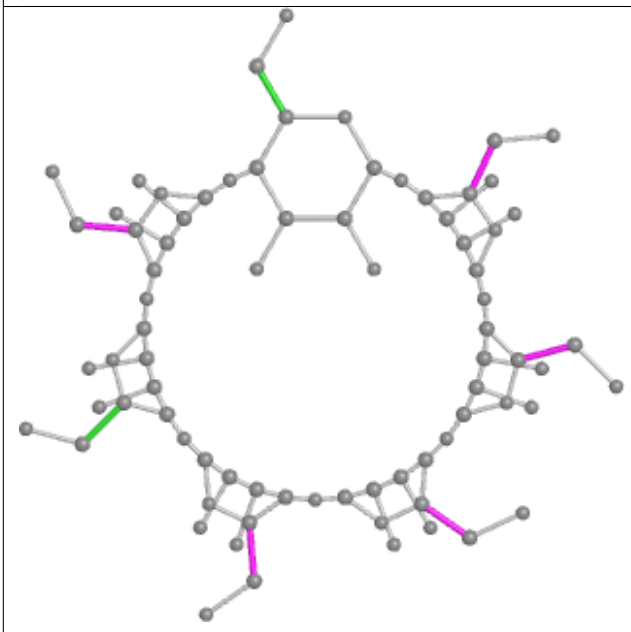
Oligosaccharide Chain D



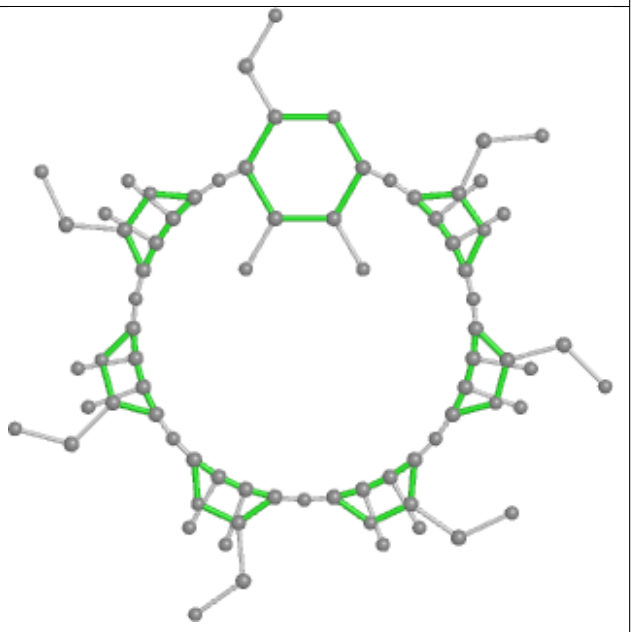
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	585/585 (100%)	-0.94	1 (0%)	95	87	7, 22, 39, 50	0
1	B	585/585 (100%)	-0.87	1 (0%)	95	87	6, 23, 39, 50	0
All	All	1170/1170 (100%)	-0.90	2 (0%)	95	87	6, 22, 39, 50	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	THR	2.5
1	A	278	THR	2.2

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	6	11/12	0.78	0.26	49,50,51,53	0
2	GLC	D	2	11/12	0.83	0.27	43,47,49,49	0
2	GLC	D	5	11/12	0.83	0.26	47,50,53,56	0
2	GLC	D	1	11/12	0.83	0.30	47,48,50,51	0
2	GLC	C	6	11/12	0.85	0.23	44,49,52,53	0
2	GLC	D	7	11/12	0.85	0.26	46,50,52,52	0
2	GLC	D	4	11/12	0.86	0.26	43,46,48,49	0

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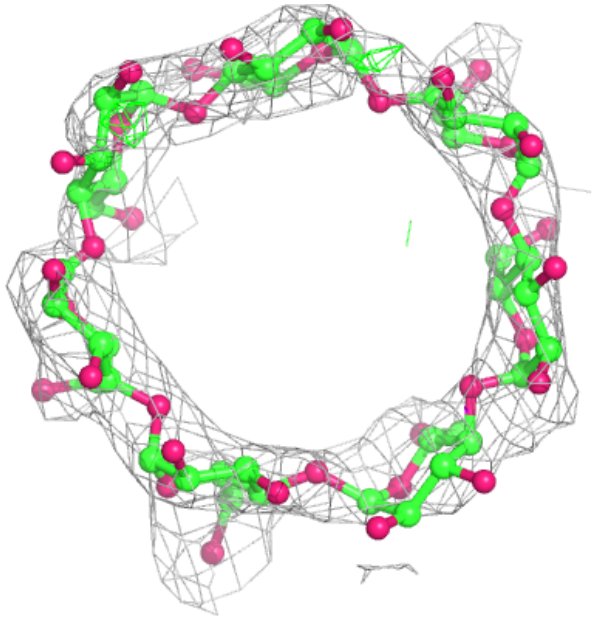
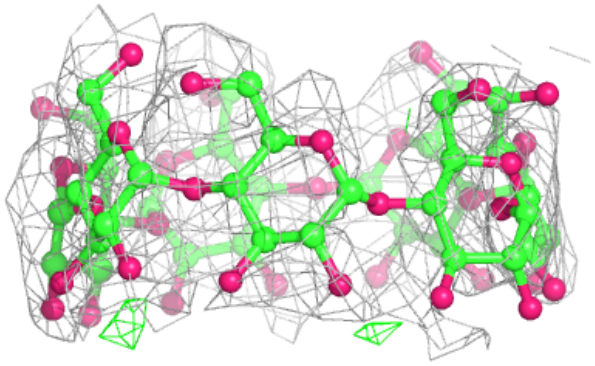
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	3	11/12	0.87	0.29	45,49,53,55	0
2	GLC	C	2	11/12	0.87	0.22	36,49,51,53	0
2	GLC	C	7	11/12	0.87	0.23	40,49,50,51	0
2	GLC	D	3	11/12	0.88	0.28	45,50,51,51	0
2	GLC	C	1	11/12	0.89	0.23	46,48,50,53	0
2	GLC	C	5	11/12	0.90	0.23	36,38,42,47	0
2	GLC	C	4	11/12	0.93	0.17	33,38,44,46	0

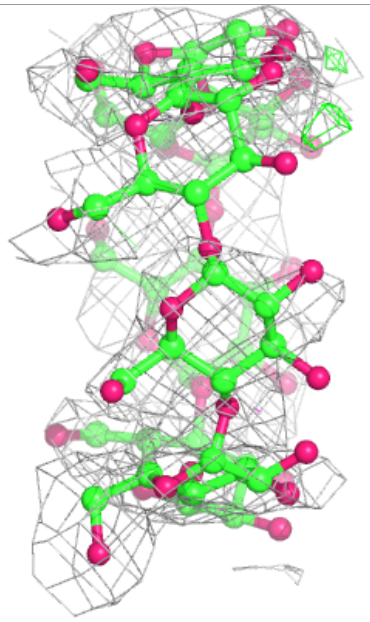
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

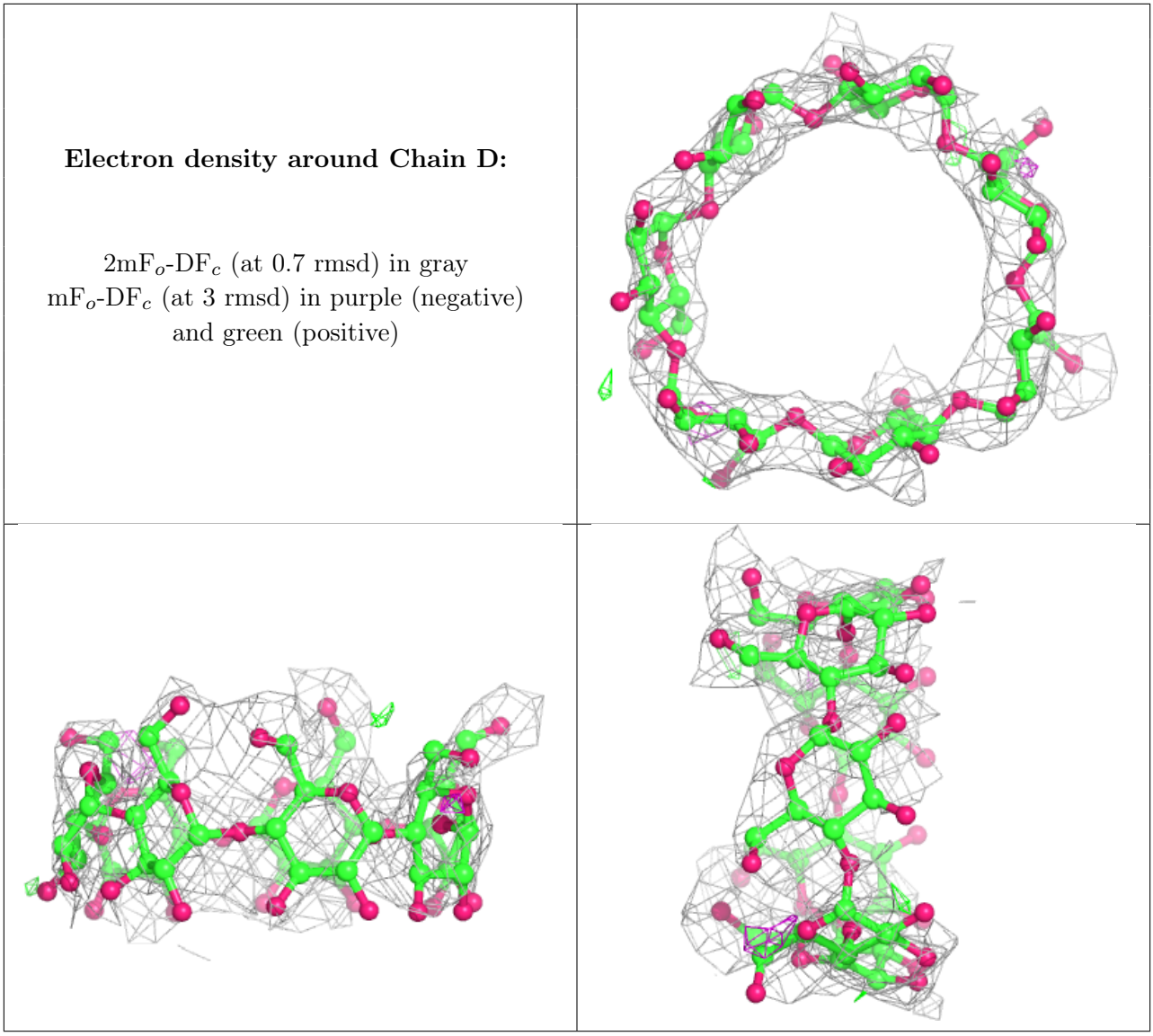






Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.